



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:53 PM UTC

PDB ID : 4I54 / pdb_00004i54
Title : Crystal structure of clade A/E 93TH057 HIV-1 gp120 H375S core in complex with DMJ-II-121
Authors : Le-Khac, M.; Hendrickson, W.A.
Deposited on : 2012-11-28
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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

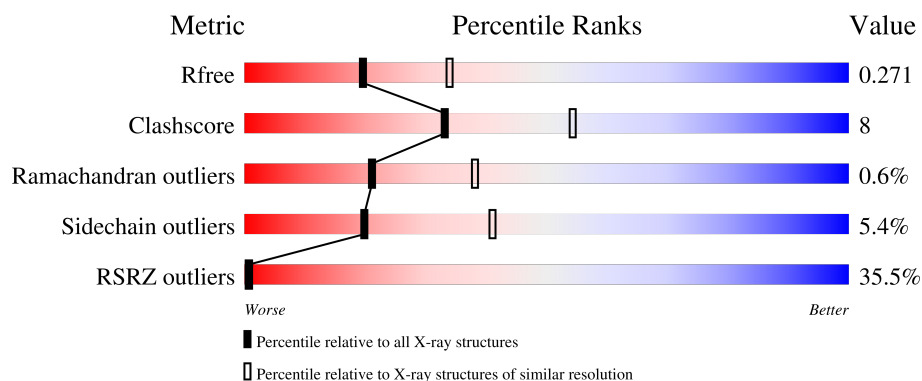
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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 $\leq 5\%$. 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	18% 82% 13% • •
1	B	353	50% 71% 23% • •

2 Entry composition [i](#)

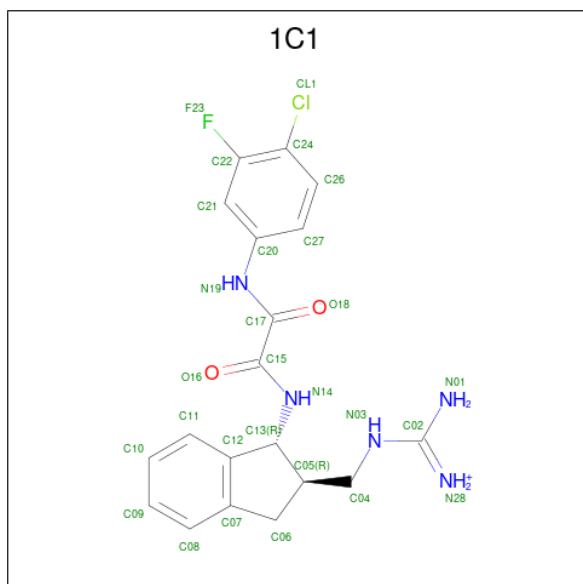
There are 5 unique types of molecules in this entry. The entry contains 5676 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HIV-1 glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2654	1666	460	507	21			
1	B	339	Total	C	N	O	S	0	5	0
			2687	1684	467	515	21			

- Molecule 2 is amino({[(1R,2R)-1-({[(4-chloro-3-fluorophenyl)amino](oxo)acetyl}amino)-2,3-dihydro-1H-inden-2-yl]methyl}amino)methaniminium (CCD ID: 1C1) (formula: C₁₉H₂₀ClFN₅O₂).





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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

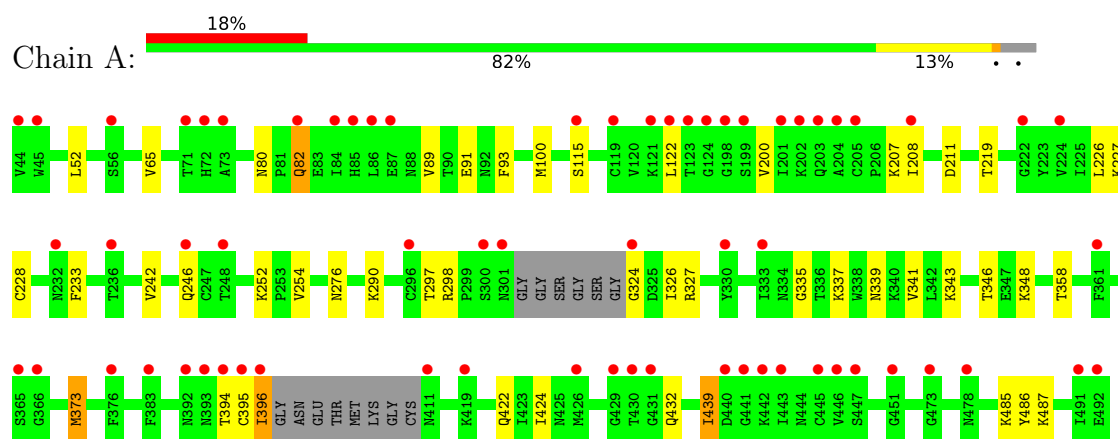
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	17	Total	O	0	0
			17	17		
5	B	8	Total	O	0	0
			8	8		

3 Residue-property plots

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 glycoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.32Å 68.78Å 94.44Å 90.00° 90.89° 90.00°	Depositor
Resolution (Å)	33.63 – 2.50 33.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (33.63-2.50) 97.9 (33.63-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.196 , 0.261 0.207 , 0.271	Depositor DCC
R_{free} test set	1849 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	-4.4	Xtriage
Anisotropy	5.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5676	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 6.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, NAG, 1C1

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	0.60	0/2709	0.90	2/3678 (0.1%)
1	B	0.48	0/2742	0.82	1/3722 (0.0%)
All	All	0.54	0/5451	0.86	3/7400 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ASP	CA-C-N	5.67	126.92	119.84
1	A	211	ASP	C-N-CA	5.67	126.92	119.84
1	B	291	SER	N-CA-C	5.22	116.92	108.41

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	2592	29	0
1	B	2687	0	2620	56	0
2	A	28	0	20	0	0
2	B	28	0	20	0	0
3	A	15	0	17	0	0
3	B	15	0	17	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	112	0	104	4	0
4	B	112	0	104	6	0
5	A	17	0	0	1	0
5	B	8	0	0	2	0
All	All	5676	0	5494	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 8.

