Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2023 – 12:38 AM EDT

PDB ID	:	4DKV
Title	:	Crystal structure of clade A/E 93TH057 HIV-1 gp120 core in complex with NBD-10007
Authors	:	Kwon, Y.D.; Debnath, A.K.; Kwong, P.D.
Deposited on	:	2012-02-04
Resolution	:	2.18 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 (i) 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 (i)) were used in the production of this report:

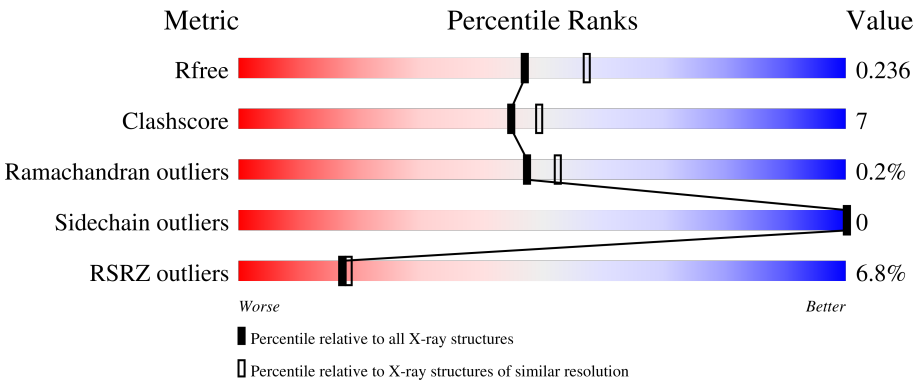
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.18 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	3% 90% 6% ·
1	B	353	10% 81% 15% ·

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	NAG	A	502	-	-	-	X
2	NAG	A	507	-	-	-	X
2	NAG	A	510	-	-	-	X
4	0KW	B	511	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5922 atoms, of which 50 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.

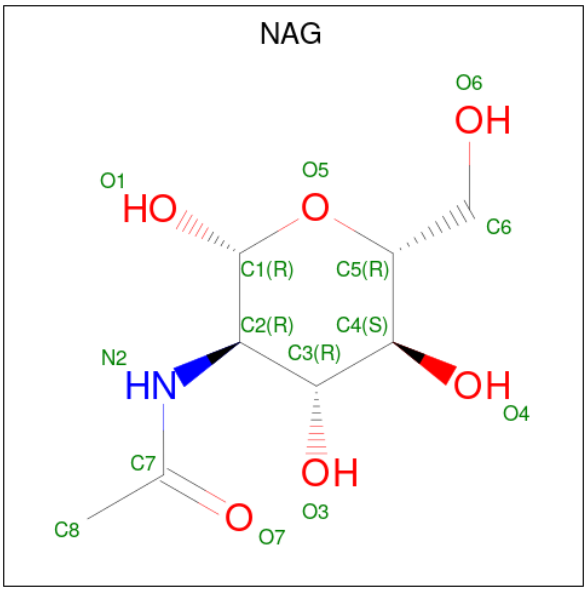
- Molecule 1 is a protein called HIV-1 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	339	2654	1666	460	507	21	0	0	0
1	B	339	2654	1666	460	507	21	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	GLY	-	linker	UNP Q0ED31
A	198	GLY	-	linker	UNP Q0ED31
A	318	GLY	-	linker	UNP Q0ED31
A	319	GLY	-	linker	UNP Q0ED31
A	320	SER	-	linker	UNP Q0ED31
A	321	GLY	-	linker	UNP Q0ED31
A	322	SER	-	linker	UNP Q0ED31
A	323	GLY	-	linker	UNP Q0ED31
A	375	SER	HIS	engineered mutation	UNP Q0ED31
B	124	GLY	-	linker	UNP Q0ED31
B	198	GLY	-	linker	UNP Q0ED31
B	318	GLY	-	linker	UNP Q0ED31
B	319	GLY	-	linker	UNP Q0ED31
B	320	SER	-	linker	UNP Q0ED31
B	321	GLY	-	linker	UNP Q0ED31
B	322	SER	-	linker	UNP Q0ED31
B	323	GLY	-	linker	UNP Q0ED31
B	375	SER	HIS	engineered mutation	UNP Q0ED31

- 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
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
			Total	C	N	O		
2	B	1	14	8	1	5	0	0
			Total	C	N	O		
2	B	1	14	8	1	5	0	0
			Total	C	N	O		
2	B	1	14	8	1	5	0	0

