



Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2021 – 02:09 PM EDT

PDB ID : 4I53
Title : Crystal structure of clade C1086 HIV-1 gp120 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 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)
Xtrriage (Phenix) : 1.13
EDS : 2.18
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) : 2.18

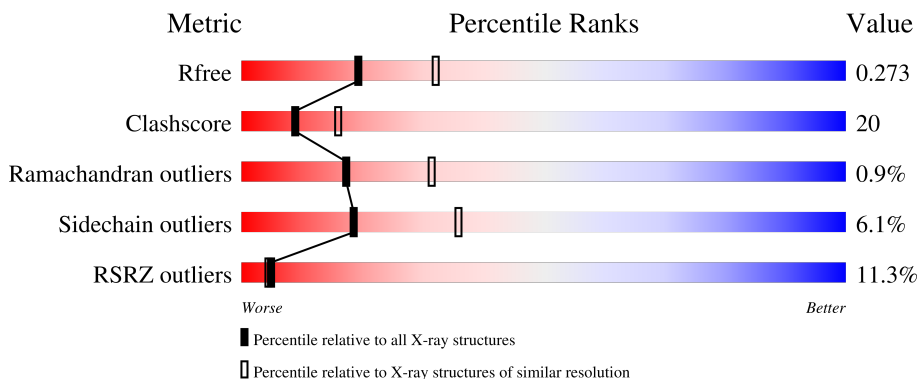
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	358	
1	B	358	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	503	-	-	X	-
4	FMT	B	502	-	-	-	X

2 Entry composition i

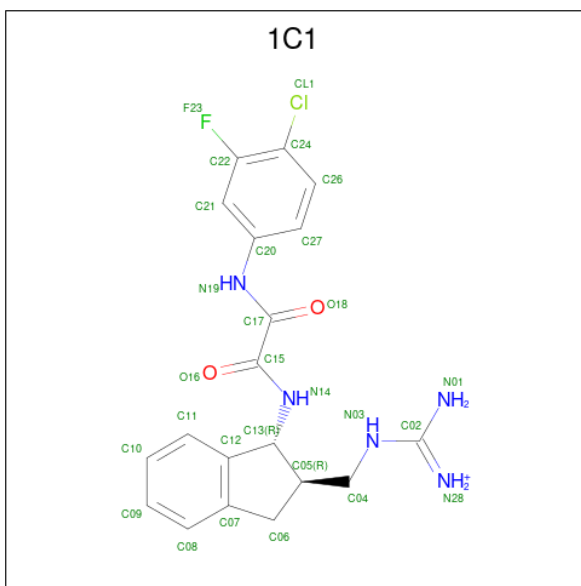
There are 5 unique types of molecules in this entry. The entry contains 5770 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	336	Total	C	N	O	S	0	1	0
			2643	1653	463	507	20			
1	B	335	Total	C	N	O	S	0	0	0
			2627	1642	459	506	20			

- Molecule 2 is amino(1-((1R,2R)-1-((4-chloro-3-fluorophenyl)amino)(oxo)acetyl)amino)-2,3-dihydro-1H-inden-2-yl)methyl)amino)methaniminium (three-letter code: 1C1) (formula: C₁₉H₂₀ClFN₅O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	F	N			O
2	A	1	Total	C	Cl	F	N	O	0	0
			28	19	1	1	5	2		
2	B	1	Total	C	Cl	F	N	O	0	0
			28	19	1	1	5	2		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 3 1 2	0	0

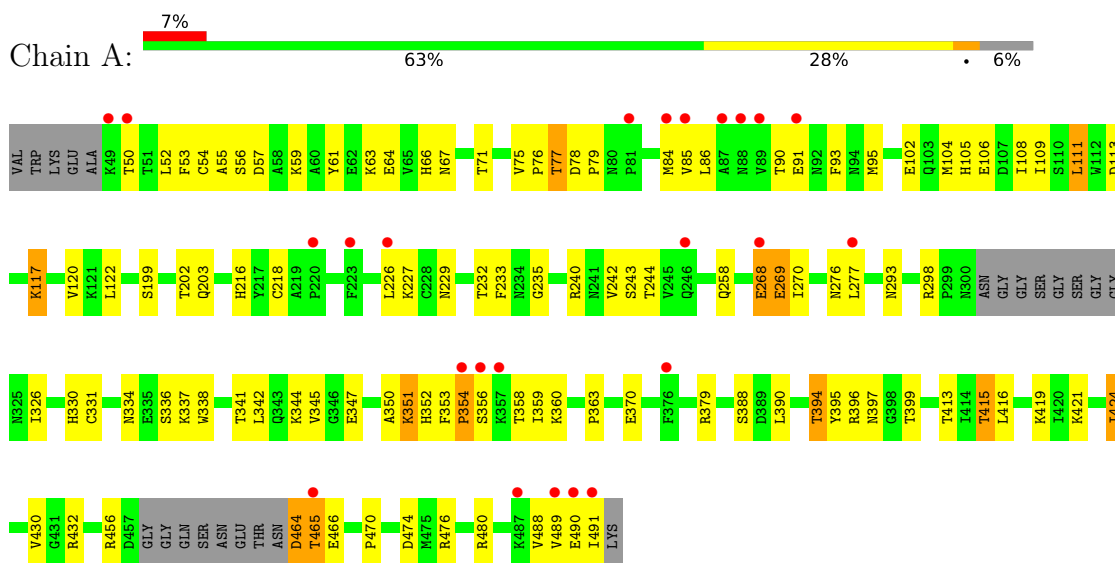
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	161	Total O 161 161	0	0
5	B	98	Total O 98 98	0	0

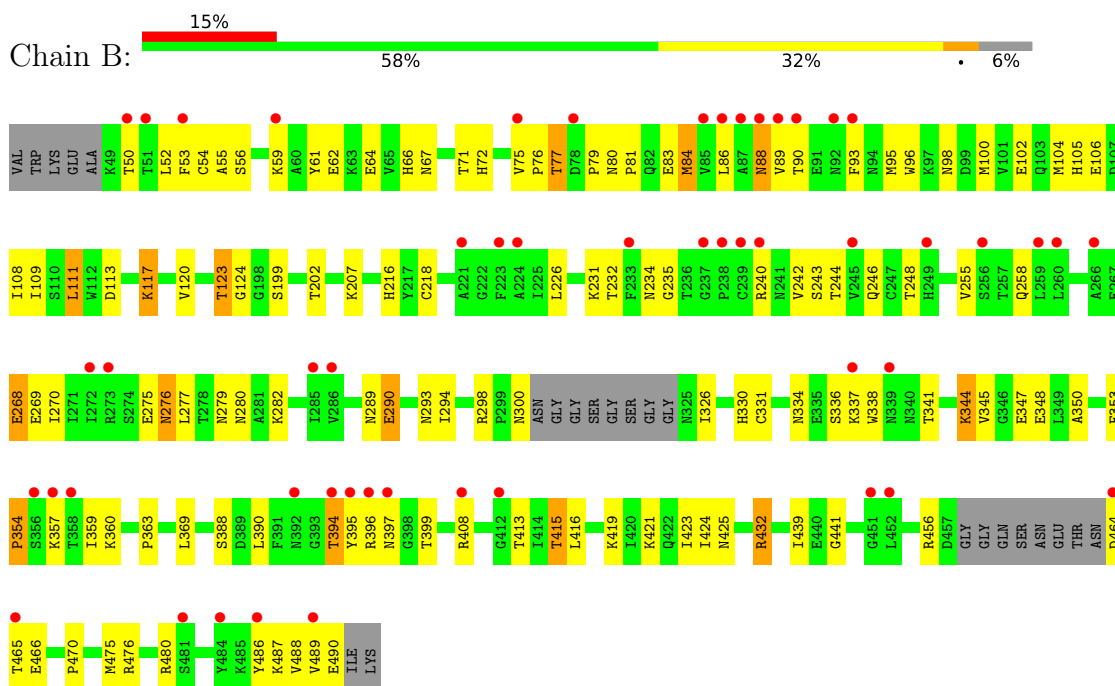
3 Residue-property plots [i](#)