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:B:234:ASN:HD22	4:B:502:NAG:C1	1.39	1.34
1:B:234:ASN:ND2	4:B:502:NAG:C2	2.48	0.77
1:A:485:LYS:HG2	1:A:485:LYS:O	1.86	0.74
1:A:91:GLU:OE1	1:A:487:LYS:NZ	2.22	0.71
1:A:228:CYS:O	1:A:485:LYS:HG3	1.89	0.71
1:B:361:PHE:O	1:B:393:ASN:ND2	2.28	0.66
1:B:265:LEU:HD21	1:B:291:SER:HB3	1.77	0.66
1:A:227:LYS:HD2	1:A:486:TYR:HE1	1.61	0.66
1:B:119:CYS:N	1:B:205:CYS:SG	2.69	0.65
1:A:335:GLY:O	1:A:339:ASN:ND2	2.28	0.65
1:B:234:ASN:OD1	1:B:234:ASN:N	2.30	0.65
1:B:59:LYS:HB3	1:B:61:HIS:CE1	2.32	0.64
1:B:234:ASN:ND2	4:B:502:NAG:H2	2.13	0.63
1:B:269:GLU:HB3	4:B:505:NAG:H61	1.81	0.62
1:B:423:ILE:HG12	1:B:434:MET:HG3	1.81	0.61
1:B:363:PRO:O	1:B:469:ARG:NH1	2.34	0.60
1:B:46:LYS:NZ	1:B:490:GLN:OE1	2.34	0.60
1:B:82:GLN:HE22	1:B:246:GLN:HG2	1.68	0.59
1:A:207:LYS:HD2	1:A:439:ILE:HG23	1.84	0.59
4:A:509:NAG:H82	1:B:252:LYS:HE3	1.86	0.58
1:A:228:CYS:O	1:A:485:LYS:CD	2.52	0.57
1:A:324:GLY:N	5:A:609:HOH:O	2.38	0.57
1:A:228:CYS:O	1:A:485:LYS:CG	2.53	0.56
1:A:65:VAL:HG11	1:A:208:ILE:HD12	1.88	0.56
1:A:91:GLU:OE1	1:A:487:LYS:CE	2.53	0.55
1:A:327:ARG:NH2	1:A:422:GLN:OE1	2.34	0.54
1:B:59:LYS:HB2	1:B:62:GLU:HG3	1.90	0.54
1:B:101:VAL:HG21	1:B:480:ARG:HG2	1.90	0.53
1:A:227:LYS:HD2	1:A:486:TYR:CE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:LEU:HD12	1:B:451:GLY:HA3	1.90	0.53
4:A:505:NAG:HN2	1:B:61:HIS:CD2	2.27	0.52
1:B:364:PRO:HG2	1:B:372:THR:HA	1.92	0.52
1:B:234:ASN:HD21	4:B:502:NAG:C1	2.14	0.52
1:A:91:GLU:HB2	1:A:242:VAL:HG21	1.91	0.52
1:B:390:LEU:HD11	1:B:416:LEU:HD11	1.92	0.52
1:B:384:TYR:CE1	1:B:421:LYS:HB2	2.45	0.52
1:B:229:ASN:HB2	1:B:241:ASN:HB2	1.91	0.51
1:B:378:CYS:HB3	1:B:383:PHE:CE1	2.46	0.51
1:A:82:GLN:OE1	1:A:246:GLN:NE2	2.44	0.51
1:B:234:ASN:HD21	4:B:502:NAG:C2	2.22	0.51
1:B:103:GLN:OE1	3:B:510:EPE:O8	2.28	0.50
1:B:264:SER:O	1:B:287:HIS:NE2	2.26	0.50
1:A:298:ARG:HD3	1:A:326:ILE:O	2.13	0.49
1:A:485:LYS:O	1:A:485:LYS:CG	2.58	0.49
1:B:91:GLU:HG3	1:B:226:LEU:HD13	1.95	0.49
1:B:103:GLN:HB3	3:B:510:EPE:O8	2.13	0.48
1:A:373:MET:HE3	4:A:510:NAG:H82	1.97	0.47
1:A:343:LYS:O	1:A:346:THR:OG1	2.31	0.47
1:B:342:LEU:O	1:B:345:VAL:HB	2.15	0.47
1:B:297:THR:OG1	5:B:608:HOH:O	2.21	0.47
1:B:341:VAL:O	1:B:345:VAL:HG23	2.15	0.47
1:A:337:LYS:O	1:A:341:VAL:HG23	2.16	0.46
1:B:426:MET:HE3	1:B:433:ALA:HB2	1.97	0.46
1:B:360:ILE:HD13	1:B:465:ASN:HB3	1.97	0.46
1:A:396:ILE:HD12	1:A:396:ILE:HA	1.81	0.46
3:B:510:EPE:H52	3:B:510:EPE:H82	1.68	0.46
1:B:384:TYR:O	5:B:607:HOH:O	2.21	0.45
1:B:258:GLN:CD	1:B:470:PRO:HB2	2.42	0.44
1:B:457:ASP:HB2	1:B:467:THR:HB	1.98	0.44
1:B:201:ILE:HG22	1:B:203:GLN:HG3	1.98	0.44
1:B:348:LYS:HD3	1:B:351:GLU:CD	2.41	0.44
1:B:229:ASN:HB2	1:B:241:ASN:CB	2.48	0.44
1:A:227:LYS:HA	1:A:485:LYS:O	2.18	0.44
1:A:52:LEU:HD11	1:A:100:MET:HG2	1.99	0.43
1:A:226:LEU:O	1:A:486:TYR:HA	2.18	0.43
1:B:274:SER:HB3	1:B:277:LEU:HG	1.99	0.43
1:B:439:ILE:HG13	1:B:443:ILE:HD11	1.99	0.43
1:A:93:PHE:HB2	1:A:233:PHE:HZ	1.84	0.43
1:B:277:LEU:HD23	1:B:277:LEU:HA	1.72	0.43
1:B:294:ILE:HD12	1:B:333:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:LEU:HD23	1:B:349:LEU:HA	1.83	0.43
1:A:122:LEU:HD23	1:A:200:VAL:HG22	2.01	0.43
1:B:57:ASP:OD1	1:B:77:THR:OG1	2.29	0.43
1:B:52:LEU:HD21	1:B:488:VAL:HG21	2.01	0.42
1:A:65:VAL:HB	1:A:115:SER:HB3	2.01	0.42
1:B:419:LYS:HA	1:B:419:LYS:HD3	1.81	0.42
1:A:290:LYS:HB2	4:A:506:NAG:H82	2.02	0.42
1:B:280:ASN:ND2	1:B:458:GLY:HA3	2.35	0.42
1:B:350:LYS:HG2	1:B:355:ASN:HA	2.01	0.41
1:B:426:MET:SD	1:B:430[A]:THR:OG1	2.77	0.41
1:B:99:ASN:O	1:B:103:GLN:HG3	2.19	0.41
1:B:392:ASN:C	1:B:394:THR:H	2.29	0.41
1:B:428[B]:GLN:OE1	1:B:428[B]:GLN:N	2.50	0.41
1:A:485:LYS:HE2	1:A:485:LYS:HB3	1.74	0.40
1:B:384:TYR:CG	1:B:421:LYS:HD3	2.56	0.40
1:B:231:LYS:HB3	1:B:268:GLU:HB2	2.03	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	333/353 (94%)	313 (94%)	19 (6%)	1 (0%)	36	55
1	B	338/353 (96%)	312 (92%)	23 (7%)	3 (1%)	14	27
All	All	671/706 (95%)	625 (93%)	42 (6%)	4 (1%)	21	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	GLU
1	B	241	ASN