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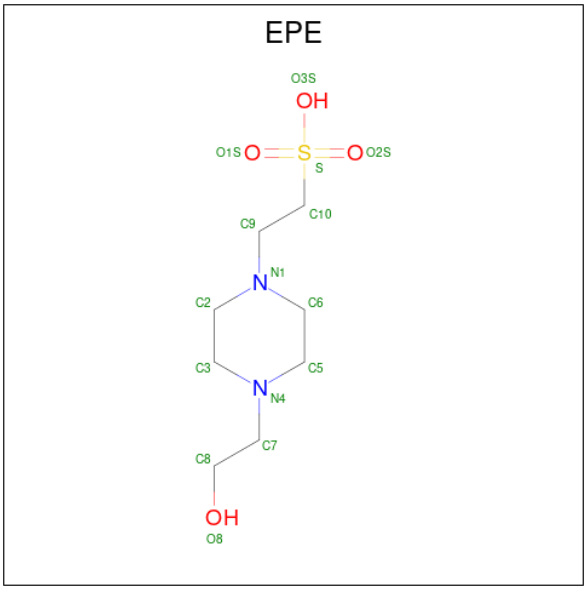
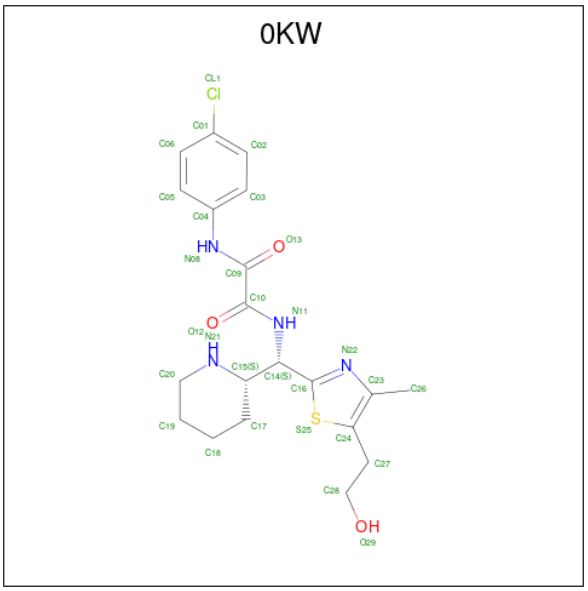
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	14	8	1	5	0	0
2	B	1	14	8	1	5	0	0
2	B	1	14	8	1	5	0	0
2	B	1	14	8	1	5	0	0
2	B	1	14	8	1	5	0	0
2	B	1	14	8	1	5	0	0

- Molecule 3 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
			Total	C	N	O	S		
3	A	1	15	8	2	4	1	0	0
3	B	1	15	8	2	4	1	0	0

- Molecule 4 is N-(4-chlorophenyl)-N'-{(S)-[5-(2-hydroxyethyl)-4-methyl-1,3-thiazol-2-yl][(2S)-piperidin-2-yl]methyl}ethanediamide (three-letter code: 0KW) (formula: $C_{20}H_{25}ClN_4O_3S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Cl	H	N	O	S		
4	A	1	54	20	1	25	4	3	1	0	0
			Total	C	Cl	H	N	O	S		
4	B	1	54	20	1	25	4	3	1	0	0

- Molecule 5 is water.

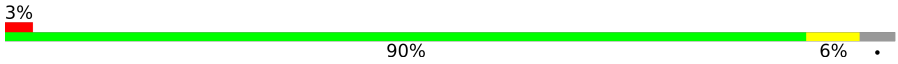
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	117	117	117	0	0
			Total	O		
5	B	79	79	79	0	0

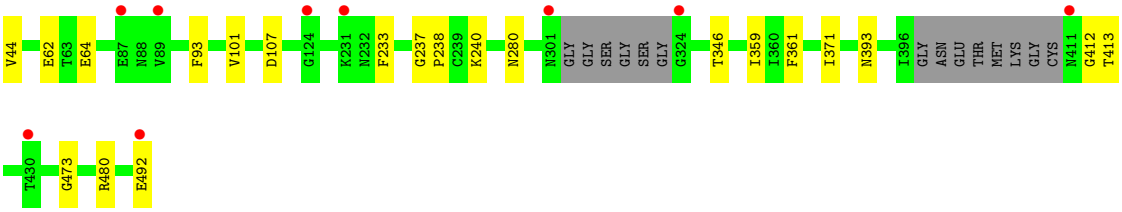
3 Residue-property plots (i)

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: HIV-1 gp120 core

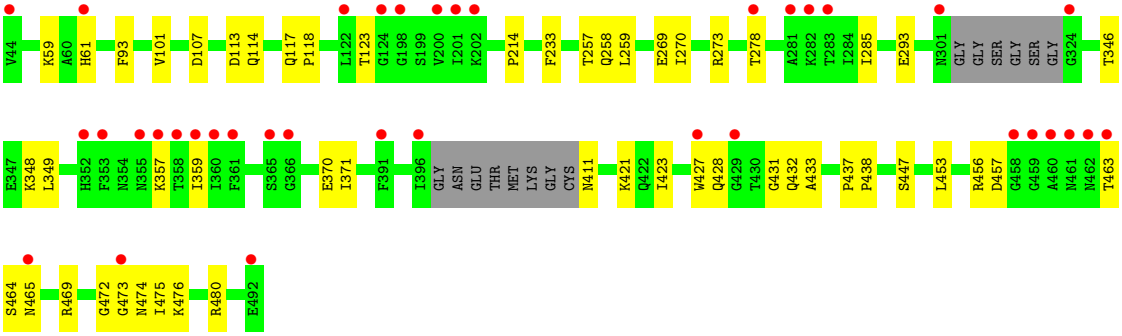
Chain A:





- Molecule 1: 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	64.33Å 68.77Å 93.85Å 90.00° 91.74° 90.00°	Depositor
Resolution (Å)	27.60 – 2.18 46.97 – 2.18	Depositor EDS
% Data completeness (in resolution range)	91.5 (27.60-2.18) 85.5 (46.97-2.18)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	0.92 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.200 , 0.235 0.202 , 0.236	Depositor DCC
R_{free} test set	1954 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	42.5	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5922	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, 0KW, 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	1/2709 (0.0%)	0.44	1/3678 (0.0%)
1	B	0.23	0/2709	0.40	0/3678
All	All	0.28	1/5418 (0.0%)	0.42	1/7356 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	PRO	N-CD	6.13	1.56	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	237	GLY	C-N-CD	5.15	139.22	128.40

