Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 01:08 PM EDT

PDB ID	:	5U6E
Title	:	Crystal structure of clade A/E HIV-1 gp120 core in complex with NBD-14010
Authors	:	Kwon, Y.D.; Debnath, A.K.; Kwong, P.D.
Deposited on	:	2016-12-07
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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

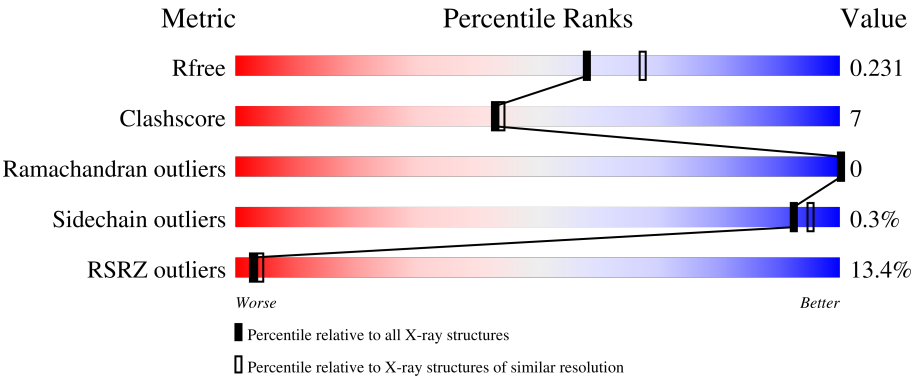
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 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	353	8% 86% 10% .
1	B	353	18% 82% 14% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5886 atoms, of which 36 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.

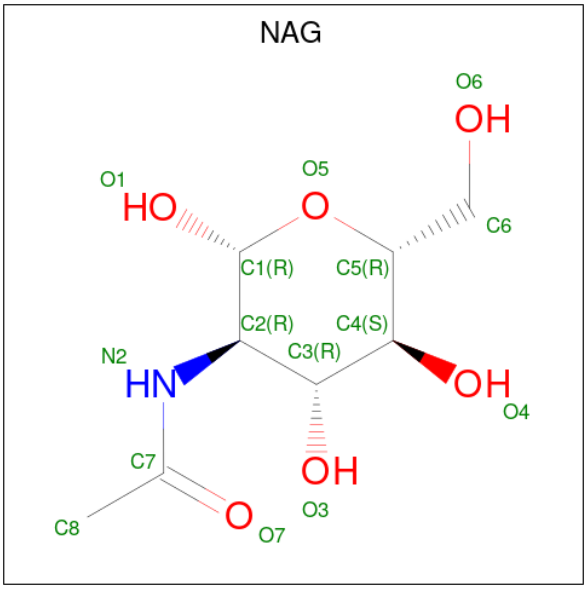
- Molecule 1 is a protein called clade A/E 93TH057 HIV-1 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2660	1669	461	508	22			
1	B	340	Total	C	N	O	S	0	0	0
			2660	1669	461	508	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9
B	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9

- 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		

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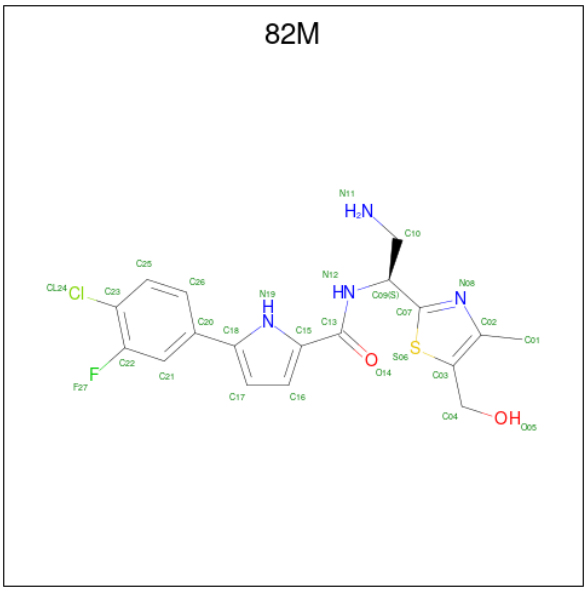
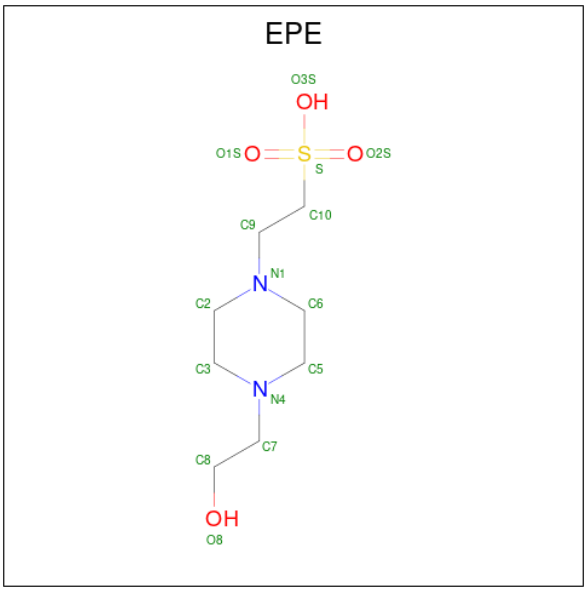
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total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

- Molecule 3 is N-{(1S)-2-amino-1-[5-(hydroxymethyl)-4-methyl-1,3-thiazol-2-yl]ethyl}-5 -(4-chloro-3-fluorophenyl)-1H-pyrrole-2-carboxamide (three-letter code: 82M) (formula: $C_{18}H_{18}ClFN_4O_2S$).



Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	H	N	O	S	0	0
			45	18	1	1	18	4	2	1		
3	B	1	Total	C	Cl	F	H	N	O	S	0	0
			45	18	1	1	18	4	2	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is water.

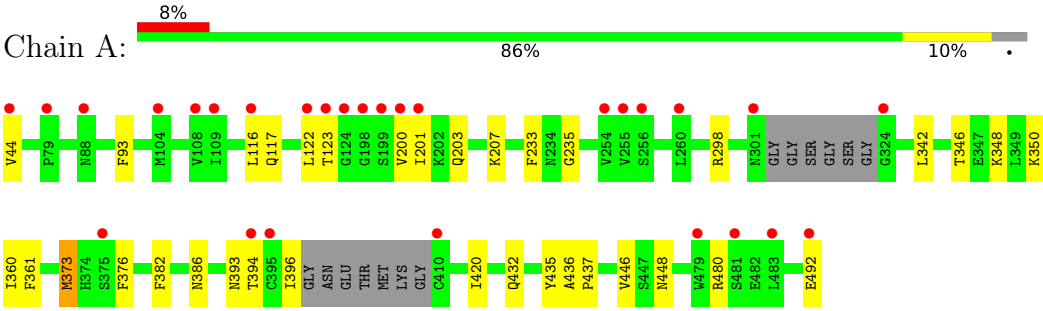
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	134	Total	O	0	0
			134	134		
5	B	60	Total	O	0	0
			60	60		

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.

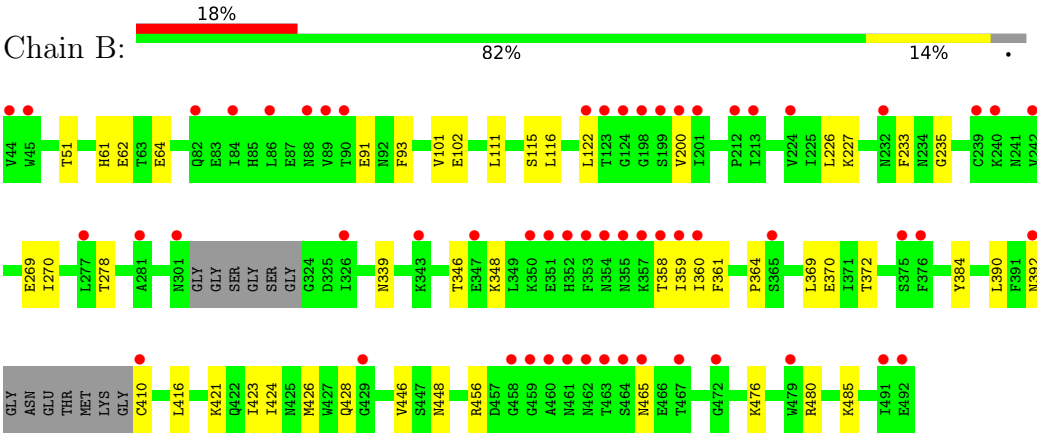
• Molecule 1: clade A/E 93TH057 HIV-1 gp120 core

Chain A:



• Molecule 1: clade A/E 93TH057 HIV-1 gp120 core

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.18Å 68.74Å 94.75Å 90.00° 91.26° 90.00°	Depositor
Resolution (Å)	37.92 – 2.10 37.92 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.1 (37.92-2.10) 96.1 (37.92-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.193 , 0.231 0.193 , 0.231	Depositor DCC
R_{free} test set	2330 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	43.6	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 59.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5886	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% 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: 82M, EPE, 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	0.33	0/2715	0.48	0/3686
1	B	0.28	0/2715	0.47	0/3686
All	All	0.31	0/5430	0.47	0/7372

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	2660	0	2592	33	0
1	B	2660	0	2596	39	0
2	A	154	0	143	9	0
2	B	98	0	91	1	0
3	A	27	18	0	0	0
3	B	27	18	0	1	0
4	A	15	0	17	0	0
4	B	15	0	17	0	0
5	A	134	0	0	7	0
5	B	60	0	0	6	0
All	All	5850	36	5456	75	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 7.