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Mol	Chain	Res	Type
1	A	276	ASN
1	B	357	LYS

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	303/311 (97%)	287 (95%)	16 (5%)	20	42
1	B	306/311 (98%)	289 (94%)	17 (6%)	19	39
All	All	609/622 (98%)	576 (95%)	33 (5%)	20	41

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	82	GLN
1	A	89	VAL
1	A	219	THR
1	A	252	LYS
1	A	254	VAL
1	A	297	THR
1	A	348	LYS
1	A	358	THR
1	A	373	MET
1	A	394	THR
1	A	395	CYS
1	A	396	ILE
1	A	424	ILE
1	A	432	GLN
1	A	439	ILE
1	B	59	LYS
1	B	80	ASN
1	B	82	GLN
1	B	111	LEU
1	B	115	SER

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Mol	Chain	Res	Type
1	B	116	LEU
1	B	208	ILE
1	B	219	THR
1	B	232	ASN
1	B	234	ASN
1	B	268	GLU
1	B	348	LYS
1	B	358	THR
1	B	379	ARG
1	B	439	ILE
1	B	455	THR
1	B	457	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	246	GLN
1	A	352	HIS
1	A	444	ASN
1	A	465	ASN
1	B	61	HIS
1	B	82	GLN
1	B	114	GLN
1	B	355	ASN
1	B	362	GLN
1	B	465	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 oligosaccharides in this entry.

5.6 Ligand geometry

20 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	EPE	B	510	-	15,15,15	0.79	1 (6%)	19,20,20	1.83	3 (15%)
4	NAG	B	502	1	14,14,15	0.47	0	17,19,21	1.14	1 (5%)
4	NAG	B	503	1	14,14,15	0.64	0	17,19,21	1.35	3 (17%)
4	NAG	A	509	1	14,14,15	0.73	0	17,19,21	2.13	3 (17%)
2	1C1	A	501	-	30,30,30	3.37	11 (36%)	36,42,42	2.38	15 (41%)
4	NAG	A	505	1	14,14,15	0.75	0	17,19,21	1.07	1 (5%)
4	NAG	A	503	1	14,14,15	0.42	0	17,19,21	1.25	2 (11%)
4	NAG	A	507	1	14,14,15	0.42	0	17,19,21	2.25	2 (11%)
3	EPE	A	502	-	15,15,15	0.60	0	19,20,20	1.77	5 (26%)
2	1C1	B	501	-	30,30,30	3.47	11 (36%)	36,42,42	1.77	7 (19%)
4	NAG	B	509	1	14,14,15	0.44	0	17,19,21	0.70	1 (5%)
4	NAG	B	506	1	14,14,15	0.58	0	17,19,21	1.31	3 (17%)
4	NAG	B	507	1	14,14,15	0.50	0	17,19,21	0.82	0
4	NAG	B	508	1	14,14,15	0.51	0	17,19,21	0.91	1 (5%)
4	NAG	A	506	1	14,14,15	0.62	0	17,19,21	1.14	3 (17%)
4	NAG	B	504	1	14,14,15	0.49	0	17,19,21	0.90	1 (5%)
4	NAG	B	505	1	14,14,15	0.53	0	17,19,21	1.71	2 (11%)
4	NAG	A	508	1	14,14,15	0.67	0	17,19,21	1.18	2 (11%)
4	NAG	A	510	1	14,14,15	0.50	0	17,19,21	0.86	0
4	NAG	A	504	1	14,14,15	0.63	0	17,19,21	1.44	3 (17%)