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	2654	0	2588	19	0
1	B	2654	0	2591	52	0
2	A	154	0	143	9	0
2	B	126	0	117	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	15	0	17	3	0
3	B	15	0	17	2	0
4	A	29	25	25	3	0
4	B	29	25	25	4	0
5	A	117	0	0	4	0
5	B	79	0	0	15	0
All	All	5872	50	5523	73	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 (73) 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:371:ILE:CD1	4:B:511:0KW:H14	1.70	1.19
1:B:411:ASN:ND2	5:B:659:HOH:O	1.89	1.06
1:B:411:ASN:CG	5:B:659:HOH:O	1.93	1.05
1:B:474:ASN:N	5:B:651:HOH:O	1.87	1.04
1:B:371:ILE:HD11	4:B:511:0KW:C19	1.86	1.04
1:B:411:ASN:N	5:B:659:HOH:O	1.96	0.97
1:B:123:THR:CG2	1:B:432:GLN:H	1.77	0.97
1:B:472:GLY:O	5:B:651:HOH:O	1.83	0.95
1:B:123:THR:HG21	1:B:432:GLN:H	1.30	0.94
2:A:503:NAG:O3	5:A:664:HOH:O	1.84	0.94
1:A:280:ASN:OD1	5:A:714:HOH:O	1.86	0.94
1:B:371:ILE:HD11	4:B:511:0KW:H14	0.93	0.93
1:B:123:THR:HG21	1:B:431:GLY:HA3	1.49	0.92
1:B:411:ASN:CA	5:B:664:HOH:O	2.18	0.92
1:A:480:ARG:NH2	5:A:663:HOH:O	2.04	0.90
1:B:357:LYS:HE3	1:B:464:SER:HA	1.56	0.88
1:B:411:ASN:N	5:B:664:HOH:O	2.06	0.87
1:B:269:GLU:OE2	5:B:678:HOH:O	1.92	0.87
1:B:293:GLU:OE2	5:B:663:HOH:O	1.93	0.86
1:B:411:ASN:CA	5:B:659:HOH:O	2.27	0.83
1:B:123:THR:HG21	1:B:432:GLN:N	1.98	0.79
1:B:411:ASN:HA	5:B:664:HOH:O	1.77	0.76
1:A:371:ILE:HD11	4:A:513:0KW:H10	1.71	0.70
1:A:361:PHE:O	1:A:393:ASN:ND2	2.24	0.70
1:B:117:GLN:O	5:B:640:HOH:O	2.11	0.69
1:B:346:THR:O	1:B:359:ILE:HD12	1.94	0.67
1:B:357:LYS:HE3	1:B:464:SER:CA	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:GLY:HA3	4:A:513:0KW:H9	1.76	0.66
1:B:123:THR:HG23	1:B:432:GLN:H	1.61	0.65
1:A:240:LYS:HD2	2:A:502:NAG:H82	1.81	0.62
1:B:370:GLU:HG2	4:B:511:0KW:N08	2.15	0.61
1:B:114:GLN:OE1	5:B:642:HOH:O	2.16	0.60
1:B:59:LYS:O	5:B:602:HOH:O	2.17	0.59
1:A:346:THR:HG23	1:A:359:ILE:HB	1.85	0.59
1:B:123:THR:HG21	1:B:431:GLY:CA	2.26	0.59
1:B:457:ASP:OD2	1:B:469:ARG:NH1	2.37	0.58
2:A:508:NAG:H62	1:B:214:PRO:HG2	1.87	0.57
3:A:512:EPE:H61	5:A:653:HOH:O	2.04	0.56
1:B:270:ILE:O	1:B:348:LYS:NZ	2.34	0.55
1:A:62:GLU:HG3	1:A:64:GLU:H	1.72	0.54
1:A:107:ASP:OD2	3:A:512:EPE:H72	2.08	0.54
1:A:413:THR:OG1	2:A:507:NAG:H81	2.06	0.54
1:A:412:GLY:C	2:A:507:NAG:H82	2.28	0.53
1:A:412:GLY:HA2	2:A:507:NAG:H82	1.91	0.52
1:B:107:ASP:OD2	3:B:510:EPE:H72	2.11	0.51
1:A:93:PHE:HB2	1:A:233:PHE:HZ	1.77	0.50
1:B:349:LEU:HB2	1:B:359:ILE:HD13	1.95	0.48
1:B:463:THR:HG23	1:B:465:ASN:H	1.77	0.48
1:B:273:ARG:HB2	1:B:285:ILE:HB	1.94	0.48
1:B:101:VAL:HG21	1:B:480:ARG:HG2	1.95	0.47
1:A:473:GLY:HA3	4:A:513:0KW:C17	2.43	0.47
1:B:421:LYS:NZ	1:B:423:ILE:O	2.47	0.47
1:B:427:TRP:HB2	1:B:475:ILE:HG13	1.97	0.46
1:B:357:LYS:HB3	1:B:464:SER:O	2.15	0.46
1:B:447:SER:HB3	2:B:503:NAG:HN2	1.81	0.46
1:B:93:PHE:HB2	1:B:233:PHE:HZ	1.81	0.45
1:A:44:VAL:HG13	1:A:492:GLU:HB2	1.98	0.44
1:A:412:GLY:CA	2:A:507:NAG:H82	2.47	0.44
1:B:278:THR:O	1:B:456:ARG:NH2	2.50	0.44
1:A:107:ASP:OD1	3:A:512:EPE:H31	2.18	0.44
1:B:113:ASP:O	1:B:117:GLN:NE2	2.40	0.44
1:B:257:THR:O	1:B:259:LEU:N	2.50	0.43
1:A:101:VAL:HG21	1:A:480:ARG:HG2	2.01	0.43
1:B:453:LEU:HD13	1:B:473:GLY:HA3	2.01	0.43
2:A:504:NAG:HN2	1:B:61:HIS:CG	2.36	0.42
1:B:438:PRO:O	5:B:632:HOH:O	2.22	0.41
1:B:59:LYS:HD3	1:B:61:HIS:CE1	2.55	0.41
1:B:118:PRO:HG3	1:B:433:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:GLN:OE1	1:B:428:GLN:N	2.52	0.41
1:B:107:ASP:OD1	3:B:510:EPE:H31	2.21	0.41
1:B:437:PRO:HA	1:B:438:PRO:HD3	1.94	0.40
1:A:413:THR:N	2:A:507:NAG:H82	2.36	0.40
1:B:476:LYS:O	1:B:480:ARG:HG3	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	333/353 (94%)	321 (96%)	12 (4%)	0	100	100
1	B	333/353 (94%)	317 (95%)	15 (4%)	1 (0%)	41	43
All	All	666/706 (94%)	638 (96%)	27 (4%)	1 (0%)	47	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	258	GLN

