Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 04:37 PM BST

PDB ID	:	1EVE
Title	:	THREE DIMENSIONAL STRUCTURE OF THE ANTI-ALZHEIMER DRUG, E2020 (ARICEPT), COMPLEXED WITH ITS TARGET ACETYL-CHOLINESTERASE
Authors	:	Kryger, G.; Silman, I.; Sussman, J.L.
Deposited on	:	1998-03-04
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

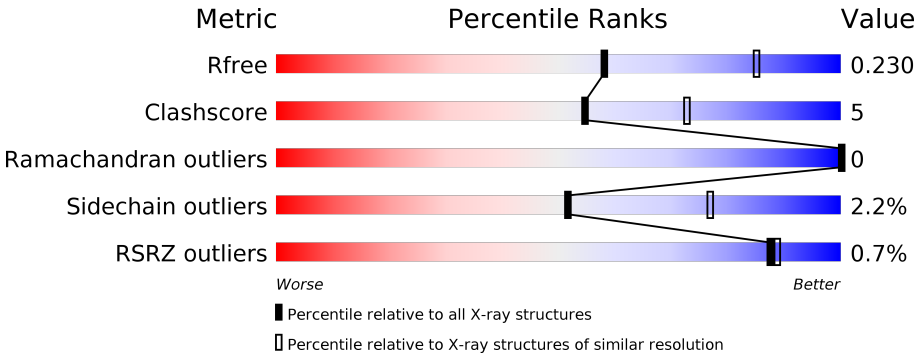
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	543	% 84% 13%
2	B	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	3004	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4748 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

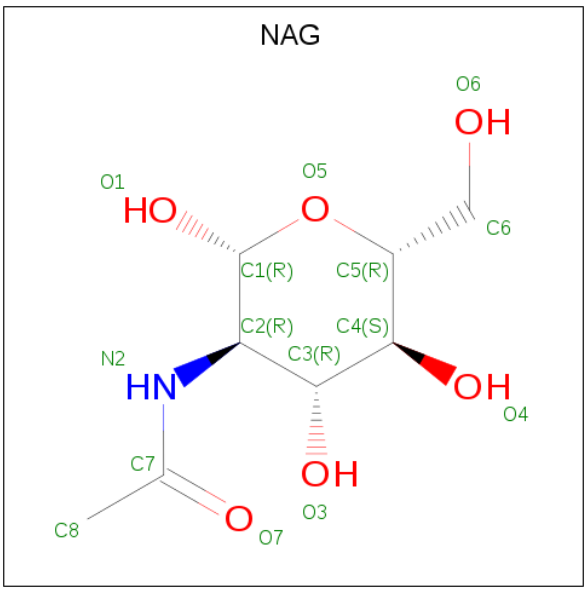
- Molecule 1 is a protein called ACETYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	534	4254	2727	722	783	22	0	0	0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

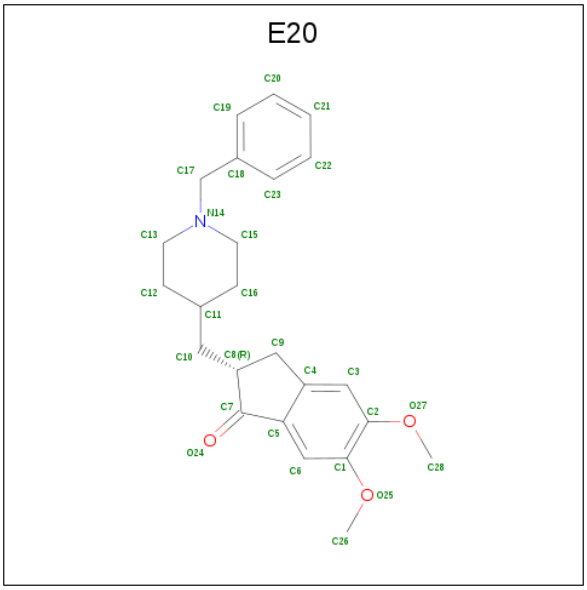
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is 1-BENZYL-4-[(5,6-DIMETHOXY-1-INDANON-2-YL)METHYL]PIPERIDIN E (three-letter code: E20) (formula: $C_{24}H_{29}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 28 24 1 3	0	0

- Molecule 5 is water.

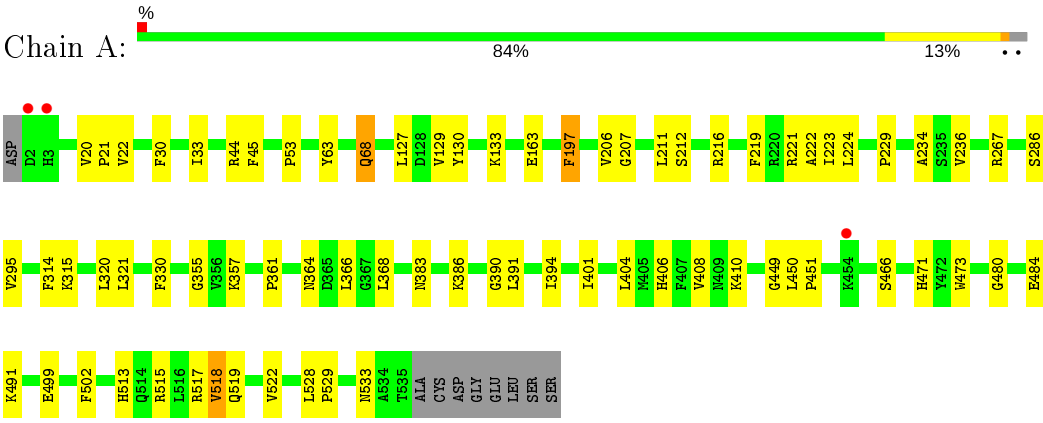
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	396	Total O 396 396	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

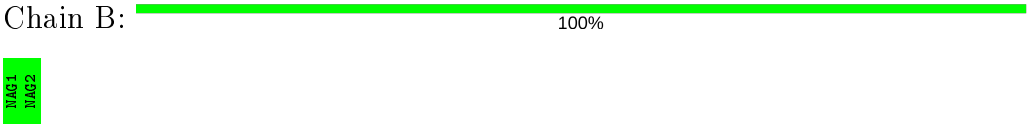
• Molecule 1: ACETYLCHOLINESTERASE

Chain A:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	111.92Å 111.92Å 136.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50 29.22 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.3 (30.00-2.50) 98.4 (29.22-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.188 , 0.228 0.191 , 0.230	Depositor DCC
R_{free} test set	1976 reflections (5.77%)	wwPDB-VP
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4748	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: E20, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.32	0/4377	0.57	0/5943

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4254	0	4097	42	0
2	B	28	0	25	0	0
3	A	42	0	39	3	0
4	A	28	0	29	0	0
5	A	396	0	0	6	0
All	All	4748	0	4190	44	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (44) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3001:NAG:H81	5:A:1323:HOH:O	1.76	0.84
3:A:3001:NAG:C8	5:A:1323:HOH:O	2.36	0.70
1:A:404:LEU:O	1:A:408:VAL:HG23	1.93	0.69
1:A:53:PRO:HG3	5:A:1332:HOH:O	1.95	0.66
1:A:401:ILE:HG21	1:A:517:ARG:HD3	1.79	0.64
1:A:406:HIS:O	1:A:410:LYS:HG2	2.00	0.62
1:A:22:VAL:HG22	1:A:133:LYS:HD2	1.80	0.62
1:A:211:LEU:HD23	1:A:314:PHE:HB3	1.87	0.57
1:A:518:VAL:O	1:A:522:VAL:HG23	2.05	0.56
1:A:487:SER:HB3	1:A:491:LYS:NZ	2.19	0.56
1:A:321:LEU:HD11	1:A:408:VAL:HG22	1.89	0.55
1:A:484:GLU:HB3	1:A:487:SER:HB2	1.91	0.53
1:A:449:GLY:HA2	1:A:466:SER:OG	2.09	0.52
1:A:355:GLY:HA3	1:A:391:LEU:HD21	1.93	0.51
1:A:515:ARG:HB3	1:A:518:VAL:CG1	2.42	0.50
1:A:163:GLU:HB3	1:A:267:ARG:HH22	1.78	0.49
1:A:471:HIS:HB3	5:A:1292:HOH:O	2.12	0.48
1:A:207:GLY:HA3	1:A:229:PRO:HD3	1.95	0.48
1:A:234:ALA:O	1:A:294:PRO:HD2	2.14	0.48
1:A:197:PHE:CB	1:A:223:ILE:HB	2.45	0.47
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.49	0.46
1:A:197:PHE:HB3	1:A:223:ILE:HB	1.97	0.46
1:A:206:VAL:CG1	1:A:222:ALA:HB1	2.45	0.46
1:A:30:PHE:HB3	1:A:33:ILE:HD11	1.97	0.46
1:A:383:ASN:HB3	1:A:386:LYS:HB2	1.97	0.45
1:A:533:ASN:OD1	3:A:3004:NAG:H2	2.16	0.45
1:A:20:VAL:HA	1:A:21:PRO:HD3	1.84	0.45
1:A:390:GLY:O	1:A:394:ILE:HG13	2.17	0.44
1:A:450:LEU:N	1:A:451:PRO:CD	2.80	0.44
1:A:68:GLN:HA	1:A:68:GLN:HE21	1.83	0.44
1:A:127:LEU:HD12	1:A:130:TYR:CE2	2.52	0.44
1:A:221:ARG:HD3	1:A:480:GLY:HA2	1.99	0.44
1:A:364:ASN:O	1:A:368:LEU:HG	2.18	0.43
1:A:223:ILE:HA	1:A:320:LEU:O	2.18	0.43
1:A:286:SER:HB3	1:A:361:PRO:HB3	2.01	0.42
1:A:499:GLU:HB2	5:A:1298:HOH:O	2.19	0.42
1:A:219:PHE:O	1:A:315:LYS:HE2	2.20	0.42
1:A:44:ARG:O	1:A:45:PHE:HB2	2.20	0.41
1:A:236:VAL:HG23	1:A:295:VAL:HG12	2.03	0.41
1:A:223:ILE:HG12	1:A:320:LEU:HB3	2.02	0.41
1:A:212:SER:O	1:A:216:ARG:HG3	2.21	0.41
1:A:528:LEU:N	1:A:529:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:HD12	1:A:224:LEU:N	2.36	0.40
1:A:519:GLN:HB2	5:A:1265:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	532/543 (98%)	501 (94%)	31 (6%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	465/474 (98%)	455 (98%)	10 (2%)	52 77

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	A	68	GLN
1	A	129	VAL
1	A	197	PHE

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Mol	Chain	Res	Type
1	A	288	PHE
1	A	330	PHE
1	A	357	LYS
1	A	366	LEU
1	A	473	TRP
1	A	518	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	65	ASN
1	A	68	GLN
1	A	519	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	B	1	1,2	14,14,15	0.44	0	17,19,21	0.69	0
2	NAG	B	2	2	14,14,15	0.41	0	17,19,21	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

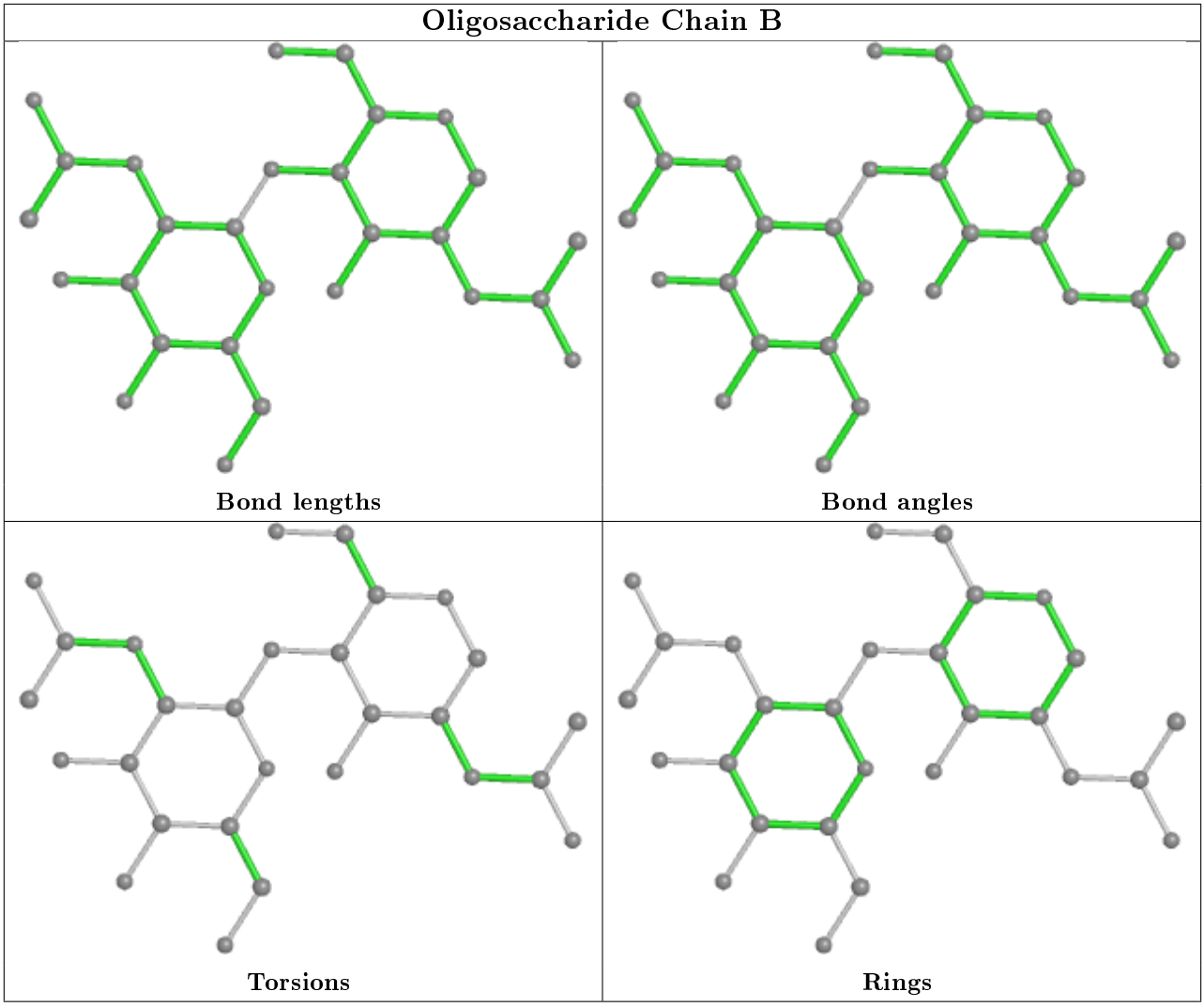
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	A	3005	1	14,14,15	0.49	0	17,19,21	0.85	1 (5%)
3	NAG	A	3004	1	14,14,15	0.43	0	17,19,21	0.72	0
3	NAG	A	3001	1	14,14,15	0.51	0	17,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	E20	A	2001	-	31,31,31	1.98	14 (45%)	39,43,43	3.65	15 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	3005	1	-	0/6/23/26	0/1/1/1
3	NAG	A	3004	1	-	0/6/23/26	0/1/1/1
3	NAG	A	3001	1	-	0/6/23/26	0/1/1/1
4	E20	A	2001	-	-	3/12/34/34	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2001	E20	C3-C4	3.72	1.45	1.39
4	A	2001	E20	C10-C11	-3.54	1.47	1.53
4	A	2001	E20	O27-C2	-3.45	1.31	1.37
4	A	2001	E20	O24-C7	3.30	1.26	1.22
4	A	2001	E20	O25-C26	3.04	1.51	1.42
4	A	2001	E20	C5-C7	-2.56	1.43	1.47
4	A	2001	E20	C6-C1	2.53	1.43	1.38
4	A	2001	E20	C20-C19	2.45	1.44	1.38
4	A	2001	E20	C17-N14	2.23	1.51	1.47
4	A	2001	E20	C22-C21	2.17	1.43	1.38
4	A	2001	E20	C22-C23	2.16	1.43	1.38
4	A	2001	E20	C19-C18	2.14	1.43	1.38
4	A	2001	E20	C3-C2	2.07	1.42	1.38
4	A	2001	E20	C23-C18	2.02	1.43	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2001	E20	O27-C2-C1	10.54	130.09	115.41
4	A	2001	E20	O27-C2-C3	-9.56	107.67	124.12
4	A	2001	E20	O24-C7-C8	7.93	129.07	124.76
4	A	2001	E20	C4-C5-C7	7.57	113.04	109.72
4	A	2001	E20	C9-C8-C7	6.02	107.63	104.68
4	A	2001	E20	C17-N14-C13	5.16	122.55	111.06
4	A	2001	E20	O25-C1-C2	5.00	122.38	115.41
4	A	2001	E20	C28-O27-C2	4.72	124.65	117.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2001	E20	C17-N14-C15	-4.58	100.86	111.06
4	A	2001	E20	C26-O25-C1	3.72	123.14	117.53
4	A	2001	E20	O25-C1-C6	-3.04	118.89	124.12
4	A	2001	E20	C6-C5-C7	-2.66	125.14	128.40
4	A	2001	E20	C9-C4-C5	-2.44	109.94	111.50
4	A	2001	E20	C3-C4-C5	-2.10	118.24	120.72
3	A	3005	NAG	C1-O5-C5	2.04	114.96	112.19
4	A	2001	E20	C15-N14-C13	2.04	113.41	108.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2001	E20	C3-C2-O27-C28
4	A	2001	E20	C1-C2-O27-C28
4	A	2001	E20	C11-C10-C8-C9

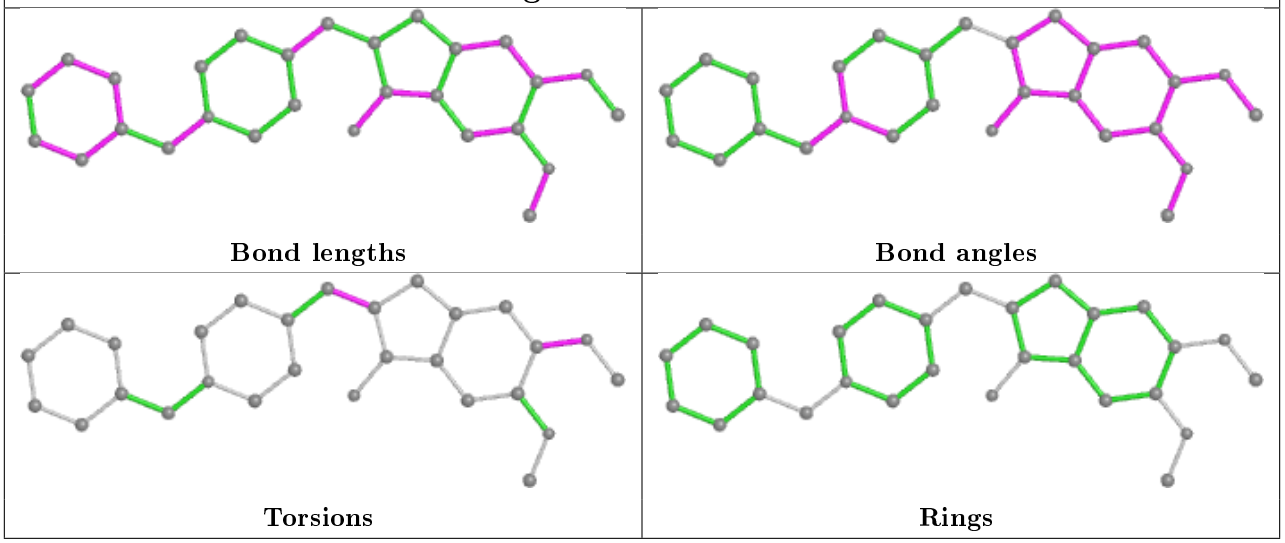
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3004	NAG	1	0
3	A	3001	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand E20 A 2001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	534/543 (98%)	-0.57	4 (0%) 87 89	9, 25, 51, 71	7 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	486	HIS	3.1
1	A	2	ASP	2.7
1	A	454	LYS	2.5
1	A	3	HIS	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

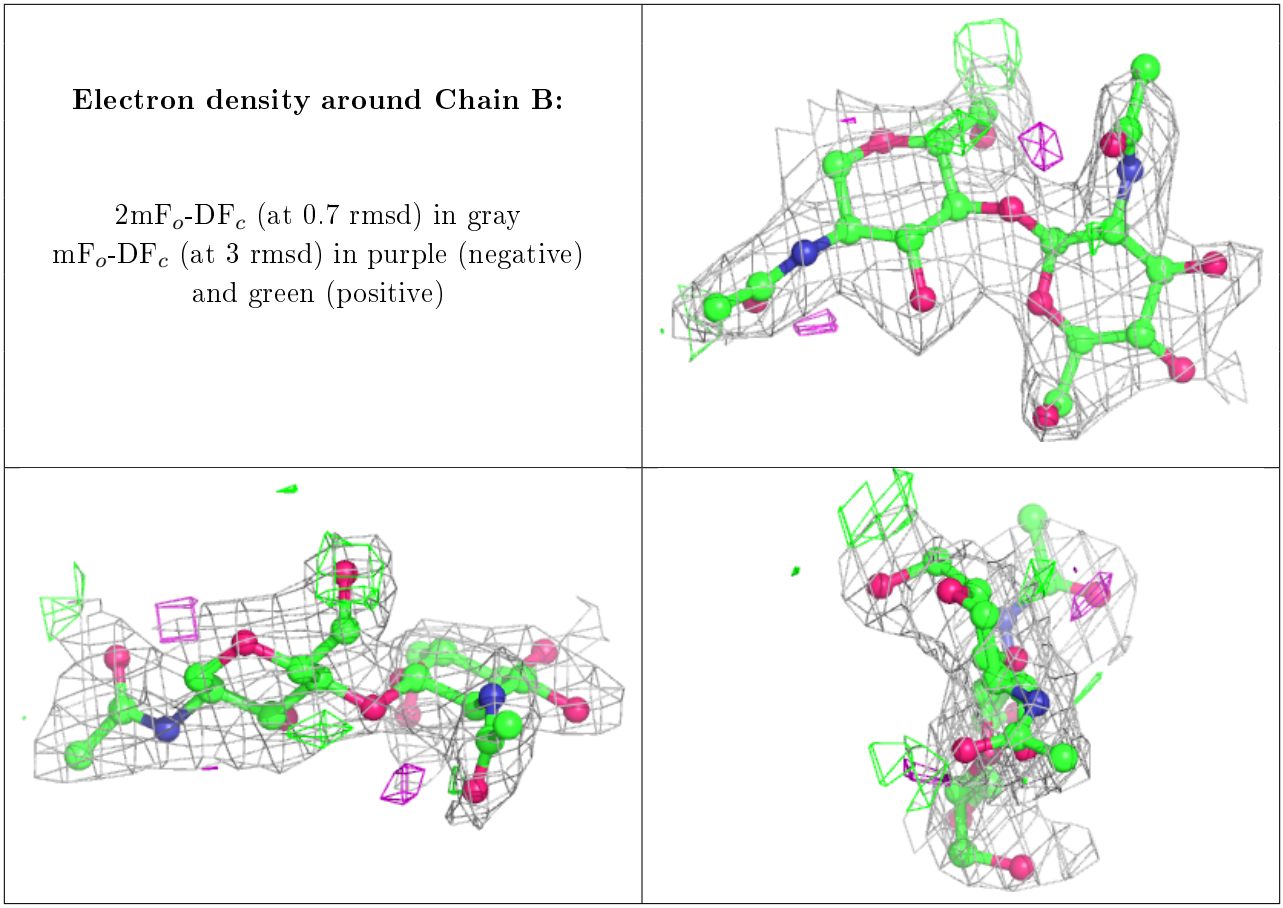
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	B	2	14/15	0.90	0.33	36,38,41,43	14
2	NAG	B	1	14/15	0.91	0.14	14,24,30,37	14