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	EPE	B	510	-	-	3/9/19/19	0/1/1/1
4	NAG	B	502	1	-	3/6/23/26	0/1/1/1
4	NAG	B	503	1	-	2/6/23/26	0/1/1/1
4	NAG	A	509	1	-	3/6/23/26	0/1/1/1
2	1C1	A	501	-	-	2/17/29/29	0/3/3/3
4	NAG	A	505	1	-	0/6/23/26	0/1/1/1
4	NAG	A	503	1	-	2/6/23/26	0/1/1/1
4	NAG	A	507	1	-	0/6/23/26	0/1/1/1
3	EPE	A	502	-	-	0/9/19/19	0/1/1/1
2	1C1	B	501	-	-	3/17/29/29	0/3/3/3
4	NAG	B	509	1	-	2/6/23/26	0/1/1/1
4	NAG	B	506	1	-	3/6/23/26	0/1/1/1
4	NAG	B	507	1	-	2/6/23/26	0/1/1/1
4	NAG	B	508	1	-	0/6/23/26	0/1/1/1
4	NAG	A	506	1	-	2/6/23/26	0/1/1/1
4	NAG	B	504	1	-	2/6/23/26	0/1/1/1
4	NAG	B	505	1	-	0/6/23/26	0/1/1/1
4	NAG	A	508	1	-	4/6/23/26	0/1/1/1
4	NAG	A	510	1	-	2/6/23/26	0/1/1/1
4	NAG	A	504	1	-	0/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	1C1	C11-C12	9.19	1.50	1.39
2	B	501	1C1	C11-C12	9.07	1.50	1.39
2	B	501	1C1	C02-N03	7.62	1.47	1.33
2	A	501	1C1	C02-N03	7.15	1.47	1.33
2	A	501	1C1	C08-C07	6.48	1.50	1.39
2	B	501	1C1	C08-C07	6.43	1.50	1.39
2	B	501	1C1	C15-N14	6.31	1.47	1.34
2	A	501	1C1	C15-N14	5.69	1.46	1.34
2	B	501	1C1	C24-C22	5.58	1.46	1.38
2	A	501	1C1	C05-C13	-5.51	1.47	1.54
2	B	501	1C1	C17-N19	5.39	1.46	1.35
2	A	501	1C1	C17-N19	5.27	1.46	1.35
2	A	501	1C1	C24-C22	4.42	1.45	1.38
2	B	501	1C1	C05-C13	-4.36	1.48	1.54
2	B	501	1C1	C21-C20	-4.26	1.32	1.39
2	A	501	1C1	C21-C20	-3.99	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	1C1	C27-C20	-3.28	1.33	1.39
2	A	501	1C1	C27-C20	-3.27	1.33	1.39
3	B	510	EPE	C10-S	2.57	1.81	1.77
2	B	501	1C1	C06-C05	-2.33	1.49	1.54
2	A	501	1C1	C10-C11	2.33	1.42	1.38
2	A	501	1C1	C06-C05	-2.25	1.49	1.54
2	B	501	1C1	C10-C11	2.09	1.42	1.38

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	507	NAG	C1-O5-C5	8.02	122.94	112.19
4	A	509	NAG	C1-O5-C5	6.76	121.25	112.19
2	A	501	1C1	C21-C22-C24	-6.53	114.01	121.66
2	A	501	1C1	C20-C21-C22	6.32	124.10	118.82
3	B	510	EPE	C5-N4-C3	5.70	121.11	108.84
2	B	501	1C1	C20-C21-C22	5.16	123.13	118.82
2	B	501	1C1	C21-C22-C24	-4.67	116.19	121.66
4	B	505	NAG	C1-O5-C5	4.62	118.38	112.19
2	A	501	1C1	C22-C24-CL1	-4.29	114.38	119.79
3	A	502	EPE	C5-N4-C3	4.25	117.99	108.84
4	B	505	NAG	C2-N2-C7	-3.92	117.64	122.90
2	A	501	1C1	C15-C17-N19	3.77	118.62	112.25
2	A	501	1C1	F23-C22-C21	3.67	125.98	118.64
4	A	508	NAG	C1-O5-C5	3.32	116.63	112.19
4	B	503	NAG	O5-C1-C2	-3.25	106.26	111.29
4	A	503	NAG	O5-C5-C6	3.21	113.91	107.66
4	A	504	NAG	C2-N2-C7	3.19	127.18	122.90
4	B	504	NAG	C1-O5-C5	3.19	116.46	112.19
2	B	501	1C1	C06-C05-C13	3.17	108.87	104.75
4	B	506	NAG	C1-C2-N2	3.12	115.34	110.43
4	A	507	NAG	O5-C5-C4	3.08	118.32	110.83
2	A	501	1C1	C26-C24-CL1	3.03	124.39	118.42
4	A	509	NAG	C6-C5-C4	-2.93	105.81	113.02
4	A	504	NAG	C1-O5-C5	2.91	116.08	112.19
2	A	501	1C1	C12-C13-N14	-2.90	106.29	114.77
4	A	509	NAG	C2-N2-C7	2.72	126.54	122.90
2	B	501	1C1	O18-C17-C15	-2.67	116.90	121.24
3	A	502	EPE	C7-N4-C5	2.66	118.34	111.24
2	A	501	1C1	C06-C05-C13	2.64	108.18	104.75
4	B	506	NAG	C4-C3-C2	-2.63	107.17	111.02
2	B	501	1C1	F23-C22-C24	2.59	122.10	118.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	EPE	C5-C6-N1	-2.56	105.48	110.65
2	A	501	1C1	C26-C24-C22	2.54	121.22	119.04
2	A	501	1C1	O18-C17-C15	-2.50	117.17	121.24
2	B	501	1C1	C15-C17-N19	2.49	116.45	112.25
2	A	501	1C1	C10-C11-C12	-2.47	118.03	120.99
3	B	510	EPE	O3S-S-C10	2.46	110.83	106.00
4	A	505	NAG	C4-C3-C2	2.43	114.58	111.02
4	A	506	NAG	C2-N2-C7	-2.40	119.68	122.90
2	B	501	1C1	C12-C13-N14	-2.40	107.76	114.77
4	B	503	NAG	C1-C2-N2	2.38	114.18	110.43
4	B	502	NAG	C1-O5-C5	2.36	115.36	112.19
4	B	508	NAG	C1-O5-C5	2.36	115.35	112.19
2	A	501	1C1	C09-C08-C07	-2.35	117.44	120.88
4	A	504	NAG	C1-C2-N2	-2.31	106.79	110.43
4	A	506	NAG	C1-O5-C5	2.31	115.28	112.19
4	A	503	NAG	C6-C5-C4	-2.28	107.43	113.02
2	A	501	1C1	C10-C09-C08	2.27	123.04	120.24
2	A	501	1C1	O16-C15-N14	-2.26	119.11	123.09
4	B	509	NAG	C1-O5-C5	2.20	115.13	112.19
4	B	506	NAG	C2-N2-C7	2.20	125.84	122.90
3	B	510	EPE	C7-N4-C3	2.19	117.07	111.24
4	A	508	NAG	C2-N2-C7	-2.17	120.00	122.90
4	B	503	NAG	C2-N2-C7	-2.13	120.04	122.90
3	A	502	EPE	O1S-S-C10	2.11	109.92	106.73
2	A	501	1C1	C27-C20-C21	2.11	122.20	119.66
4	A	506	NAG	C6-C5-C4	-2.10	107.87	113.02
3	A	502	EPE	C2-C3-N4	2.04	114.77	110.65