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	303/311 (97%)	303 (100%)	0	100	100
1	B	303/311 (97%)	303 (100%)	0	100	100
All	All	606/622 (97%)	606 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	114	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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

24 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	505	1	14,14,15	0.49	0	17,19,21	0.85	1 (5%)
2	NAG	B	506	1	14,14,15	0.55	0	17,19,21	0.56	0
2	NAG	A	507	1	14,14,15	0.61	0	17,19,21	1.00	1 (5%)
2	NAG	A	504	1	14,14,15	0.51	0	17,19,21	0.70	0
2	NAG	B	502	1	14,14,15	0.64	0	17,19,21	1.06	1 (5%)
2	NAG	A	506	1	14,14,15	0.54	0	17,19,21	0.59	0
2	NAG	A	509	1	14,14,15	0.51	0	17,19,21	0.76	0
2	NAG	B	501	1	14,14,15	0.55	0	17,19,21	0.63	0
2	NAG	A	503	1	14,14,15	0.48	0	17,19,21	0.81	0
2	NAG	A	510	1	14,14,15	0.50	0	17,19,21	0.89	1 (5%)
2	NAG	B	503	1	14,14,15	0.46	0	17,19,21	0.91	0
3	EPE	B	510	-	15,15,15	2.46	4 (26%)	18,20,20	3.81	5 (27%)
2	NAG	B	505	1	14,14,15	0.57	0	17,19,21	0.97	0
4	0KW	A	513	-	28,31,31	2.19	11 (39%)	30,42,42	2.02	6 (20%)
2	NAG	A	508	1	14,14,15	0.66	0	17,19,21	0.74	0
3	EPE	A	512	-	15,15,15	2.44	4 (26%)	18,20,20	3.72	6 (33%)
2	NAG	B	508	1	14,14,15	0.49	0	17,19,21	0.76	0
2	NAG	B	507	1	14,14,15	0.49	0	17,19,21	0.77	0
2	NAG	A	502	1	14,14,15	0.64	0	17,19,21	1.06	1 (5%)
2	NAG	B	509	1	14,14,15	0.51	0	17,19,21	0.64	0
2	NAG	A	511	1	14,14,15	0.52	0	17,19,21	1.03	1 (5%)
2	NAG	B	504	1	14,14,15	1.17	0	17,19,21	1.25	2 (11%)
2	NAG	A	501	1	14,14,15	0.55	0	17,19,21	0.60	0
4	0KW	B	511	-	28,31,31	2.21	11 (39%)	30,42,42	2.01	6 (20%)