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.4 Ligands

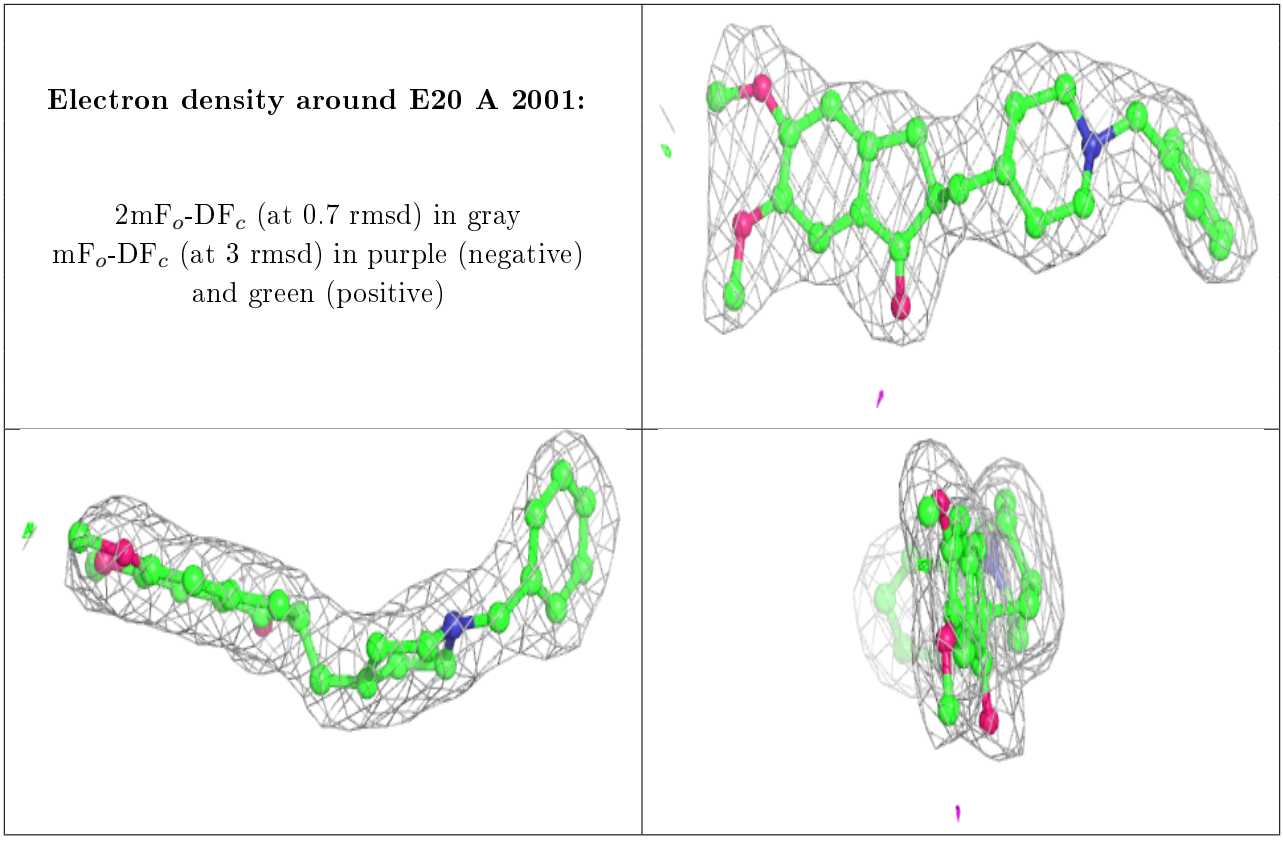
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	A	3004	14/15	0.76	0.49	63,69,72,74	14
3	NAG	A	3005	14/15	0.81	0.31	47,53,55,57	14
3	NAG	A	3001	14/15	0.81	0.20	46,49,52,60	14
4	E20	A	2001	28/28	0.98	0.10	13,19,28,31	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around E20 A 2001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 05:53 AM BST

PDB ID	:	1E66
Title	:	STRUCTURE OF ACETYLCHOLINESTERASE COMPLEXED WITH (-)-HUPRINE X AT 2.1A RESOLUTION
Authors	:	Dvir, H.; Harel, M.; Silman, I.; Sussman, J.L.
Deposited on	:	2000-08-08
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

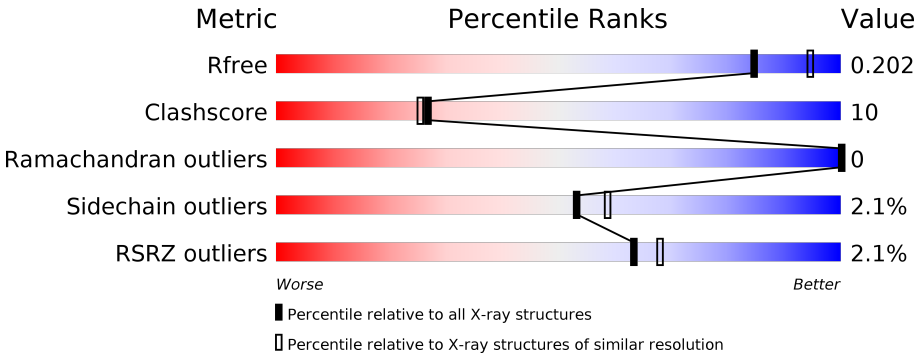
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	543	2% 87% 9%

2 Entry composition

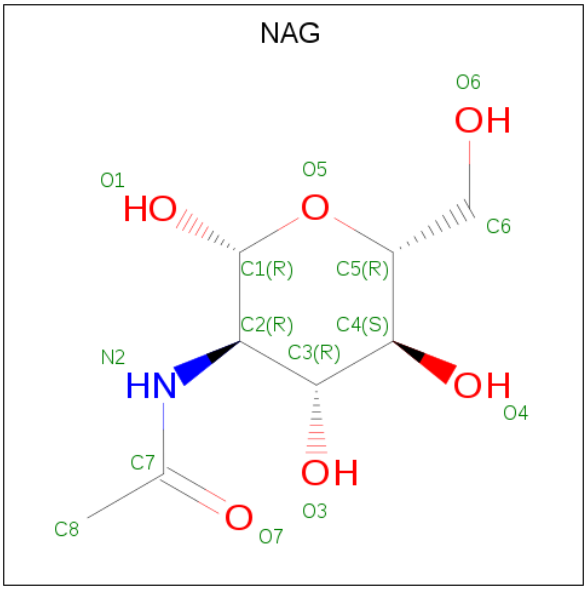
There are 4 unique types of molecules in this entry. The entry contains 4818 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ACETYLCHOLINESTERASE.

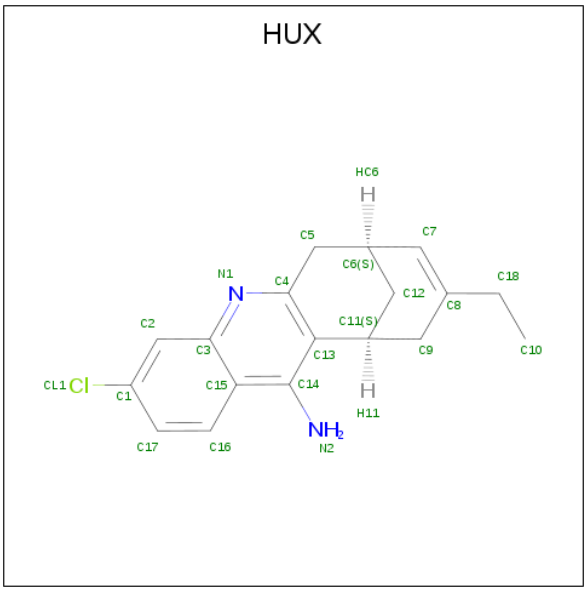
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	14	1
			4272	2747	721	779	25			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 3-CHLORO-9-ETHYL-6,7,8,9,10,11-HEXAHYDRO-7,11-METHANOCYCLOOCTA[B]QUINOLIN-12-AMINE (three-letter code: HUX) (formula: $C_{18}H_{19}ClN_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			21	18	1	2		

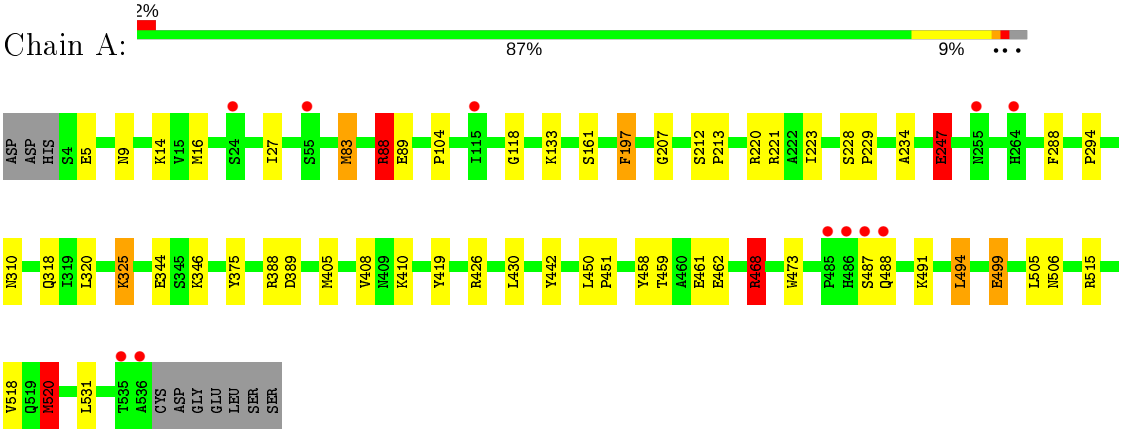
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	497	Total	O	0	0
			497	497		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ACETYLCHOLINESTERASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	112.33Å 112.33Å 138.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.42 – 2.10 29.42 – 2.09	Depositor EDS
% Data completeness (in resolution range)	76.0 (29.42-2.10) 75.5 (29.42-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.177 , 0.205 0.172 , 0.202	Depositor DCC
R_{free} test set	4542 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å^2)	27.0	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 64.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4818	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HUX, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	7.21	26/4395 (0.6%)	3.74	31/5975 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	468[A]	ARG	CZ-NH2	194.03	3.85	1.33
1	A	468[B]	ARG	CZ-NH2	194.03	3.85	1.33
1	A	88[A]	ARG	CZ-NH1	172.87	3.57	1.33
1	A	88[B]	ARG	CZ-NH1	172.87	3.57	1.33
1	A	247[A]	GLU	CD-OE1	147.56	2.88	1.25
1	A	247[B]	GLU	CD-OE1	147.56	2.88	1.25
1	A	88[A]	ARG	CZ-NH2	135.61	3.09	1.33
1	A	88[B]	ARG	CZ-NH2	135.61	3.09	1.33
1	A	468[A]	ARG	CZ-NH1	41.93	1.87	1.33
1	A	468[B]	ARG	CZ-NH1	41.93	1.87	1.33
1	A	247[A]	GLU	CD-OE2	38.69	1.68	1.25
1	A	247[B]	GLU	CD-OE2	38.69	1.68	1.25
1	A	325[A]	LYS	CE-NZ	34.20	2.34	1.49
1	A	325[B]	LYS	CE-NZ	34.20	2.34	1.49
1	A	88[A]	ARG	CG-CD	-25.03	0.89	1.51
1	A	88[B]	ARG	CG-CD	-25.03	0.89	1.51
1	A	83[A]	MET	CB-CG	-13.20	1.09	1.51
1	A	83[B]	MET	CB-CG	-13.20	1.09	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	520[A]	MET	SD-CE	-12.65	1.07	1.77
1	A	520[B]	MET	SD-CE	-12.65	1.07	1.77
1	A	83[A]	MET	SD-CE	-11.93	1.11	1.77
1	A	83[B]	MET	SD-CE	-11.93	1.11	1.77
1	A	16[A]	MET	CG-SD	-9.81	1.55	1.81
1	A	16[B]	MET	CG-SD	-9.81	1.55	1.81
1	A	228[A]	SER	CA-CB	-5.00	1.45	1.52
1	A	228[B]	SER	CA-CB	-5.00	1.45	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	88[A]	ARG	NE-CZ-NH1	-96.03	72.29	120.30
1	A	88[B]	ARG	NE-CZ-NH1	-96.03	72.29	120.30
1	A	468[A]	ARG	NE-CZ-NH2	-92.89	73.85	120.30
1	A	468[B]	ARG	NE-CZ-NH2	-92.89	73.85	120.30
1	A	468[A]	ARG	NH1-CZ-NH2	-86.25	24.52	119.40
1	A	468[B]	ARG	NH1-CZ-NH2	-86.25	24.52	119.40
1	A	88[A]	ARG	NH1-CZ-NH2	-72.67	39.46	119.40
1	A	88[B]	ARG	NH1-CZ-NH2	-72.67	39.46	119.40
1	A	247[A]	GLU	OE1-CD-OE2	-61.59	49.39	123.30
1	A	247[B]	GLU	OE1-CD-OE2	-61.59	49.39	123.30
1	A	468[A]	ARG	NE-CZ-NH1	-56.89	91.85	120.30
1	A	468[B]	ARG	NE-CZ-NH1	-56.89	91.85	120.30
1	A	88[A]	ARG	NE-CZ-NH2	-33.54	103.53	120.30
1	A	88[B]	ARG	NE-CZ-NH2	-33.54	103.53	120.30
1	A	520[A]	MET	CG-SD-CE	19.71	131.73	100.20
1	A	520[B]	MET	CG-SD-CE	19.71	131.73	100.20
1	A	88[A]	ARG	CB-CG-CD	16.40	154.25	111.60
1	A	88[B]	ARG	CB-CG-CD	16.40	154.25	111.60
1	A	247[A]	GLU	CG-CD-OE1	-12.80	92.71	118.30
1	A	247[B]	GLU	CG-CD-OE1	-12.80	92.71	118.30
1	A	88[A]	ARG	CG-CD-NE	-11.90	86.81	111.80
1	A	88[B]	ARG	CG-CD-NE	-11.90	86.81	111.80
1	A	247[A]	GLU	CG-CD-OE2	11.75	141.80	118.30
1	A	247[B]	GLU	CG-CD-OE2	11.75	141.80	118.30
1	A	83[A]	MET	CG-SD-CE	11.28	118.25	100.20
1	A	83[B]	MET	CG-SD-CE	11.28	118.25	100.20
1	A	83[A]	MET	CA-CB-CG	7.81	126.57	113.30
1	A	83[B]	MET	CA-CB-CG	7.81	126.57	113.30
1	A	16[A]	MET	CB-CG-SD	6.75	132.66	112.40
1	A	16[B]	MET	CB-CG-SD	6.75	132.66	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	494	LEU	CA-CB-CG	5.21	127.29	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	247[A]	GLU	Sidechain
1	A	442	TYR	Sidechain
1	A	468[A]	ARG	Sidechain
1	A	88[A]	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4272	0	4052	81	0
2	A	28	0	26	5	0
3	A	21	0	19	1	0
4	A	497	0	0	5	0
All	All	4818	0	4097	86	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (86) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83[B]:MET:CG	1:A:83[B]:MET:CB	1.95	1.40
1:A:468[A]:ARG:NH1	1:A:468[A]:ARG:CZ	1.87	1.37
1:A:247[A]:GLU:CD	1:A:247[A]:GLU:OE2	1.68	1.32
1:A:83[A]:MET:SD	1:A:83[A]:MET:CE	1.11	1.19
1:A:468[B]:ARG:NH1	1:A:468[B]:ARG:CZ	2.08	1.16
1:A:520[A]:MET:SD	1:A:520[A]:MET:CE	1.07	1.16
1:A:468[B]:ARG:HH11	1:A:468[B]:ARG:NH2	1.47	1.12
1:A:83[A]:MET:SD	1:A:83[A]:MET:HE2	1.70	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83[A]:MET:SD	1:A:83[A]:MET:HE3	1.70	1.08
1:A:520[A]:MET:SD	1:A:520[A]:MET:HE2	1.66	1.07
1:A:520[A]:MET:SD	1:A:520[A]:MET:HE1	1.66	1.06
1:A:520[A]:MET:SD	1:A:520[A]:MET:HE3	1.66	1.06
1:A:83[A]:MET:SD	1:A:83[A]:MET:HE1	1.70	1.04
1:A:468[A]:ARG:HD2	1:A:468[A]:ARG:HH11	1.19	1.03
1:A:88[B]:ARG:CG	1:A:88[B]:ARG:CD	2.42	0.98
1:A:88[A]:ARG:NH1	1:A:88[A]:ARG:HD2	1.82	0.95
1:A:88[B]:ARG:NH2	1:A:88[B]:ARG:HH11	1.66	0.94
1:A:468[A]:ARG:NH2	1:A:468[A]:ARG:HH11	1.67	0.91
1:A:325[A]:LYS:NZ	1:A:325[A]:LYS:CE	2.34	0.90
1:A:468[A]:ARG:NH1	1:A:468[A]:ARG:CD	2.35	0.90
1:A:83[A]:MET:CG	1:A:83[A]:MET:CE	2.51	0.89
1:A:468[A]:ARG:NH1	1:A:468[A]:ARG:HD2	1.85	0.88
1:A:247[B]:GLU:OE2	1:A:247[B]:GLU:HG3	1.73	0.87
1:A:88[A]:ARG:NH1	1:A:88[A]:ARG:CD	2.43	0.81
1:A:88[A]:ARG:NH1	1:A:88[A]:ARG:NH2	2.29	0.80
1:A:468[A]:ARG:HH11	1:A:468[A]:ARG:CD	1.90	0.80
1:A:468[A]:ARG:NH1	1:A:468[A]:ARG:NH2	2.28	0.80
1:A:88[B]:ARG:NH2	1:A:88[B]:ARG:NH1	2.30	0.79
1:A:468[B]:ARG:NH1	1:A:468[B]:ARG:NH2	2.30	0.78
1:A:468[A]:ARG:NH1	1:A:468[A]:ARG:NE	2.33	0.77
2:A:801:NAG:H82	2:A:801:NAG:H3	1.69	0.75
1:A:88[B]:ARG:NH2	1:A:88[B]:ARG:HE	1.84	0.75
1:A:88[A]:ARG:NH1	1:A:88[A]:ARG:HH21	1.91	0.68
2:A:801:NAG:H82	2:A:801:NAG:C3	2.24	0.67
1:A:520[A]:MET:HG2	4:A:1113:HOH:O	1.94	0.67
1:A:88[B]:ARG:CB	1:A:88[B]:ARG:CD	2.74	0.66
1:A:247[B]:GLU:CG	1:A:247[B]:GLU:OE2	2.45	0.65
1:A:310:ASN:HD21	1:A:410:LYS:NZ	1.97	0.63
1:A:221:ARG:HD3	1:A:318:GLN:OE1	2.00	0.62
1:A:468[A]:ARG:NH2	1:A:468[A]:ARG:HD2	2.16	0.61
1:A:247[B]:GLU:OE1	1:A:247[B]:GLU:OE2	2.20	0.60
1:A:83[B]:MET:CG	1:A:83[B]:MET:CA	2.77	0.60
1:A:247[A]:GLU:OE2	1:A:247[A]:GLU:OE1	2.19	0.59
1:A:468[B]:ARG:HD3	1:A:468[B]:ARG:NH2	2.19	0.57
1:A:89:GLU:CG	4:A:1372:HOH:O	2.54	0.54
1:A:344:GLU:OE2	1:A:346:LYS:HE3	2.08	0.54
1:A:223:ILE:HA	1:A:320:LEU:O	2.07	0.54
1:A:5:GLU:OE2	1:A:104:PRO:HA	2.09	0.52
1:A:499:GLU:HG3	4:A:1296:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88[B]:ARG:HD3	1:A:88[B]:ARG:HA	1.92	0.51
1:A:9[A]:ASN:ND2	1:A:14:LYS:HG2	2.26	0.51
1:A:375:TYR:CZ	1:A:520[B]:MET:SD	3.04	0.51
1:A:468[A]:ARG:NH2	1:A:468[A]:ARG:CD	2.74	0.51
1:A:405:MET:HA	1:A:408:VAL:HG12	1.92	0.50
1:A:197:PHE:CB	1:A:223:ILE:HB	2.41	0.50
2:A:801:NAG:C8	2:A:801:NAG:C3	2.87	0.50
1:A:451:PRO:HA	1:A:458:TYR:CD1	2.46	0.50
1:A:459:THR:OG1	1:A:462:GLU:HG3	2.12	0.50
1:A:419:TYR:CZ	1:A:494:LEU:HD13	2.46	0.50
1:A:310:ASN:ND2	1:A:410:LYS:HZ2	2.12	0.48
1:A:88[B]:ARG:HA	1:A:88[B]:ARG:CD	2.44	0.48
1:A:310:ASN:ND2	1:A:410:LYS:NZ	2.62	0.47
1:A:488:GLN:CG	4:A:1263:HOH:O	2.63	0.47
1:A:247[A]:GLU:HB2	1:A:247[A]:GLU:OE1	2.15	0.46
1:A:515:ARG:HB3	1:A:518:VAL:HB	1.96	0.46
1:A:118:GLY:HA2	3:A:803:HUX:C8	2.46	0.46
1:A:88[B]:ARG:NE	1:A:88[B]:ARG:NH2	2.57	0.46
1:A:531:LEU:HD23	1:A:531:LEU:C	2.37	0.45
1:A:491:LYS:HA	1:A:491:LYS:HD3	1.79	0.45
1:A:310:ASN:HD21	1:A:410:LYS:HZ1	1.62	0.45
1:A:220:ARG:HG3	1:A:221:ARG:HG3	1.98	0.45
1:A:197:PHE:HB3	1:A:223:ILE:HB	1.99	0.45
1:A:207:GLY:HA3	1:A:229:PRO:HD3	1.99	0.45
1:A:388:ARG:HD2	1:A:389:ASP:OD1	2.16	0.45
1:A:88[A]:ARG:NH1	1:A:88[A]:ARG:HD3	2.27	0.45
1:A:506:ASN:HB2	4:A:1115:HOH:O	2.17	0.44
1:A:426:ARG:CZ	1:A:430:LEU:HD23	2.47	0.44
1:A:212:SER:HA	1:A:213:PRO:HD3	1.88	0.44
1:A:27:ILE:HD11	1:A:133:LYS:HB2	2.00	0.43
1:A:468[B]:ARG:NH1	1:A:468[B]:ARG:HD3	2.34	0.42
1:A:461:GLU:OE1	1:A:461:GLU:N	2.41	0.41
2:A:801:NAG:C8	2:A:801:NAG:O3	2.68	0.41
1:A:520[A]:MET:CE	1:A:520[A]:MET:HA	2.50	0.41
1:A:234:ALA:O	1:A:294:PRO:HD2	2.21	0.41
1:A:450:LEU:N	1:A:451:PRO:CD	2.84	0.40
2:A:801:NAG:H82	2:A:801:NAG:O3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	545/543 (100%)	520 (95%)	25 (5%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	451/474 (95%)	440 (98%)	11 (2%)	49 53

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88[A]	ARG
1	A	88[B]	ARG
1	A	161	SER
1	A	197	PHE
1	A	288	PHE
1	A	473	TRP
1	A	487	SER
1	A	499	GLU
1	A	505	LEU
1	A	520[A]	MET
1	A	520[B]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	310	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	A	802	1	14,14,15	0.71	0	17,19,21	0.77	1 (5%)
2	NAG	A	801	1	14,14,15	1.02	1 (7%)	17,19,21	1.16	3 (17%)
3	HUX	A	803	-	23,24,24	3.95	12 (52%)	23,36,36	3.58	13 (56%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	802	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	801	1	-	3/6/23/26	0/1/1/1
3	HUX	A	803	-	-	0/2/22/22	0/5/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	HUX	C5-C4	10.41	1.62	1.51
3	A	803	HUX	C17-C1	6.90	1.51	1.38
3	A	803	HUX	C2-C1	6.32	1.48	1.36
3	A	803	HUX	C6-C7	5.88	1.67	1.51
3	A	803	HUX	C3-N1	5.40	1.46	1.37
3	A	803	HUX	C12-C11	4.79	1.59	1.53
3	A	803	HUX	C16-C15	4.42	1.51	1.42
3	A	803	HUX	C13-C4	-3.72	1.38	1.42
3	A	803	HUX	C1-CL1	-3.53	1.66	1.74
2	A	801	NAG	C1-C2	3.32	1.57	1.52
3	A	803	HUX	C15-C3	-2.81	1.37	1.42
3	A	803	HUX	C4-N1	2.49	1.35	1.32
3	A	803	HUX	C2-C3	-2.07	1.38	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	803	HUX	C13-C4-N1	7.89	127.19	123.66
3	A	803	HUX	C2-C3-C15	7.53	128.32	119.65
3	A	803	HUX	C9-C11-C13	-6.60	104.42	111.33
3	A	803	HUX	C1-C2-C3	-4.88	115.38	119.50
3	A	803	HUX	C2-C3-N1	-4.87	111.29	118.72
3	A	803	HUX	C17-C1-C2	-3.98	117.28	121.99
3	A	803	HUX	C16-C17-C1	3.94	123.79	119.21
3	A	803	HUX	C13-C14-N2	-3.17	117.11	121.11
3	A	803	HUX	C2-C1-CL1	2.92	123.29	119.64
3	A	803	HUX	C12-C11-C13	2.87	114.96	111.64
3	A	803	HUX	C17-C16-C15	-2.58	117.55	121.13
2	A	801	NAG	C1-C2-N2	2.47	114.71	110.49
3	A	803	HUX	C15-C3-N1	-2.30	120.37	122.81
2	A	801	NAG	C8-C7-N2	2.26	119.92	116.10
2	A	801	NAG	O7-C7-C8	-2.15	118.06	122.06
2	A	802	NAG	C2-N2-C7	-2.15	119.84	122.90
3	A	803	HUX	C5-C4-N1	-2.09	113.07	116.34

