



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:36 PM UTC

PDB ID : 5L2A / pdb_00005l2a
Title : Structure of CNTnw N149S,F366A in an outward-facing state
Authors : Hirschi, M.; Johnson, Z.L.; Lee, S.-Y.
Deposited on : 2016-07-31
Resolution : 3.45 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

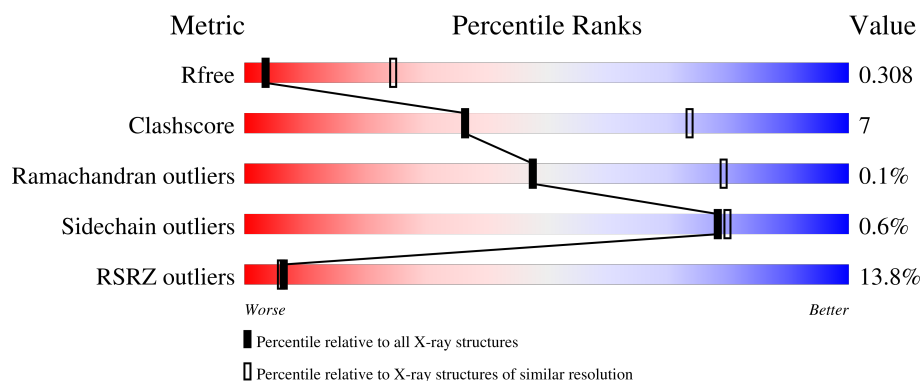
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	431	9% 87% 11% .
1	B	431	14% 84% 13% ..
1	C	431	17% 69% 24% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8963 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 Nucleoside permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3024	1982	492	533	17			
1	B	422	Total	C	N	O	S	0	0	0
			3017	1970	492	539	16			
1	C	406	Total	C	N	O	S	0	0	0
			2869	1883	460	510	16			

There are 24 discrepancies between the modelled and reference sequences:

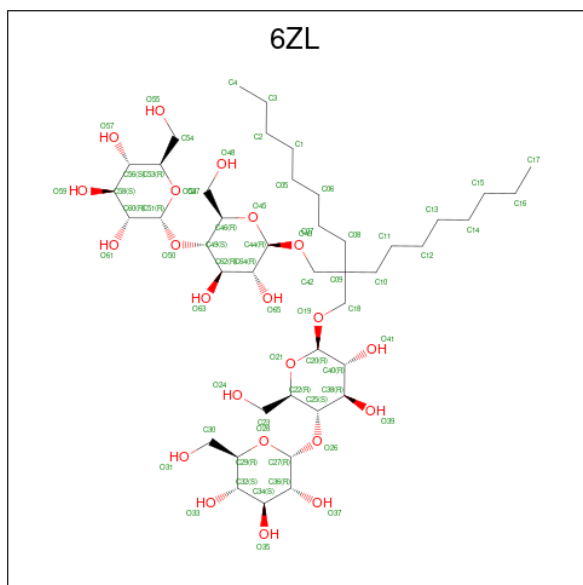
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP G4CRQ5
A	-4	PRO	-	expression tag	UNP G4CRQ5
A	-3	ALA	-	expression tag	UNP G4CRQ5
A	-2	VAL	-	expression tag	UNP G4CRQ5
A	-1	PRO	-	expression tag	UNP G4CRQ5
A	0	ARG	-	expression tag	UNP G4CRQ5
A	149	SER	ASN	engineered mutation	UNP G4CRQ5
A	366	ALA	PHE	engineered mutation	UNP G4CRQ5
B	-5	GLY	-	expression tag	UNP G4CRQ5
B	-4	PRO	-	expression tag	UNP G4CRQ5
B	-3	ALA	-	expression tag	UNP G4CRQ5
B	-2	VAL	-	expression tag	UNP G4CRQ5
B	-1	PRO	-	expression tag	UNP G4CRQ5
B	0	ARG	-	expression tag	UNP G4CRQ5
B	149	SER	ASN	engineered mutation	UNP G4CRQ5
B	366	ALA	PHE	engineered mutation	UNP G4CRQ5
C	-5	GLY	-	expression tag	UNP G4CRQ5
C	-4	PRO	-	expression tag	UNP G4CRQ5
C	-3	ALA	-	expression tag	UNP G4CRQ5
C	-2	VAL	-	expression tag	UNP G4CRQ5
C	-1	PRO	-	expression tag	UNP G4CRQ5
C	0	ARG	-	expression tag	UNP G4CRQ5
C	149	SER	ASN	engineered mutation	UNP G4CRQ5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	366	ALA	PHE	engineered mutation	UNP G4CRQ5