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	505	1	-	0/6/23/26	0/1/1/1
2	NAG	B	506	1	-	0/6/23/26	0/1/1/1
2	NAG	A	507	1	-	4/6/23/26	0/1/1/1
2	NAG	A	504	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	506	1	-	0/6/23/26	0/1/1/1
2	NAG	A	509	1	-	0/6/23/26	0/1/1/1
2	NAG	B	501	1	-	4/6/23/26	0/1/1/1
2	NAG	A	503	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	510	1	-	4/6/23/26	0/1/1/1
2	NAG	B	503	1	-	0/6/23/26	0/1/1/1
3	EPE	B	510	-	-	3/9/19/19	0/1/1/1
2	NAG	B	505	1	-	2/6/23/26	0/1/1/1
4	0KW	A	513	-	-	5/18/31/31	0/3/3/3
2	NAG	A	508	1	-	3/6/23/26	0/1/1/1
3	EPE	A	512	-	-	2/9/19/19	0/1/1/1
2	NAG	B	508	1	-	0/6/23/26	0/1/1/1
2	NAG	B	507	1	-	3/6/23/26	0/1/1/1
2	NAG	A	502	1	-	0/6/23/26	0/1/1/1
2	NAG	B	509	1	-	2/6/23/26	0/1/1/1
2	NAG	A	511	1	-	3/6/23/26	0/1/1/1
2	NAG	B	504	1	-	0/6/23/26	0/1/1/1
2	NAG	A	501	1	-	0/6/23/26	0/1/1/1
4	0KW	B	511	-	-	5/18/31/31	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	511	0KW	C10-N11	5.55	1.45	1.34
4	A	513	0KW	C10-N11	5.54	1.45	1.34
3	B	510	EPE	O2S-S	5.07	1.60	1.45
3	A	512	EPE	O2S-S	5.05	1.59	1.45
3	B	510	EPE	O1S-S	4.99	1.59	1.45
3	A	512	EPE	O1S-S	4.91	1.59	1.45
4	B	511	0KW	C27-C24	4.38	1.52	1.50
3	B	510	EPE	O3S-S	4.30	1.62	1.47
3	A	512	EPE	O3S-S	4.25	1.62	1.47
4	A	513	0KW	C27-C24	4.23	1.52	1.50
3	B	510	EPE	O8-C8	-3.88	1.22	1.42
3	A	512	EPE	O8-C8	-3.87	1.22	1.42
4	A	513	0KW	C17-C15	-3.16	1.47	1.53
4	B	511	0KW	C17-C15	-3.15	1.47	1.53
4	B	511	0KW	C09-N08	3.12	1.42	1.35
4	A	513	0KW	C09-N08	3.10	1.42	1.35
4	B	511	0KW	C14-C15	-3.05	1.50	1.54
4	A	513	0KW	C14-C15	-3.01	1.50	1.54
4	B	511	0KW	C03-C04	-2.70	1.34	1.39
4	A	513	0KW	C03-C04	-2.67	1.34	1.39
4	B	511	0KW	O13-C09	-2.48	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	513	0KW	O13-C09	-2.45	1.18	1.23
4	A	513	0KW	C06-C01	-2.39	1.33	1.38
4	B	511	0KW	C06-C01	-2.32	1.33	1.38
4	B	511	0KW	C05-C04	-2.29	1.35	1.39
4	A	513	0KW	C05-C04	-2.26	1.35	1.39
4	B	511	0KW	C01-CL1	-2.25	1.69	1.74
4	A	513	0KW	C01-CL1	-2.25	1.69	1.74
4	B	511	0KW	C06-C05	-2.08	1.35	1.38
4	A	513	0KW	C06-C05	-2.03	1.35	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	510	EPE	O1S-S-C10	10.71	119.81	106.92
3	A	512	EPE	O1S-S-C10	10.26	119.27	106.92
3	B	510	EPE	O2S-S-C10	8.41	117.04	106.92
3	A	512	EPE	O2S-S-C10	8.35	116.97	106.92
3	B	510	EPE	O3S-S-O2S	-5.58	97.65	111.27
4	A	513	0KW	C17-C15-C14	5.46	118.41	112.61
4	B	511	0KW	C17-C15-C14	5.45	118.40	112.61
3	A	512	EPE	O3S-S-O2S	-5.36	98.19	111.27
4	B	511	0KW	C17-C15-N21	-5.15	104.34	111.90
4	A	513	0KW	C17-C15-N21	-5.14	104.35	111.90
3	A	512	EPE	O3S-S-O1S	-4.88	99.35	111.27
3	B	510	EPE	O3S-S-O1S	-4.78	99.58	111.27
4	A	513	0KW	C10-C09-N08	4.56	119.52	112.31
4	B	511	0KW	C10-C09-N08	4.55	119.51	112.31
2	B	504	NAG	C4-C3-C2	-3.21	106.31	111.02
2	A	511	NAG	O5-C5-C6	3.18	112.19	107.20
3	A	512	EPE	O8-C8-C7	2.85	122.98	111.19
3	B	510	EPE	O8-C8-C7	2.83	122.94	111.19
4	B	511	0KW	C09-C10-N11	2.71	120.23	113.73
4	A	513	0KW	C09-C10-N11	2.71	120.22	113.73
2	B	504	NAG	C2-N2-C7	-2.64	119.14	122.90
2	A	502	NAG	C4-C3-C2	2.56	114.77	111.02
2	B	502	NAG	C4-C3-C2	2.54	114.74	111.02
4	A	513	0KW	C19-C18-C17	2.33	116.16	111.42
2	A	510	NAG	C1-O5-C5	2.31	115.33	112.19
4	B	511	0KW	C19-C18-C17	2.30	116.10	111.42
4	B	511	0KW	C04-N08-C09	-2.24	123.64	127.53
4	A	513	0KW	C04-N08-C09	-2.24	123.64	127.53
2	A	505	NAG	C1-O5-C5	2.19	115.16	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	512	EPE	C9-N1-C6	2.09	116.58	111.23
2	A	507	NAG	C4-C3-C2	2.06	114.04	111.02