All (75) 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:384:TYR:OH	1:B:424:ILE:HD12	1.79	0.83
1:A:342:LEU:HD23	1:A:396:ILE:HD11	1.68	0.75
1:B:269:GLU:O	5:B:601:HOH:O	2.04	0.75
2:A:507:NAG:H3	2:A:507:NAG:H83	1.69	0.74
1:A:373:MET:HE2	1:A:386:ASN:HA	1.73	0.70
1:A:480:ARG:NH2	5:A:601:HOH:O	2.24	0.70
1:A:354:ASN:HA	2:A:508:NAG:H81	1.74	0.69
1:B:270:ILE:O	1:B:348:LYS:HE2	1.94	0.68
1:B:423:ILE:O	1:B:424:ILE:HD13	1.94	0.68
1:A:44:VAL:HG13	1:A:492:GLU:HB3	1.76	0.67
1:A:360:ILE:HG23	1:A:393:ASN:ND2	2.09	0.67
1:B:62:GLU:HG3	1:B:64:GLU:H	1.61	0.65
1:A:348:LYS:HG2	5:A:631:HOH:O	1.97	0.65
1:A:346:THR:HG23	1:A:359:ILE:HB	1.79	0.64
1:B:101:VAL:HG21	1:B:480:ARG:HG2	1.81	0.62
2:A:511:NAG:O6	1:B:62:GLU:OE2	2.11	0.62
1:B:227:LYS:HE3	1:B:485:LYS:HD2	1.82	0.62
1:B:448:ASN:ND2	5:B:602:HOH:O	2.19	0.62
1:B:446:VAL:HG21	2:B:505:NAG:H82	1.82	0.61
1:B:426:MET:HE3	5:B:617:HOH:O	2.01	0.60
1:A:116:LEU:HG	1:A:435:TYR:CE2	2.37	0.59
1:A:373:MET:CE	1:A:386:ASN:HA	2.31	0.59
2:A:507:NAG:C1	2:A:507:NAG:H82	2.32	0.59
1:A:203:GLN:NE2	5:A:607:HOH:O	2.37	0.58
1:B:51:THR:HB	5:B:607:HOH:O	2.03	0.58
1:A:207:LYS:NZ	5:A:608:HOH:O	2.37	0.57
1:B:360:ILE:HG23	1:B:393:ASN:ND2	2.20	0.57
2:A:504:NAG:H3	1:B:61:HIS:CD2	2.39	0.56
1:B:339:ASN:ND2	1:B:410:CYS:O	2.39	0.56
1:B:390:LEU:HD11	1:B:416:LEU:HD11	1.88	0.55
1:A:207:LYS:HE2	1:A:436:ALA:HB3	1.89	0.55
1:B:395:CYS:HB3	1:B:410:CYS:N	2.21	0.55
1:B:122:LEU:HD22	1:B:200:VAL:HG22	1.90	0.53
1:A:342:LEU:CD2	1:A:396:ILE:HD11	2.38	0.53
1:A:123:THR:HG23	1:A:123:THR:O	2.09	0.53
1:B:278:THR:O	1:B:456:ARG:NH2	2.42	0.52
1:A:116:LEU:HG	1:A:435:TYR:HE2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLN:NE2	1:A:117:GLN:HA	2.24	0.52
1:B:102:GLU:HG3	1:B:476:LYS:NZ	2.25	0.51
1:A:116:LEU:HD21	1:A:382:PHE:CZ	2.46	0.50
2:A:507:NAG:C1	2:A:507:NAG:C8	2.90	0.49
1:A:448:ASN:HD22	2:A:510:NAG:H83	1.77	0.49
1:B:361:PHE:H	1:B:393:ASN:HD21	1.60	0.48
1:A:446:VAL:HG21	2:A:506:NAG:H82	1.94	0.48
1:B:122:LEU:CD2	1:B:200:VAL:HG22	2.43	0.48
1:B:233:PHE:CE2	1:B:235:GLY:HA2	2.48	0.48
1:A:122:LEU:HD12	1:A:432:GLN:HB2	1.94	0.48
1:B:485:LYS:NZ	5:B:605:HOH:O	2.41	0.47
1:A:348:LYS:HD3	2:A:505:NAG:O6	2.14	0.47
1:B:346:THR:HG23	1:B:359:ILE:HB	1.97	0.47
1:A:207:LYS:HE3	1:A:437:PRO:O	2.15	0.46
1:B:364:PRO:HG2	1:B:372:THR:HA	1.97	0.46
1:A:93:PHE:HB2	1:A:233:PHE:HZ	1.80	0.45
1:B:370:GLU:HG2	3:B:508:82M:C26	2.46	0.45
1:B:428:GLN:NE2	5:B:608:HOH:O	2.46	0.45
1:A:361:PHE:N	1:A:393:ASN:HD21	2.14	0.45
1:B:392:ASN:C	1:B:394:THR:H	2.19	0.45
1:B:91:GLU:HG3	1:B:226:LEU:HD13	1.99	0.45
1:A:350:LYS:NZ	5:A:615:HOH:O	2.50	0.44
1:A:200:VAL:O	1:A:201:ILE:HD13	2.18	0.44
1:A:298:ARG:HG3	1:A:420:ILE:CD1	2.48	0.44
1:B:115:SER:HB2	1:B:116:LEU:HD12	2.00	0.44
1:B:384:TYR:CZ	1:B:424:ILE:HD12	2.52	0.44
1:A:376:PHE:HB2	5:A:628:HOH:O	2.18	0.43
1:B:360:ILE:HG23	1:B:393:ASN:HD21	1.81	0.43
1:B:116:LEU:HD12	1:B:116:LEU:N	2.34	0.43
1:B:358:THR:HB	1:B:465:ASN:OD1	2.19	0.42
1:B:111:LEU:C	1:B:111:LEU:HD23	2.40	0.42
1:A:348:LYS:HD2	5:A:623:HOH:O	2.19	0.42
1:A:233:PHE:CE2	1:A:235:GLY:HA2	2.54	0.41
1:B:369:LEU:HD12	1:B:421:LYS:HE2	2.01	0.41
1:B:421:LYS:HE3	1:B:423:ILE:O	2.20	0.41
1:B:93:PHE:HB2	1:B:233:PHE:HZ	1.85	0.41
1:A:360:ILE:HG23	1:A:393:ASN:HD21	1.85	0.40
1:A:361:PHE:H	1:A:393:ASN:HD21	1.68	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	334/353 (95%)	326 (98%)	8 (2%)	0	100	100
1	B	334/353 (95%)	321 (96%)	13 (4%)	0	100	100
All	All	668/706 (95%)	647 (97%)	21 (3%)	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	304/311 (98%)	302 (99%)	2 (1%)	84	88
1	B	304/311 (98%)	304 (100%)	0	100	100
All	All	608/622 (98%)	606 (100%)	2 (0%)	92	95