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 glycoprotein



- Molecule 1: HIV-1 glycoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	67.45Å 127.67Å 192.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 2.50 29.82 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.82-2.50) 98.5 (29.82-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.44 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.254 , 0.273 0.255 , 0.273	Depositor DCC
R_{free} test set	1087 reflections (3.78%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtrriage
Anisotropy	0.050	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5770	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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: FMT, 1C1, 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	0.41	0/2701	0.54	3/3665 (0.1%)
1	B	0.35	0/2682	0.46	0/3640
All	All	0.38	0/5383	0.50	3/7305 (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	268	GLU	N-CA-C	-7.17	91.65	111.00
1	A	276	ASN	CB-CA-C	5.61	121.62	110.40
1	A	276	ASN	N-CA-C	-5.19	96.99	111.00

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	2643	0	2564	98	0
1	B	2627	0	2543	120	0
2	A	28	0	20	2	0
2	B	28	0	20	0	0
3	A	98	0	91	8	0
3	B	84	0	78	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	3	0	1	1	0
5	A	161	0	0	6	0
5	B	98	0	0	3	0
All	All	5770	0	5317	219	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 20.

All (219) 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:HD21	3:B:503:NAG:C1	1.58	1.14
1:B:432:ARG:HG3	1:B:432:ARG:HH11	1.18	1.08
1:B:100:MET:HE1	1:B:486:TYR:HB3	1.38	1.04
1:A:269:GLU:HB2	3:A:505:NAG:H62	1.43	0.99
1:A:90:THR:HG22	1:A:240:ARG:HA	1.43	0.97
1:B:84:MET:HB3	1:B:244:THR:HB	1.47	0.95
1:A:293:ASN:H	1:A:337:LYS:NZ	1.66	0.94
1:B:432:ARG:HG3	1:B:432:ARG:NH1	1.84	0.89
1:B:226:LEU:HD13	1:B:489:VAL:HG11	1.54	0.88
1:B:100:MET:HE1	1:B:486:TYR:CB	2.04	0.87
1:B:100:MET:HE3	1:B:486:TYR:HB2	1.57	0.86
1:B:100:MET:CE	1:B:486:TYR:CB	2.54	0.86
1:B:79:PRO:O	1:B:81:PRO:HD3	1.75	0.86
1:A:293:ASN:H	1:A:337:LYS:HZ1	1.20	0.85
1:A:226:LEU:HD13	1:A:489:VAL:HG11	1.62	0.82
1:B:226:LEU:HD13	1:B:489:VAL:CG1	2.13	0.77
1:B:75:VAL:HG13	1:B:76:PRO:HD2	1.65	0.77
3:B:505:NAG:H3	3:B:505:NAG:H83	1.66	0.76
1:B:50:THR:HG23	1:B:52:LEU:HD12	1.68	0.75
1:A:424:ILE:O	1:A:424:ILE:HG13	1.86	0.75
1:A:75:VAL:HG13	1:A:76:PRO:HD2	1.66	0.75
1:A:50:THR:HG23	1:A:52:LEU:HD12	1.67	0.75
1:B:59:LYS:HB3	1:B:61:TYR:CE1	2.22	0.75
1:B:226:LEU:CD1	1:B:489:VAL:HG11	2.15	0.74
1:A:50:THR:HG22	1:A:488:VAL:HG21	1.70	0.73
1:A:67:ASN:O	1:A:71:THR:HG23	1.88	0.73
1:B:242:VAL:HG12	1:B:243:SER:N	2.04	0.73
1:B:357:LYS:HZ2	1:B:464:ASP:N	1.87	0.72
1:B:298:ARG:HD2	1:B:326:ILE:O	1.89	0.72
1:A:242:VAL:HG12	1:A:243:SER:N	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:MET:CE	1:B:486:TYR:HB2	2.20	0.71
1:B:55:ALA:HA	1:B:75:VAL:O	1.91	0.71
1:A:59:LYS:HB3	1:A:61:TYR:CE1	2.26	0.71
1:A:270:ILE:H	3:A:505:NAG:H61	1.56	0.70
1:A:55:ALA:HA	1:A:75:VAL:O	1.91	0.69
1:B:67:ASN:O	1:B:71:THR:HG23	1.91	0.69
1:A:277:LEU:HD12	3:A:502:NAG:H81	1.75	0.69
1:B:123:THR:HB	5:B:612:HOH:O	1.92	0.69
1:B:432:ARG:HH11	1:B:432:ARG:CG	2.00	0.68
1:A:270:ILE:HD12	1:A:344:LYS:HB3	1.76	0.67
1:A:277:LEU:CD1	3:A:502:NAG:H81	2.24	0.67
1:B:270:ILE:HD12	1:B:344:LYS:HB3	1.76	0.67
1:A:396:ARG:HG2	1:A:397:ASN:HD22	1.59	0.66
1:A:111:LEU:HD12	1:A:111:LEU:O	1.94	0.66
1:B:98:ASN:OD1	1:B:100:MET:HG3	1.94	0.66
1:B:396:ARG:HG2	1:B:397:ASN:HD22	1.59	0.66
1:A:50:THR:CG2	1:A:488:VAL:HG21	2.25	0.65
1:A:298:ARG:HD2	1:A:326:ILE:O	1.96	0.65
1:B:100:MET:CE	1:B:486:TYR:HB3	2.15	0.65
1:B:234:ASN:HD21	3:B:503:NAG:C2	2.09	0.65
1:A:334:ASN:HB3	1:A:337:LYS:HD3	1.78	0.65
1:B:111:LEU:HD12	1:B:111:LEU:O	1.97	0.64