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	508	NAG	C3-C2-N2-C7
2	A	508	NAG	C8-C7-N2-C2
2	A	508	NAG	O7-C7-N2-C2
2	A	510	NAG	C8-C7-N2-C2
2	A	510	NAG	O7-C7-N2-C2
2	B	509	NAG	C8-C7-N2-C2
2	B	509	NAG	O7-C7-N2-C2
3	A	512	EPE	C10-C9-N1-C6
3	B	510	EPE	C10-C9-N1-C2
3	B	510	EPE	C10-C9-N1-C6
4	A	513	0KW	N11-C14-C15-C17
4	A	513	0KW	N11-C14-C15-N21
4	A	513	0KW	C16-C14-C15-C17
4	A	513	0KW	C16-C14-C15-N21
4	B	511	0KW	N11-C14-C15-C17
4	B	511	0KW	N11-C14-C15-N21
4	B	511	0KW	C16-C14-C15-C17
4	B	511	0KW	C16-C14-C15-N21
2	A	507	NAG	C8-C7-N2-C2
2	B	501	NAG	O5-C5-C6-O6
2	A	507	NAG	O7-C7-N2-C2
2	A	511	NAG	C8-C7-N2-C2
2	A	511	NAG	O7-C7-N2-C2
2	A	510	NAG	O5-C5-C6-O6
2	A	510	NAG	C4-C5-C6-O6
2	B	507	NAG	C8-C7-N2-C2
2	B	507	NAG	O7-C7-N2-C2
2	B	505	NAG	C4-C5-C6-O6
2	B	501	NAG	C4-C5-C6-O6
2	B	505	NAG	O5-C5-C6-O6
2	A	507	NAG	C4-C5-C6-O6
2	B	507	NAG	O5-C5-C6-O6
3	A	512	EPE	C10-C9-N1-C2
2	A	507	NAG	O5-C5-C6-O6
3	B	510	EPE	C9-C10-S-O1S

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Mol	Chain	Res	Type	Atoms
2	B	501	NAG	C8-C7-N2-C2
2	A	511	NAG	C4-C5-C6-O6
2	B	501	NAG	O7-C7-N2-C2
4	A	513	0KW	C23-C24-C27-C28
4	B	511	0KW	C23-C24-C27-C28

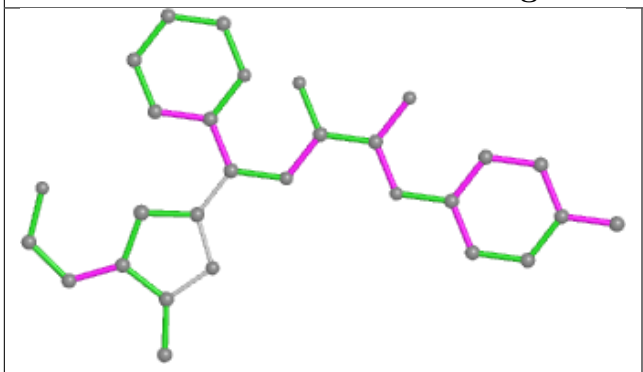
There are no ring outliers.

10 monomers are involved in 22 short contacts:

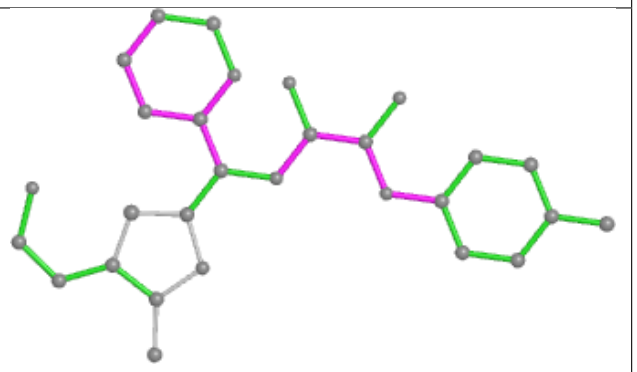
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	507	NAG	5	0
2	A	504	NAG	1	0
2	A	503	NAG	1	0
2	B	503	NAG	1	0
3	B	510	EPE	2	0
4	A	513	0KW	3	0
2	A	508	NAG	1	0
3	A	512	EPE	3	0
2	A	502	NAG	1	0
4	B	511	0KW	4	0

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.