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAG	C3-C2-N2-C7
2	A	801	NAG	C8-C7-N2-C2
2	A	801	NAG	O7-C7-N2-C2
2	A	802	NAG	O5-C5-C6-O6
2	A	802	NAG	C4-C5-C6-O6

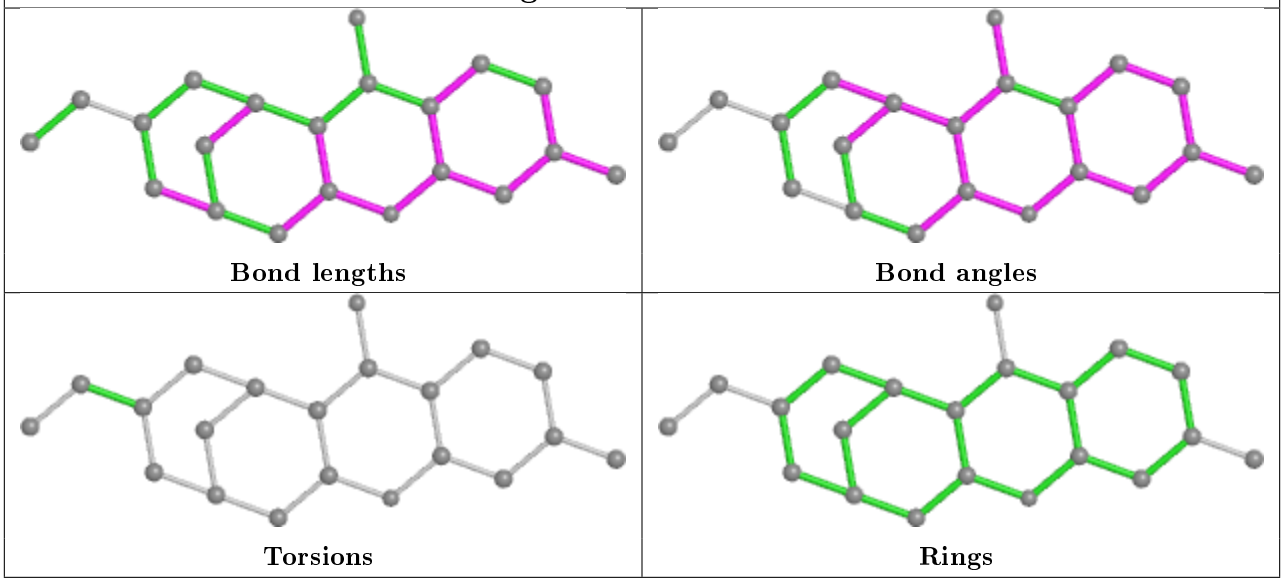
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAG	5	0
3	A	803	HUX	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HUX A 803



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	533/543 (98%)	-0.41	11 (2%) 63 68	21, 31, 47, 70	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	536	ALA	5.3
1	A	485	PRO	5.1
1	A	535	THR	4.5
1	A	486	HIS	4.2
1	A	55[A]	SER	3.6
1	A	487	SER	3.0
1	A	488	GLN	2.9
1	A	24[A]	SER	2.7
1	A	264	HIS	2.2
1	A	255	ASN	2.1
1	A	115	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

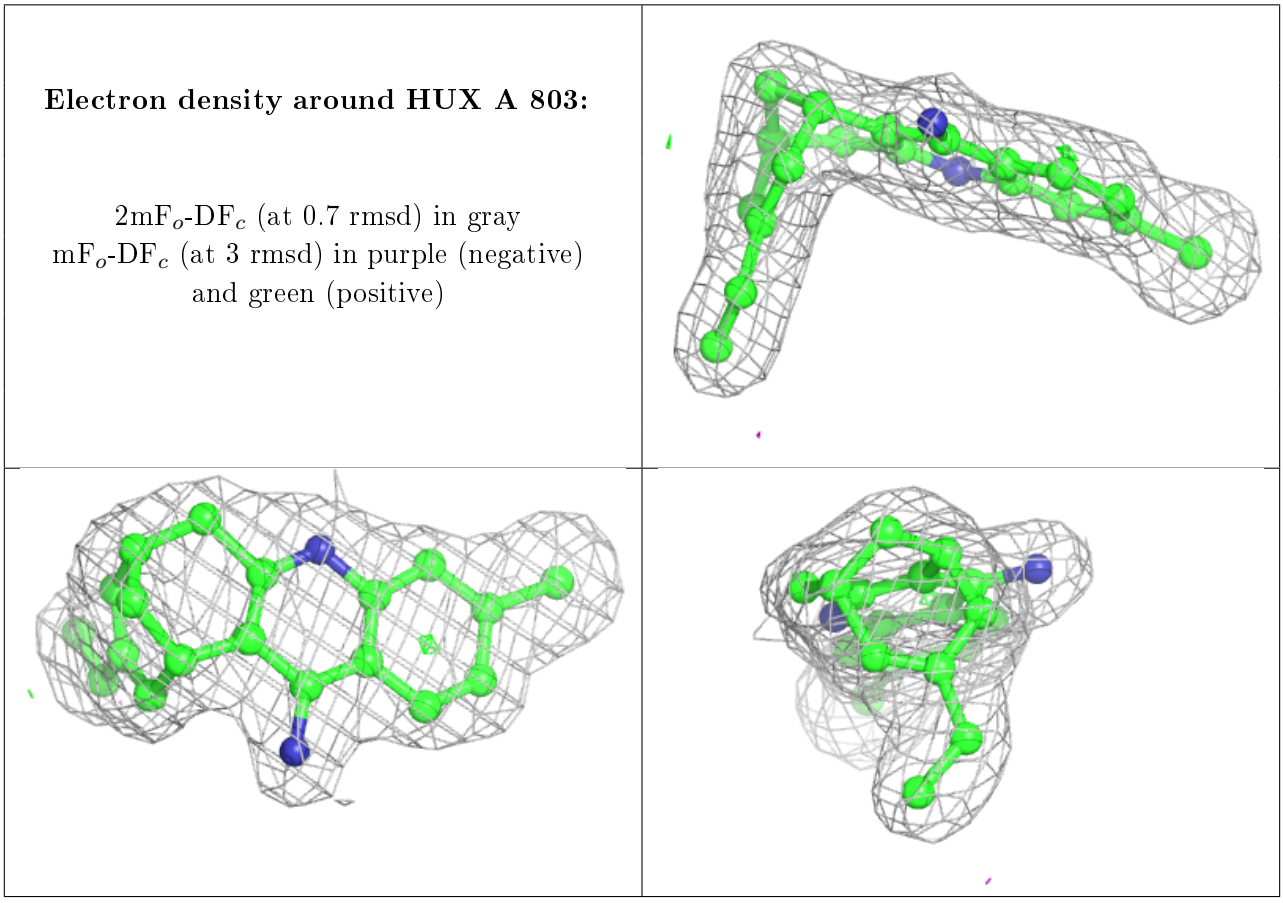
6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	A	801	14/15	0.80	0.25	67,72,74,74	0
2	NAG	A	802	14/15	0.88	0.23	46,49,53,54	0
3	HUX	A	803	21/21	0.96	0.10	24,26,27,28	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers (i)

There are no such residues in this entry.

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 07:32 AM EDT

PDB ID	:	1HW8
Title	:	COMPLEX OF THE CATALYTIC PORTION OF HUMAN HMG-COA REDUCTASE WITH COMPACTIN (ALSO KNOWN AS MEVASTATIN)
Authors	:	Istvan, E.S.; Deisenhofer, J.
Deposited on	:	2001-01-09
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

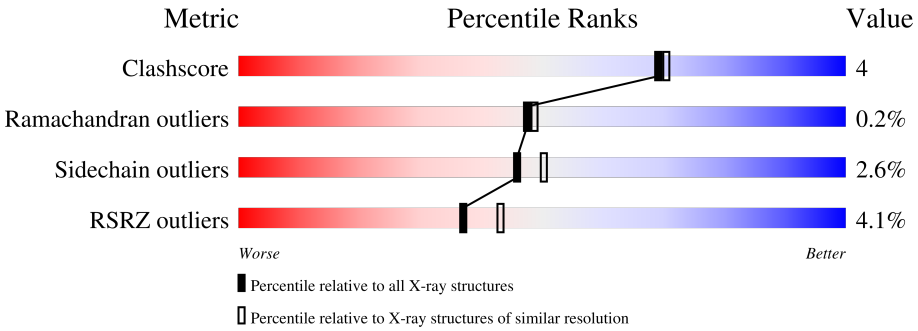
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	467	7% 75% 11% • 13%
1	B	467	2% 81% 7% 12%
1	C	467	3% 74% 5% 20%
1	D	467	2% 74% 5% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	114	A	2	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12022 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

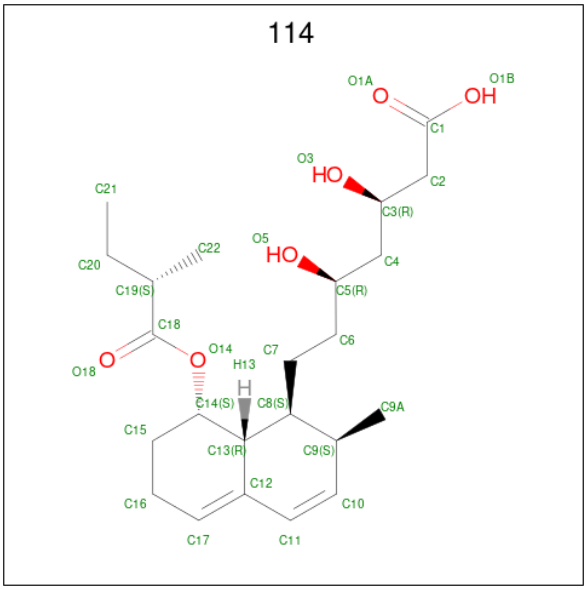
- Molecule 1 is a protein called HMG-COA REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3004	1867	527	580	30			
1	B	410	Total	C	N	O	S	0	0	0
			3055	1904	536	585	30			
1	C	373	Total	C	N	O	S	0	0	0
			2755	1711	487	528	29			
1	D	372	Total	C	N	O	S	0	0	0
			2751	1709	486	527	29			

There are 20 discrepancies between the modelled and reference sequences:

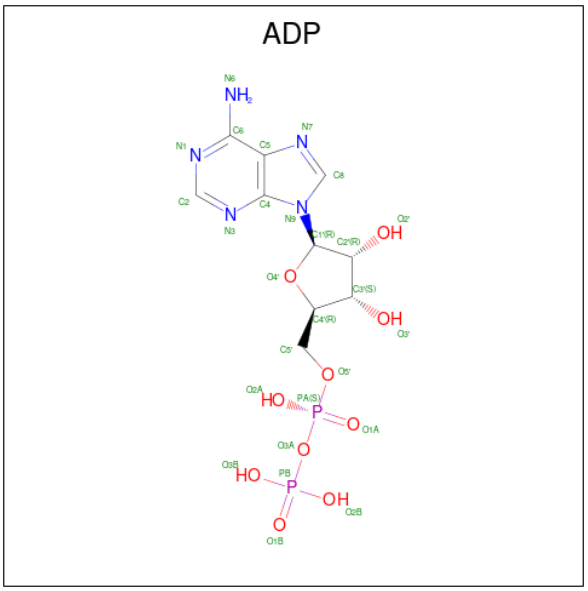
Chain	Residue	Modelled	Actual	Comment	Reference
A	422	GLY	-	insertion	UNP P04035
A	423	ALA	-	insertion	UNP P04035
A	424	MET	-	insertion	UNP P04035
A	425	ALA	-	insertion	UNP P04035
A	485	ILE	MET	engineered mutation	UNP P04035
B	422	GLY	-	insertion	UNP P04035
B	423	ALA	-	insertion	UNP P04035
B	424	MET	-	insertion	UNP P04035
B	425	ALA	-	insertion	UNP P04035
B	485	ILE	MET	engineered mutation	UNP P04035
C	422	GLY	-	insertion	UNP P04035
C	423	ALA	-	insertion	UNP P04035
C	424	MET	-	insertion	UNP P04035
C	425	ALA	-	insertion	UNP P04035
C	485	ILE	MET	engineered mutation	UNP P04035
D	422	GLY	-	insertion	UNP P04035
D	423	ALA	-	insertion	UNP P04035
D	424	MET	-	insertion	UNP P04035
D	425	ALA	-	insertion	UNP P04035
D	485	ILE	MET	engineered mutation	UNP P04035

- Molecule 2 is (3R,5R)-3,5-dihydroxy-7-[(1S,2S,8S,8aR)-2-methyl-8-{[(2S)-2-methylbutanoyl]oxy}-1,2,6,7,8,8a-hexahydronaphthalen-1-yl]h eptanoic acid (three-letter code: 114) (formula: $C_{23}H_{36}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 29 23 6	0	0
2	B	1	Total C O 29 23 6	0	0
2	C	1	Total C O 29 23 6	0	0
2	D	1	Total C O 29 23 6	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is water.

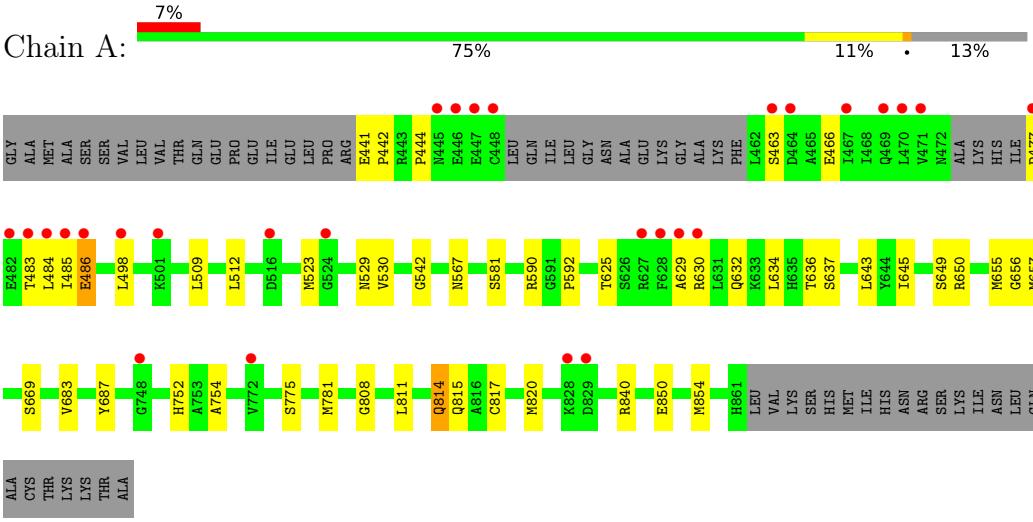
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total	O	0	0
			66	66		
4	B	79	Total	O	0	0
			79	79		
4	C	67	Total	O	0	0
			67	67		
4	D	75	Total	O	0	0
			75	75		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

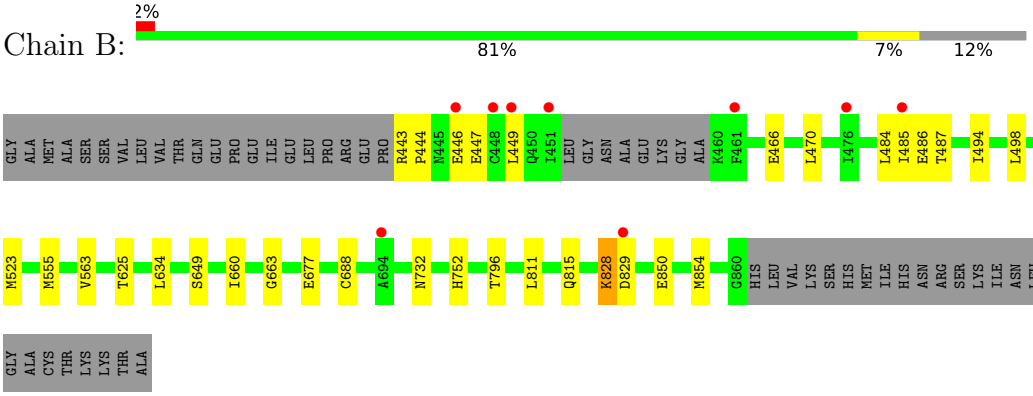
• Molecule 1: HMG-COA REDUCTASE

Chain A:



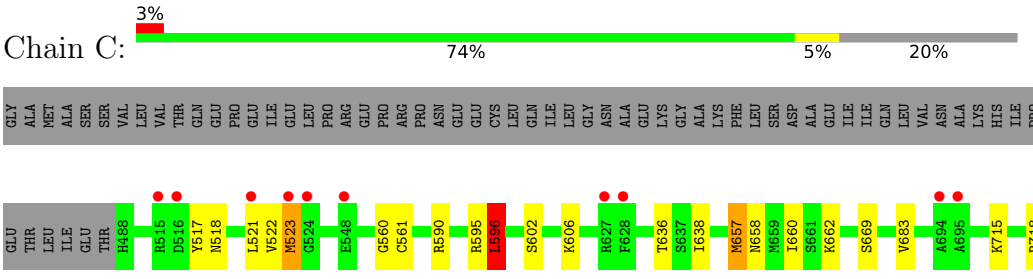
• Molecule 1: HMG-COA REDUCTASE

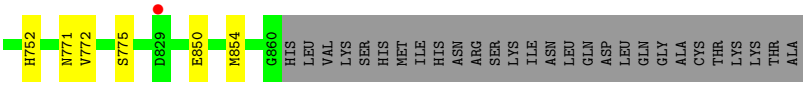
Chain B:



• Molecule 1: HMG-COA REDUCTASE

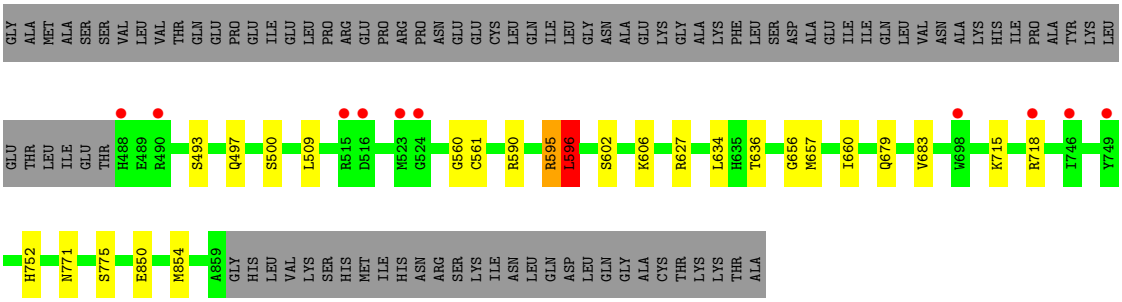
Chain C:





• Molecule 1: HMG-COA REDUCTASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.83Å 173.00Å 75.18Å 90.00° 118.38° 90.00°	Depositor
Resolution (Å)	43.13 – 2.10 52.54 – 2.09	Depositor EDS
% Data completeness (in resolution range)	92.7 (43.13-2.10) 88.2 (52.54-2.09)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 2.08Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.191 , 0.223 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.006 for -h-l,k,h 0.006 for l,k,-h-l 0.028 for h,-k,-h-l 0.029 for -h-l,-k,l 0.019 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12022	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, 114

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.49	0/3046	0.68	0/4117
1	B	0.52	0/3098	0.68	0/4187
1	C	0.50	0/2794	0.67	1/3776 (0.0%)
1	D	0.53	0/2790	0.70	1/3771 (0.0%)
All	All	0.51	0/11728	0.68	2/15851 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	596	LEU	CA-CB-CG	-6.27	100.89	115.30
1	D	596	LEU	CA-CB-CG	-6.14	101.18	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3004	0	3026	38	0
1	B	3055	0	3094	18	0
1	C	2755	0	2784	20	0
1	D	2751	0	2781	13	0
2	A	29	0	35	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	29	0	35	0	0
2	C	29	0	35	2	0
2	D	29	0	35	1	0
3	B	27	0	12	3	0
3	D	27	0	12	1	0
4	A	66	0	0	0	0
4	B	79	0	0	0	0
4	C	67	0	0	1	0
4	D	75	0	0	0	0
All	All	12022	0	11849	87	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (87) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:828:LYS:HD2	1:B:828:LYS:H	1.19	1.08
1:B:828:LYS:HD2	1:B:828:LYS:N	1.99	0.74
1:B:555:MET:HE3	1:B:563:VAL:HG22	1.71	0.73
1:A:529:ASN:ND2	3:B:101:ADP:H2	1.88	0.72
1:A:581:SER:OG	1:A:840:ARG:HD2	1.94	0.67
1:B:828:LYS:H	1:B:828:LYS:CD	1.90	0.66
1:A:683:VAL:HG11	2:A:2:114:H221	1.77	0.66
1:A:529:ASN:HD22	3:B:101:ADP:H2	1.40	0.66
1:A:655:MET:SD	1:A:657:MET:HG2	2.36	0.66
1:D:596:LEU:HD13	1:D:602:SER:HA	1.81	0.63
1:D:595:ARG:HD2	1:D:679:GLN:OE1	1.98	0.63
1:C:518:ASN:HD21	1:C:521:LEU:HD13	1.64	0.60
1:A:542:GLY:H	1:A:567:ASN:ND2	2.00	0.59
1:A:636:THR:CG2	1:A:643:LEU:HD11	2.34	0.58
1:A:529:ASN:ND2	3:B:101:ADP:C2	2.72	0.57
1:A:625:THR:CG2	1:A:666:LYS:HG3	2.33	0.57
1:A:590:ARG:NH2	1:A:657:MET:HE3	2.20	0.56
1:A:817:CYS:HA	1:A:820:MET:HE3	1.87	0.56
1:A:523:MET:HE1	1:A:530:VAL:HG21	1.88	0.56
1:A:656:GLY:O	1:A:660:ILE:HG12	2.07	0.55
1:C:850:GLU:O	1:C:854:MET:HG2	2.07	0.54
1:A:811:LEU:HB2	1:A:814:GLN:HG2	1.91	0.53
1:A:632:GLN:NE2	1:A:650:ARG:HG2	2.23	0.53
1:C:658:ASN:O	1:C:662:LYS:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:GLY:H	1:A:567:ASN:HD22	1.57	0.52
1:A:683:VAL:CG1	2:A:2:114:H221	2.39	0.52
1:D:850:GLU:O	1:D:854:MET:HG2	2.09	0.52
1:B:446:GLU:O	1:B:449:LEU:HG	2.09	0.52
1:B:649:SER:HB3	1:B:660:ILE:CD1	2.40	0.51
1:C:596:LEU:HD13	1:C:602:SER:HA	1.92	0.51
1:A:625:THR:HG22	1:A:666:LYS:HG3	1.92	0.50
1:C:518:ASN:ND2	1:C:521:LEU:HD13	2.27	0.50
1:A:781:MET:CE	1:A:854:MET:HG3	2.42	0.50
1:D:606:LYS:HG3	1:D:636:THR:OG1	2.12	0.50
1:D:715:LYS:HG3	1:D:718:ARG:NH2	2.26	0.49
1:A:485:ILE:CG2	1:A:486:GLU:N	2.76	0.49
1:C:523:MET:HE1	4:C:1172:HOH:O	2.13	0.49
1:A:477:PRO:O	1:A:478:ALA:HB3	2.13	0.49
1:A:441:GLU:N	1:A:442:PRO:CD	2.76	0.48
1:A:754:ALA:HA	1:A:775:SER:OG	2.14	0.48
1:C:606:LYS:HG3	1:C:636:THR:OG1	2.14	0.48
1:B:485:ILE:HD13	1:B:494:ILE:HD12	1.94	0.47
1:C:683:VAL:HG11	2:C:4:114:H221	1.95	0.47
1:C:715:LYS:HG3	1:C:718:ARG:NH2	2.29	0.47
1:D:683:VAL:HG11	2:D:3:114:H221	1.95	0.47
1:A:480:LYS:O	1:A:483:THR:HG22	2.15	0.47
1:B:498:LEU:O	1:B:501:LYS:HG2	2.14	0.47
1:C:715:LYS:HB3	1:C:715:LYS:NZ	2.30	0.47
1:D:715:LYS:HB3	1:D:715:LYS:NZ	2.29	0.47
1:A:484:LEU:HD22	1:A:485:ILE:HD12	1.97	0.46
1:B:850:GLU:O	1:B:854:MET:HG2	2.16	0.46
1:D:590:ARG:HA	1:D:590:ARG:HD3	1.75	0.45
1:C:517:TYR:HE2	1:C:522:VAL:HG21	1.82	0.45
1:B:811:LEU:O	1:B:815:GLN:HG3	2.17	0.45
1:A:850:GLU:O	1:A:854:MET:HG2	2.17	0.45
1:A:629:ALA:O	1:A:630:ARG:HD2	2.16	0.45
1:B:466:GLU:O	1:B:470:LEU:HD13	2.16	0.45
1:B:449:LEU:HD23	1:B:449:LEU:HA	1.82	0.44
1:C:657:MET:HA	1:C:657:MET:CE	2.47	0.44
1:D:771:ASN:OD1	1:D:775:SER:OG	2.34	0.44
1:B:447:GLU:C	1:B:449:LEU:H	2.20	0.44
1:A:592:PRO:HD2	1:A:645:ILE:O	2.17	0.44
1:A:590:ARG:HD3	1:A:590:ARG:HA	1.61	0.43
1:A:479:TYR:HB3	1:A:529:ASN:HD21	1.84	0.43
1:B:732:ASN:HA	1:B:854:MET:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:GLY:O	1:C:561:CYS:HB2	2.18	0.43
1:A:629:ALA:C	1:A:630:ARG:HD2	2.39	0.43
1:C:590:ARG:HB2	1:C:660:ILE:HG22	2.00	0.43
1:B:677:GLU:H	1:B:677:GLU:CD	2.21	0.43
1:C:772:VAL:HG23	1:D:771:ASN:ND2	2.34	0.43
1:A:630:ARG:O	1:A:632:GLN:NE2	2.52	0.43
1:C:771:ASN:OD1	1:C:775:SER:OG	2.36	0.43
1:A:463:SER:OG	1:A:466:GLU:HG3	2.19	0.43
1:C:590:ARG:HA	1:C:590:ARG:HD3	1.72	0.42
1:A:649:SER:HB3	1:A:660:ILE:HD12	2.01	0.41
1:D:493:SER:O	1:D:497:GLN:HG3	2.19	0.41
1:C:523:MET:HA	1:C:523:MET:CE	2.50	0.41
1:D:656:GLY:HA2	3:D:102:ADP:O1B	2.21	0.41
1:A:781:MET:HE3	1:A:854:MET:HG3	2.01	0.41
1:B:625:THR:HG21	1:B:663:GLY:HA2	2.01	0.41
1:A:811:LEU:O	1:A:815:GLN:HG3	2.21	0.41
1:A:637:SER:HB2	1:A:687:TYR:OH	2.21	0.41
1:A:808:GLY:O	1:A:814:GLN:HG3	2.22	0.40
1:B:796:THR:HG21	1:C:638:ILE:O	2.20	0.40
1:B:443:ARG:HA	1:B:444:PRO:HD3	1.95	0.40
1:D:560:GLY:O	1:D:561:CYS:HB2	2.20	0.40
1:C:683:VAL:CG1	2:C:4:114:H221	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	398/467 (85%)	381 (96%)	14 (4%)	3 (1%)	19 15
1	B	406/467 (87%)	389 (96%)	17 (4%)	0	100 100
1	C	371/467 (79%)	359 (97%)	12 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	370/467 (79%)	356 (96%)	14 (4%)	0	100 100
All	All	1545/1868 (83%)	1485 (96%)	57 (4%)	3 (0%)	47 49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	478	ALA
1	A	486	GLU
1	A	444	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	323/375 (86%)	316 (98%)	7 (2%)	52 57
1	B	328/375 (88%)	318 (97%)	10 (3%)	41 44
1	C	294/375 (78%)	288 (98%)	6 (2%)	55 60
1	D	294/375 (78%)	285 (97%)	9 (3%)	40 43
All	All	1239/1500 (83%)	1207 (97%)	32 (3%)	46 50