1:A:226:LEU:HD13	1:A:489:VAL:CG1	2.26	0.64
1:B:100:MET:HE3	1:B:486:TYR:CB	2.23	0.64
1:B:83:GLU:HG3	1:B:243:SER:OG	1.98	0.64
1:A:50:THR:HG23	1:A:52:LEU:CD1	2.28	0.63
1:B:242:VAL:CG1	1:B:243:SER:N	2.61	0.63
1:A:242:VAL:CG1	1:A:243:SER:N	2.62	0.63
1:B:50:THR:HG22	1:B:488:VAL:HG21	1.81	0.62
1:B:50:THR:HG23	1:B:52:LEU:CD1	2.29	0.62
1:A:90:THR:CG2	1:A:240:ARG:HA	2.26	0.61
1:B:100:MET:CE	1:B:486:TYR:C	2.68	0.61
1:A:350:ALA:O	1:A:351:LYS:O	2.18	0.61
1:B:293:ASN:H	1:B:337:LYS:NZ	1.97	0.61
1:B:100:MET:CE	1:B:487:LYS:N	2.64	0.60
1:A:226:LEU:CD1	1:A:489:VAL:HG11	2.29	0.60
1:B:344:LYS:HG2	3:B:506:NAG:H5	1.82	0.60
1:A:476:ARG:HB3	1:A:480:ARG:NH1	2.16	0.60
1:B:77:THR:O	1:B:79:PRO:HD3	2.01	0.60
1:A:351:LYS:O	1:A:353:PHE:N	2.35	0.59
1:B:363:PRO:HG3	1:B:388:SER:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ASN:HD22	3:B:506:NAG:H83	1.66	0.59
1:A:491:ILE:O	1:A:491:ILE:HG22	2.03	0.59
1:A:396:ARG:O	1:A:399:THR:HG22	2.04	0.58
1:B:396:ARG:O	1:B:399:THR:HG22	2.03	0.58
1:B:50:THR:CG2	1:B:488:VAL:HG21	2.33	0.58
1:B:55:ALA:HB1	1:B:77:THR:HA	1.85	0.58
1:B:56:SER:C	1:B:77:THR:HG22	2.25	0.57
1:A:104:MET:O	1:A:108:ILE:HG12	2.04	0.57
1:B:88:ASN:OD1	1:B:88:ASN:N	2.37	0.57
1:B:331:CYS:O	1:B:415:THR:HA	2.06	0.56
1:A:430:VAL:HA	2:A:501:1C1:N28	2.21	0.56
1:A:56:SER:C	1:A:77:THR:HG22	2.26	0.56
1:A:379[B]:ARG:NH1	5:A:755:HOH:O	2.37	0.56
1:A:456:ARG:HD2	1:A:466:GLU:OE2	2.05	0.55
1:A:363:PRO:HG3	1:A:388:SER:HA	1.89	0.55
1:A:269:GLU:HB2	3:A:505:NAG:C6	2.26	0.55
1:A:293:ASN:H	1:A:337:LYS:HZ3	1.51	0.54
1:B:489:VAL:HG22	1:B:490:GLU:N	2.23	0.54
1:A:489:VAL:HG22	1:A:490:GLU:N	2.23	0.54
1:B:242:VAL:CG1	1:B:243:SER:H	2.19	0.54
1:B:95:MET:SD	1:B:235:GLY:HA3	2.47	0.54
1:A:350:ALA:HA	1:A:359:ILE:HD11	1.88	0.54
1:B:408:ARG:HH11	1:B:408:ARG:HG3	1.71	0.54
1:A:242:VAL:CG1	1:A:243:SER:H	2.20	0.54
1:B:232:THR:HG22	1:B:232:THR:O	2.08	0.54
1:B:100:MET:HE1	1:B:487:LYS:N	2.23	0.53
1:B:104:MET:O	1:B:108:ILE:HG12	2.08	0.53
1:B:289:ASN:OD1	1:B:290:GLU:HG2	2.08	0.53
1:A:424:ILE:HD11	5:A:752:HOH:O	2.08	0.53
1:B:350:ALA:HA	1:B:359:ILE:HD11	1.90	0.53
1:A:90:THR:HG22	1:A:240:ARG:CA	2.28	0.53
1:A:232:THR:HG22	1:A:232:THR:O	2.07	0.53
1:B:231:LYS:HD2	1:B:268:GLU:OE1	2.09	0.53
1:A:331:CYS:O	1:A:415:THR:HA	2.09	0.52
1:B:268:GLU:O	3:B:506:NAG:H83	2.09	0.52
1:B:280:ASN:HB2	1:B:456:ARG:O	2.09	0.52
1:A:90:THR:CG2	1:A:240:ARG:HG3	2.40	0.52
1:A:105:HIS:O	1:A:109:ILE:HG13	2.09	0.52
1:A:111:LEU:HD12	1:A:111:LEU:C	2.29	0.52
1:A:476:ARG:O	1:A:480:ARG:HG3	2.10	0.52
1:A:90:THR:HG22	1:A:240:ARG:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:ARG:HH11	1:B:408:ARG:CG	2.23	0.51
1:B:111:LEU:HD12	1:B:111:LEU:C	2.30	0.51
1:B:234:ASN:CG	3:B:503:NAG:C1	2.78	0.51
1:B:75:VAL:HG13	1:B:76:PRO:CD	2.39	0.51
1:B:102:GLU:O	1:B:106:GLU:HG2	2.09	0.51
1:A:424:ILE:CD1	5:A:752:HOH:O	2.58	0.51
1:A:293:ASN:N	1:A:337:LYS:NZ	2.48	0.50
1:A:258:GLN:HG2	1:A:470:PRO:HB2	1.93	0.50
1:B:90:THR:O	1:B:90:THR:OG1	2.30	0.50
1:B:276:ASN:ND2	1:B:279:ASN:HB2	2.27	0.50
1:B:120:VAL:HG22	1:B:202:THR:HG22	1.93	0.49
1:B:476:ARG:O	1:B:480:ARG:HG3	2.12	0.49
1:B:270:ILE:CD1	1:B:344:LYS:HB3	2.43	0.49
1:B:423:ILE:C	1:B:424:ILE:HD12	2.33	0.49
1:B:100:MET:HE2	1:B:487:LYS:N	2.29	0.48
1:B:334:ASN:OD1	1:B:336:SER:HB2	2.14	0.48
1:A:53:PHE:CZ	1:A:218:CYS:HB2	2.49	0.48
1:B:64:GLU:OE1	1:B:66:HIS:HB2	2.14	0.48
1:B:242:VAL:HG12	1:B:243:SER:H	1.79	0.47
1:A:270:ILE:H	3:A:505:NAG:C6	2.25	0.47
1:A:298:ARG:CD	1:A:326:ILE:O	2.61	0.47
1:A:476:ARG:HB3	1:A:480:ARG:HH12	1.77	0.47
1:B:106:GLU:OE1	5:B:672:HOH:O	2.20	0.47
1:B:90:THR:HG22	1:B:240:ARG:HG3	1.97	0.46
1:A:75:VAL:HG13	1:A:76:PRO:CD	2.41	0.46
1:A:358:THR:HB	1:A:465:THR:HB	1.98	0.46
1:A:270:ILE:CD1	1:A:344:LYS:HB3	2.42	0.46
1:A:270:ILE:N	3:A:505:NAG:H61	2.28	0.46