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	1C1	C15-C17-N19-C20
3	B	510	EPE	C10-C9-N1-C2
4	A	508	NAG	C8-C7-N2-C2
4	A	508	NAG	O7-C7-N2-C2
4	B	502	NAG	C8-C7-N2-C2
4	B	502	NAG	O7-C7-N2-C2
4	B	504	NAG	C8-C7-N2-C2
4	B	504	NAG	O7-C7-N2-C2
4	B	506	NAG	C1-C2-N2-C7
3	B	510	EPE	N4-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
4	A	509	NAG	C8-C7-N2-C2
4	A	510	NAG	O5-C5-C6-O6
4	A	509	NAG	O7-C7-N2-C2
2	B	501	1C1	O16-C15-N14-C13
3	B	510	EPE	C8-C7-N4-C5
4	B	506	NAG	C8-C7-N2-C2
4	B	509	NAG	C8-C7-N2-C2
4	B	509	NAG	O7-C7-N2-C2
4	A	503	NAG	O5-C5-C6-O6
4	B	506	NAG	O7-C7-N2-C2
2	B	501	1C1	O18-C17-N19-C20
4	A	508	NAG	O5-C5-C6-O6
4	A	510	NAG	C4-C5-C6-O6
2	B	501	1C1	O16-C15-C17-N19
4	B	503	NAG	C4-C5-C6-O6
4	A	508	NAG	C4-C5-C6-O6
4	B	503	NAG	O5-C5-C6-O6
4	B	507	NAG	C8-C7-N2-C2
4	A	503	NAG	C4-C5-C6-O6
4	A	506	NAG	C8-C7-N2-C2
4	B	507	NAG	O7-C7-N2-C2
4	A	506	NAG	O7-C7-N2-C2
4	B	502	NAG	O5-C5-C6-O6
2	A	501	1C1	O16-C15-N14-C13
4	A	509	NAG	O5-C5-C6-O6

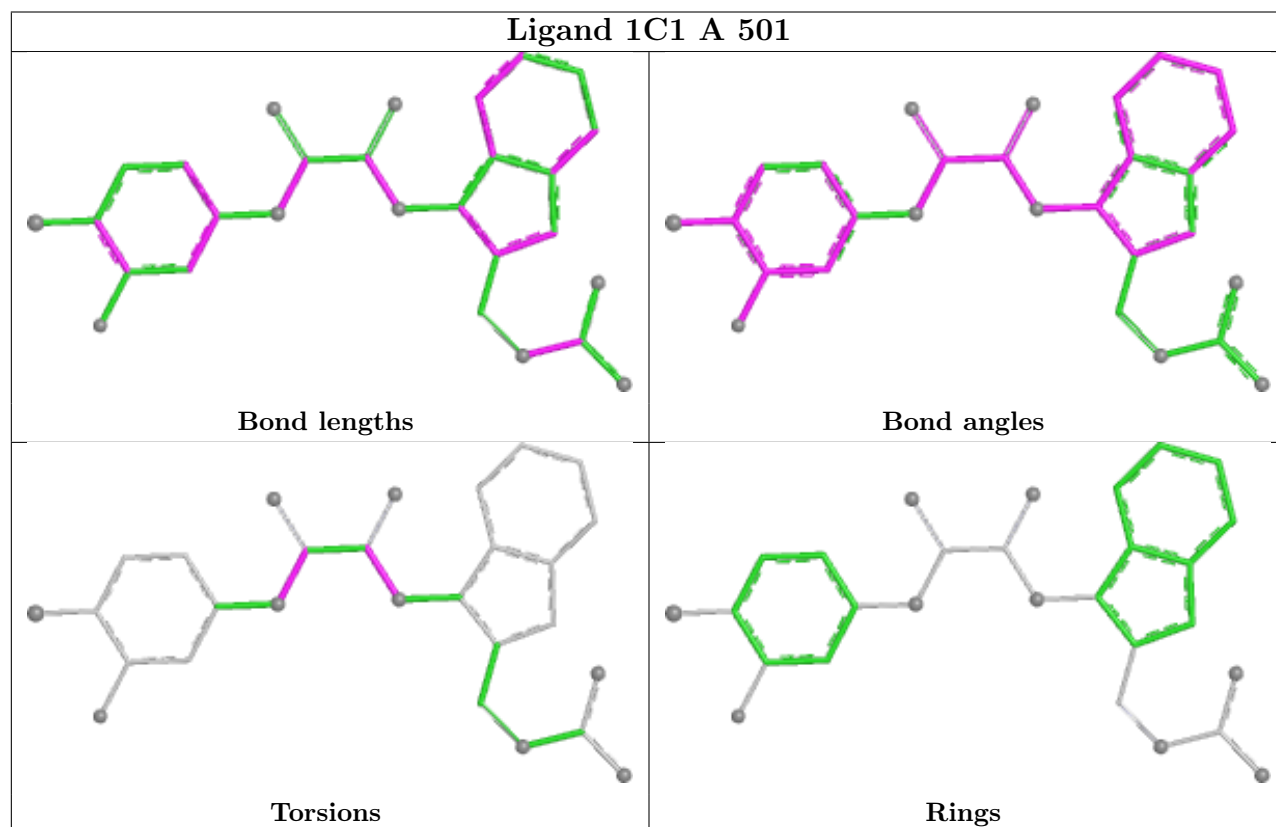
There are no ring outliers.