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

Mol	Chain	Res	Type
1	A	373	MET
1	A	394	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	393	ASN

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

22 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	506	1	14,14,15	0.31	0	17,19,21	0.52	0
2	NAG	A	504	1	14,14,15	0.49	0	17,19,21	0.40	0
2	NAG	A	511	1	14,14,15	0.51	0	17,19,21	0.68	1 (5%)
2	NAG	A	510	1	14,14,15	0.16	0	17,19,21	0.72	1 (5%)
2	NAG	B	505	1	14,14,15	0.23	0	17,19,21	0.64	0
2	NAG	B	501	1	14,14,15	0.25	0	17,19,21	0.36	0
2	NAG	A	501	1	14,14,15	0.40	0	17,19,21	0.35	0
2	NAG	B	506	1	14,14,15	0.27	0	17,19,21	0.44	0
2	NAG	B	504	1	14,14,15	0.41	0	17,19,21	0.49	0
2	NAG	A	505	1	14,14,15	0.40	0	17,19,21	0.66	1 (5%)
2	NAG	A	509	1	14,14,15	0.36	0	17,19,21	0.46	0
4	EPE	B	509	-	15,15,15	0.91	1 (6%)	18,20,20	1.74	4 (22%)
2	NAG	A	503	1	14,14,15	0.38	0	17,19,21	0.65	1 (5%)
2	NAG	B	502	1	14,14,15	0.22	0	17,19,21	0.37	0
2	NAG	A	508	1	14,14,15	0.61	1 (7%)	17,19,21	0.71	1 (5%)
2	NAG	B	507	1	14,14,15	0.31	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	82M	A	512	-	25,29,29	2.25	5 (20%)	21,41,41	1.57	5 (23%)
2	NAG	B	503	1	14,14,15	0.52	0	17,19,21	0.83	1 (5%)
4	EPE	A	513	-	15,15,15	0.96	1 (6%)	18,20,20	1.61	5 (27%)
2	NAG	A	507	1	14,14,15	0.31	0	17,19,21	0.71	0
3	82M	B	508	-	25,29,29	2.25	7 (28%)	21,41,41	1.35	3 (14%)
2	NAG	A	502	1	14,14,15	0.26	0	17,19,21	0.59	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	A	506	1	-	0/6/23/26	0/1/1/1
2	NAG	A	504	1	-	2/6/23/26	0/1/1/1
2	NAG	A	511	1	-	2/6/23/26	0/1/1/1
2	NAG	A	510	1	-	4/6/23/26	0/1/1/1
2	NAG	B	505	1	-	0/6/23/26	0/1/1/1
2	NAG	B	501	1	-	2/6/23/26	0/1/1/1
2	NAG	A	501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	506	1	-	0/6/23/26	0/1/1/1
2	NAG	B	504	1	-	2/6/23/26	0/1/1/1
2	NAG	A	505	1	-	0/6/23/26	0/1/1/1
2	NAG	A	509	1	-	2/6/23/26	0/1/1/1
4	EPE	B	509	-	-	0/9/19/19	0/1/1/1
2	NAG	A	503	1	-	0/6/23/26	0/1/1/1
2	NAG	B	502	1	-	0/6/23/26	0/1/1/1
2	NAG	A	508	1	-	2/6/23/26	0/1/1/1
2	NAG	B	507	1	-	2/6/23/26	0/1/1/1
3	82M	A	512	-	-	1/10/20/20	0/3/3/3
2	NAG	B	503	1	-	0/6/23/26	0/1/1/1
4	EPE	A	513	-	-	0/9/19/19	0/1/1/1
2	NAG	A	507	1	-	6/6/23/26	0/1/1/1
3	82M	B	508	-	-	1/10/20/20	0/3/3/3
2	NAG	A	502	1	-	0/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	512	82M	C03-S06	-7.47	1.60	1.74
3	B	508	82M	C03-S06	-7.40	1.60	1.74
3	B	508	82M	C13-N12	5.17	1.45	1.34
3	A	512	82M	C13-N12	5.00	1.45	1.34
3	A	512	82M	C07-S06	-3.49	1.62	1.73
4	A	513	EPE	C10-S	3.47	1.82	1.77
3	B	508	82M	C07-S06	-3.41	1.63	1.73
4	B	509	EPE	C10-S	3.22	1.82	1.77
3	A	512	82M	C04-C03	2.93	1.53	1.50
3	B	508	82M	C20-C18	2.63	1.53	1.48
3	B	508	82M	C04-C03	2.52	1.53	1.50
3	A	512	82M	C20-C18	2.34	1.52	1.48
3	B	508	82M	C23-CL24	2.22	1.78	1.73
2	A	508	NAG	C1-C2	2.10	1.55	1.52
3	B	508	82M	O14-C13	-2.09	1.19	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	509	EPE	C5-N4-C3	4.20	118.27	108.83
4	A	513	EPE	C5-N4-C3	4.19	118.26	108.83
4	B	509	EPE	O3S-S-C10	3.79	111.90	105.77
2	B	503	NAG	C1-O5-C5	2.84	116.04	112.19
3	A	512	82M	C20-C18-N19	2.72	125.36	120.78
4	A	513	EPE	C7-N4-C5	2.67	118.07	111.23
3	B	508	82M	C20-C18-N19	2.61	125.17	120.78
2	A	510	NAG	C1-O5-C5	2.51	115.59	112.19
2	A	508	NAG	C1-O5-C5	2.47	115.54	112.19
3	A	512	82M	C09-N12-C13	-2.45	119.18	122.34
4	A	513	EPE	O3S-S-C10	2.45	109.73	105.77
3	A	512	82M	C15-C13-N12	2.44	119.74	115.20
4	B	509	EPE	C7-N4-C5	2.44	117.48	111.23
3	A	512	82M	C25-C23-C22	2.43	120.89	118.94
3	B	508	82M	C15-C13-N12	2.33	119.53	115.20
4	B	509	EPE	C7-N4-C3	2.29	117.10	111.23
4	A	513	EPE	C7-N4-C3	2.23	116.94	111.23
2	A	511	NAG	C1-O5-C5	2.20	115.17	112.19
3	A	512	82M	C17-C18-C20	-2.12	126.79	128.77
2	A	505	NAG	C1-O5-C5	2.11	115.05	112.19
3	B	508	82M	C09-N12-C13	-2.11	119.62	122.34
2	A	503	NAG	C1-O5-C5	2.09	115.03	112.19
4	A	513	EPE	C2-C3-N4	2.01	114.77	110.64