1:A:419:LYS:O	1:A:419:LYS:HG3	2.15	0.46
1:B:300:ASN:OD1	1:B:441:GLY:HA2	2.14	0.46
1:B:298:ARG:CD	1:B:326:ILE:O	2.62	0.46
1:A:64:GLU:OE1	1:A:66:HIS:HB2	2.15	0.46
1:A:258:GLN:CG	1:A:470:PRO:HB2	2.45	0.46
1:B:270:ILE:HB	1:B:348:GLU:HG3	1.98	0.45
1:A:240:ARG:HB2	1:A:240:ARG:NH1	2.31	0.45
1:A:341:THR:O	1:A:345:VAL:HG23	2.17	0.45
1:B:113:ASP:O	1:B:117:LYS:HE3	2.17	0.45
1:B:277:LEU:CD1	3:B:503:NAG:H81	2.47	0.45
1:B:258:GLN:HG2	1:B:470:PRO:HB2	1.98	0.45
1:A:102:GLU:O	1:A:106:GLU:HG2	2.17	0.45
1:B:234:ASN:OD1	3:B:503:NAG:C1	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PHE:HB2	1:A:233:PHE:CZ	2.51	0.44
1:B:53:PHE:CZ	1:B:218:CYS:HB2	2.52	0.44
1:A:57:ASP:OD2	5:A:644:HOH:O	2.21	0.44
1:A:95:MET:SD	1:A:235:GLY:HA3	2.58	0.44
1:A:474:ASP:OD1	1:A:476:ARG:HB2	2.18	0.43
1:B:258:GLN:CG	1:B:470:PRO:HB2	2.48	0.43
1:A:269:GLU:HA	3:A:505:NAG:O5	2.18	0.43
1:A:334:ASN:OD1	1:A:336:SER:HB2	2.19	0.43
1:B:98:ASN:OD1	1:B:100:MET:CG	2.66	0.43
1:B:293:ASN:H	1:B:337:LYS:HZ3	1.66	0.43
1:A:293:ASN:N	1:A:337:LYS:HZ1	2.01	0.43
1:B:456:ARG:HD2	1:B:466:GLU:OE2	2.19	0.43
1:A:52:LEU:HD12	1:A:52:LEU:N	2.34	0.43
1:A:354:PRO:HB2	1:A:356:SER:H	1.69	0.43
1:B:330:HIS:HA	1:B:416:LEU:O	2.19	0.43
1:B:408:ARG:CG	1:B:408:ARG:NH1	2.80	0.43
1:B:421:LYS:HB3	1:B:421:LYS:HE2	1.82	0.42
1:A:330:HIS:HA	1:A:416:LEU:O	2.19	0.42
1:B:248:THR:HG22	1:B:486:TYR:CD1	2.54	0.42
1:B:353:PHE:HA	1:B:354:PRO:HD2	1.71	0.42
1:B:360:LYS:HG2	1:B:394:THR:HB	2.01	0.42
1:B:66:HIS:CD2	1:B:111:LEU:HD21	2.54	0.42
1:B:240:ARG:HB2	1:B:240:ARG:CZ	2.49	0.42
1:B:240:ARG:HB2	1:B:240:ARG:NH1	2.33	0.42
1:A:78:ASP:HA	1:A:79:PRO:HD3	1.88	0.42
1:A:240:ARG:NH2	5:A:698:HOH:O	2.51	0.42
1:B:52:LEU:HD12	1:B:52:LEU:N	2.35	0.42
1:B:105:HIS:O	1:B:109:ILE:HG13	2.19	0.42
1:A:113:ASP:O	1:A:117:LYS:HE3	2.20	0.42
1:A:240:ARG:HB2	1:A:240:ARG:CZ	2.50	0.42
1:B:54:CYS:HA	1:B:216:HIS:O	2.20	0.42
1:B:84:MET:SD	1:B:86:LEU:HG	2.59	0.42
1:B:294:ILE:HG23	1:B:294:ILE:O	2.19	0.42
1:A:227:LYS:NZ	1:A:229:ASN:ND2	2.68	0.42
1:A:347:GLU:HG2	1:A:395:TYR:OH	2.20	0.42
1:B:79:PRO:C	1:B:81:PRO:HD3	2.35	0.42
1:B:207:LYS:HG3	1:B:439:ILE:HG22	2.00	0.42
1:A:360:LYS:HG2	1:A:394:THR:HB	2.02	0.41
1:A:421:LYS:HB3	1:A:421:LYS:HE2	1.84	0.41
1:B:298:ARG:NH2	1:B:441:GLY:O	2.45	0.41
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ASN:ND2	4:B:502:FMT:O1	2.53	0.41
1:A:54:CYS:HA	1:A:216:HIS:O	2.20	0.41
1:B:93:PHE:CE2	1:B:487:LYS:HB3	2.55	0.41
1:B:279:ASN:ND2	1:B:282:LYS:HG2	2.35	0.41
1:A:120:VAL:HG22	1:A:202:THR:HG22	2.03	0.41
1:B:59:LYS:HB2	1:B:62:GLU:HB2	2.02	0.41
1:B:234:ASN:ND2	3:B:503:NAG:C2	2.77	0.41
1:B:334:ASN:OD1	1:B:337:LYS:HG3	2.21	0.41
1:A:338:TRP:CZ2	1:A:390:LEU:HG	2.55	0.41
1:A:370:GLU:HG2	2:A:501:1C1:N19	2.36	0.41
1:A:85:VAL:O	1:A:86:LEU:HD23	2.20	0.41
1:A:397:ASN:N	5:A:706:HOH:O	2.38	0.41
1:B:234:ASN:HD21	3:B:503:NAG:H2	1.83	0.41
1:B:341:THR:O	1:B:345:VAL:HG23	2.21	0.41
1:B:347:GLU:HG2	1:B:395:TYR:OH	2.20	0.41
1:B:432:ARG:NH2	5:B:685:HOH:O	2.53	0.41
1:A:55:ALA:HB1	1:A:77:THR:HA	2.02	0.41
1:A:464:ASP:OD2	1:A:465:THR:HG22	2.21	0.41
1:B:338:TRP:CZ2	1:B:390:LEU:HG	2.56	0.41
1:B:96:TRP:CD1	1:B:275:GLU:HA	2.56	0.40
1:A:122:LEU:HD12	1:A:199:SER:O	2.21	0.40
1:B:72:HIS:ND1	1:B:72:HIS:C	2.75	0.40
1:B:246:GLN:OE1	1:B:246:GLN:HA	2.22	0.40
1:A:91:GLU:HG3	1:A:226:LEU:CD2	2.52	0.40
1:B:255:VAL:HG13	1:B:475:MET:SD	2.61	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	331/358 (92%)	314 (95%)	14 (4%)	3 (1%)	17 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	329/358 (92%)	306 (93%)	20 (6%)	3 (1%)	17	31
All	All	660/716 (92%)	620 (94%)	34 (5%)	6 (1%)	17	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	351	LYS
1	A	352	HIS
1	A	354	PRO
1	B	354	PRO
1	B	276	ASN
1	B	124	GLY