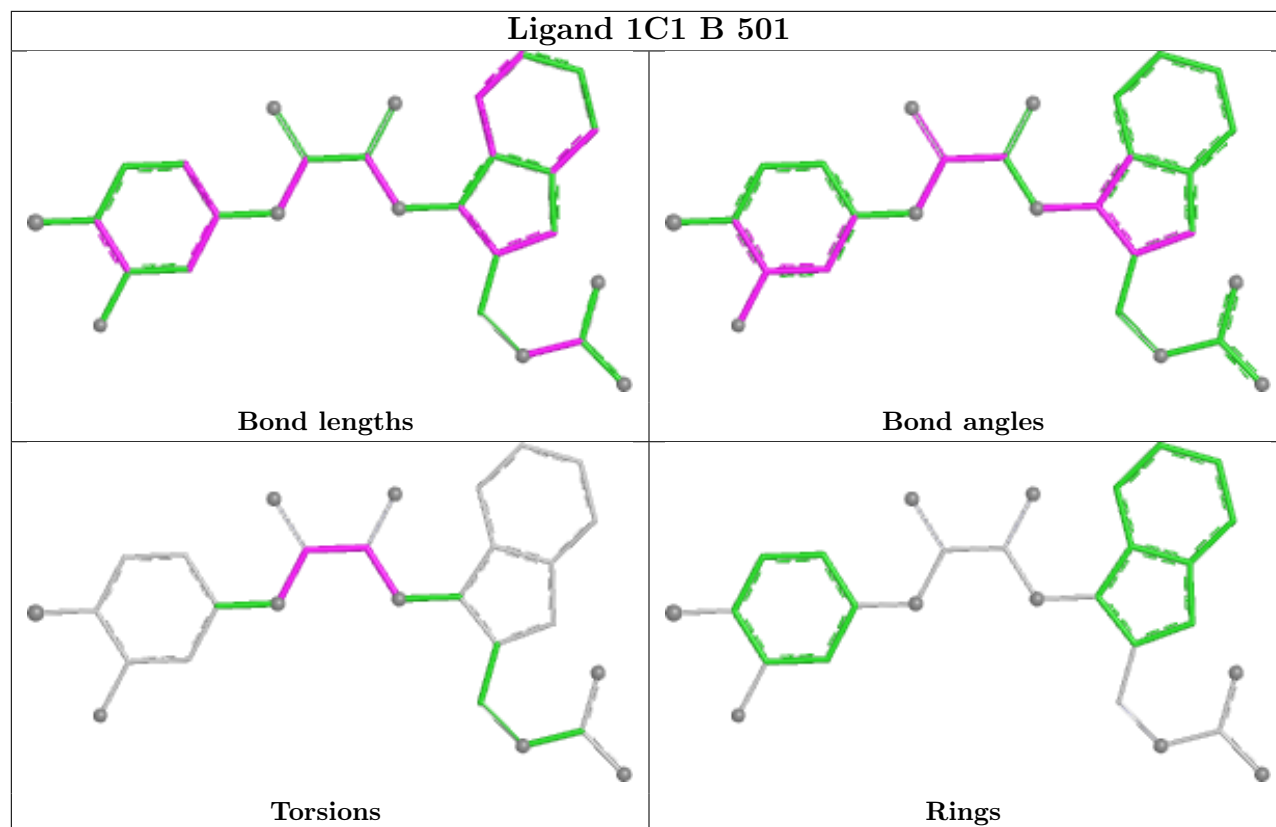
7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	510	EPE	3	0
4	B	502	NAG	5	0
4	A	509	NAG	1	0
4	A	505	NAG	1	0
4	A	506	NAG	1	0
4	B	505	NAG	1	0
4	A	510	NAG	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 than 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.





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, 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%)	1.32	65 (19%) 3 2	28, 43, 78, 107	0
1	B	339/353 (96%)	2.19	176 (51%) 0 0	29, 68, 114, 138	5 (1%)
All	All	678/706 (96%)	1.75	241 (35%) 1 1	28, 54, 105, 138	5 (0%)