- Molecule 2 is 2-[[[(4-O-alpha-D-glucopyranosyl-beta-D-glucopyranosyl)oxy]methyl}-2-octyldecyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (CCD ID: 6ZL) (formula: $C_{43}H_{80}O_{22}$).

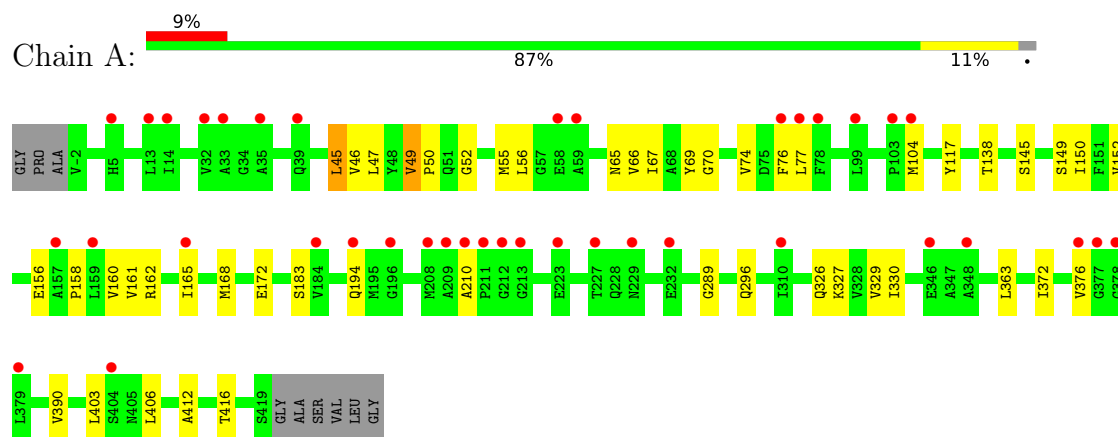


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			53	36	17		

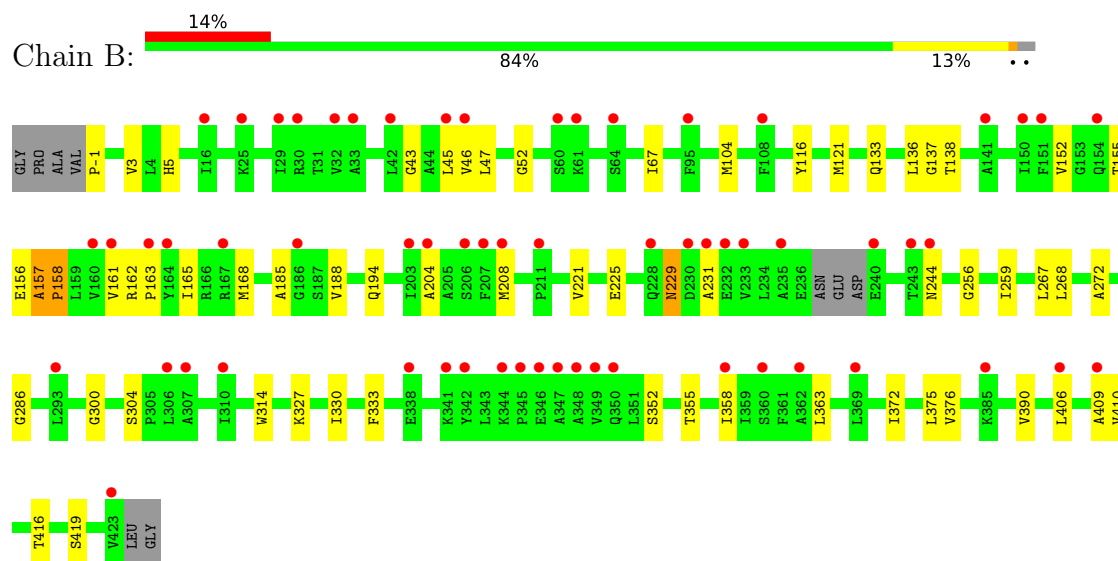
3 Residue-property plots [i](#)