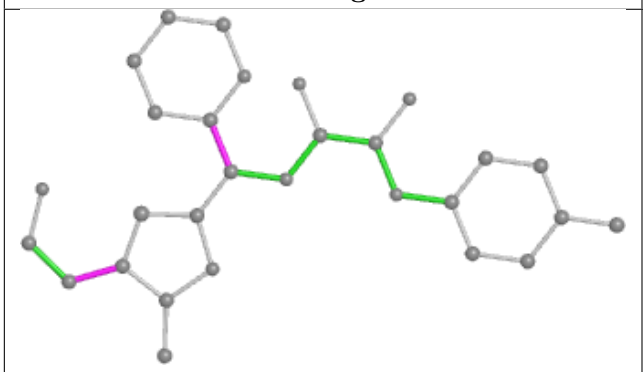
Ligand 0KW A 513



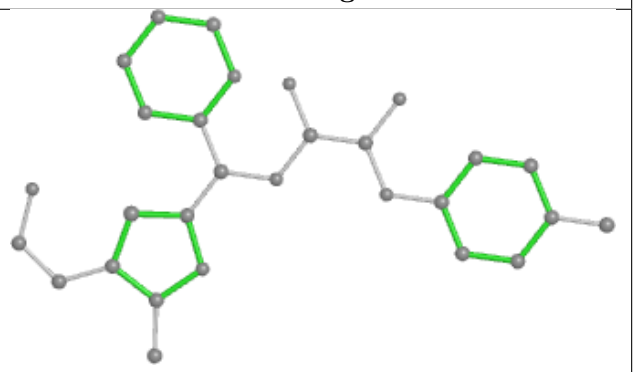
Bond lengths



Bond angles

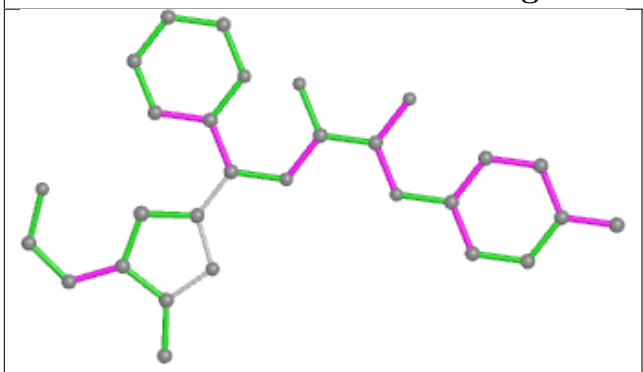


Torsions

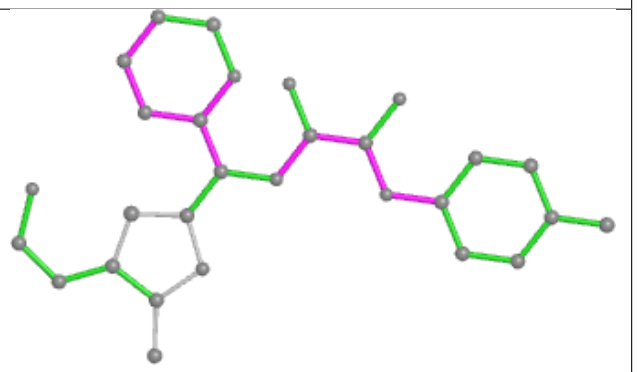


Rings

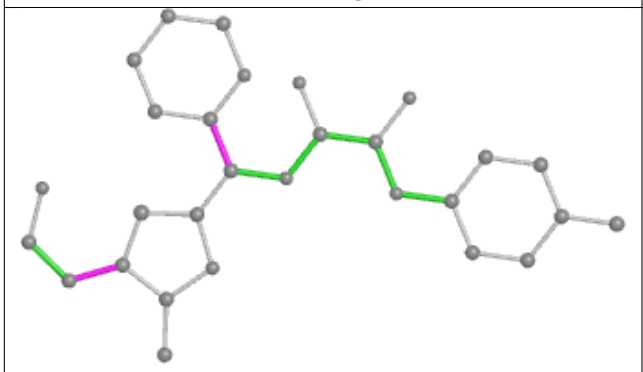
Ligand 0KW B 511



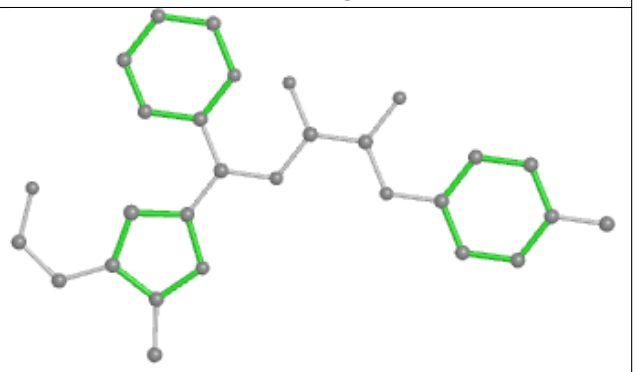
Bond lengths



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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	339/353 (96%)	0.15	9 (2%) 54 55	28, 44, 89, 122	0
1	B	339/353 (96%)	0.70	37 (10%) 5 6	32, 63, 117, 161	0
All	All	678/706 (96%)	0.42	46 (6%) 17 18	28, 52, 109, 161	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	GLY	8.4
1	B	124	GLY	7.3
1	B	460	ALA	7.1
1	B	200	VAL	6.8
1	B	461	ASN	6.6
1	B	44	VAL	6.3
1	B	473	GLY	5.3
1	B	353	PHE	5.2
1	B	278	THR	4.7
1	A	124	GLY	4.6
1	B	358	THR	4.1
1	B	459	GLY	3.9
1	B	462	ASN	3.9
1	B	365	SER	3.9
1	B	301	ASN	3.8
1	B	360	ILE	3.8
1	B	122	LEU	3.6
1	A	411	ASN	3.5
1	B	492	GLU	3.4
1	B	281	ALA	3.4
1	B	359	ILE	3.3
1	A	492	GLU	3.2
1	B	357	LYS	3.2
1	B	355	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	396	ILE	2.9
1	B	458	GLY	2.9
1	B	202	LYS	2.8
1	A	430	THR	2.8
1	B	361	PHE	2.7
1	B	324	GLY	2.7
1	A	89	VAL	2.6
1	B	198	GLY	2.6
1	A	301	ASN	2.6
1	B	465	ASN	2.6
1	B	61	HIS	2.5
1	B	352	HIS	2.5
1	B	429	GLY	2.5
1	B	201	ILE	2.3
1	B	283	THR	2.2
1	B	391	PHE	2.1
1	B	463	THR	2.1
1	B	366	GLY	2.1
1	A	87	GLU	2.1
1	A	231	LYS	2.1
1	B	427	TRP	2.0
1	B	282	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 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, 95th 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	0.39	0.78	134,143,153,155	0