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	430[A]	THR	6.8
1	B	359	ILE	6.3
1	A	123	THR	5.7
1	B	122	LEU	5.6
1	A	396	ILE	5.6
1	A	430	THR	5.5
1	B	350	LYS	5.3
1	B	396	ILE	5.3
1	B	349	LEU	5.1
1	B	358	THR	5.1
1	B	124	GLY	5.1
1	B	232	ASN	5.0
1	B	353	PHE	4.9
1	B	481	SER	4.9
1	A	492	GLU	4.8
1	A	392	ASN	4.8
1	B	394	THR	4.6
1	A	324	GLY	4.6
1	B	419	LYS	4.5
1	B	123	THR	4.4
1	A	393	ASN	4.4
1	A	124	GLY	4.3
1	B	393	ASN	4.2
1	B	395	CYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	101	VAL	4.1
1	B	355	ASN	4.1
1	B	392	ASN	4.1
1	B	463	THR	4.1
1	B	265	LEU	4.0
1	A	122	LEU	4.0
1	B	242	VAL	4.0
1	B	461	ASN	3.9
1	B	89	VAL	3.9
1	B	411	ASN	3.9
1	B	243	SER	3.9
1	B	200	VAL	3.9
1	A	203	GLN	3.8
1	A	121	LYS	3.8
1	B	357	LYS	3.8
1	A	246	GLN	3.8
1	B	60	ALA	3.8
1	A	394	THR	3.7
1	A	395	CYS	3.7
1	B	361	PHE	3.7
1	B	277	LEU	3.7
1	A	202	LYS	3.7
1	B	233	PHE	3.7
1	B	263	GLY	3.7
1	B	468	PHE	3.6
1	B	360	ILE	3.6
1	B	224	VAL	3.6
1	B	88	ASN	3.6
1	B	271	ILE	3.5
1	B	44	VAL	3.5
1	B	245	VAL	3.4
1	B	230	ASP	3.4
1	B	462	ASN	3.4
1	A	82	GLN	3.4
1	A	491	ILE	3.4
1	A	440	ASP	3.4
1	B	389	GLN	3.4
1	B	113	ASP	3.4
1	B	325	ASP	3.4
1	B	326	ILE	3.4
1	B	241	ASN	3.3
1	B	235	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	416	LEU	3.3
1	B	492	GLU	3.3
1	A	73	ALA	3.3
1	B	199	SER	3.3
1	B	246	GLN	3.3
1	A	301	ASN	3.3
1	B	429[A]	GLY	3.3
1	B	391	PHE	3.3
1	B	92	ASN	3.3
1	B	228	CYS	3.3
1	A	419	LYS	3.3
1	B	115	SER	3.2
1	B	488	VAL	3.2
1	A	199	SER	3.2
1	A	446	VAL	3.2
1	B	106	GLU	3.1
1	B	484	TYR	3.1
1	B	201	ILE	3.1
1	B	93	PHE	3.1
1	A	72	HIS	3.1
1	B	85	HIS	3.1
1	B	61	HIS	3.1
1	B	264	SER	3.1
1	B	96	TRP	3.1
1	B	436	ALA	3.1
1	A	86	LEU	3.1
1	B	82	GLN	3.0
1	B	428[A]	GLN	3.0
1	B	354	ASN	3.0
1	A	429	GLY	3.0
1	B	45	TRP	3.0
1	A	383	PHE	3.0
1	B	464	SER	3.0
1	B	489	VAL	3.0
1	B	365	SER	3.0
1	A	198	GLY	3.0
1	B	275	GLU	2.9
1	A	376	PHE	2.9
1	B	274	SER	2.9
1	A	361	PHE	2.9
1	B	91	GLU	2.9
1	B	217	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	465	ASN	2.9
1	B	272	ILE	2.9
1	A	296	CYS	2.9
1	B	240	LYS	2.9
1	B	247	CYS	2.9
1	B	279	ASN	2.8
1	B	390	LEU	2.8
1	B	417	PRO	2.8
1	B	52	LEU	2.8
1	A	84	ILE	2.8
1	B	280	ASN	2.8
1	B	104	MET	2.8
1	B	72	HIS	2.8
1	B	491	ILE	2.8
1	B	234	ASN	2.8
1	B	276	ASN	2.7
1	B	334	ASN	2.7
1	B	84	ILE	2.7
1	B	236	THR	2.7
1	B	203	GLN	2.7
1	B	455	THR	2.7
1	B	456	ARG	2.7
1	B	460	ALA	2.7
1	B	103	GLN	2.7
1	B	80	ASN	2.7
1	B	97	LYS	2.7
1	B	487	LYS	2.7
1	B	292	VAL	2.7
1	B	108	VAL	2.6
1	A	236	THR	2.6
1	B	90	THR	2.6
1	A	201	ILE	2.6
1	B	218	CYS	2.6
1	A	426	MET	2.6
1	B	351	GLU	2.6
1	B	329	ALA	2.6
1	A	330	TYR	2.6
1	A	87	GLU	2.5
1	B	260	LEU	2.5
1	A	71	THR	2.5
1	B	259	LEU	2.5
1	A	85	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	278	THR	2.5
1	B	467	THR	2.5
1	B	459	GLY	2.5
1	A	445	CYS	2.5
1	A	441	GLY	2.5
1	B	208	ILE	2.5
1	B	77	THR	2.5
1	B	118	PRO	2.4
1	B	282	LYS	2.4
1	A	300	SER	2.4
1	A	222	GLY	2.4
1	B	362	GLN	2.4
1	B	244	SER	2.4
1	B	454	LEU	2.4
1	B	486	TYR	2.4
1	A	44	VAL	2.4
1	B	345	VAL	2.4
1	B	301	ASN	2.4
1	A	204	ALA	2.4
1	B	110	SER	2.4
1	B	476	LYS	2.4
1	B	482	GLU	2.4
1	B	372	THR	2.3
1	B	81	PRO	2.3
1	A	431	GLY	2.3
1	B	412	GLY	2.3
1	B	254	VAL	2.3
1	B	388	THR	2.3
1	B	109	ILE	2.3
1	B	423	ILE	2.3
1	B	231	LYS	2.3
1	A	119	CYS	2.3
1	B	239	CYS	2.3
1	A	473	GLY	2.3
1	B	458	GLY	2.3
1	B	347	GLU	2.3
1	A	232	ASN	2.2
1	B	105	GLN	2.2
1	B	335	GLY	2.2
1	A	45	TRP	2.2
1	B	120	VAL	2.2
1	B	206	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	286	VAL	2.2
1	B	51	THR	2.2
1	B	374	HIS	2.2
1	B	59	LYS	2.2
1	A	56	SER	2.2
1	A	365	SER	2.2
1	B	225	ILE	2.2
1	B	363	PRO	2.2
1	A	478	ASN	2.2
1	A	366	GLY	2.2
1	A	451	GLY	2.2
1	B	330	TYR	2.2
1	B	284	ILE	2.2
1	B	452	ILE	2.2
1	B	102	GLU	2.2
1	B	434	MET	2.1
1	B	71	THR	2.1
1	B	86	LEU	2.1
1	B	431[A]	GLY	2.1
1	B	472	GLY	2.1
1	A	333	ILE	2.1
1	B	414	ILE	2.1
1	B	340	LYS	2.1
1	B	281	ALA	2.1
1	B	50	THR	2.1
1	B	198	GLY	2.1
1	B	413	THR	2.1
1	B	332	GLU	2.1
1	A	411	ASN	2.1
1	B	471	GLY	2.1
1	A	248	THR	2.1
1	A	443	ILE	2.1
1	A	115	SER	2.1
1	A	447	SER	2.1
1	A	205	CYS	2.1
1	A	224	VAL	2.0
1	B	98	ASN	2.0
1	B	289	ASN	2.0
1	A	208	ILE	2.0
1	A	442	LYS	2.0
1	B	49	ASP	2.0
1	B	369	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	442	LYS	2.0
1	B	485	LYS	2.0
1	B	294	ILE	2.0
1	B	346	THR	2.0
1	B	387	THR	2.0
1	B	209	SER	2.0
1	B	256	SER	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 oligosaccharides 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
4	NAG	A	508	14/15	0.47	0.23	62,74,81,83	0
4	NAG	B	504	14/15	0.55	0.19	87,97,102,105	0
4	NAG	B	508	14/15	0.55	0.22	75,99,120,124	0
4	NAG	B	509	14/15	0.55	0.24	64,89,101,106	0
4	NAG	B	506	14/15	0.60	0.21	46,69,87,91	0
4	NAG	B	505	14/15	0.64	0.19	58,65,84,86	0
4	NAG	B	502	14/15	0.64	0.24	82,95,99,99	0
4	NAG	A	507	14/15	0.65	0.16	46,62,74,74	0
4	NAG	A	503	14/15	0.71	0.16	47,62,74,77	0
4	NAG	A	505	14/15	0.71	0.14	41,61,66,67	0
4	NAG	B	507	14/15	0.73	0.20	70,79,90,91	0
4	NAG	A	510	14/15	0.81	0.15	44,63,73,76	0
3	EPE	B	510	15/15	0.82	0.18	43,65,81,93	0
4	NAG	A	509	14/15	0.82	0.14	33,43,48,61	0
4	NAG	A	506	14/15	0.83	0.16	34,58,72,73	0
2	1C1	B	501	28/28	0.85	0.17	48,58,91,97	0