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: Nucleoside permease

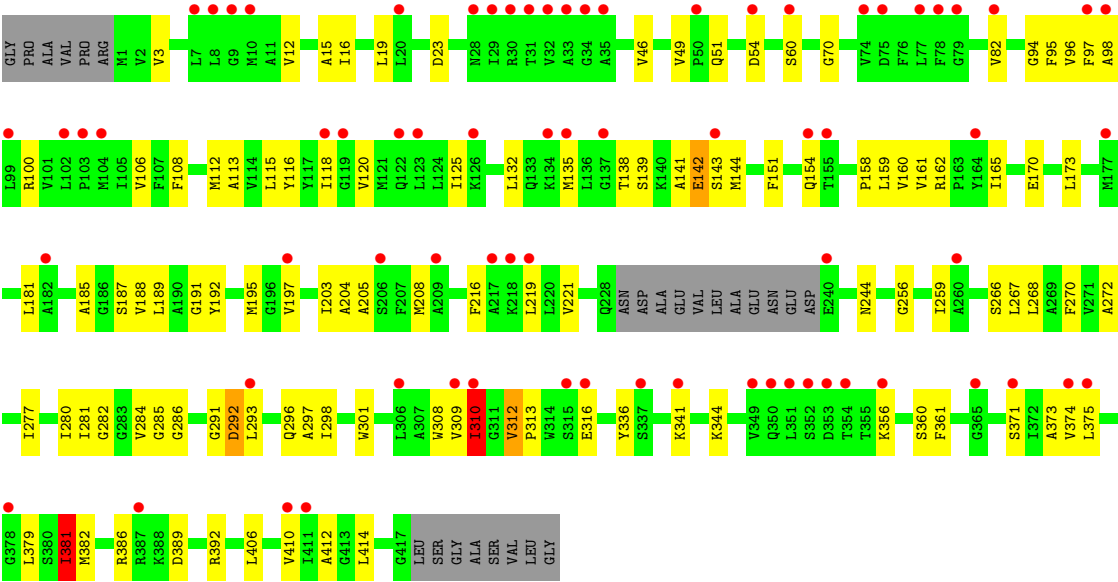


• Molecule 1: Nucleoside permease



• Molecule 1: Nucleoside permease





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	119.08Å 119.08Å 276.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.98 – 3.45 38.98 – 3.45	Depositor EDS
% Data completeness (in resolution range)	92.5 (38.98-3.45) 94.8 (38.98-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.272 , 0.307 0.277 , 0.308	Depositor DCC
R_{free} test set	1948 reflections (6.67%)	wwPDB-VP
Wilson B-factor (Å ²)	74.1	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.062 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	8963	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 6ZL