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	512	82M	N12-C09-C10-N11
3	B	508	82M	N12-C09-C10-N11
2	A	507	NAG	C4-C5-C6-O6
2	A	507	NAG	O5-C5-C6-O6
2	A	510	NAG	O5-C5-C6-O6
2	B	501	NAG	O5-C5-C6-O6
2	A	510	NAG	C4-C5-C6-O6
2	A	507	NAG	C8-C7-N2-C2
2	A	507	NAG	O7-C7-N2-C2
2	A	510	NAG	C8-C7-N2-C2
2	A	510	NAG	O7-C7-N2-C2
2	B	501	NAG	C4-C5-C6-O6
2	A	508	NAG	C4-C5-C6-O6
2	A	511	NAG	O5-C5-C6-O6
2	A	509	NAG	O5-C5-C6-O6
2	B	504	NAG	O5-C5-C6-O6
2	A	508	NAG	O5-C5-C6-O6
2	A	509	NAG	C4-C5-C6-O6
2	A	511	NAG	C4-C5-C6-O6
2	B	504	NAG	C4-C5-C6-O6
2	A	507	NAG	C3-C2-N2-C7
2	A	507	NAG	C1-C2-N2-C7
2	A	504	NAG	C4-C5-C6-O6
2	A	504	NAG	O5-C5-C6-O6
2	B	507	NAG	C4-C5-C6-O6
2	B	507	NAG	O5-C5-C6-O6

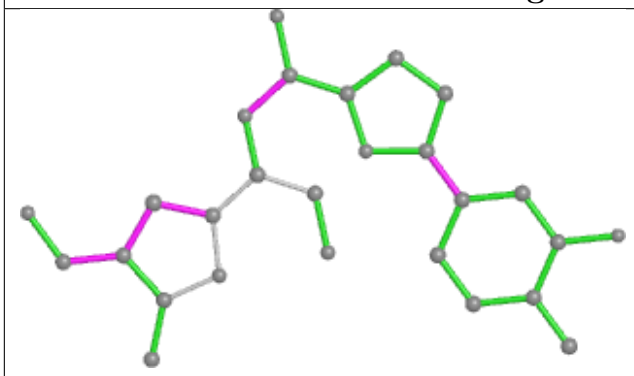
There are no ring outliers.

9 monomers are involved in 11 short contacts:

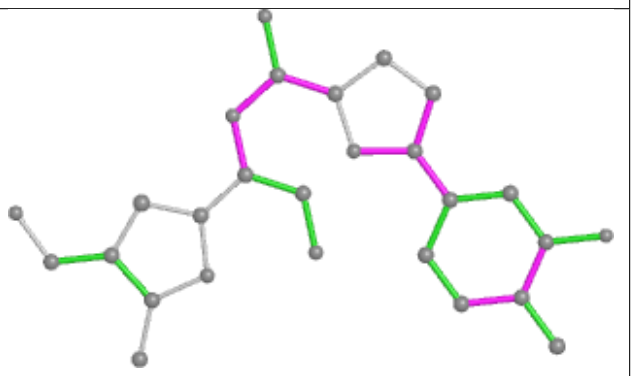
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	506	NAG	1	0
2	A	504	NAG	1	0
2	A	511	NAG	1	0
2	A	510	NAG	1	0
2	B	505	NAG	1	0
2	A	505	NAG	1	0
2	A	508	NAG	1	0
2	A	507	NAG	3	0
3	B	508	82M	1	0

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.