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	498	LEU
1	A	509	LEU
1	A	512	LEU
1	A	634	LEU
1	A	669	SER
1	A	752	HIS
1	A	814	GLN
1	B	484	LEU
1	B	486	GLU
1	B	487	THR
1	B	505	GLU

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Mol	Chain	Res	Type
1	B	523	MET
1	B	634	LEU
1	B	688	CYS
1	B	752	HIS
1	B	828	LYS
1	B	829	ASP
1	C	523	MET
1	C	595	ARG
1	C	596	LEU
1	C	657	MET
1	C	669	SER
1	C	752	HIS
1	D	500	SER
1	D	509	LEU
1	D	595	ARG
1	D	596	LEU
1	D	627	ARG
1	D	634	LEU
1	D	657	MET
1	D	660	ILE
1	D	752	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	488	HIS
1	A	518	ASN
1	A	529	ASN
1	A	567	ASN
1	A	632	GLN
1	B	472	ASN
1	B	488	HIS
1	B	510	GLN
1	B	635	HIS
1	D	642	ASN
1	D	672	HIS
1	D	788	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ADP	D	102	-	24,29,29	1.42	3 (12%)	29,45,45	0.81	1 (3%)
2	114	A	2	-	27,30,30	1.68	5 (18%)	34,41,41	1.07	3 (8%)
2	114	B	1	-	27,30,30	1.71	8 (29%)	34,41,41	1.18	5 (14%)
2	114	C	4	-	27,30,30	1.67	5 (18%)	34,41,41	1.22	5 (14%)
2	114	D	3	-	27,30,30	1.74	5 (18%)	34,41,41	1.14	2 (5%)
3	ADP	B	101	-	24,29,29	1.27	2 (8%)	29,45,45	0.77	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	D	102	-	-	5/12/32/32	0/3/3/3
2	114	A	2	-	1/1/10/13	4/21/50/50	0/2/2/2
2	114	B	1	-	-	2/21/50/50	0/2/2/2
2	114	C	4	-	-	2/21/50/50	0/2/2/2
2	114	D	3	-	-	0/21/50/50	0/2/2/2
3	ADP	B	101	-	-	2/12/32/32	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	114	C9-C8	4.49	1.59	1.54
2	B	1	114	C9-C8	4.24	1.58	1.54
2	D	3	114	C13-C12	4.14	1.57	1.52
2	C	4	114	C9-C8	4.02	1.58	1.54
2	A	2	114	C9-C8	3.83	1.58	1.54
2	C	4	114	C13-C12	3.83	1.57	1.52
2	A	2	114	C13-C12	3.64	1.57	1.52
3	B	101	ADP	C8-N7	-3.50	1.28	1.34
2	B	1	114	C13-C12	3.44	1.57	1.52
3	D	102	ADP	C8-N7	-3.32	1.28	1.34
3	D	102	ADP	O4'-C4'	3.14	1.52	1.45
2	C	4	114	C9-C10	3.14	1.55	1.50
2	C	4	114	C13-C8	2.75	1.58	1.54
2	A	2	114	C9-C10	2.72	1.54	1.50
2	D	3	114	C9-C10	2.71	1.54	1.50
2	B	1	114	C13-C8	2.57	1.58	1.54
2	A	2	114	C13-C8	2.48	1.58	1.54
3	B	101	ADP	O4'-C4'	2.42	1.50	1.45
2	D	3	114	C11-C12	-2.27	1.36	1.43
2	B	1	114	C9-C10	2.26	1.53	1.50
2	B	1	114	C15-C14	2.23	1.56	1.52
2	D	3	114	C13-C8	2.19	1.57	1.54
2	B	1	114	O14-C18	2.15	1.39	1.34
2	A	2	114	C15-C14	2.11	1.56	1.52
2	C	4	114	C11-C12	-2.03	1.37	1.43
2	B	1	114	C11-C10	2.03	1.37	1.33
3	D	102	ADP	C2'-C3'	2.02	1.58	1.53
2	B	1	114	C11-C12	-2.02	1.37	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	3	114	C7-C8-C9	3.64	115.21	112.87
2	D	3	114	C9A-C9-C10	-2.87	106.33	110.85
2	C	4	114	C7-C8-C9	2.82	114.68	112.87
2	A	2	114	C9A-C9-C10	-2.71	106.57	110.85
2	C	4	114	C13-C8-C9	-2.69	109.27	110.70
2	B	1	114	C7-C8-C9	2.62	114.56	112.87
2	C	4	114	C9A-C9-C10	-2.56	106.81	110.85
2	B	1	114	C7-C8-C13	2.44	115.82	112.50
2	C	4	114	O14-C14-C15	2.41	112.90	108.46
2	B	1	114	C9A-C9-C10	-2.37	107.11	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2	114	C7-C8-C9	2.33	114.36	112.87
2	B	1	114	C13-C8-C9	2.29	111.91	110.70
2	B	1	114	C15-C16-C17	2.17	115.46	111.85
2	A	2	114	C15-C16-C17	2.15	115.44	111.85
3	D	102	ADP	C5-C6-N6	2.12	123.57	120.35
2	C	4	114	C15-C16-C17	2.12	115.38	111.85
3	B	101	ADP	C5-C6-N6	2.06	123.49	120.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2	114	C19

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	114	C22-C19-C20-C21
3	B	101	ADP	O4'-C4'-C5'-O5'
3	B	101	ADP	C3'-C4'-C5'-O5'
3	D	102	ADP	PA-O3A-PB-O3B
3	D	102	ADP	C3'-C4'-C5'-O5'
2	A	2	114	C18-C19-C20-C21
2	C	4	114	C18-C19-C20-C21
2	A	2	114	C22-C19-C20-C21
3	D	102	ADP	O4'-C4'-C5'-O5'
2	A	2	114	O14-C18-C19-C20
2	B	1	114	C18-C19-C20-C21
2	A	2	114	O18-C18-C19-C20
3	D	102	ADP	C4'-C5'-O5'-PA
2	B	1	114	C22-C19-C20-C21
3	D	102	ADP	PA-O3A-PB-O1B

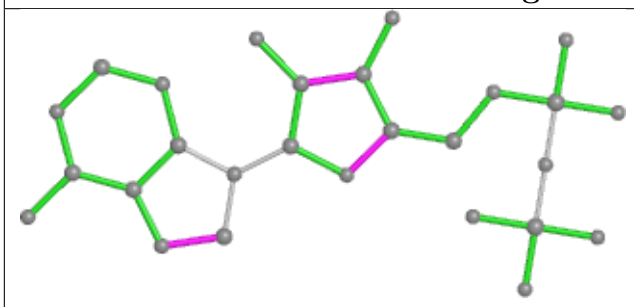
There are no ring outliers.

5 monomers are involved in 9 short contacts:

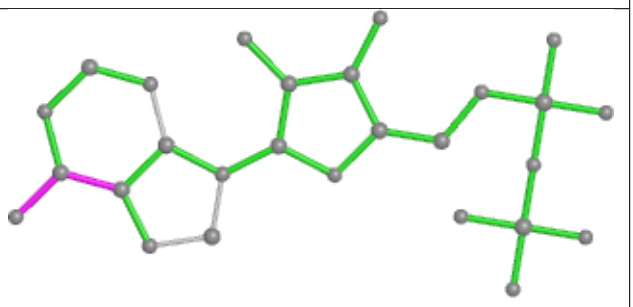
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	102	ADP	1	0
2	A	2	114	2	0
2	C	4	114	2	0
2	D	3	114	1	0
3	B	101	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