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	299/312 (96%)	283 (95%)	16 (5%)	22	42
1	B	297/312 (95%)	277 (93%)	20 (7%)	16	31
All	All	596/624 (96%)	560 (94%)	36 (6%)	18	37

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	77	THR
1	A	84	MET
1	A	111	LEU
1	A	117	LYS
1	A	203	GLN
1	A	244	THR
1	A	268	GLU
1	A	269	GLU
1	A	394	THR

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Mol	Chain	Res	Type
1	A	413	THR
1	A	415	THR
1	A	424	ILE
1	A	432	ARG
1	A	464	ASP
1	A	465	THR
1	B	77	THR
1	B	80	ASN
1	B	84	MET
1	B	88	ASN
1	B	89	VAL
1	B	111	LEU
1	B	117	LYS
1	B	123	THR
1	B	199	SER
1	B	268	GLU
1	B	269	GLU
1	B	290	GLU
1	B	344	LYS
1	B	369	LEU
1	B	394	THR
1	B	413	THR
1	B	415	THR
1	B	419	LYS
1	B	432	ARG
1	B	465	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	GLN
1	A	229	ASN
1	A	397	ASN
1	A	425	ASN
1	B	229	ASN
1	B	397	ASN
1	B	425	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	503	1	14,14,15	0.49	0	17,19,21	0.80	0
2	1C1	A	501	-	30,30,30	3.35	13 (43%)	37,42,42	2.71	13 (35%)
2	1C1	B	501	-	30,30,30	3.35	12 (40%)	37,42,42	2.69	13 (35%)
3	NAG	A	507	1	14,14,15	0.56	0	17,19,21	0.69	0
3	NAG	A	503	1	14,14,15	0.54	0	17,19,21	0.65	0
3	NAG	B	504	1	14,14,15	0.56	0	17,19,21	0.91	0
3	NAG	A	505	1	14,14,15	0.53	0	17,19,21	1.03	2 (11%)
3	NAG	B	507	1	14,14,15	0.52	0	17,19,21	0.68	0
3	NAG	A	504	1	14,14,15	0.59	0	17,19,21	0.78	1 (5%)
3	NAG	B	506	1	14,14,15	0.51	0	17,19,21	0.74	0
3	NAG	B	508	1	14,14,15	0.38	0	17,19,21	0.66	0
3	NAG	B	505	1	14,14,15	0.48	0	17,19,21	0.61	0
4	FMT	B	502	-	0,2,2	0.00	-	0,1,1	0.00	-
3	NAG	A	506	1	14,14,15	0.29	0	17,19,21	0.61	0
3	NAG	A	508	1	14,14,15	0.52	0	17,19,21	0.81	0
3	NAG	A	502	1	14,14,15	0.57	0	17,19,21	0.62	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	503	1	-	0/6/23/26	0/1/1/1
2	1C1	A	501	-	-	3/17/29/29	0/3/3/3
2	1C1	B	501	-	-	4/17/29/29	0/3/3/3
3	NAG	A	507	1	-	0/6/23/26	0/1/1/1
3	NAG	A	503	1	-	0/6/23/26	0/1/1/1
3	NAG	B	504	1	-	0/6/23/26	0/1/1/1
3	NAG	A	505	1	-	3/6/23/26	0/1/1/1
3	NAG	B	507	1	-	2/6/23/26	0/1/1/1
3	NAG	A	504	1	-	2/6/23/26	0/1/1/1
3	NAG	B	506	1	-	2/6/23/26	0/1/1/1
3	NAG	B	508	1	-	2/6/23/26	0/1/1/1
3	NAG	B	505	1	-	3/6/23/26	0/1/1/1
3	NAG	A	506	1	-	0/6/23/26	0/1/1/1
3	NAG	A	508	1	-	2/6/23/26	0/1/1/1
3	NAG	A	502	1	-	0/6/23/26	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	1C1	C11-C12	7.74	1.49	1.39
2	A	501	1C1	C11-C12	7.68	1.49	1.39
2	A	501	1C1	C05-C13	-7.16	1.45	1.54
2	B	501	1C1	C05-C13	-7.14	1.45	1.54
2	A	501	1C1	C02-N03	6.63	1.46	1.33
2	B	501	1C1	C02-N03	6.61	1.46	1.33
2	A	501	1C1	C21-C20	-6.01	1.29	1.39
2	B	501	1C1	C21-C20	-5.97	1.29	1.39
2	B	501	1C1	C15-N14	5.39	1.44	1.34
2	A	501	1C1	C15-N14	5.35	1.44	1.34
2	A	501	1C1	C08-C07	5.31	1.48	1.39
2	B	501	1C1	C08-C07	5.28	1.48	1.39
2	A	501	1C1	C27-C20	-3.94	1.32	1.39
2	B	501	1C1	C27-C20	-3.90	1.32	1.39
2	A	501	1C1	C17-N19	3.74	1.43	1.35
2	B	501	1C1	C17-N19	3.68	1.43	1.35
2	A	501	1C1	C17-C15	-3.66	1.47	1.53
2	B	501	1C1	C17-C15	-3.65	1.47	1.53
2	A	501	1C1	C24-C22	3.60	1.43	1.38
2	B	501	1C1	C24-C22	3.59	1.43	1.38
2	A	501	1C1	C07-C12	-2.68	1.34	1.39
2	B	501	1C1	C07-C12	-2.60	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	1C1	O16-C15	-2.44	1.18	1.23
2	A	501	1C1	O16-C15	-2.44	1.19	1.23
2	A	501	1C1	F23-C22	-2.03	1.30	1.35

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	1C1	C21-C22-C24	-8.57	113.45	121.72
2	B	501	1C1	C21-C22-C24	-8.51	113.51	121.72
2	B	501	1C1	C20-C21-C22	7.97	125.28	118.76
2	A	501	1C1	C20-C21-C22	7.92	125.24	118.76
2	B	501	1C1	C12-C13-N14	-4.93	106.70	114.61
2	A	501	1C1	C12-C13-N14	-4.90	106.75	114.61
2	A	501	1C1	F23-C22-C24	4.44	123.08	118.98
2	B	501	1C1	F23-C22-C24	4.36	123.00	118.98
2	B	501	1C1	C12-C13-C05	3.49	107.67	104.38
2	A	501	1C1	C12-C13-C05	3.48	107.67	104.38
2	A	501	1C1	C22-C24-CL1	-3.11	116.01	119.78
2	B	501	1C1	C22-C24-CL1	-3.09	116.04	119.78
2	A	501	1C1	O18-C17-C15	-2.84	117.83	121.30
2	B	501	1C1	O18-C17-C15	-2.84	117.83	121.30
2	A	501	1C1	N01-C02-N03	2.66	125.33	119.19
2	B	501	1C1	N01-C02-N03	2.61	125.21	119.19
3	A	504	NAG	C1-O5-C5	2.55	115.65	112.19
2	B	501	1C1	C26-C24-CL1	2.52	123.47	118.41
2	A	501	1C1	C26-C24-CL1	2.52	123.46	118.41
2	B	501	1C1	F23-C22-C21	2.43	123.45	118.61
2	A	501	1C1	F23-C22-C21	2.42	123.43	118.61
2	A	501	1C1	C10-C11-C12	-2.32	118.06	121.01
2	A	501	1C1	C07-C12-C13	-2.29	108.31	110.22
2	B	501	1C1	C10-C11-C12	-2.28	118.11	121.01
2	B	501	1C1	C07-C12-C13	-2.22	108.37	110.22
2	A	501	1C1	C13-N14-C15	2.17	125.82	122.32
2	B	501	1C1	C13-N14-C15	2.16	125.81	122.32
3	A	505	NAG	C2-N2-C7	-2.12	119.89	122.90
3	A	505	NAG	O5-C1-C2	-2.08	108.01	111.29