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	0.38	3/3077 (0.1%)	0.79	5/4184 (0.1%)
1	B	0.45	4/3069 (0.1%)	0.81	8/4170 (0.2%)
1	C	0.39	0/2918	0.95	10/3971 (0.3%)
All	All	0.41	7/9064 (0.1%)	0.85	23/12325 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	3
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	138	THR	C-N	8.37	1.45	1.33
1	B	286	GLY	C-N	8.09	1.45	1.33
1	B	314	TRP	C-N	-6.78	1.24	1.34
1	A	138	THR	C-N	5.75	1.41	1.33
1	B	229	ASN	C-N	-5.40	1.26	1.33
1	A	76	PHE	C-N	-5.26	1.26	1.33
1	A	117	TYR	C-N	-5.02	1.27	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	292	ASP	N-CA-C	-16.55	91.17	113.18
1	C	142	GLU	N-CA-C	-8.49	102.10	111.36
1	C	284	VAL	N-CA-C	-7.24	103.24	110.62
1	B	136	LEU	O-C-N	6.84	130.20	122.27
1	C	162	ARG	CA-C-N	-6.83	112.67	120.04
1	C	162	ARG	C-N-CA	-6.83	112.67	120.04
1	B	416	THR	CA-C-N	6.27	128.18	120.22
1	B	416	THR	C-N-CA	6.27	128.18	120.22
1	C	310	ILE	CB-CA-C	-6.18	103.79	111.94
1	A	49	VAL	CA-C-O	6.17	125.18	119.62
1	C	187	SER	N-CA-C	-5.91	104.42	111.69
1	B	157	ALA	CA-C-N	-5.77	112.64	119.05
1	B	157	ALA	C-N-CA	-5.77	112.64	119.05
1	A	49	VAL	O-C-N	5.66	127.25	121.14
1	C	221	VAL	N-CA-C	5.65	113.83	109.19
1	B	419	SER	CB-CA-C	-5.39	110.38	116.63
1	A	45	LEU	N-CA-C	5.36	118.28	111.69
1	C	381	ILE	N-CA-C	5.31	116.09	110.72
1	C	113	ALA	N-CA-C	-5.22	107.28	113.97
1	B	330	ILE	CB-CA-C	-5.15	102.84	111.29
1	B	225	GLU	N-CA-C	-5.09	102.92	110.46
1	A	162	ARG	CA-C-N	-5.03	115.70	120.83
1	A	162	ARG	C-N-CA	-5.03	115.70	120.83