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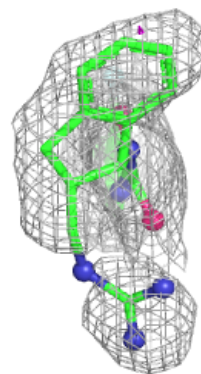
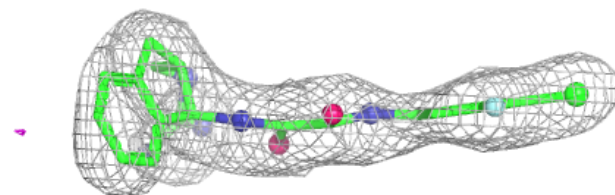
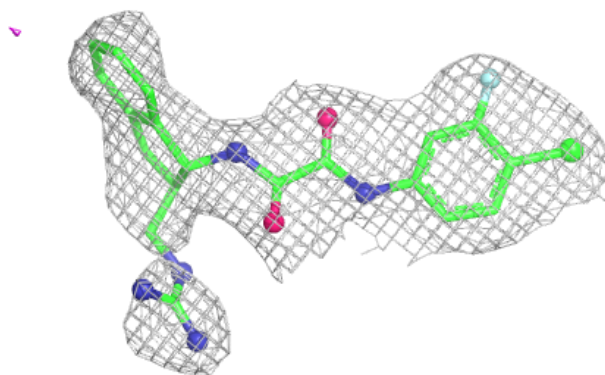
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	1C1	A	501	28/28	0.85	0.17	28,41,59,64	0
4	NAG	B	503	14/15	0.88	0.13	37,44,53,54	0
4	NAG	A	504	14/15	0.89	0.11	28,42,45,47	0
3	EPE	A	502	15/15	0.93	0.11	32,37,52,65	0

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.

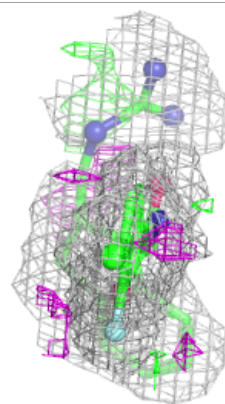
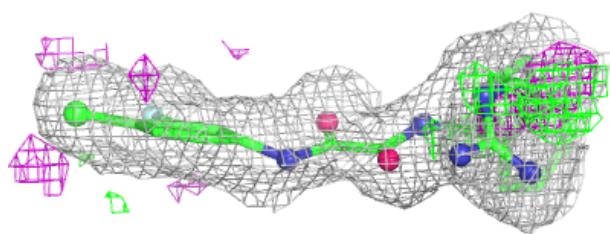
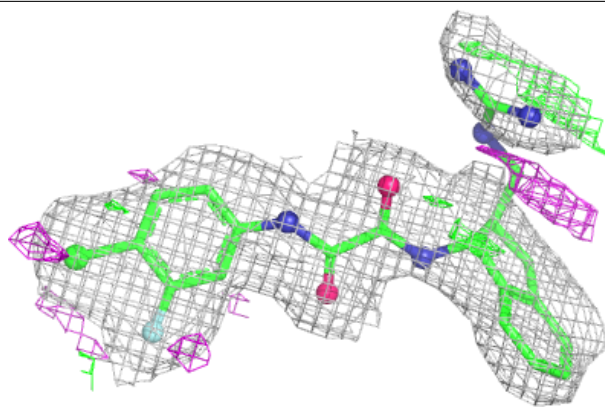
Electron density around 1C1 B 501:

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 1C1 A 501:

$2mF_o-DF_c$ (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.