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	1C1	N03-C04-C05-C06

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Mol	Chain	Res	Type	Atoms
2	A	501	1C1	N03-C04-C05-C13
3	A	508	NAG	C8-C7-N2-C2
3	A	508	NAG	O7-C7-N2-C2
3	B	505	NAG	C3-C2-N2-C7
3	B	505	NAG	C8-C7-N2-C2
3	B	505	NAG	O7-C7-N2-C2
2	B	501	1C1	O16-C15-C17-N19
3	A	505	NAG	C8-C7-N2-C2
3	A	505	NAG	O7-C7-N2-C2
3	B	506	NAG	C8-C7-N2-C2
3	B	506	NAG	O7-C7-N2-C2
3	B	507	NAG	C8-C7-N2-C2
3	B	508	NAG	C8-C7-N2-C2
3	B	508	NAG	O7-C7-N2-C2
3	B	507	NAG	O7-C7-N2-C2
2	A	501	1C1	O16-C15-C17-N19
3	A	505	NAG	O5-C5-C6-O6
3	A	504	NAG	O5-C5-C6-O6
3	A	504	NAG	C4-C5-C6-O6
2	B	501	1C1	N03-C04-C05-C06
2	B	501	1C1	N03-C04-C05-C13
2	B	501	1C1	O16-C15-C17-O18

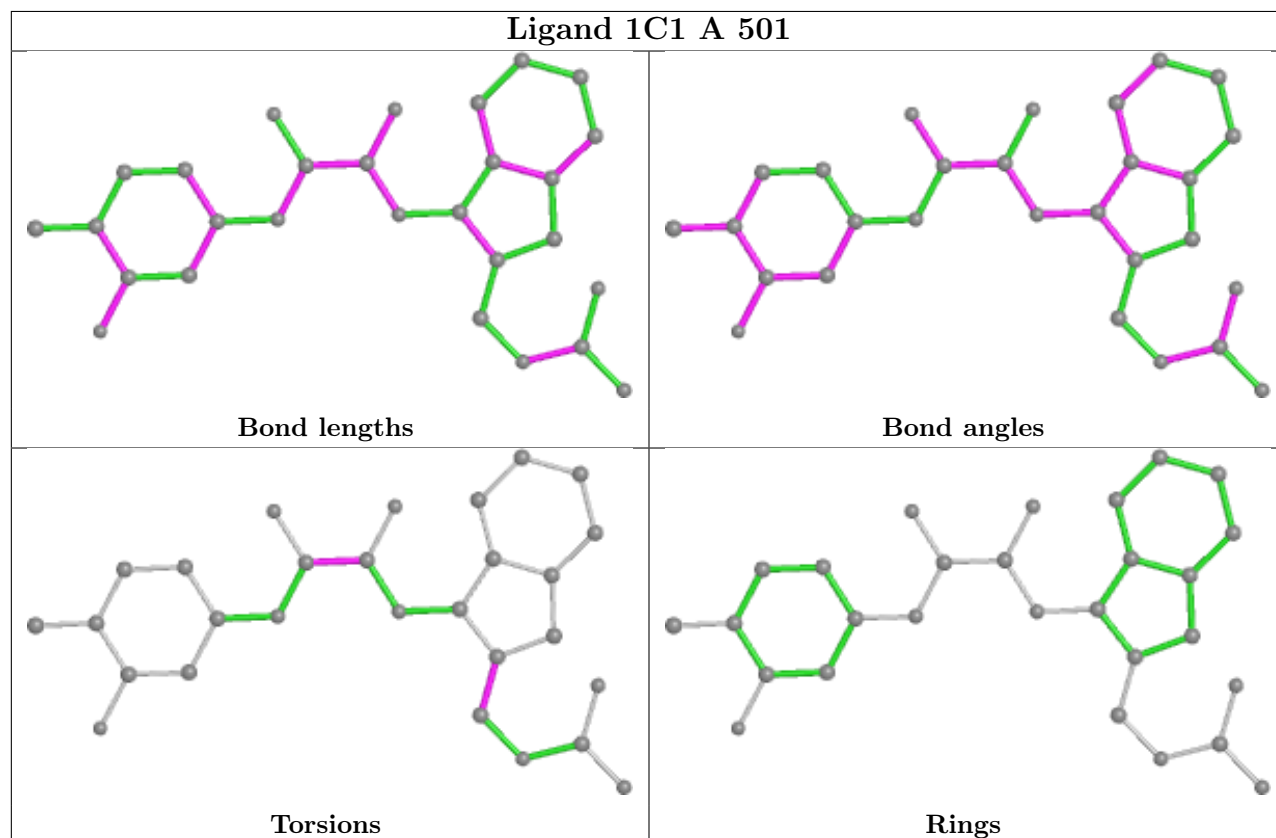
There are no ring outliers.