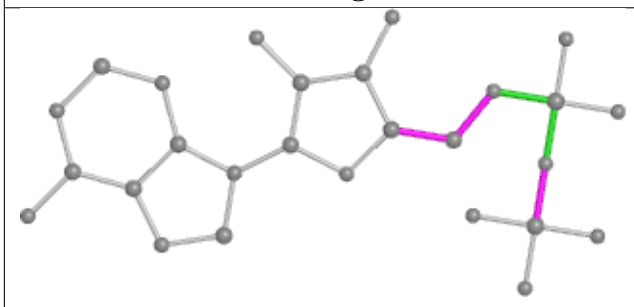
Ligand ADP D 102



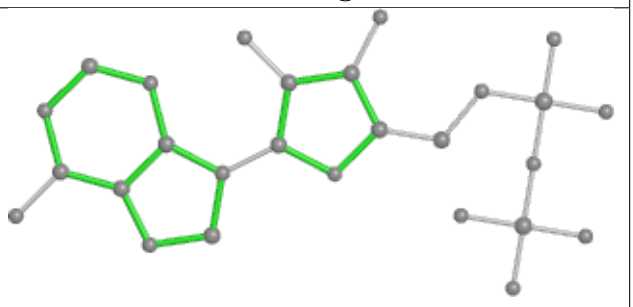
Bond lengths



Bond angles

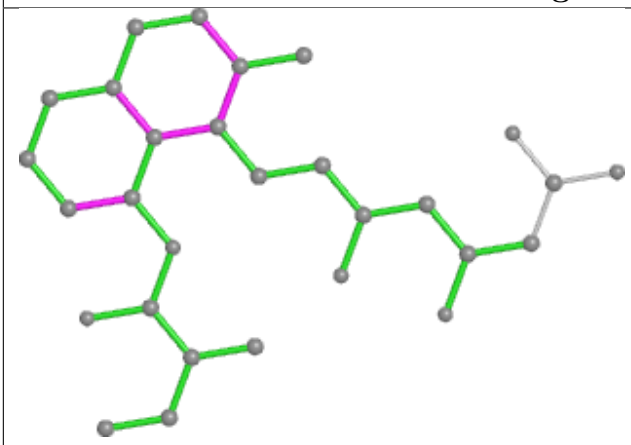


Torsions

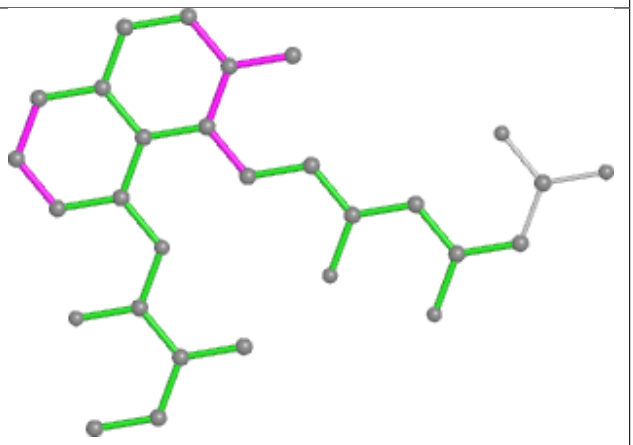


Rings

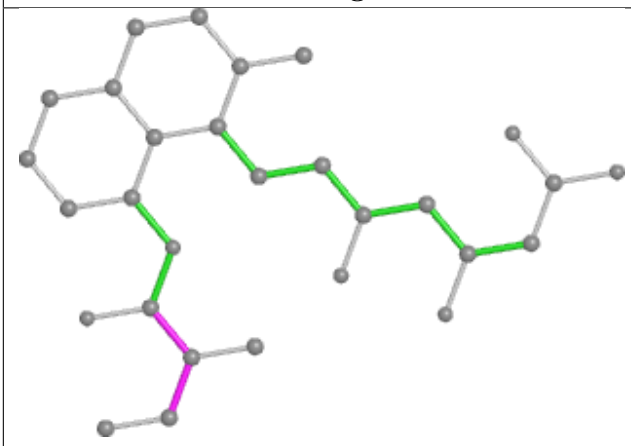
Ligand 114 A 2



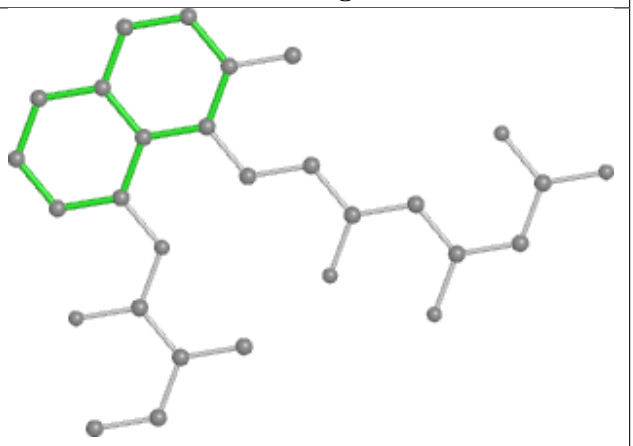
Bond lengths



Bond angles

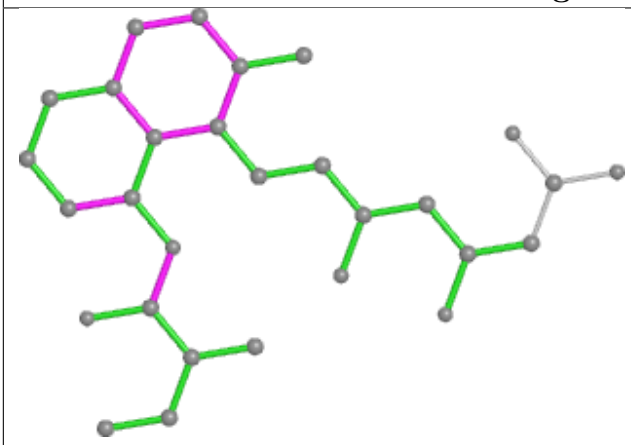


Torsions

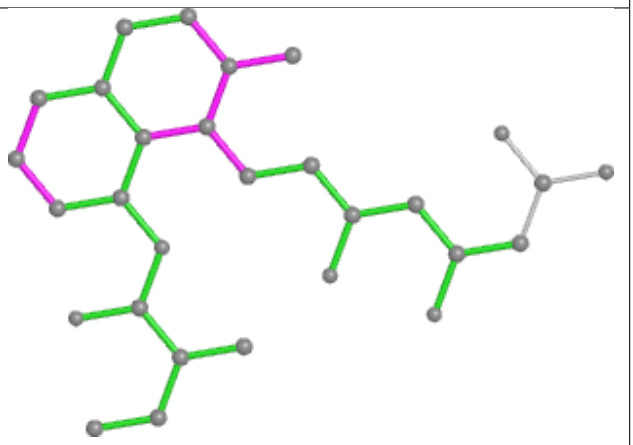


Rings

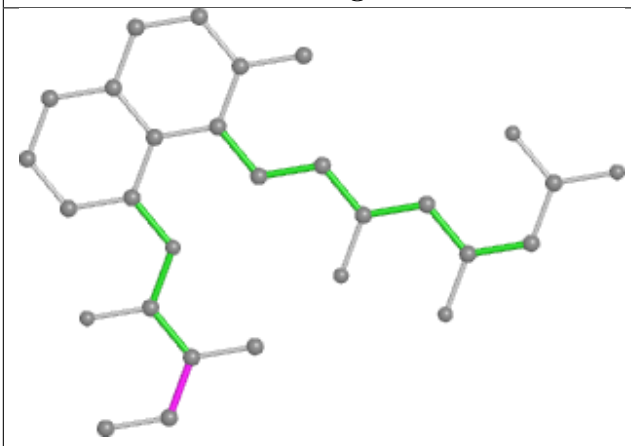
Ligand 114 B 1



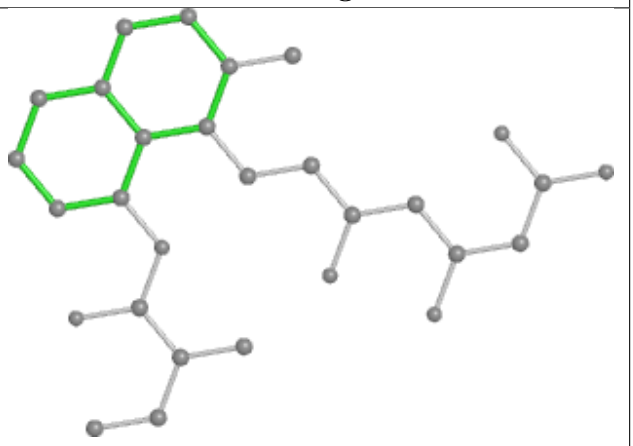
Bond lengths



Bond angles

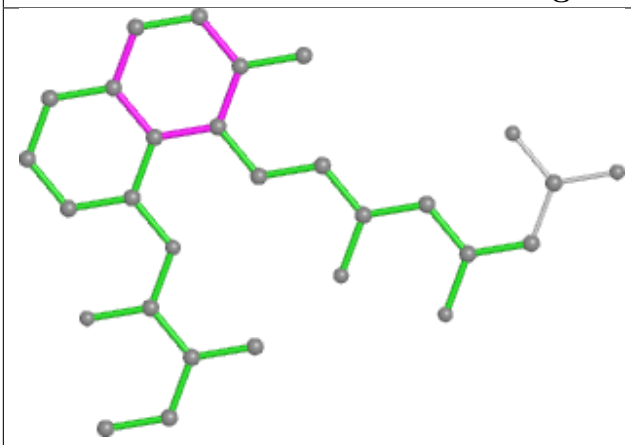


Torsions

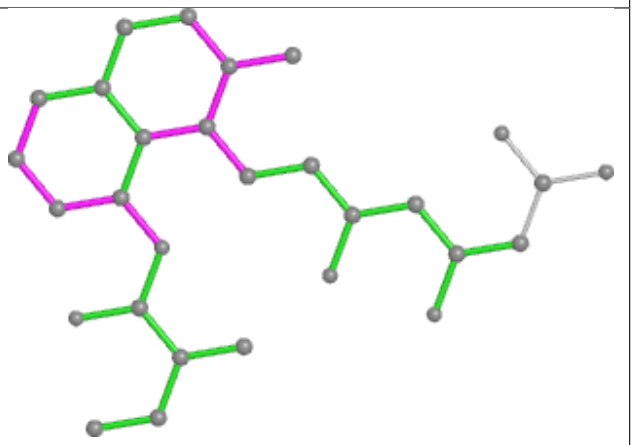


Rings

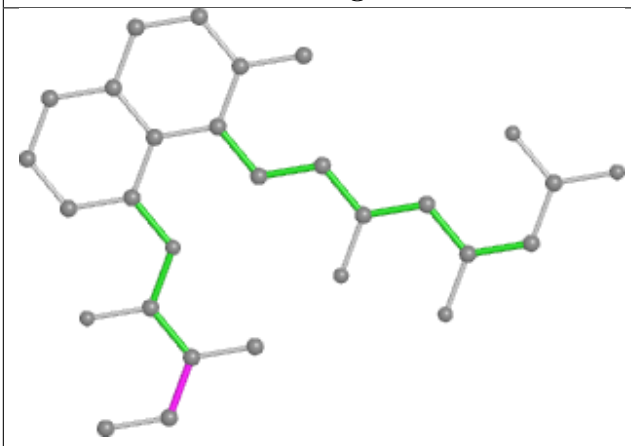
Ligand 114 C 4



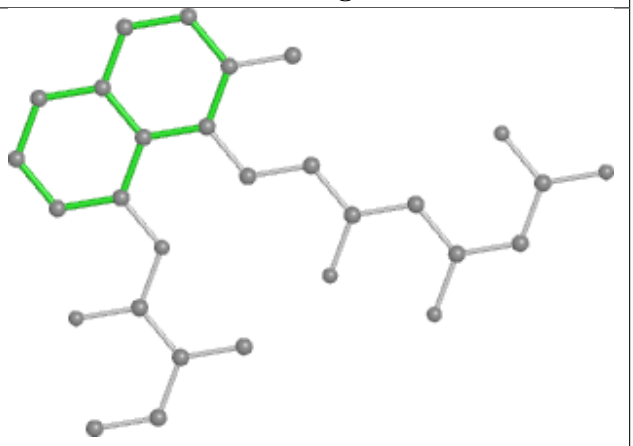
Bond lengths



Bond angles

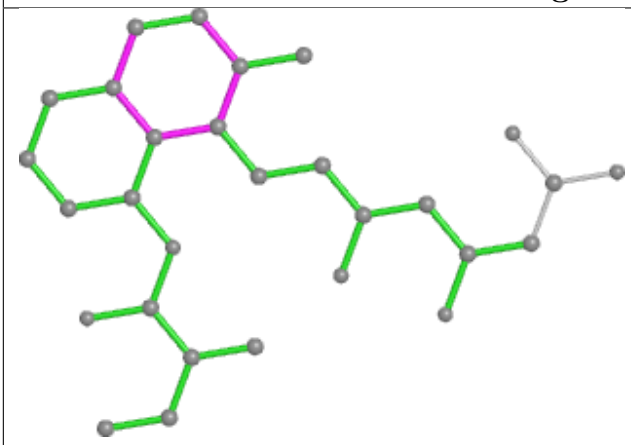


Torsions

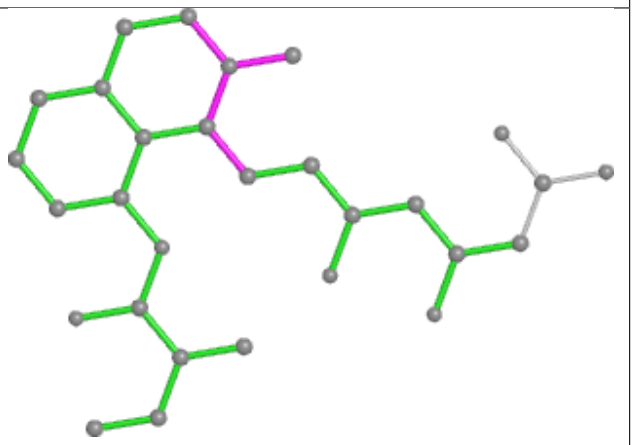


Rings

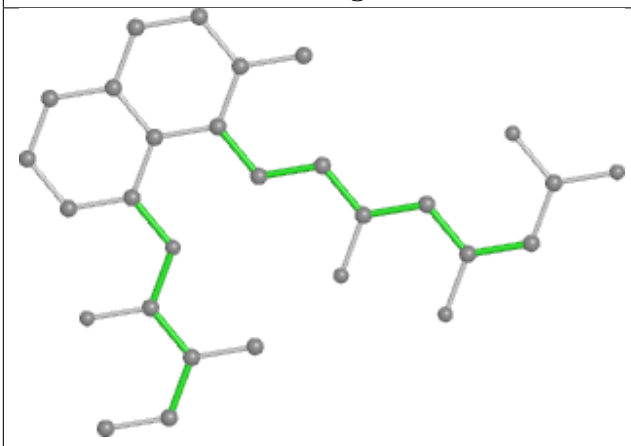
Ligand 114 D 3



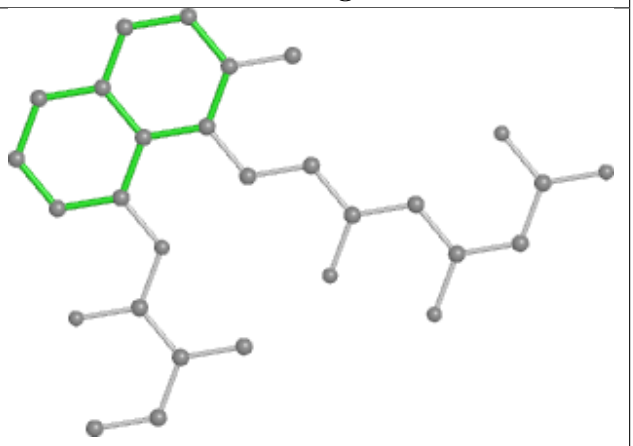
Bond lengths



Bond angles

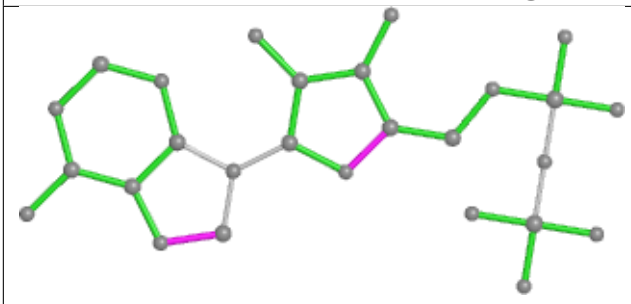


Torsions

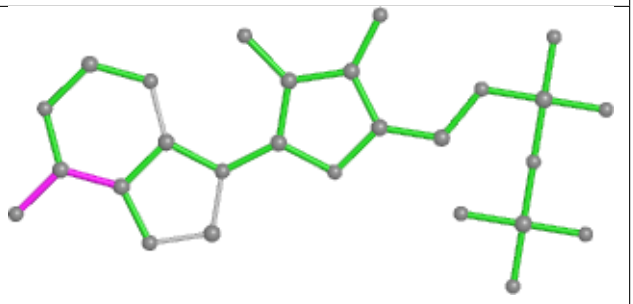


Rings

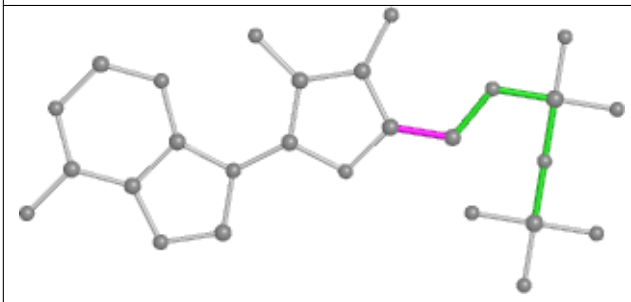
Ligand ADP B 101



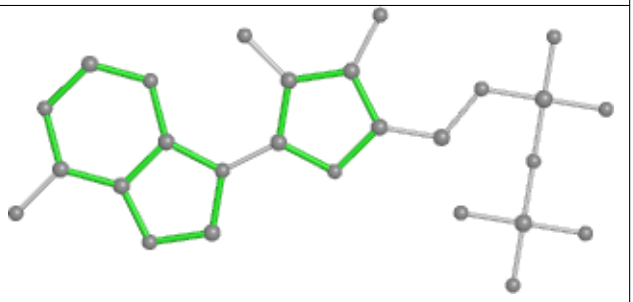
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	404/467 (86%)	0.13	32 (7%)	12	16	20, 34, 69, 99	0
1	B	410/467 (87%)	-0.07	9 (2%)	62	66	20, 33, 60, 88	0
1	C	373/467 (79%)	0.05	13 (3%)	44	50	20, 33, 54, 80	0
1	D	372/467 (79%)	-0.13	10 (2%)	54	60	21, 32, 50, 61	0
All	All	1559/1868 (83%)	-0.00	64 (4%)	37	43	20, 33, 57, 99	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	LEU	9.0
1	C	524	GLY	7.1
1	A	448	CYS	5.1
1	A	470	LEU	5.1
1	A	829	ASP	4.8
1	A	482	GLU	4.6
1	A	446	GLU	4.2
1	A	479	TYR	4.2
1	D	523	MET	3.9
1	B	448	CYS	3.7
1	A	447	GLU	3.6
1	A	445	ASN	3.5
1	D	746	ILE	3.5
1	A	478	ALA	3.3
1	D	524	GLY	3.3
1	B	449	LEU	3.3
1	A	628	PHE	3.2
1	A	485	ILE	3.2
1	C	523	MET	3.1
1	A	486	GLU	3.1
1	A	464	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	471	VAL	3.0
1	B	446	GLU	2.9
1	C	627	ARG	2.9
1	A	828	LYS	2.9
1	A	477	PRO	2.8
1	A	627	ARG	2.8
1	A	501	LYS	2.8
1	C	746	ILE	2.7
1	B	461	PHE	2.7
1	D	490	ARG	2.7
1	A	467	ILE	2.7
1	A	483	THR	2.7
1	A	480	LYS	2.6
1	A	524	GLY	2.5
1	A	516	ASP	2.5
1	D	718	ARG	2.5
1	C	749	TYR	2.4
1	C	829	ASP	2.4
1	A	772	VAL	2.3
1	C	695	ALA	2.3
1	D	516	ASP	2.2
1	B	694	ALA	2.2
1	A	630	ARG	2.2
1	B	451	ILE	2.2
1	C	628	PHE	2.2
1	B	476	ILE	2.1
1	D	488	HIS	2.1
1	D	749	TYR	2.1
1	B	829	ASP	2.1
1	C	694	ALA	2.1
1	C	548	GLU	2.1
1	A	498	LEU	2.1
1	C	516	ASP	2.1
1	A	748	GLY	2.1
1	A	463	SER	2.1
1	B	485	ILE	2.1
1	A	481	LEU	2.1
1	A	629	ALA	2.1
1	D	515	ARG	2.1
1	D	698	TRP	2.1
1	C	515	ARG	2.0
1	A	469	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	521	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

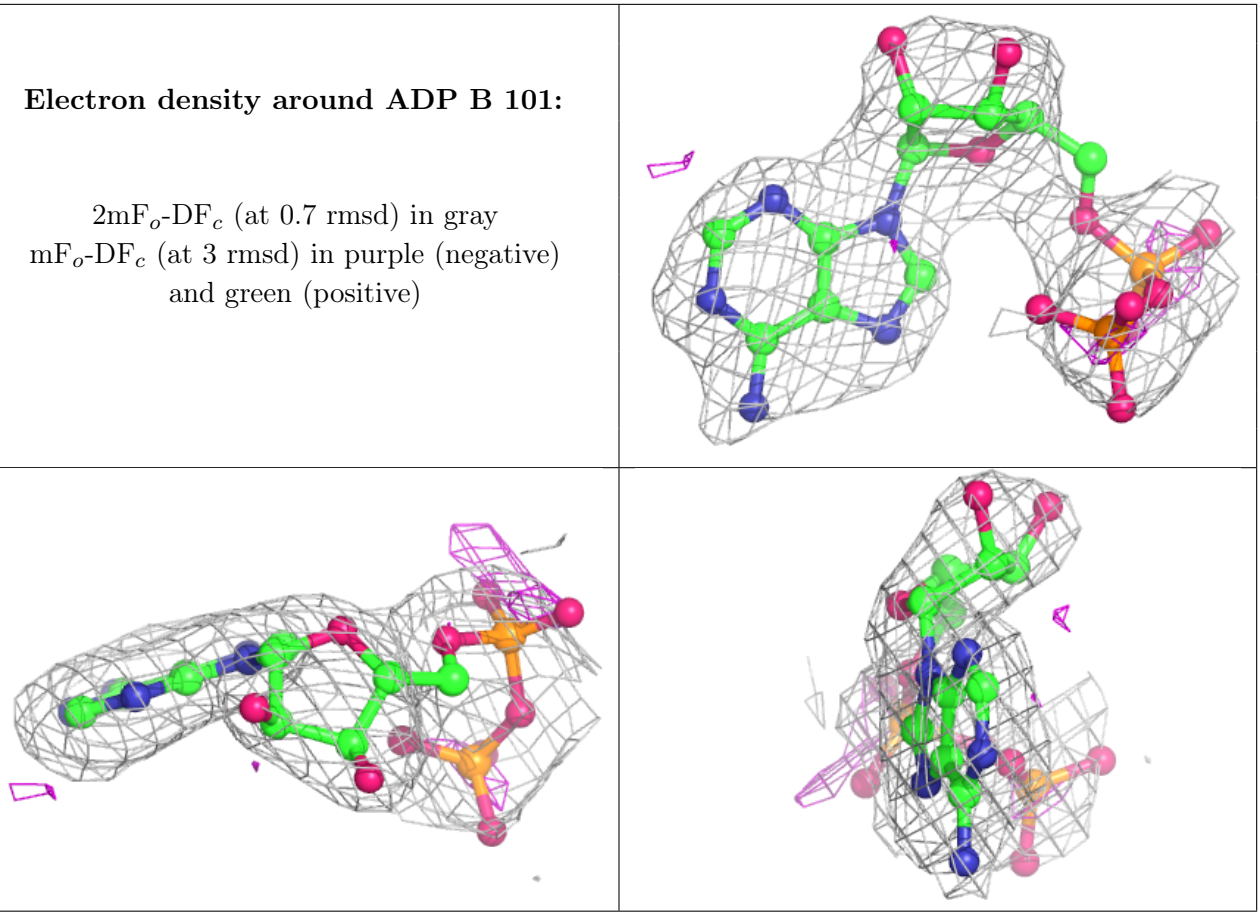
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	B	101	27/27	0.71	0.24	83,90,100,100	0
3	ADP	D	102	27/27	0.83	0.16	58,67,80,81	0
2	114	C	4	29/29	0.87	0.13	30,40,47,48	0
2	114	A	2	29/29	0.91	0.12	33,40,47,49	0
2	114	B	1	29/29	0.93	0.11	28,36,46,47	0
2	114	D	3	29/29	0.93	0.12	29,41,49,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

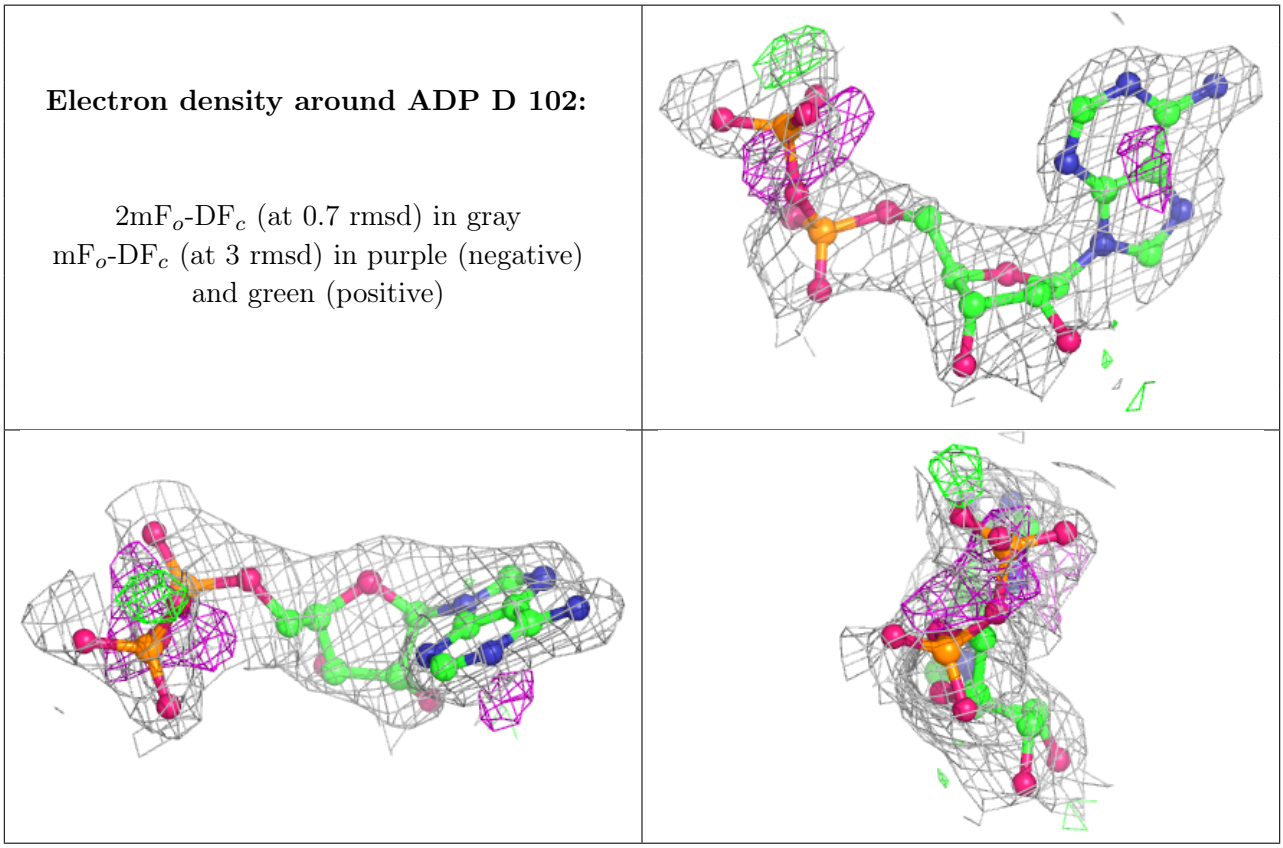
Electron density around ADP B 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



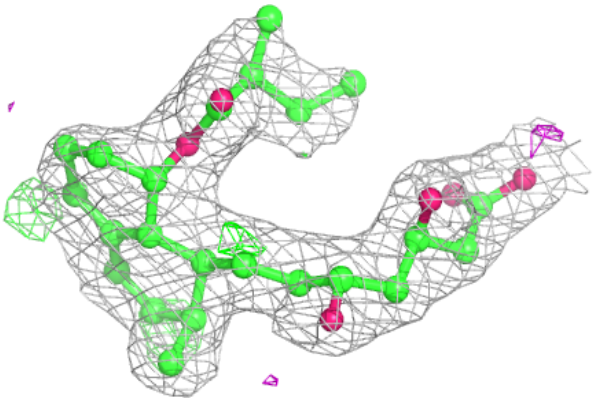
Electron density around ADP D 102:

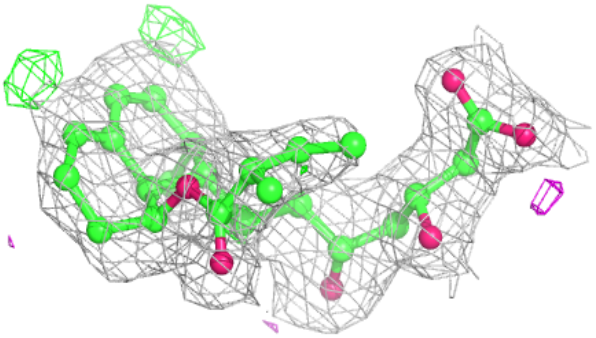
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

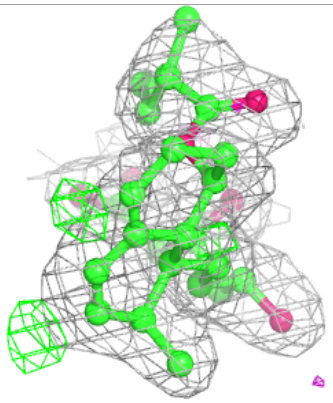


Electron density around 114 C 4:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

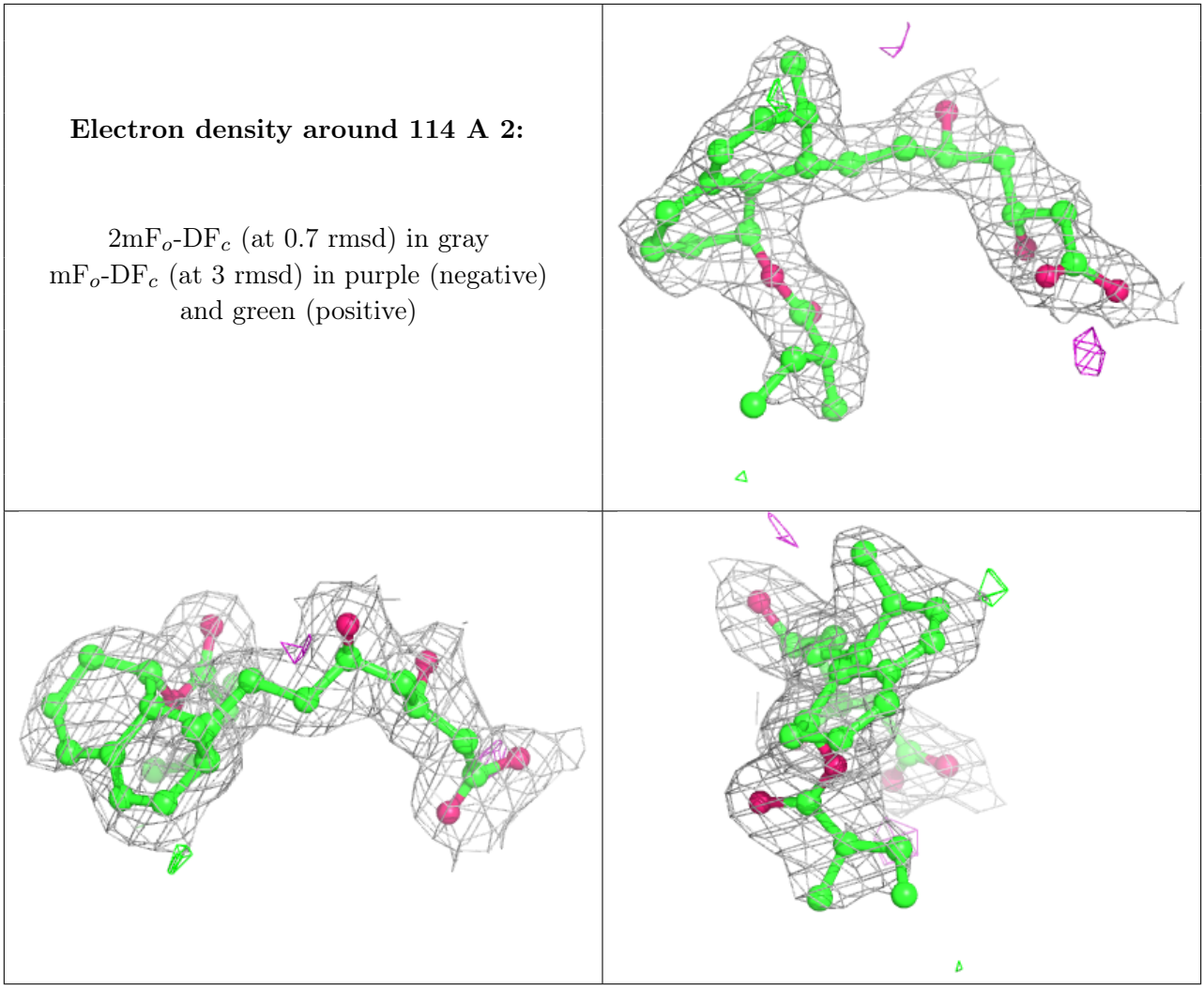






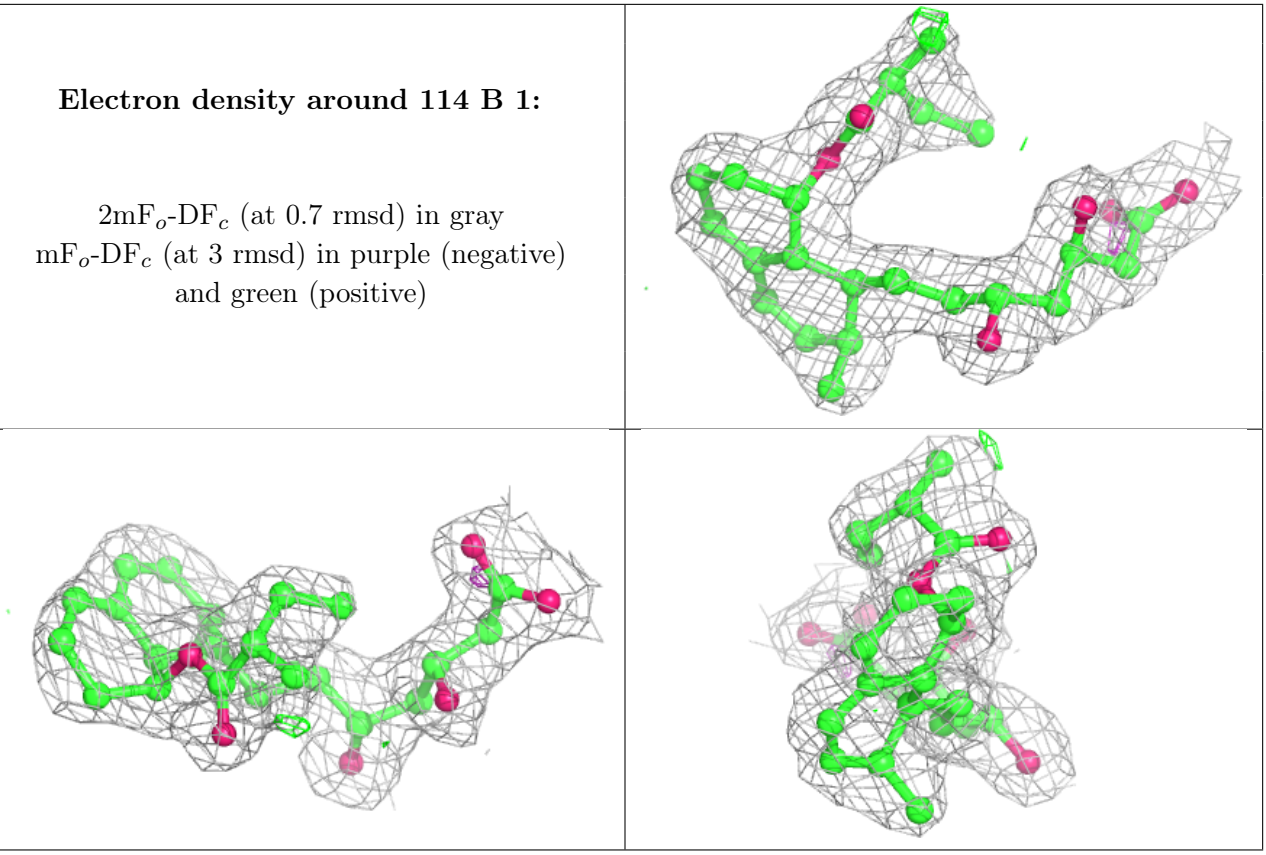
Electron density around 114 A 2:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