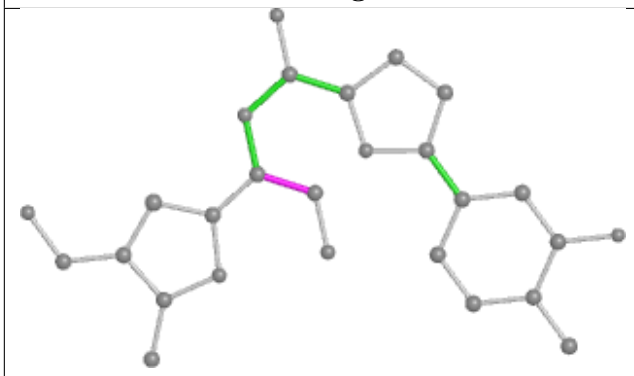
Ligand 82M A 512



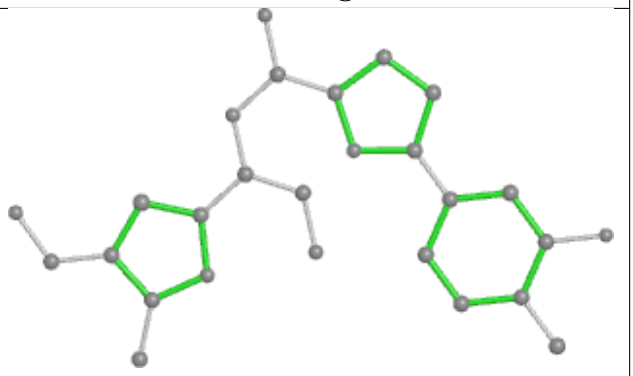
Bond lengths



Bond angles

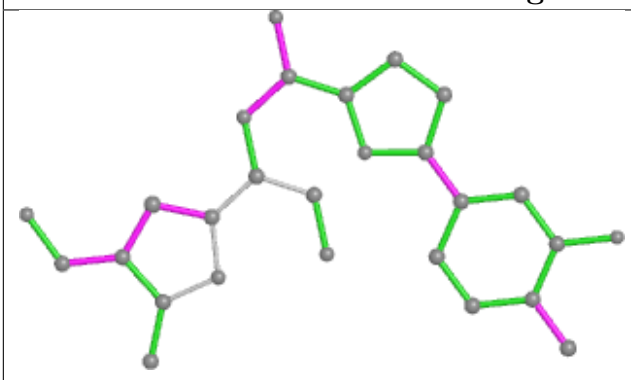


Torsions

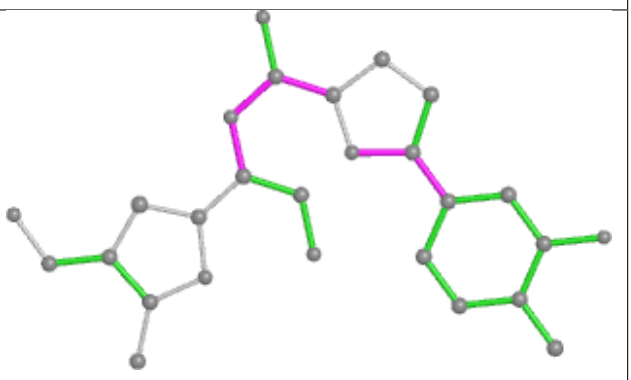


Rings

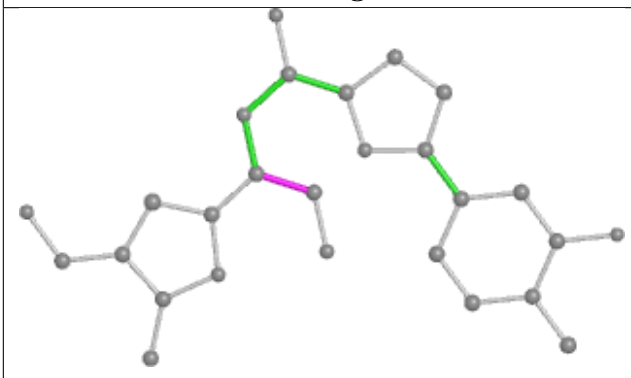
Ligand 82M B 508



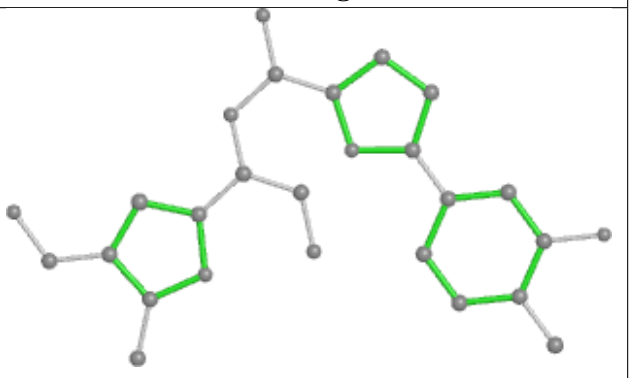
Bond lengths



Bond angles



Torsions



Rings

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	340/353 (96%)	0.29	28 (8%)	11	15	31, 48, 92, 127	0
1	B	340/353 (96%)	0.98	63 (18%)	1	1	38, 76, 131, 185	0
All	All	680/706 (96%)	0.64	91 (13%)	3	4	31, 59, 119, 185	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	GLY	9.7
1	B	123	THR	9.1
1	B	44	VAL	8.9
1	B	462	ASN	7.0
1	A	199	SER	7.0
1	A	124	GLY	6.8
1	B	460	ALA	6.5
1	B	396	ILE	6.1
1	A	301	ASN	5.7
1	B	465	ASN	5.6
1	B	358	THR	5.5
1	A	198	GLY	5.4
1	B	200	VAL	5.3
1	B	353	PHE	5.3
1	B	492	GLU	5.2
1	B	354	ASN	5.2
1	B	464	SER	5.0
1	B	394	THR	4.8
1	B	89	VAL	4.7
1	A	492	GLU	4.7
1	A	123	THR	4.6
1	B	301	ASN	4.3
1	B	491	ILE	4.3
1	B	240	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	459	GLY	4.2
1	B	350	LYS	4.1
1	A	201	ILE	4.0
1	A	122	LEU	4.0
1	B	461	ASN	4.0
1	A	44	VAL	4.0
1	B	410	CYS	3.9
1	B	198	GLY	3.9
1	B	467	THR	3.8
1	B	343	LYS	3.7
1	B	463	THR	3.7
1	A	108	VAL	3.6
1	B	261	LEU	3.5
1	A	255	VAL	3.5
1	B	90	THR	3.5
1	B	392	ASN	3.4
1	A	479	TRP	3.4
1	B	199	SER	3.3
1	B	86	LEU	3.3
1	A	200	VAL	3.3
1	B	45	TRP	3.2
1	A	410	CYS	3.2
1	B	122	LEU	3.2
1	B	277	LEU	3.2
1	B	201	ILE	3.2
1	B	242	VAL	3.2
1	B	263	GLY	3.0
1	B	360	ILE	3.0
1	B	347	GLU	2.9
1	A	254	VAL	2.9
1	B	359	ILE	2.9
1	B	479	TRP	2.8
1	B	365	SER	2.8
1	A	88	ASN	2.8
1	B	239	CYS	2.7
1	B	262	ASN	2.7
1	B	84	ILE	2.7
1	A	483	LEU	2.7
1	A	116	LEU	2.7
1	B	326	ILE	2.6