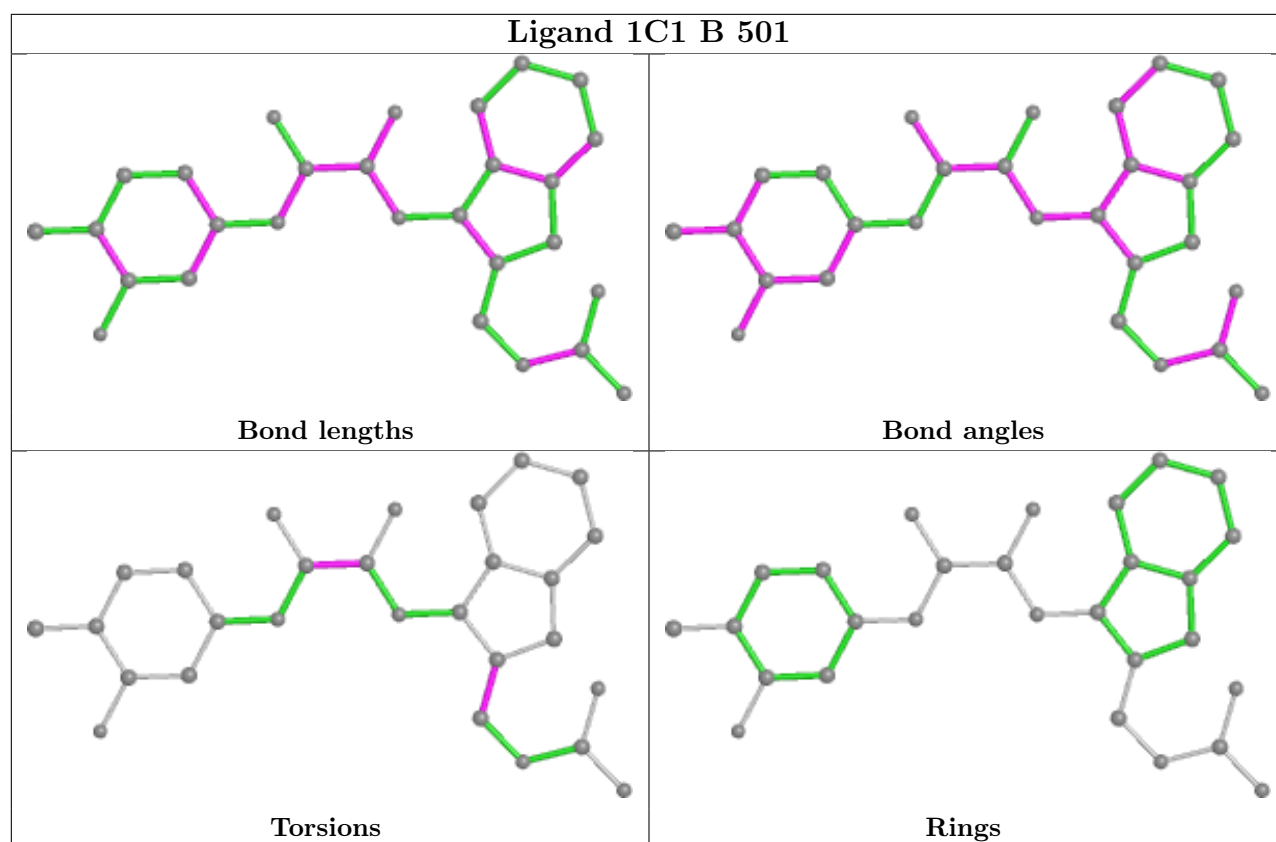
7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	NAG	7	0
2	A	501	1C1	2	0
3	A	505	NAG	6	0
3	B	506	NAG	3	0
3	B	505	NAG	1	0
4	B	502	FMT	1	0
3	A	502	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	336/358 (93%)	0.37	24 (7%) 16 16	4, 28, 74, 129	0
1	B	335/358 (93%)	0.95	52 (15%) 2 1	10, 45, 87, 127	0
All	All	671/716 (93%)	0.66	76 (11%) 5 4	4, 36, 82, 129	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	88	ASN	6.7
1	B	88	ASN	6.2
1	B	87	ALA	6.1
1	B	239	CYS	5.2
1	A	87	ALA	5.0
1	B	221	ALA	4.9
1	A	491	ILE	4.6
1	B	285	ILE	3.9
1	B	92	ASN	3.7
1	B	89	VAL	3.7
1	B	223	PHE	3.7
1	A	89	VAL	3.7
1	A	489	VAL	3.6
1	B	90	THR	3.6
1	B	240	ARG	3.5
1	A	354	PRO	3.4
1	A	357	LYS	3.3
1	A	81	PRO	3.2
1	A	490	GLU	3.2
1	A	85	VAL	3.1
1	B	464	ASP	3.1
1	A	220	PRO	3.1
1	B	93	PHE	3.0
1	B	256	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	412	GLY	3.0
1	B	486	TYR	2.9
1	A	49	LYS	2.8
1	B	259	LEU	2.8
1	B	465	THR	2.8
1	B	51	THR	2.8
1	B	237	GLY	2.7
1	B	50	THR	2.7
1	B	86	LEU	2.7
1	B	339	ASN	2.7
1	B	272	ILE	2.7
1	B	357	LYS	2.7
1	B	484	TYR	2.7
1	B	266	ALA	2.6
1	A	84	MET	2.6
1	B	452	LEU	2.6
1	B	238	PRO	2.6
1	B	233	PHE	2.5
1	B	408	ARG	2.5
1	A	50	THR	2.5
1	A	465	THR	2.5
1	B	396	ARG	2.5
1	B	224	ALA	2.5
1	B	394	THR	2.5
1	B	358	THR	2.5
1	B	286	VAL	2.4
1	A	356	SER	2.4
1	B	78	ASP	2.4
1	B	397	ASN	2.4
1	A	268	GLU	2.4
1	B	85	VAL	2.3
1	B	59	LYS	2.3
1	B	260	LEU	2.3
1	B	395	TYR	2.3
1	B	249	HIS	2.3
1	A	91	GLU	2.2
1	A	223	PHE	2.2
1	A	376	PHE	2.2
1	B	356	SER	2.2
1	A	277	LEU	2.2
1	A	487	LYS	2.2
1	B	273	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	53	PHE	2.2
1	A	226	LEU	2.1
1	B	75	VAL	2.1
1	B	337	LYS	2.1
1	B	245	VAL	2.1
1	B	481	SER	2.0
1	B	489	VAL	2.0
1	B	451	GLY	2.0
1	A	246	GLN	2.0
1	B	392	ASN	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.