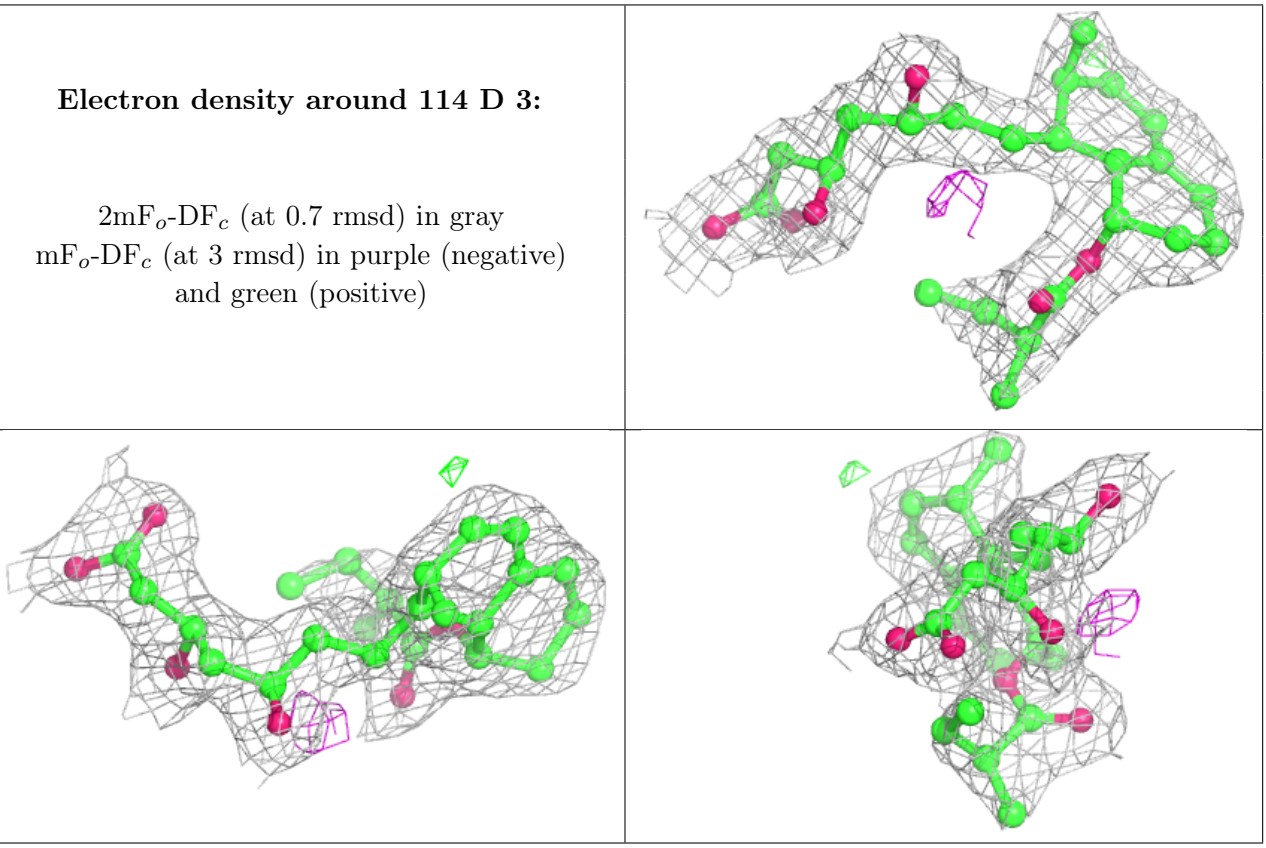
Electron density around 114 B 1:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 114 D 3:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 07:50 AM EDT

PDB ID	:	3CCW
Title	:	Thermodynamic and structure guided design of statin hmg-coa reductase inhibitors
Authors	:	Pavlovsky, A.; Sarver, R.W.; Harris, M.S.; Finzel, B.C.
Deposited on	:	2008-02-26
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

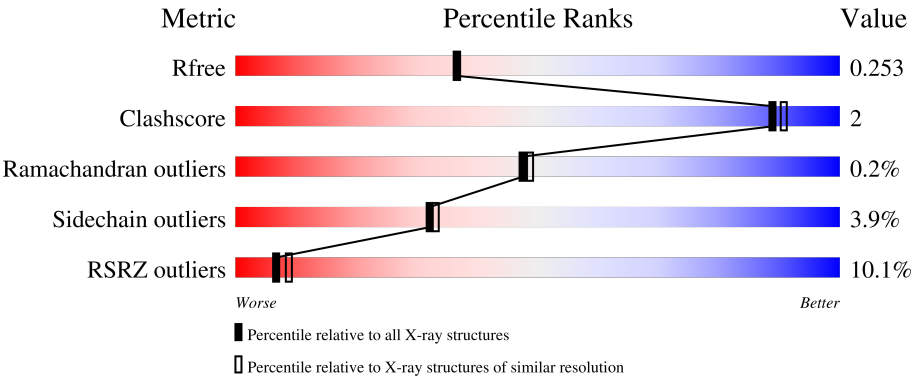
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	441	14% 87% 7% • 5%
1	B	441	7% 86% 9% 5%
1	C	441	9% 88% 5% 6%
1	D	441	9% 83% 6% 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12823 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3-hydroxy-3-methylglutaryl-coenzyme A reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3133	1951	551	601	30			
1	B	421	Total	C	N	O	S	0	0	0
			3133	1951	551	601	30			
1	C	414	Total	C	N	O	S	0	0	0
			3073	1915	538	590	30			
1	D	394	Total	C	N	O	S	0	0	0
			2920	1818	514	559	29			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	435	HIS	-	expression tag	UNP P04035
A	436	HIS	-	expression tag	UNP P04035
A	437	HIS	-	expression tag	UNP P04035
A	438	HIS	-	expression tag	UNP P04035
A	439	HIS	-	expression tag	UNP P04035
A	440	HIS	-	expression tag	UNP P04035
A	485	ILE	MET	engineered mutation	UNP P04035
B	435	HIS	-	expression tag	UNP P04035
B	436	HIS	-	expression tag	UNP P04035
B	437	HIS	-	expression tag	UNP P04035
B	438	HIS	-	expression tag	UNP P04035
B	439	HIS	-	expression tag	UNP P04035
B	440	HIS	-	expression tag	UNP P04035
B	485	ILE	MET	engineered mutation	UNP P04035
C	435	HIS	-	expression tag	UNP P04035
C	436	HIS	-	expression tag	UNP P04035
C	437	HIS	-	expression tag	UNP P04035
C	438	HIS	-	expression tag	UNP P04035
C	439	HIS	-	expression tag	UNP P04035
C	440	HIS	-	expression tag	UNP P04035
C	485	ILE	MET	engineered mutation	UNP P04035

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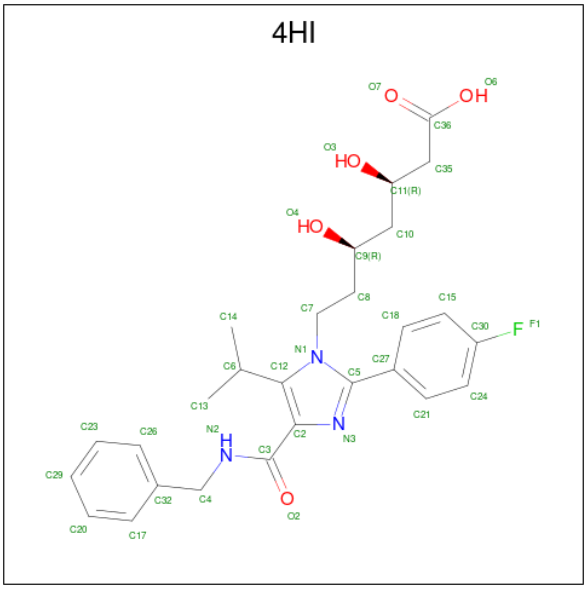
Chain	Residue	Modelled	Actual	Comment	Reference
D	435	HIS	-	expression tag	UNP P04035
D	436	HIS	-	expression tag	UNP P04035
D	437	HIS	-	expression tag	UNP P04035
D	438	HIS	-	expression tag	UNP P04035
D	439	HIS	-	expression tag	UNP P04035
D	440	HIS	-	expression tag	UNP P04035
D	485	ILE	MET	engineered mutation	UNP P04035

- Molecule 2 is (3R,5R)-7-[4-(benzylcarbamoyl)-2-(4-fluorophenyl)-5-(1-methylethyl)-1H-imidazol-1-yl]-3,5-dihydroxyheptanoic acid (three-letter code: 4HI) (formula: $C_{27}H_{32}FN_3O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			36	27	1	3	5		
2	B	1	Total	C	F	N	O	0	0
			36	27	1	3	5		
2	C	1	Total	C	F	N	O	0	0
			36	27	1	3	5		
2	D	1	Total	C	F	N	O	0	0
			36	27	1	3	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	109	Total	O	0	0
			109	109		

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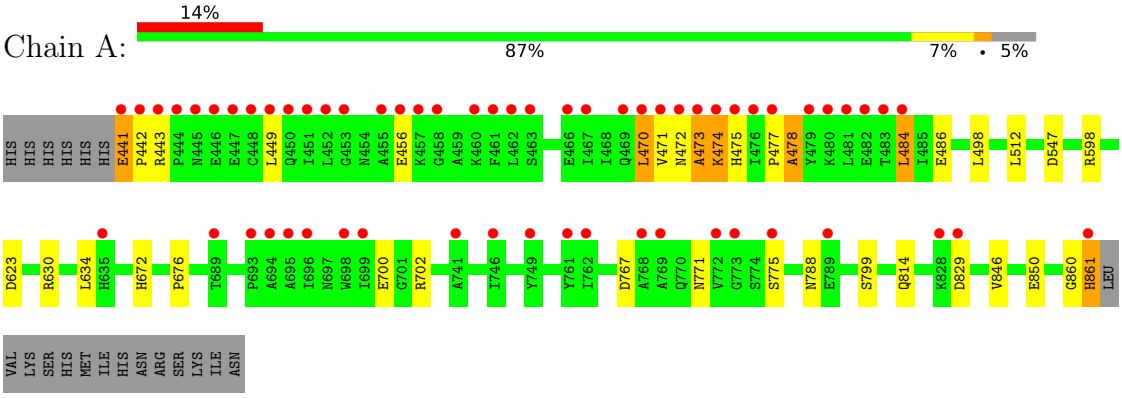
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	113	Total O 113 113	0	0
3	C	89	Total O 89 89	0	0
3	D	109	Total O 109 109	0	0

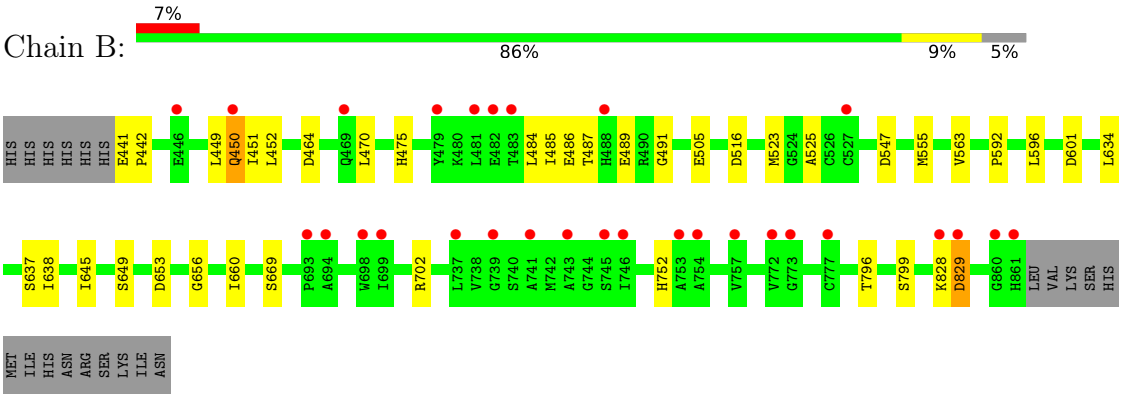
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

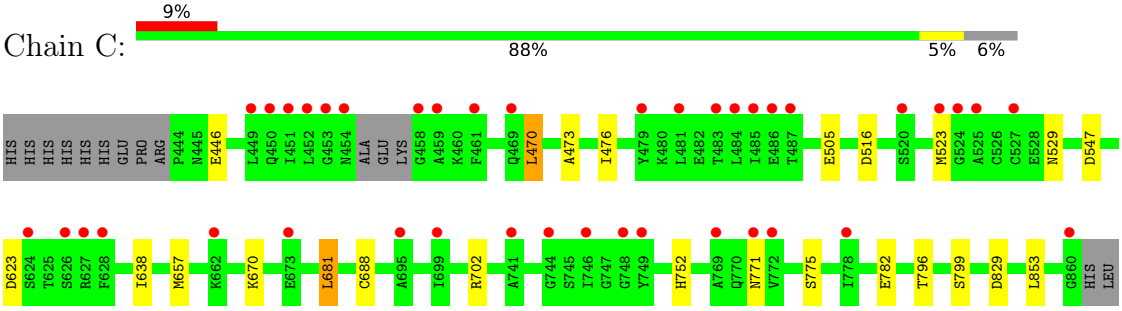
• Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



• Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase

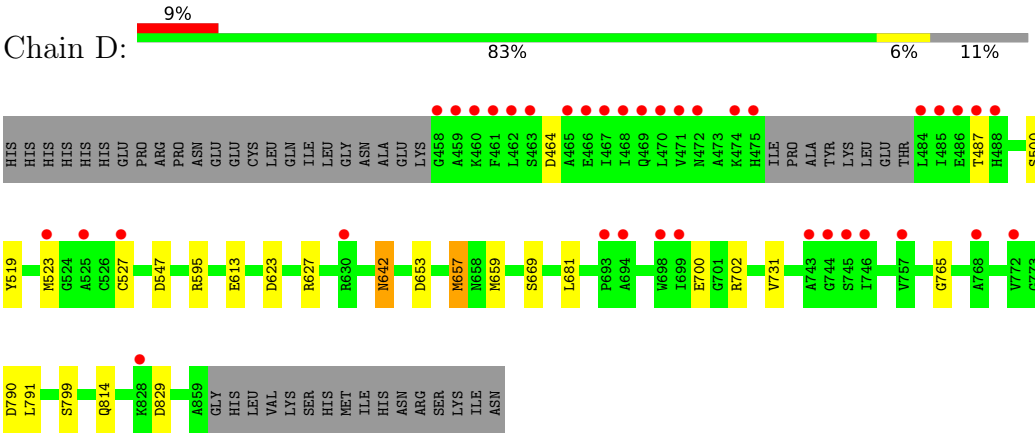


• Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



• Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.93Å 174.38Å 76.08Å 90.00° 118.83° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 38.16 – 2.10	Depositor EDS
% Data completeness (in resolution range)	88.4 (50.00-2.10) 88.4 (38.16-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.217 , 0.252 0.220 , 0.253	Depositor DCC
R_{free} test set	2647 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -h-l,k,h 0.006 for l,k,-h-l 0.027 for h,-k,-h-l 0.027 for -h-l,-k,l 0.029 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12823	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4HI

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.37	0/3179	0.63	4/4298 (0.1%)
1	B	0.37	0/3179	0.63	5/4298 (0.1%)
1	C	0.34	0/3116	0.60	4/4211 (0.1%)
1	D	0.36	0/2960	0.64	7/3999 (0.2%)
All	All	0.36	0/12434	0.62	20/16806 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	623	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	547	ASP	CB-CG-OD2	5.84	123.56	118.30
1	D	547	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	653	ASP	CB-CG-OD2	5.68	123.41	118.30
1	D	653	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	464	ASP	CB-CG-OD2	5.53	123.28	118.30
1	C	623	ASP	CB-CG-OD2	5.47	123.22	118.30
1	D	829	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	767	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	516	ASP	CB-CG-OD2	5.32	123.08	118.30
1	D	790	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	829	ASP	CB-CG-OD2	5.27	123.04	118.30
1	D	464	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	623	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	516	ASP	CB-CG-OD2	5.16	122.95	118.30
1	B	547	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	829	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	547	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	829	ASP	CB-CG-OD2	5.01	122.81	118.30
1	C	516	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3133	0	3167	15	0
1	B	3133	0	3167	14	0
1	C	3073	0	3110	8	0
1	D	2920	0	2957	10	0
2	B	72	0	62	3	0
2	C	36	0	31	0	0
2	D	36	0	31	0	0
3	A	109	0	0	0	0
3	B	113	0	0	0	0
3	C	89	0	0	1	0
3	D	109	0	0	2	0
All	All	12823	0	12525	46	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:LEU:O	1:A:474:LYS:O	2.07	0.72
1:C:771:ASN:OD1	1:C:775:SER:OG	2.11	0.67
1:B:555:MET:HE1	1:B:563:VAL:HA	1.81	0.60
1:A:471:VAL:HG11	1:A:498:LEU:HD21	1.83	0.60
1:C:681:LEU:HD22	1:D:731:VAL:HG22	1.86	0.57
1:D:595:ARG:HD2	1:D:681:LEU:HD22	1.86	0.57
1:A:860:GLY:O	1:A:861:HIS:HB2	2.05	0.57
1:D:642:ASN:HD22	1:D:642:ASN:N	2.01	0.57
2:B:2:4HI:H7	2:B:2:4HI:H13B	1.87	0.55
1:A:477:PRO:O	1:A:478:ALA:HB2	2.08	0.54
1:B:555:MET:CE	1:B:563:VAL:HA	2.38	0.54
1:D:657:MET:HG3	3:D:197:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:ASN:OD1	1:A:775:SER:OG	2.27	0.53
1:A:472:ASN:O	1:A:473:ALA:CB	2.57	0.52
2:B:2:4HI:H8A	2:B:2:4HI:H14B	1.92	0.52
1:A:441:GLU:N	1:A:442:PRO:CD	2.72	0.52
1:A:474:LYS:O	1:A:475:HIS:HB2	2.09	0.52
1:B:449:LEU:HD11	1:B:475:HIS:ND1	2.26	0.50
1:A:477:PRO:O	1:A:478:ALA:CB	2.59	0.49
1:A:700:GLU:OE2	1:D:700:GLU:OE2	2.29	0.49
1:B:485:ILE:HD12	1:B:491:GLY:HA2	1.95	0.48
1:B:450:GLN:HG3	1:B:451:ILE:N	2.29	0.48
1:A:702:ARG:O	1:A:799:SER:HA	2.14	0.48
1:C:529:ASN:ND2	3:C:252:HOH:O	2.48	0.46
1:C:470:LEU:O	1:C:473:ALA:O	2.34	0.46
1:B:796:THR:HG21	1:C:638:ILE:O	2.16	0.46
1:B:555:MET:CE	1:B:563:VAL:HG22	2.46	0.46
1:B:638:ILE:O	1:C:796:THR:HG21	2.16	0.45
1:C:702:ARG:O	1:C:799:SER:HA	2.17	0.45
2:B:1:4HI:H7	2:B:1:4HI:H13B	1.98	0.45
1:B:592:PRO:HD2	1:B:645:ILE:O	2.17	0.45
1:D:519:TYR:O	1:D:523:MET:HG2	2.17	0.45
1:A:846:VAL:O	1:A:850:GLU:HG2	2.17	0.45
1:A:471:VAL:HG11	1:A:498:LEU:CD2	2.45	0.44
1:A:672:HIS:CD2	1:A:676:PRO:HA	2.52	0.44
1:D:700:GLU:OE1	3:D:369:HOH:O	2.21	0.44
1:D:774:SER:HA	1:D:799:SER:O	2.19	0.43
1:B:702:ARG:O	1:B:799:SER:HA	2.19	0.43
1:A:449:LEU:HD11	1:A:475:HIS:ND1	2.34	0.43
1:C:752:HIS:CD2	1:C:853:LEU:HD23	2.53	0.43
1:B:656:GLY:O	1:B:660:ILE:HG12	2.19	0.42
1:D:702:ARG:O	1:D:799:SER:HA	2.20	0.42
1:B:596:LEU:HB3	1:B:601:ASP:HB2	2.02	0.41
1:D:765:GLY:HA2	1:D:814:GLN:HG2	2.03	0.41
1:B:441:GLU:N	1:B:442:PRO:CD	2.85	0.40
1:B:555:MET:HE2	1:B:563:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	419/441 (95%)	398 (95%)	18 (4%)	3 (1%)	22	18
1	B	419/441 (95%)	406 (97%)	12 (3%)	1 (0%)	47	49
1	C	410/441 (93%)	397 (97%)	13 (3%)	0	100	100
1	D	390/441 (88%)	377 (97%)	13 (3%)	0	100	100
All	All	1638/1764 (93%)	1578 (96%)	56 (3%)	4 (0%)	47	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	473	ALA
1	A	478	ALA
1	A	484	LEU
1	B	525	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/355 (94%)	321 (96%)	14 (4%)	30	30
1	B	335/355 (94%)	319 (95%)	16 (5%)	25	24
1	C	329/355 (93%)	319 (97%)	10 (3%)	41	44
1	D	312/355 (88%)	301 (96%)	11 (4%)	36	38
All	All	1311/1420 (92%)	1260 (96%)	51 (4%)	32	33

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	441	GLU
1	A	443	ARG
1	A	456	GLU
1	A	470	LEU
1	A	474	LYS
1	A	484	LEU
1	A	486	GLU
1	A	512	LEU
1	A	598	ARG
1	A	630	ARG
1	A	634	LEU
1	A	788	ASN
1	A	814	GLN
1	A	861	HIS
1	B	450	GLN
1	B	452	LEU
1	B	470	LEU
1	B	484	LEU
1	B	486	GLU
1	B	487	THR
1	B	489	GLU
1	B	505	GLU
1	B	523	MET
1	B	634	LEU
1	B	637	SER
1	B	649	SER
1	B	669	SER
1	B	752	HIS
1	B	828	LYS
1	B	829	ASP
1	C	446	GLU
1	C	470	LEU
1	C	476	ILE
1	C	505	GLU
1	C	523	MET
1	C	657	MET
1	C	670	LYS
1	C	681	LEU
1	C	688	CYS
1	C	782	GLU
1	D	487	THR
1	D	500	SER

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Mol	Chain	Res	Type
1	D	527	CYS
1	D	613	GLU
1	D	627	ARG
1	D	642	ASN
1	D	657	MET
1	D	659	MET
1	D	669	SER
1	D	788	ASN
1	D	791	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	GLN
1	A	518	ASN
1	A	567	ASN
1	A	632	GLN
1	A	635	HIS
1	A	672	HIS
1	B	472	ASN
1	B	510	GLN
1	B	529	ASN
1	B	632	GLN
1	C	469	GLN
1	C	472	ASN
1	C	672	HIS
1	C	679	GLN
1	C	824	GLN
1	D	472	ASN
1	D	518	ASN
1	D	632	GLN
1	D	642	ASN
1	D	788	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	4HI	B	2	-	30,38,38	0.56	0	40,52,52	1.41	4 (10%)
2	4HI	B	1	-	30,38,38	0.60	0	40,52,52	1.37	5 (12%)
2	4HI	D	3	-	30,38,38	0.53	0	40,52,52	1.36	4 (10%)
2	4HI	C	4	-	30,38,38	0.53	0	40,52,52	1.44	3 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4HI	B	2	-	-	3/25/30/30	0/3/3/3
2	4HI	B	1	-	-	5/25/30/30	0/3/3/3
2	4HI	D	3	-	-	5/25/30/30	0/3/3/3
2	4HI	C	4	-	-	5/25/30/30	0/3/3/3

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	4HI	C12-C2-C3	-4.46	122.62	131.18
2	C	4	4HI	C12-C2-C3	-3.99	123.53	131.18
2	D	3	4HI	C12-C2-C3	-3.86	123.77	131.18
2	B	1	4HI	C12-C2-C3	-3.67	124.14	131.18
2	C	4	4HI	C2-C12-C6	-3.66	123.89	129.87
2	B	2	4HI	C2-C12-C6	-3.57	124.05	129.87
2	D	3	4HI	C2-C12-C6	-3.56	124.06	129.87
2	B	1	4HI	C2-C12-C6	-2.95	125.06	129.87
2	D	3	4HI	C4-N2-C3	2.59	127.94	121.81
2	B	2	4HI	C4-N2-C3	2.40	127.49	121.81
2	B	2	4HI	N3-C5-N1	-2.20	109.58	115.11
2	C	4	4HI	C4-N2-C3	2.20	127.02	121.81
2	B	1	4HI	C24-C30-C15	-2.15	119.97	122.83
2	B	1	4HI	C4-N2-C3	2.13	126.86	121.81
2	D	3	4HI	N3-C5-N1	-2.12	109.80	115.11
2	B	1	4HI	N3-C5-N1	-2.07	109.91	115.11

There are no chirality outliers.