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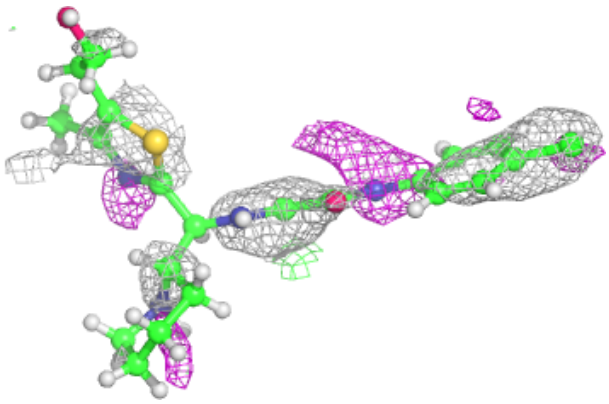
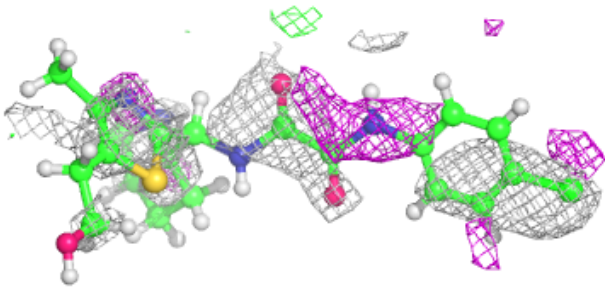
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	A	507	14/15	0.53	0.71	99,118,121,125	0
4	0KW	B	511	29/29	0.62	0.48	90,123,147,199	0
2	NAG	A	502	14/15	0.68	0.56	96,107,111,116	0
2	NAG	A	511	14/15	0.71	0.28	63,77,88,93	0
2	NAG	B	502	14/15	0.75	0.36	84,107,115,121	0
2	NAG	B	509	14/15	0.77	0.26	80,90,104,106	0
2	NAG	B	504	14/15	0.79	0.35	79,90,100,101	0
2	NAG	B	506	14/15	0.83	0.15	49,70,81,82	0
2	NAG	B	507	14/15	0.83	0.37	71,99,111,111	0
4	0KW	A	513	29/29	0.86	0.22	49,91,133,159	0
2	NAG	B	505	14/15	0.86	0.13	69,79,86,88	0
2	NAG	A	508	14/15	0.88	0.15	47,54,80,89	0
2	NAG	A	506	14/15	0.88	0.24	40,69,76,78	0
2	NAG	B	508	14/15	0.88	0.13	66,81,83,86	0
2	NAG	A	505	14/15	0.89	0.12	44,53,64,70	0
2	NAG	B	501	14/15	0.90	0.23	67,80,85,86	0
2	NAG	A	501	14/15	0.91	0.14	46,66,74,82	0
2	NAG	A	504	14/15	0.94	0.12	52,57,66,72	0
2	NAG	A	509	14/15	0.94	0.10	55,69,76,83	0
3	EPE	B	510	15/15	0.96	0.18	31,47,59,59	0
2	NAG	A	503	14/15	0.96	0.09	31,36,41,49	0
2	NAG	B	503	14/15	0.96	0.14	29,36,44,46	0
3	EPE	A	512	15/15	0.98	0.15	31,35,44,44	0

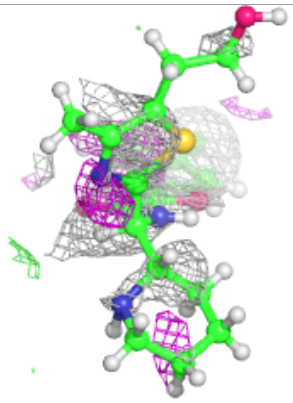
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 0KW B 511:

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

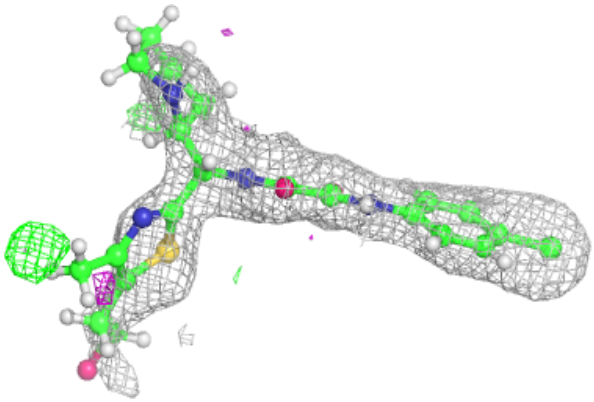


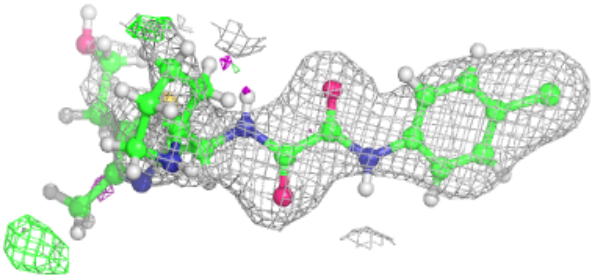


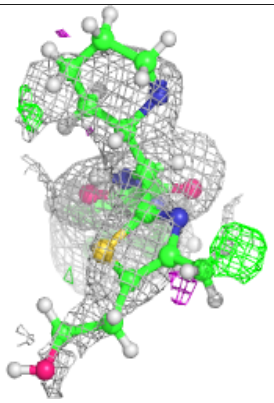


Electron density around 0KW A 513:

$2mF_o$-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.