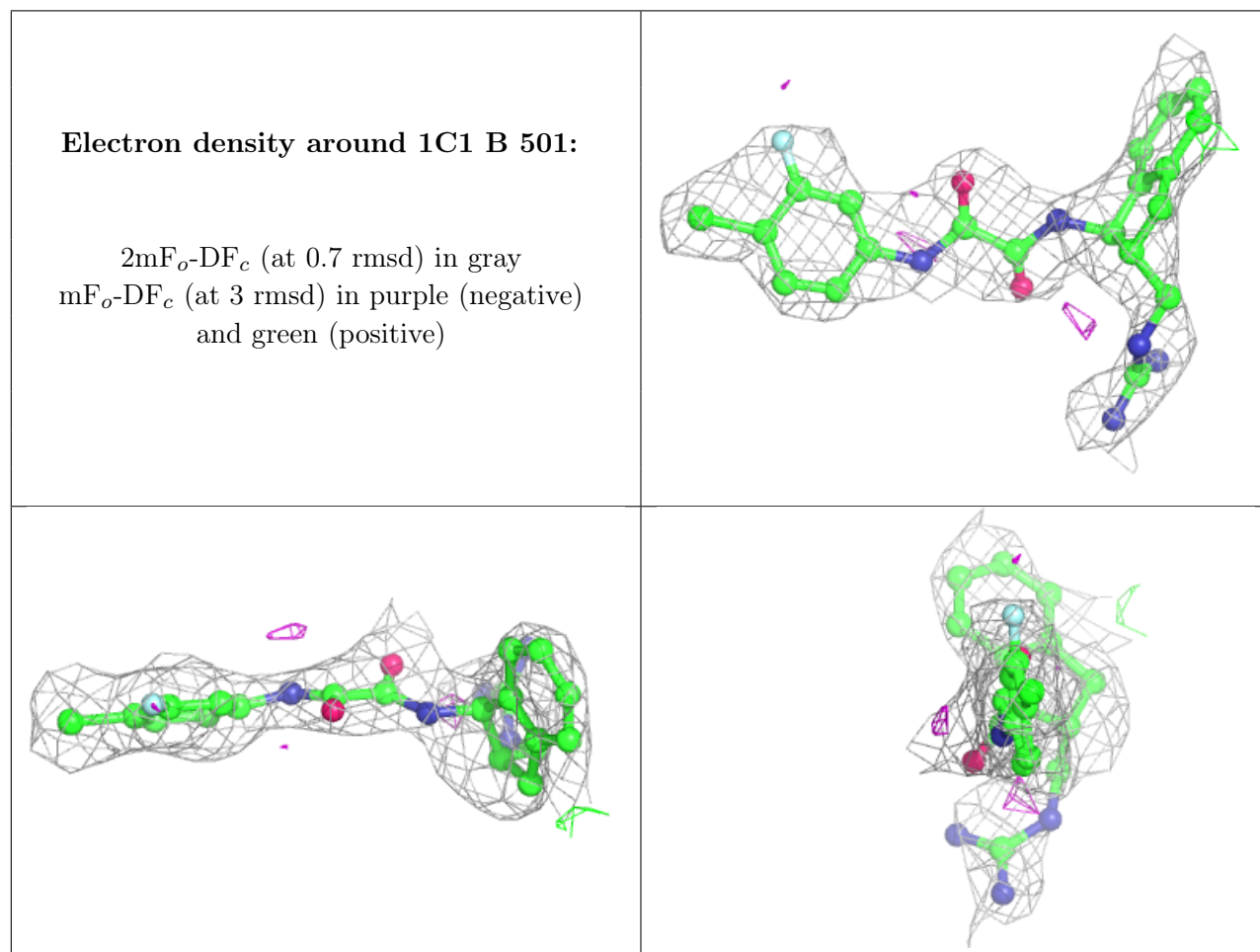
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	505	14/15	0.65	0.21	76,76,76,76	0
3	NAG	B	503	14/15	0.69	0.24	86,86,86,86	0
3	NAG	A	502	14/15	0.71	0.30	77,77,77,77	0
3	NAG	A	505	14/15	0.72	0.24	58,58,58,58	0
4	FMT	B	502	3/3	0.74	0.45	46,46,46,46	0
3	NAG	A	506	14/15	0.79	0.27	44,44,44,44	0
3	NAG	B	506	14/15	0.79	0.21	57,57,57,57	0
2	1C1	B	501	28/28	0.79	0.30	53,53,53,53	0
3	NAG	B	508	14/15	0.80	0.22	55,55,55,55	0
2	1C1	A	501	28/28	0.82	0.26	53,53,53,53	0
3	NAG	A	504	14/15	0.86	0.24	53,53,53,53	0
3	NAG	B	507	14/15	0.89	0.22	47,47,47,47	0
3	NAG	A	507	14/15	0.89	0.17	32,32,32,32	0

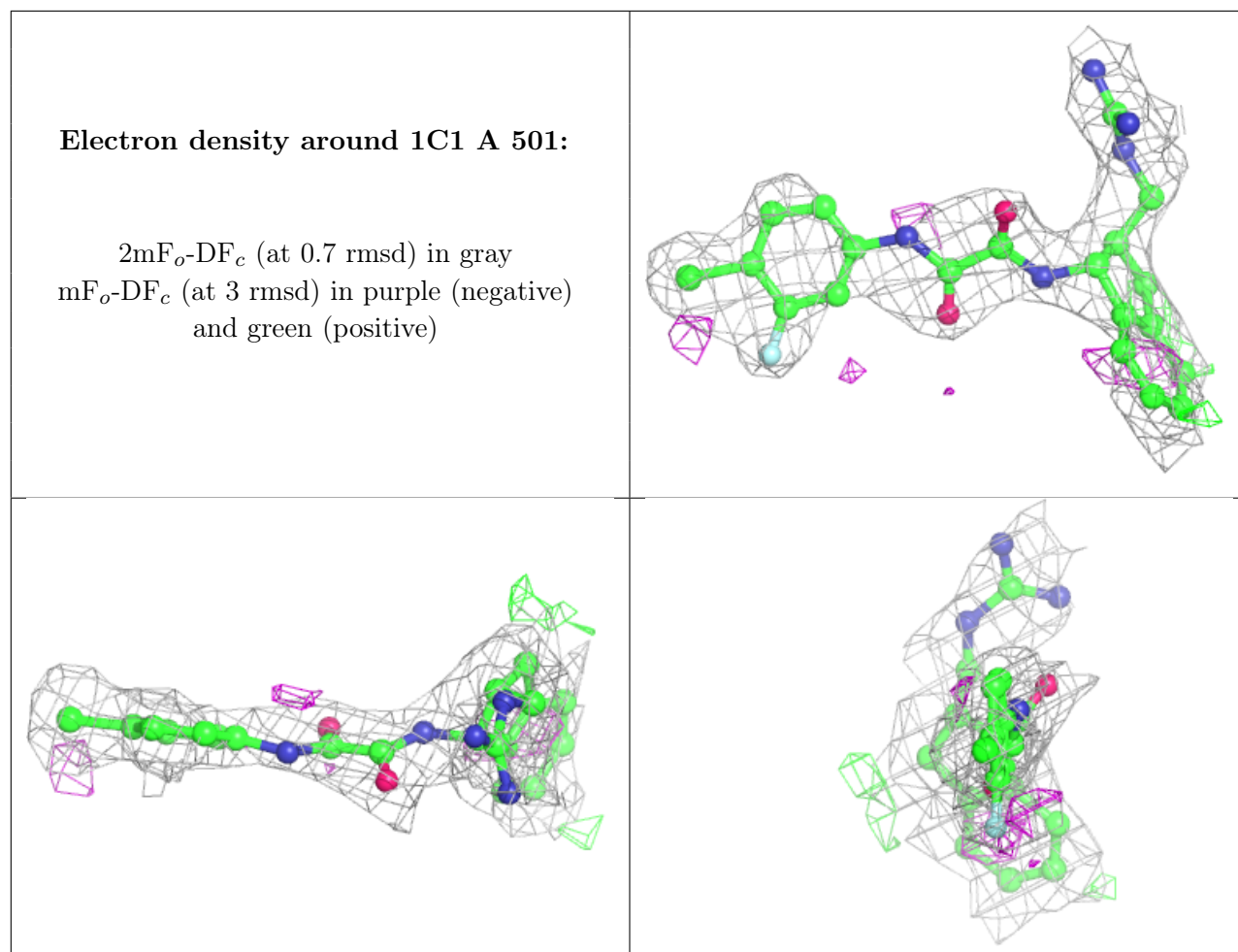
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	504	14/15	0.89	0.17	30,30,30,30	0
3	NAG	A	508	14/15	0.92	0.15	20,20,20,20	0
3	NAG	A	503	14/15	0.94	0.12	9,9,9,9	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.