All (18) torsion outliers are listed below:

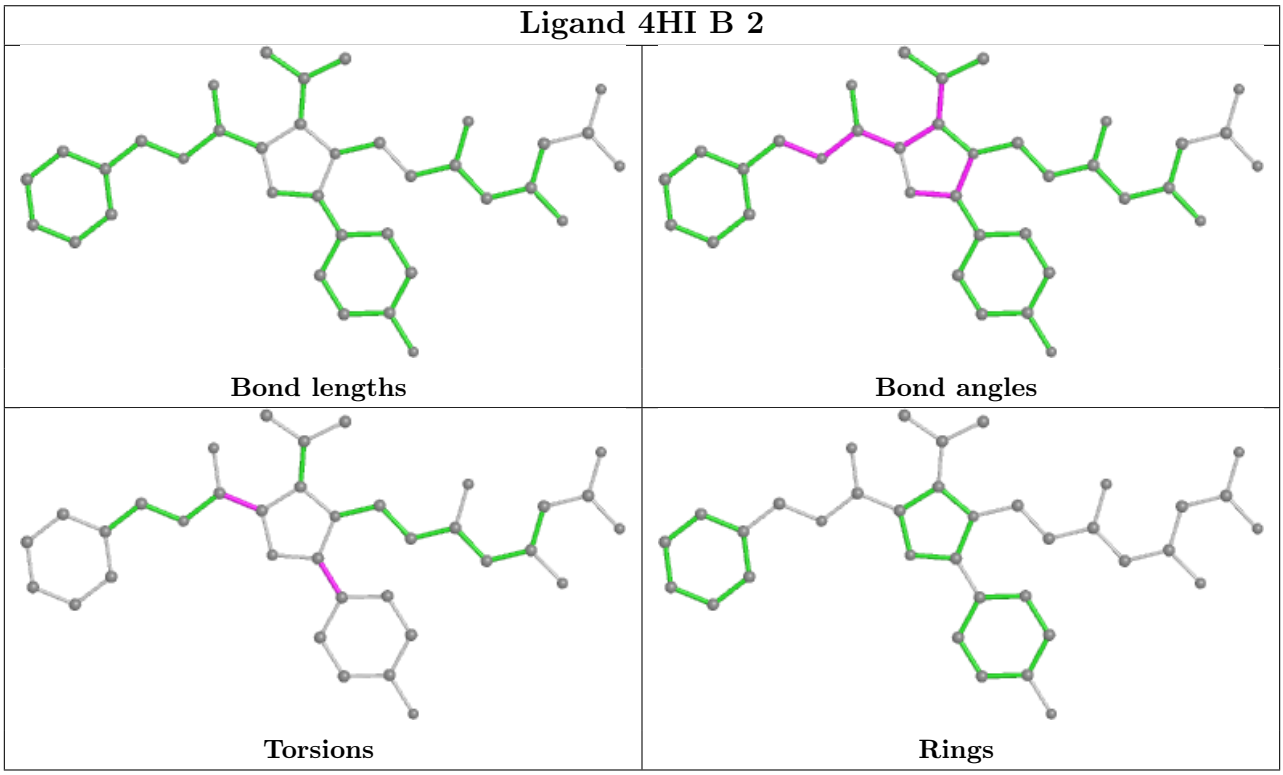
Mol	Chain	Res	Type	Atoms
2	B	1	4HI	C12-C2-C3-O2
2	B	2	4HI	C12-C2-C3-O2
2	C	4	4HI	C21-C27-C5-N1
2	C	4	4HI	C12-C2-C3-O2
2	D	3	4HI	C21-C27-C5-N1
2	D	3	4HI	C18-C27-C5-N1
2	D	3	4HI	C12-C2-C3-O2
2	D	3	4HI	C18-C27-C5-N3
2	C	4	4HI	C18-C27-C5-N3
2	D	3	4HI	C21-C27-C5-N3
2	B	1	4HI	C21-C27-C5-N3
2	C	4	4HI	C21-C27-C5-N3
2	B	1	4HI	C18-C27-C5-N3
2	B	1	4HI	C21-C27-C5-N1
2	B	1	4HI	C18-C27-C5-N1
2	C	4	4HI	C18-C27-C5-N1
2	B	2	4HI	C18-C27-C5-N3
2	B	2	4HI	C21-C27-C5-N3

There are no ring outliers.

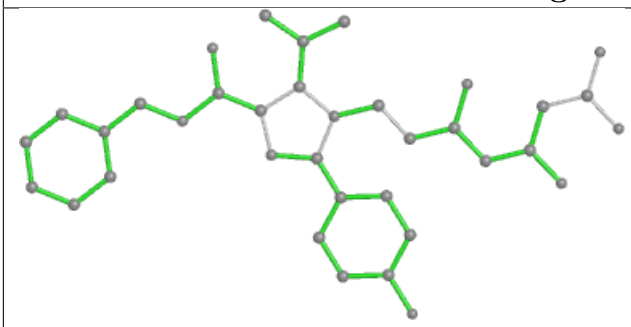
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	4HI	2	0
2	B	1	4HI	1	0

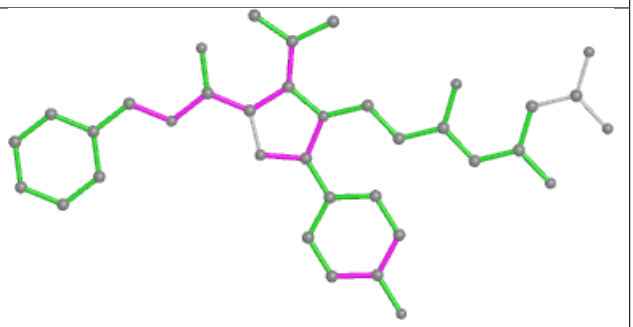
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



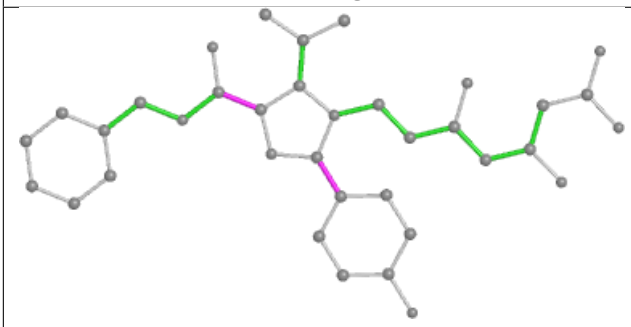
Ligand 4HI B 1



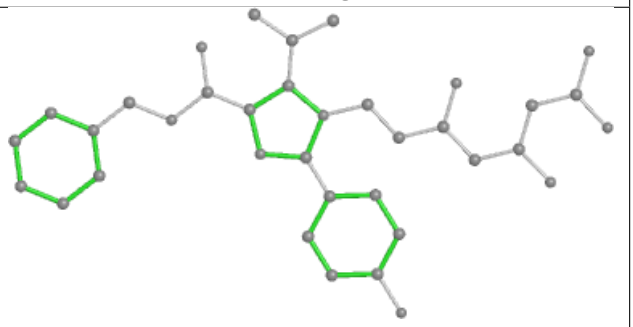
Bond lengths



Bond angles

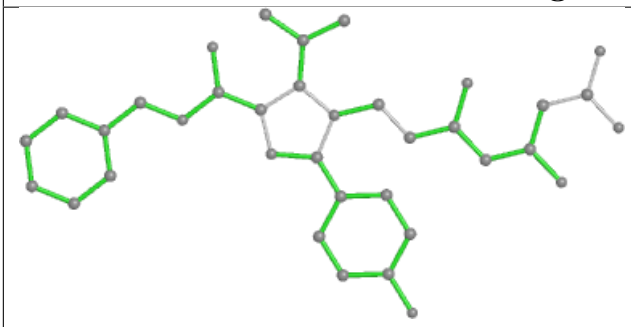


Torsions

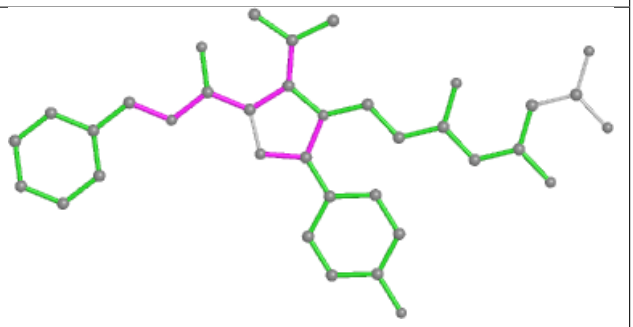


Rings

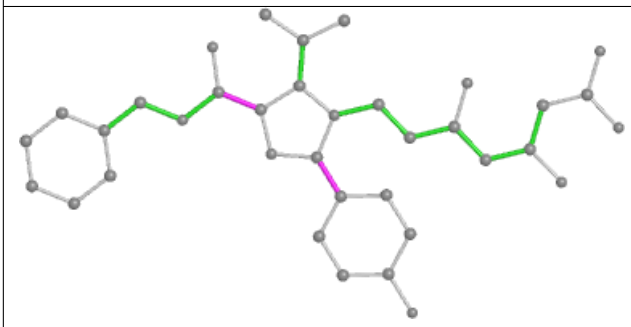
Ligand 4HI D 3



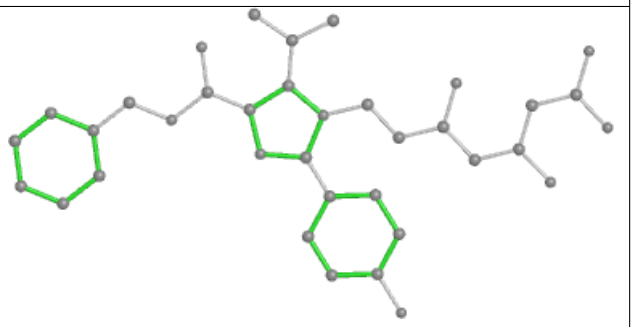
Bond lengths



Bond angles

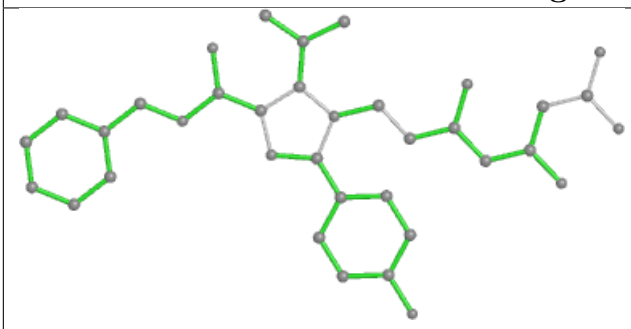


Torsions

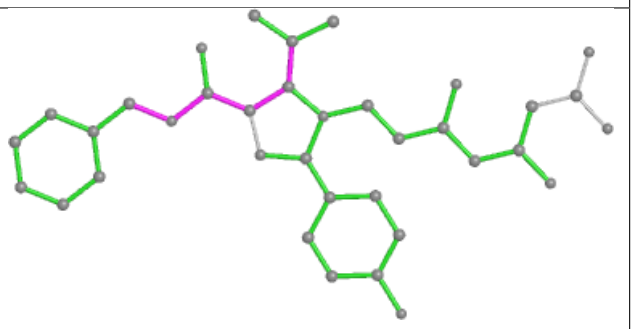


Rings

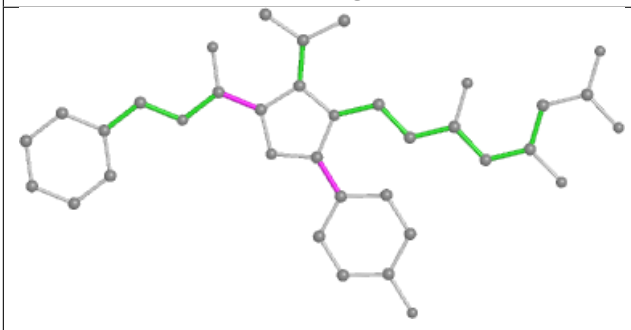
Ligand 4HI C 4



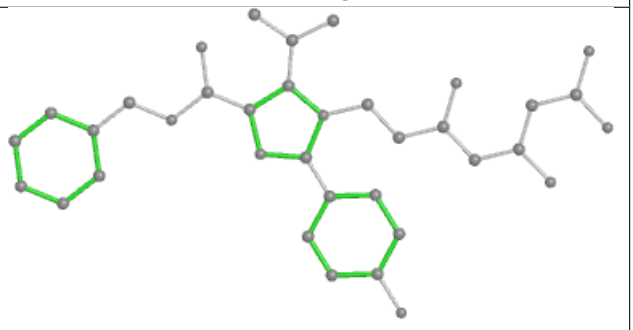
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	421/441 (95%)	0.55	60 (14%) 2 3	29, 42, 62, 69	0
1	B	421/441 (95%)	0.32	29 (6%) 16 21	29, 43, 56, 72	0
1	C	414/441 (93%)	0.57	40 (9%) 7 10	30, 46, 83, 103	0
1	D	394/441 (89%)	0.42	38 (9%) 8 10	29, 43, 82, 108	0
All	All	1650/1764 (93%)	0.46	167 (10%) 7 9	29, 43, 66, 108	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	458	GLY	11.5
1	D	461	PHE	7.9
1	D	470	LEU	7.6
1	C	452	LEU	7.5
1	B	861	HIS	6.9
1	D	475	HIS	6.7
1	C	525	ALA	6.6
1	D	459	ALA	6.6
1	C	453	GLY	6.4
1	C	524	GLY	6.4
1	A	479	TYR	6.2
1	A	452	LEU	6.2
1	C	481	LEU	6.0
1	D	527	CYS	5.9
1	D	485	ILE	5.9
1	D	484	LEU	5.6
1	D	486	GLU	5.6
1	C	484	LEU	5.6
1	C	483	THR	5.4
1	A	861	HIS	5.2
1	A	446	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	461	PHE	5.2
1	D	471	VAL	5.1
1	D	474	LYS	5.0
1	A	448	CYS	4.8
1	D	460	LYS	4.7
1	A	462	LEU	4.7
1	A	476	ILE	4.6
1	A	475	HIS	4.6
1	C	523	MET	4.5
1	A	467	ILE	4.5
1	A	455	ALA	4.5
1	C	527	CYS	4.4
1	A	445	ASN	4.3
1	C	461	PHE	4.3
1	D	469	GLN	4.3
1	C	451	ILE	4.2
1	B	828	LYS	4.1
1	A	473	ALA	4.0
1	A	450	GLN	3.9
1	A	470	LEU	3.9
1	A	447	GLU	3.9
1	C	450	GLN	3.9
1	C	487	THR	3.8
1	D	523	MET	3.8
1	C	746	ILE	3.7
1	C	748	GLY	3.6
1	A	444	PRO	3.6
1	C	454	ASN	3.5
1	B	772	VAL	3.5
1	B	829	ASP	3.5
1	C	485	ILE	3.5
1	A	477	PRO	3.5
1	A	449	LEU	3.5
1	D	462	LEU	3.5
1	A	474	LYS	3.5
1	A	746	ILE	3.5
1	C	449	LEU	3.4
1	A	828	LYS	3.4
1	A	463	SER	3.3
1	A	481	LEU	3.3
1	A	471	VAL	3.3
1	C	486	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	488	HIS	3.3
1	D	525	ALA	3.3
1	A	772	VAL	3.2
1	B	446	GLU	3.2
1	B	699	ILE	3.2
1	D	746	ILE	3.2
1	A	457	LYS	3.2
1	A	451	ILE	3.2
1	C	458	GLY	3.2
1	C	628	PHE	3.1
1	A	689	THR	3.1
1	B	527	CYS	3.1
1	A	773	GLY	3.1
1	D	463	SER	3.1
1	C	772	VAL	3.1
1	A	443	ARG	3.0
1	A	741	ALA	3.0
1	A	458	GLY	3.0
1	A	469	GLN	3.0
1	D	772	VAL	3.0
1	A	483	THR	3.0
1	D	744	GLY	3.0
1	A	442	PRO	3.0
1	A	456	GLU	2.9
1	A	480	LYS	2.8
1	C	479	TYR	2.8
1	B	698	TRP	2.8
1	A	484	LEU	2.7
1	A	696	ILE	2.7
1	C	778	ILE	2.7
1	C	627	ARG	2.7
1	A	775	SER	2.7
1	B	746	ILE	2.7
1	A	460	LYS	2.7
1	A	693	PRO	2.7
1	D	693	PRO	2.7
1	B	482	GLU	2.6
1	A	769	ALA	2.6
1	D	745	SER	2.6
1	D	768	ALA	2.6
1	D	828	LYS	2.5
1	D	472	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	699	ILE	2.5
1	A	694	ALA	2.5
1	B	757	VAL	2.5
1	A	441	GLU	2.5
1	B	479	TYR	2.5
1	C	662	LYS	2.5
1	C	520	SER	2.5
1	B	481	LEU	2.5
1	C	469	GLN	2.5
1	B	741	ALA	2.5
1	D	515	ARG	2.4
1	A	698	TRP	2.4
1	C	626	SER	2.4
1	C	771	ASN	2.4
1	B	743	ALA	2.4
1	D	465	ALA	2.4
1	C	624	SER	2.4
1	A	761	TYR	2.4
1	A	695	ALA	2.4
1	B	693	PRO	2.4
1	D	694	ALA	2.4
1	D	467	ILE	2.4
1	C	699	ILE	2.3
1	A	789	GLU	2.3
1	A	635	HIS	2.3
1	B	777	CYS	2.3
1	A	482	GLU	2.3
1	B	860	GLY	2.3
1	C	741	ALA	2.3
1	B	739	GLY	2.3
1	A	453	GLY	2.2
1	D	698	TRP	2.2
1	A	829	ASP	2.2
1	B	483	THR	2.2
1	B	754	ALA	2.2
1	D	488	HIS	2.2
1	D	757	VAL	2.2
1	A	466	GLU	2.2
1	B	450	GLN	2.2
1	A	749	TYR	2.2
1	A	768	ALA	2.1
1	D	468	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	749	TYR	2.1
1	C	769	ALA	2.1
1	D	630	ARG	2.1
1	A	762	ILE	2.1
1	B	773	GLY	2.1
1	B	745	SER	2.1
1	B	694	ALA	2.1
1	C	744	GLY	2.1
1	B	469	GLN	2.1
1	B	753	ALA	2.1
1	D	743	ALA	2.1
1	C	673	GLU	2.0
1	D	466	GLU	2.0
1	D	699	ILE	2.0
1	C	459	ALA	2.0
1	A	472	ASN	2.0
1	B	737	LEU	2.0
1	C	695	ALA	2.0
1	D	487	THR	2.0
1	C	860	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	4HI	C	4	36/36	0.87	0.15	33,45,47,51	0
2	4HI	D	3	36/36	0.89	0.14	31,41,44,47	0
2	4HI	B	1	36/36	0.94	0.11	32,41,42,44	0

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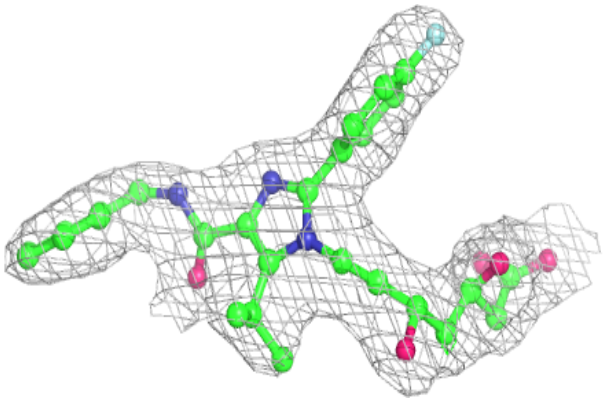
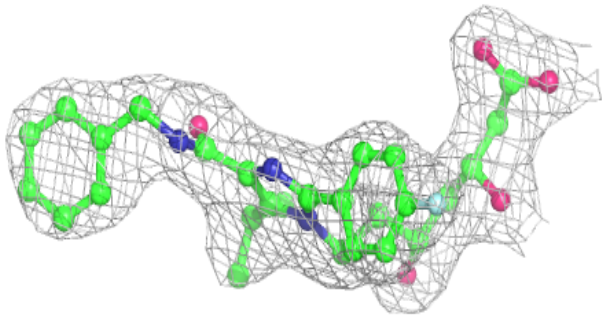
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	4HI	B	2	36/36	0.94	0.13	29,37,43,46	0

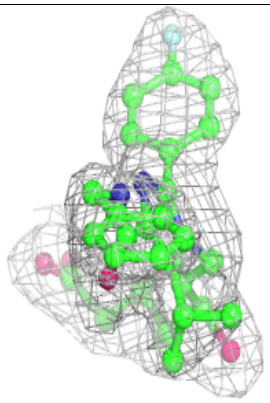
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 4HI C 4:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