1	B	213	ILE	2.6
1	B	458	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	355	ASN	2.5
1	B	224	VAL	2.4
1	A	256	SER	2.4
1	B	376	PHE	2.4
1	B	281	ALA	2.4
1	A	481	SER	2.3
1	B	393	ASN	2.3
1	B	88	ASN	2.3
1	B	232	ASN	2.3
1	A	324	GLY	2.2
1	B	472	GLY	2.2
1	B	82	GLN	2.2
1	A	395	CYS	2.2
1	B	212	PRO	2.2
1	A	260	LEU	2.2
1	B	351	GLU	2.2
1	B	352	HIS	2.1
1	A	394	THR	2.1
1	B	375	SER	2.1
1	B	429	GLY	2.1
1	A	375	SER	2.1
1	B	357	LYS	2.1
1	A	104	MET	2.1
1	A	79	PRO	2.1
1	A	109	ILE	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)

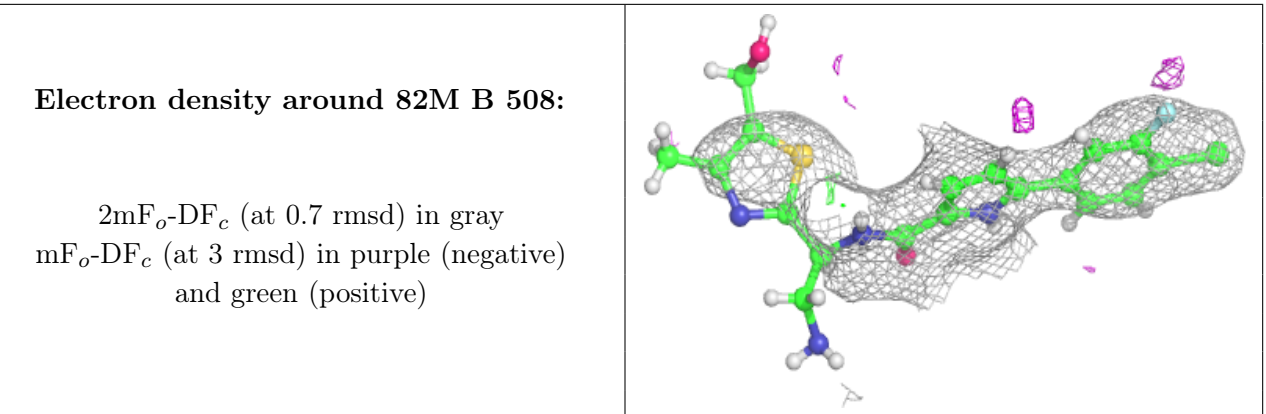
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

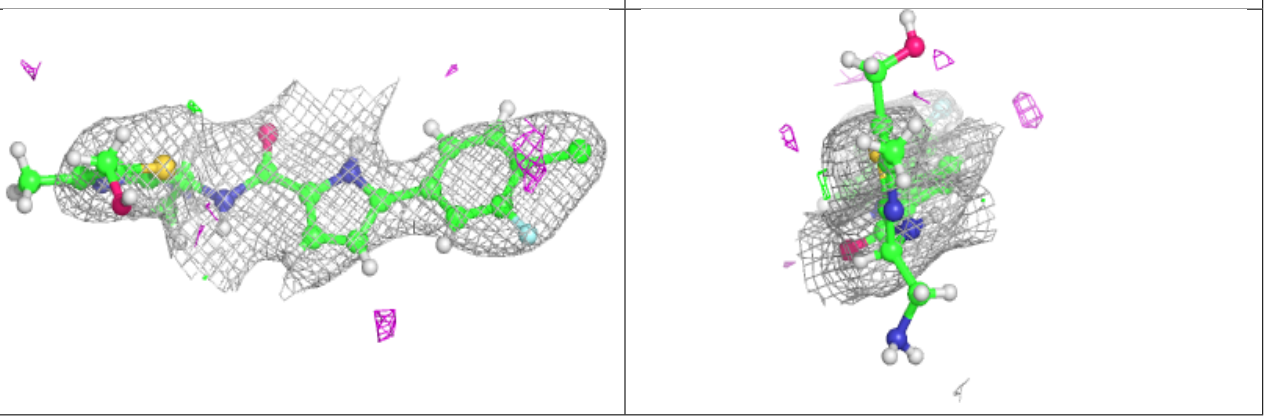
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	A	510	14/15	0.65	0.24	74,88,94,97	0
3	82M	B	508	27/27	0.72	0.24	74,104,152,153	0
2	NAG	B	506	14/15	0.77	0.29	74,95,105,107	0
2	NAG	A	511	14/15	0.78	0.30	76,95,104,111	0
2	NAG	A	502	14/15	0.80	0.27	87,103,108,109	0
3	82M	A	512	27/27	0.81	0.19	47,77,117,121	0
2	NAG	B	507	14/15	0.85	0.23	68,87,93,97	0
2	NAG	B	502	14/15	0.86	0.30	75,96,99,101	0
2	NAG	B	505	14/15	0.86	0.20	55,72,80,85	0
2	NAG	B	504	14/15	0.87	0.25	71,82,94,96	0
2	NAG	A	507	14/15	0.88	0.22	61,78,81,86	0
2	NAG	B	501	14/15	0.91	0.16	63,77,83,84	0
2	NAG	A	509	14/15	0.91	0.17	51,68,74,75	0
2	NAG	A	501	14/15	0.92	0.11	54,69,73,73	0
2	NAG	A	504	14/15	0.93	0.18	49,58,64,64	0
2	NAG	A	506	14/15	0.93	0.16	55,66,77,80	0
2	NAG	A	505	14/15	0.94	0.12	42,54,59,66	0
2	NAG	A	503	14/15	0.95	0.10	39,45,51,54	0
2	NAG	A	508	14/15	0.96	0.11	41,51,71,78	0
2	NAG	B	503	14/15	0.97	0.17	36,40,43,46	0
4	EPE	B	509	15/15	0.98	0.10	49,58,65,68	0
4	EPE	A	513	15/15	0.99	0.17	38,43,46,48	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 82M B 508:

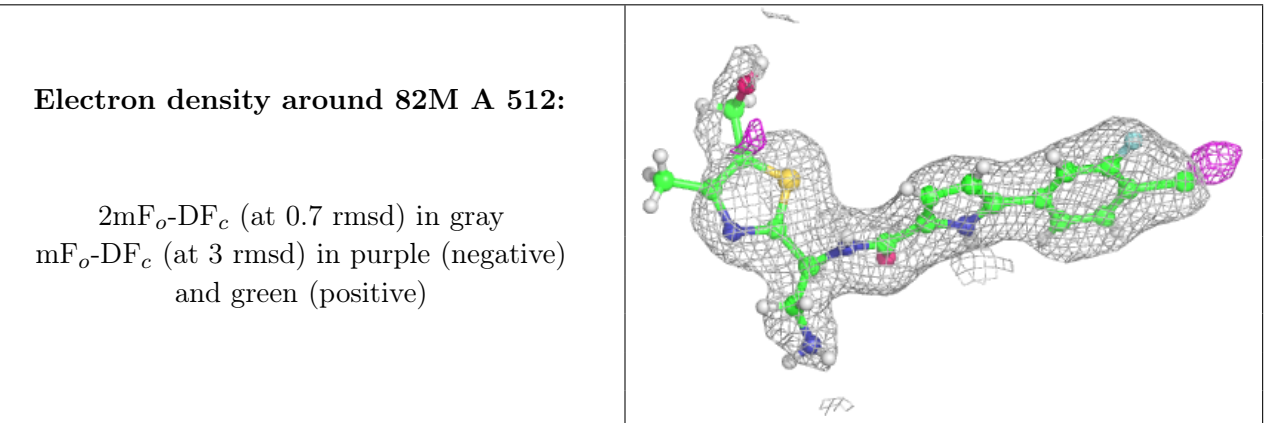
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

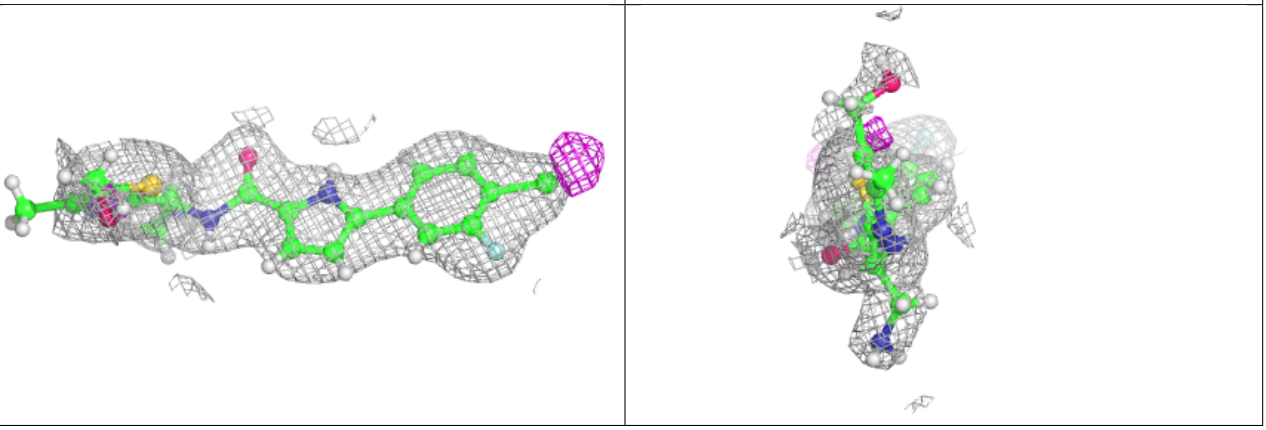




Electron density around 82M A 512:

$2mF_o$-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.