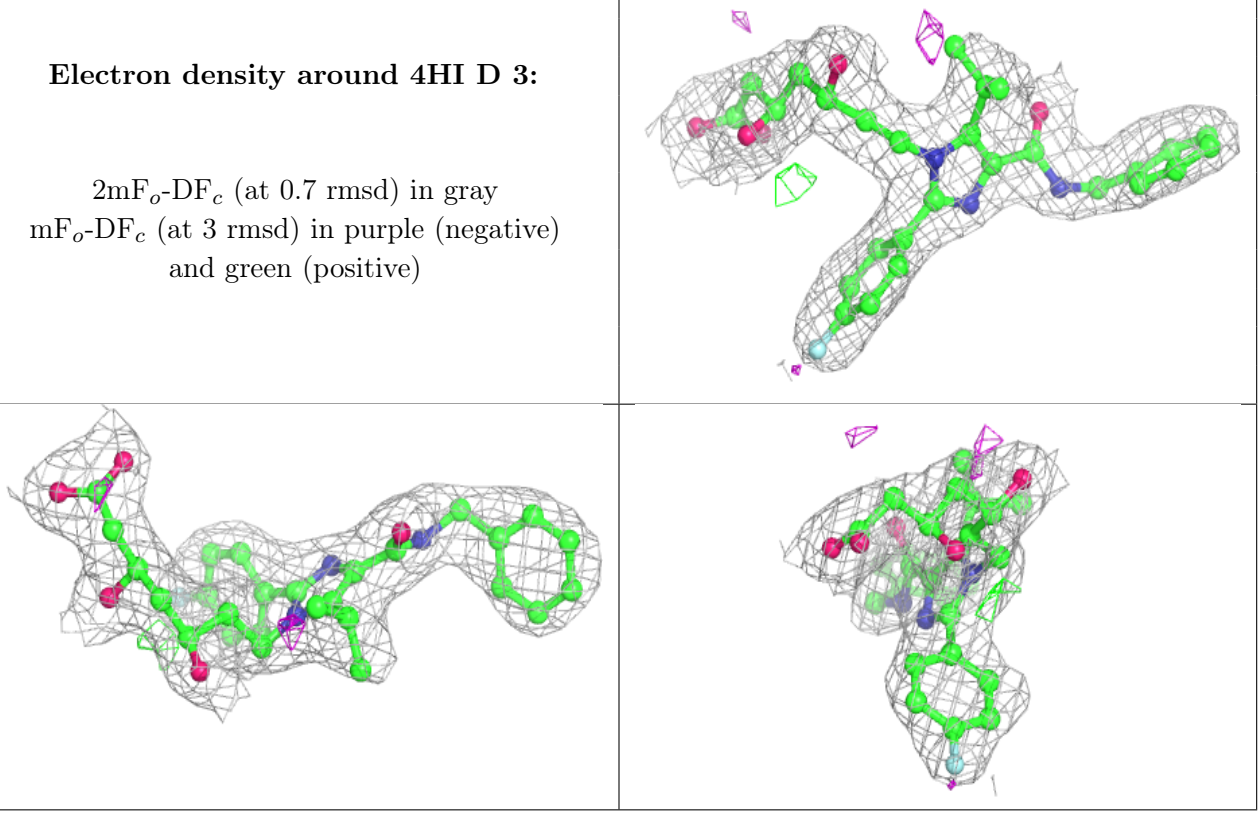






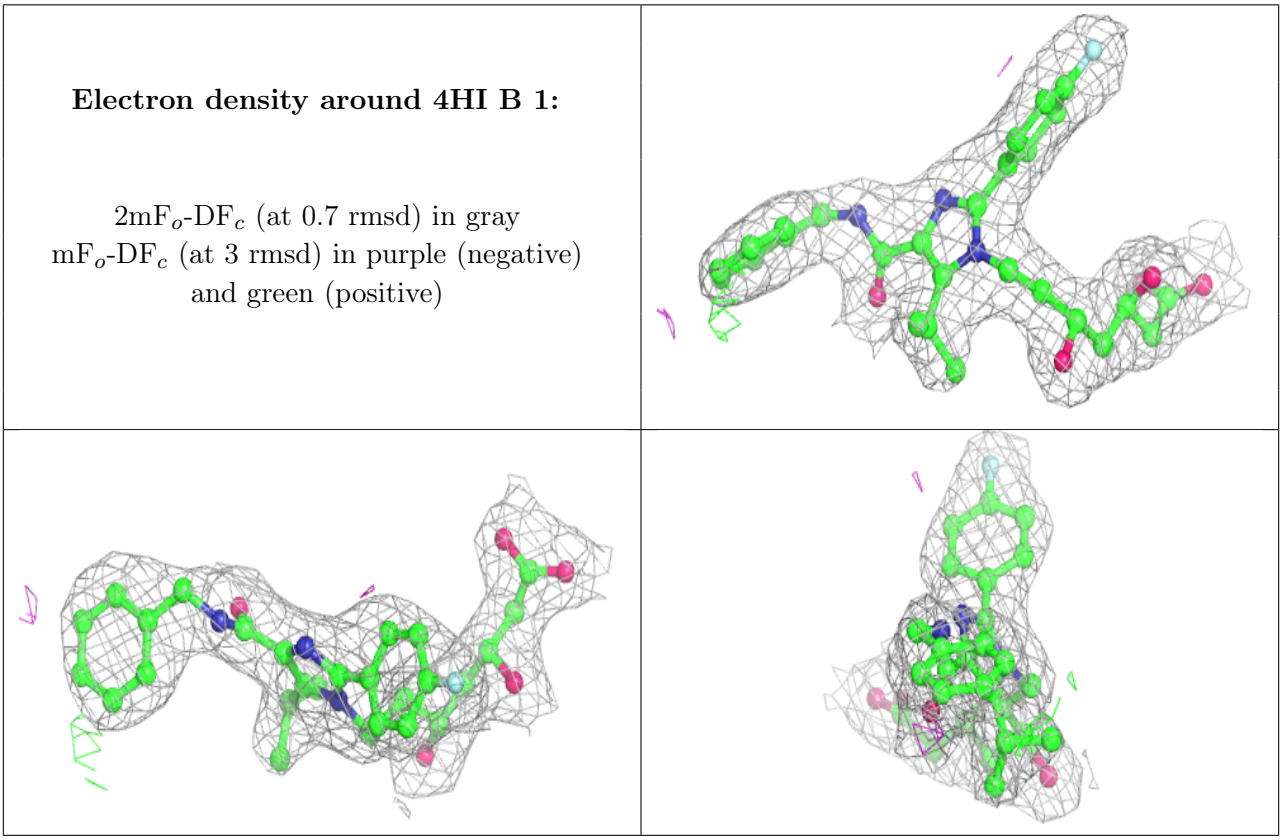
Electron density around 4HI D 3:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



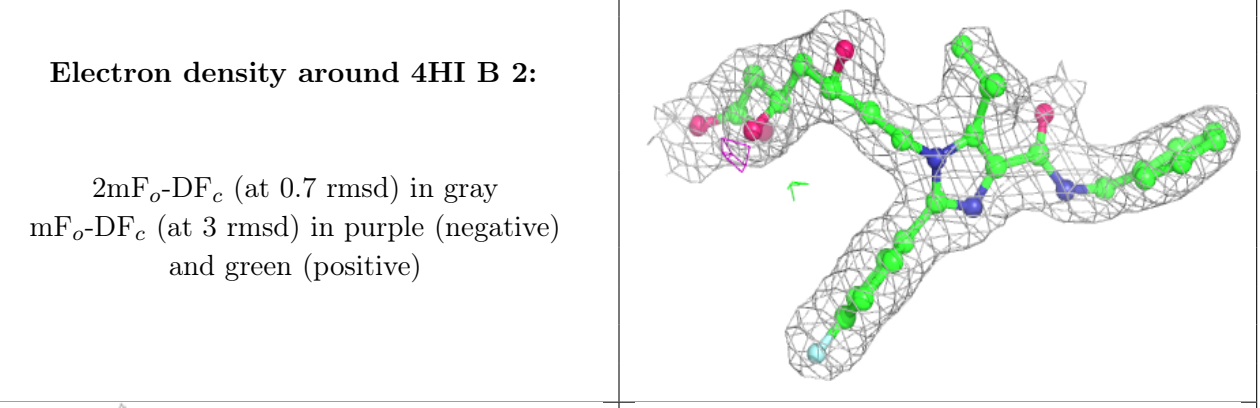
Electron density around 4HI B 1:

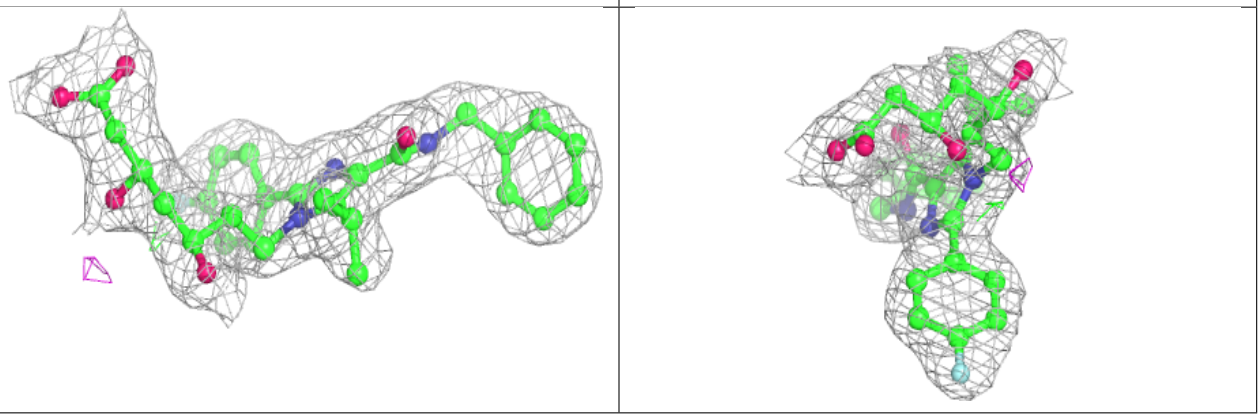
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 4HI B 2:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





6.5 Other polymers (i)

There are no such residues in this entry.

Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:26 am BST

PDB ID	:	2P54
Title	:	a crystal structure of PPAR alpha bound with SRC1 peptide and GW735
Authors	:	Xu, R.X.; Xu, H.E.; Sierra, M.L.; Montana, V.G.; Lambert, M.H.; Pianetti, P.M.
Deposited on	:	2007-03-14
Resolution	:	1.79 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

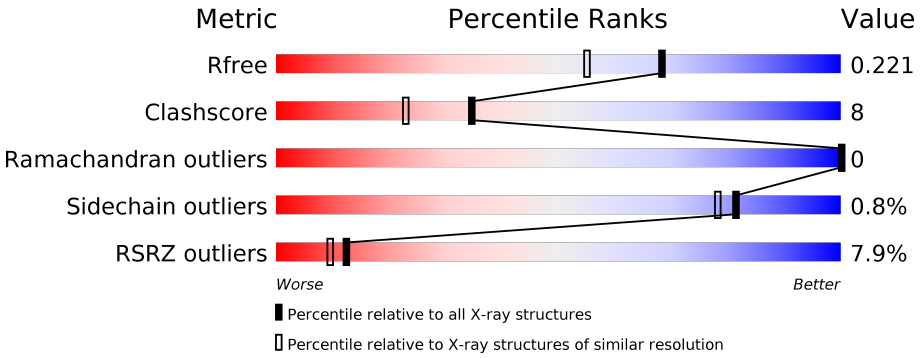
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	267	7% 82% 17%
2	B	12	25% 75% 25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2517 atoms, of which 20 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Peroxisome proliferator-activated receptor alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2099	1349	352	380	18			

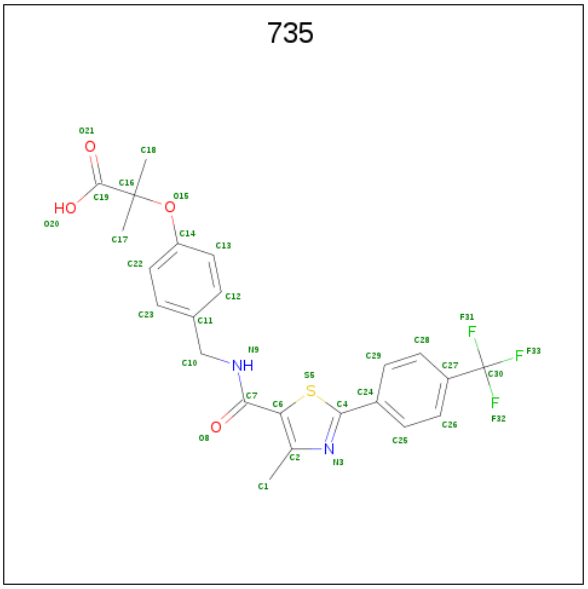
- Molecule 2 is a protein called Nuclear receptor coactivator 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	0	0	0
			97	61	20	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	685	ALA	-	CLONING ARTIFACT	UNP Q15788

- Molecule 3 is 2-METHYL-2-(4-{[({4-METHYL-2-[4-(TRIFLUOROMETHYL)PHENYL]-1,3-THIAZOL-5-YL}CARBONYL)AMINO]METHYL}PHENOXY)PROPANOIC ACID (three-letter code: 735) (formula: $C_{23}H_{21}F_3N_2O_4S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	F	H	N	O	S	0	0
			53	23	3	20	2	4	1		

- Molecule 4 is water.

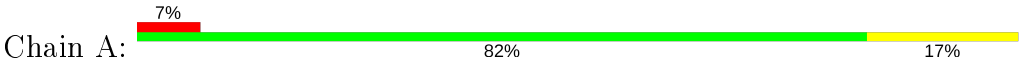
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	264	Total	O	0	0
			264	264		
4	B	4	Total	O	0	0
			4	4		

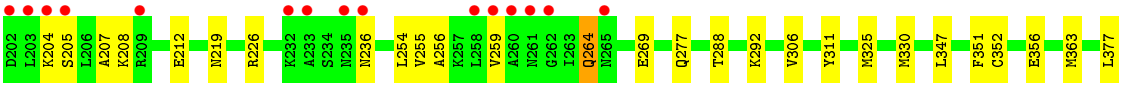
3 Residue-property plots (i)

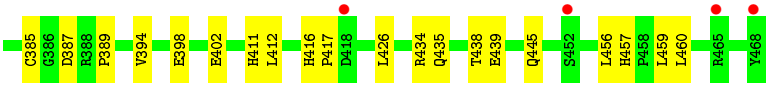
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Peroxisome proliferator-activated receptor alpha

Chain A:

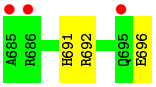






- Molecule 2: Nuclear receptor coactivator 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	61.26Å 103.53Å 49.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.79 19.77 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.5 (20.00-1.79) 97.7 (19.77-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	4.36 (at 1.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.227 0.199 , 0.221	Depositor DCC
R_{free} test set	1789 reflections (5.94%)	wwPDB-VP
Wilson B-factor (Å^2)	23.3	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2517	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 735

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.28	0/2136	0.55	0/2879
2	B	0.32	0/98	0.46	0/130
All	All	0.28	0/2234	0.54	0/3009

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2099	0	2140	35	0
2	B	97	0	93	2	0
3	A	33	20	20	1	0
4	A	264	0	0	9	0
4	B	4	0	0	0	0
All	All	2497	20	2253	37	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:GLU:O	1:A:402:GLU:HG3	1.79	0.82
1:A:204:LYS:HB2	4:A:728:HOH:O	1.82	0.79
1:A:277:GLN:HE22	1:A:456:LEU:HA	1.59	0.68
1:A:277:GLN:HE21	1:A:460:LEU:HD12	1.60	0.67
1:A:256:ALA:O	1:A:259:VAL:HG22	1.96	0.66
1:A:457:HIS:HD2	1:A:459:LEU:H	1.43	0.65
1:A:394:VAL:O	1:A:398:GLU:HG3	2.01	0.60
1:A:205:SER:HA	4:A:554:HOH:O	2.03	0.58
1:A:434:ARG:O	1:A:438:THR:HG23	2.03	0.58
1:A:264:GLN:H	1:A:264:GLN:HE21	1.54	0.56
1:A:363:MET:HE2	4:A:730:HOH:O	2.06	0.55
1:A:288:THR:O	1:A:292:LYS:HG3	2.06	0.55
1:A:457:HIS:CD2	1:A:459:LEU:H	2.24	0.55
3:A:469:735:H41	3:A:469:735:H34	1.72	0.54
1:A:363:MET:CE	4:A:730:HOH:O	2.56	0.54
1:A:356:GLU:HB2	4:A:709:HOH:O	2.07	0.53
1:A:306:VAL:HG21	2:B:691:HIS:CE1	2.45	0.52
1:A:277:GLN:HE22	1:A:457:HIS:H	1.56	0.51
1:A:325:MET:HG2	1:A:330:MET:HB3	1.93	0.51
1:A:445:GLN:HG2	4:A:671:HOH:O	2.11	0.51
1:A:311:TYR:CZ	1:A:389:PRO:HG2	2.46	0.50
1:A:208:LYS:O	1:A:212:GLU:HG3	2.11	0.49
1:A:219:ASN:HB2	4:A:577:HOH:O	2.13	0.48
1:A:236:ASN:HB3	4:A:643:HOH:O	2.13	0.47
1:A:412:LEU:HD11	1:A:426:LEU:HD12	1.97	0.46
1:A:277:GLN:NE2	1:A:457:HIS:H	2.13	0.46
1:A:363:MET:HA	1:A:363:MET:CE	2.47	0.45
1:A:435:GLN:O	1:A:439:GLU:HG3	2.17	0.45
1:A:411:HIS:HD2	4:A:626:HOH:O	1.99	0.44
2:B:692:ARG:O	2:B:696:GLU:HG3	2.17	0.43
1:A:385:CYS:SG	1:A:387:ASP:OD1	2.76	0.43
1:A:255:VAL:HG23	1:A:255:VAL:O	2.20	0.42
1:A:416:HIS:N	1:A:417:PRO:HD3	2.35	0.41
1:A:207:ALA:HA	1:A:377:LEU:HD21	2.03	0.41
1:A:226:ARG:HA	1:A:226:ARG:HD3	1.88	0.41
1:A:269:GLU:HB3	1:A:351:PHE:CD2	2.55	0.41
1:A:347:LEU:O	1:A:352:CYS:HB3	2.21	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	265/267 (99%)	261 (98%)	4 (2%)	0	100	100
2	B	10/12 (83%)	10 (100%)	0	0	100	100
All	All	275/279 (99%)	271 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	229/234 (98%)	227 (99%)	2 (1%)	78	75
2	B	9/11 (82%)	9 (100%)	0	100	100
All	All	238/245 (97%)	236 (99%)	2 (1%)	81	78

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	LEU
1	A	264	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	GLN

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Mol	Chain	Res	Type
1	A	277	GLN
1	A	299	ASN
1	A	366	ASN
1	A	401	GLN
1	A	411	HIS
1	A	442	GLN
1	A	457	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	735	A	469	-	27,35,35	1.12	2 (7%)	34,52,52	1.55	4 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	735	A	469	-	-	2/20/30/30	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	469	735	C4-N3	2.29	1.34	1.31
3	A	469	735	C4-S5	2.08	1.76	1.73

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	469	735	C6-C7-N9	5.99	121.55	115.62
3	A	469	735	F33-C30-C27	-3.06	106.21	112.93
3	A	469	735	C17-C16-C19	-2.99	104.87	111.86
3	A	469	735	O15-C16-C18	2.32	114.99	105.72

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	469	735	C22-C14-O15-C16
3	A	469	735	C13-C14-O15-C16

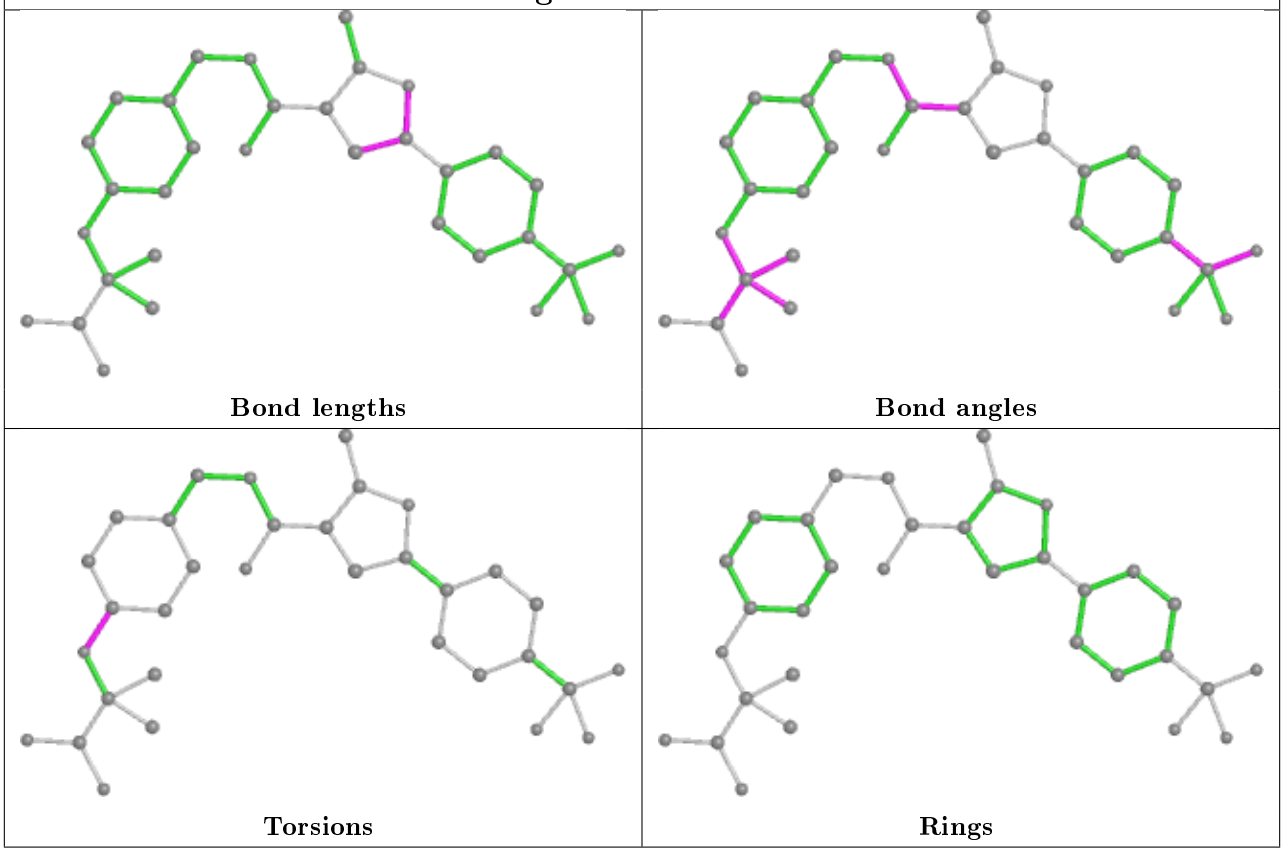
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	469	735	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 735 A 469



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	267/267 (100%)	0.40	19 (7%) 16 12	13, 23, 42, 57	0
2	B	12/12 (100%)	2.35	3 (25%) 0 0	33, 41, 53, 58	0
All	All	279/279 (100%)	0.48	22 (7%) 12 9	13, 23, 44, 58	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	685	ALA	12.6
1	A	468	TYR	6.9
1	A	235	ASN	4.8
1	A	261	ASN	4.2
1	A	262	GLY	3.9
1	A	259	VAL	3.8
1	A	236	ASN	3.6
1	A	258	LEU	3.6
1	A	465	ARG	3.3
1	A	233	ALA	3.2
1	A	418	ASP	3.2
1	A	232	LYS	3.1
2	B	695	GLN	3.0
1	A	452	SER	2.9
2	B	686	ARG	2.8
1	A	202	ASP	2.8
1	A	205	SER	2.7
1	A	203	LEU	2.5
1	A	260	ALA	2.4
1	A	265	ASN	2.2
1	A	209	ARG	2.2
1	A	204	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

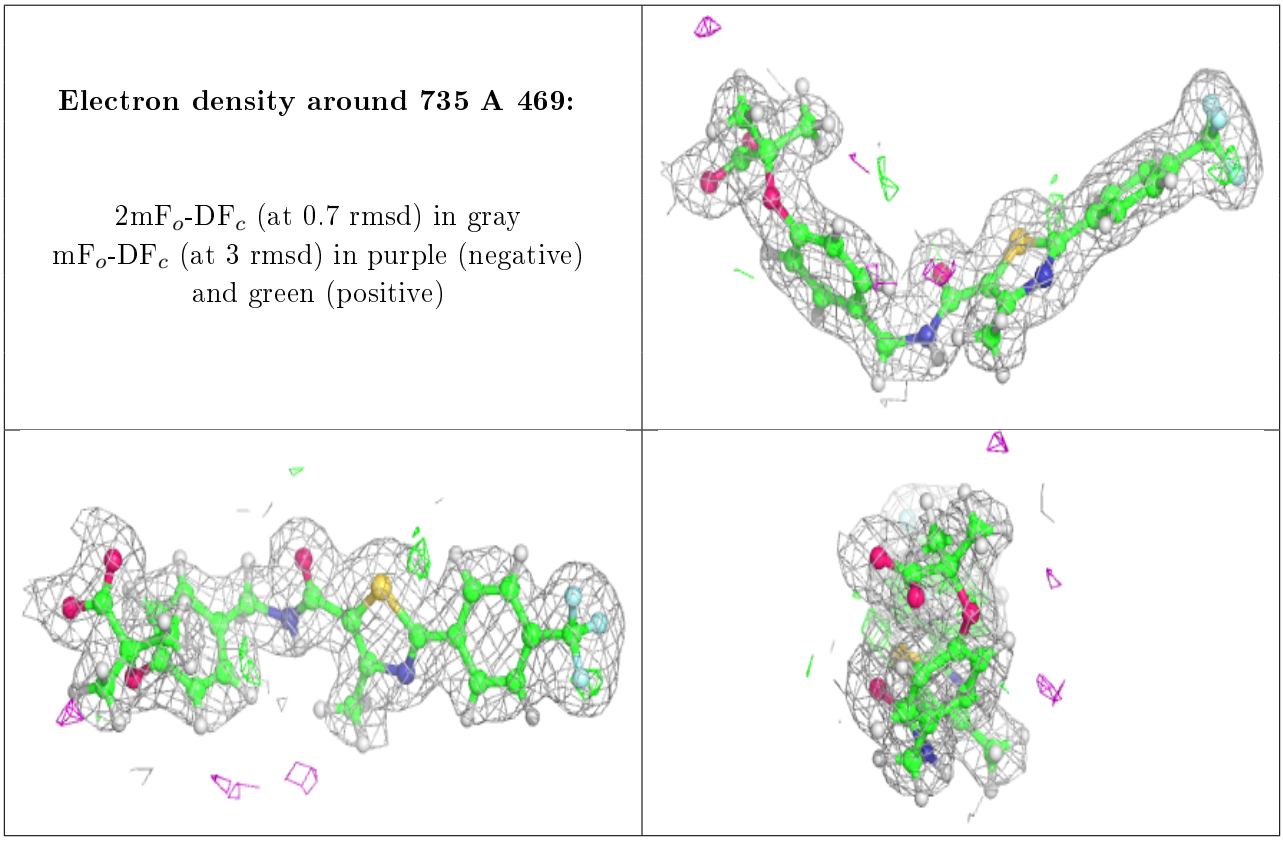
There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	735	A	469	33/33	0.97	0.09	13,17,28,32	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers (i)

There are no such residues in this entry.