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	GLY	Peptide
1	B	157	ALA	Peptide
1	B	158	PRO	Peptide
1	C	292	ASP	Peptide
1	C	310	ILE	Peptide
1	C	312	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3024	0	3142	29	0
1	B	3017	0	3112	33	0
1	C	2869	0	2959	77	0
2	A	53	0	0	2	0
All	All	8963	0	9213	131	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 (131) 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:C:308:TRP:HD1	1:C:313:PRO:HA	1.38	0.88
1:A:168:MET:HE2	1:A:172:GLU:HB3	1.64	0.77
1:C:158:PRO:HB2	1:C:382:MET:HE1	1.66	0.76
1:C:170:GLU:OE2	1:C:392:ARG:NH2	2.20	0.75
1:B:158:PRO:O	1:B:161:VAL:N	2.18	0.75
1:C:308:TRP:CD1	1:C:313:PRO:HA	2.21	0.73
1:C:310:ILE:HG12	1:C:410:VAL:HG22	1.70	0.73
1:B:256:GLY:HA2	1:B:259:ILE:HD12	1.70	0.72
1:C:181:LEU:HD11	1:C:375:LEU:HD11	1.70	0.71
1:C:141:ALA:O	1:C:144:MET:N	2.24	0.70
1:C:181:LEU:HD11	1:C:375:LEU:CD1	2.24	0.68
1:C:181:LEU:HD22	1:C:371:SER:OG	1.93	0.67
1:C:282:GLY:O	1:C:286:GLY:N	2.29	0.66
1:C:141:ALA:O	1:C:144:MET:HB3	1.95	0.66
1:C:270:PHE:CD2	1:C:373:ALA:HB2	2.29	0.65
1:B:5:HIS:O	1:B:5:HIS:ND1	2.28	0.65
1:C:95:PHE:CD1	1:C:100:ARG:HD2	2.31	0.65
1:C:185:ALA:O	1:C:188:VAL:HG12	1.98	0.64
1:A:327:LYS:HD2	1:A:363:LEU:HA	1.79	0.63
1:A:65:ASN:HB3	1:A:69:TYR:CE2	2.33	0.63
1:C:381:ILE:HD12	1:C:381:ILE:N	2.13	0.62
1:B:185:ALA:HB3	1:B:188:VAL:HG22	1.80	0.62
1:C:154:GLN:NE2	1:C:371:SER:OG	2.33	0.61
1:A:329:VAL:HG23	1:A:330:ILE:HG12	1.84	0.60
1:C:296:GLN:OE1	1:C:296:GLN:N	2.32	0.60
1:C:132:LEU:HA	1:C:135:MET:HB2	1.85	0.59
1:B:67:ILE:HG23	1:B:104:MET:HE2	1.85	0.59
1:C:285:GLY:HA3	1:C:291:GLY:HA3	1.85	0.58
1:C:256:GLY:HA2	1:C:259:ILE:HD12	1.84	0.58
1:C:266:SER:HB3	1:C:373:ALA:HB1	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:LEU:CD1	1:C:375:LEU:HD11	2.37	0.55
2:A:501:6ZL:C06	2:A:501:6ZL:C11	2.86	0.54
1:B:358:ILE:HG23	1:B:409:ALA:HB1	1.90	0.53
1:B:152:VAL:HG11	1:B:156:GLU:O	2.08	0.53
1:B:204:ALA:HB1	1:B:208:MET:HE3	1.89	0.53
1:A:77:LEU:HD12	1:C:97:PHE:CD2	2.42	0.53
1:C:108:PHE:HD1	1:C:112:MET:HE2	1.73	0.53
1:A:77:LEU:HG	1:C:98:ALA:HB2	1.89	0.52
1:C:115:LEU:HA	1:C:118:ILE:HG12	1.91	0.52
1:B:165:ILE:HA	1:B:168:MET:HE3	1.91	0.52
1:B:158:PRO:O	1:B:162:ARG:N	2.42	0.52
1:A:77:LEU:HD12	1:C:97:PHE:HD2	1.75	0.52
1:C:381:ILE:N	1:C:381:ILE:CD1	2.73	0.51
1:B:327:LYS:HD3	1:B:363:LEU:HA	1.92	0.51
1:A:152:VAL:HG11	1:A:156:GLU:HB3	1.91	0.50
1:B:43:GLY:HA2	1:B:208:MET:HE2	1.94	0.50
1:C:173:LEU:HD22	1:C:386:ARG:HD2	1.91	0.50
1:C:139:SER:C	1:C:141:ALA:H	2.19	0.50
1:A:296:GLN:HG3	1:A:326:GLN:NE2	2.26	0.50
1:C:161:VAL:O	1:C:165:ILE:HG13	2.12	0.50
1:C:375:LEU:O	1:C:379:LEU:HD23	2.12	0.49
1:A:161:VAL:O	1:A:165:ILE:HG13	2.12	0.49
1:B:5:HIS:HD1	1:B:5:HIS:C	2.20	0.49
1:A:70:GLY:HA2	1:C:272:ALA:HB1	1.94	0.49
1:C:291:GLY:HA2	1:C:293:LEU:HB2	1.96	0.48
1:B:-1:PRO:O	1:B:3:VAL:HG23	2.13	0.48
1:B:267:LEU:HD21	1:B:333:PHE:HB3	1.95	0.48
1:B:116:TYR:CD2	1:B:121:MET:HG3	2.49	0.48
1:C:266:SER:CB	1:C:373:ALA:HB1	2.43	0.48
1:C:12:VAL:O	1:C:16:ILE:HG13	2.14	0.48
1:A:46:VAL:HG23	1:A:47:LEU:HG	1.95	0.47
1:C:293:LEU:HG	1:C:298:ILE:HD11	1.94	0.47
1:A:45:LEU:O	1:A:52:GLY:HA3	2.13	0.47
1:B:5:HIS:ND1	1:B:5:HIS:C	2.73	0.47
1:A:104:MET:HG3	1:A:194:GLN:HG3	1.97	0.47
1:C:181:LEU:HD21	1:C:375:LEU:HG	1.96	0.47
1:C:139:SER:H	1:C:142:GLU:HG2	1.79	0.47
1:A:55:MET:HE2	2:A:501:6ZL:C05	2.45	0.47
1:C:118:ILE:HG13	1:C:120:VAL:HG23	1.97	0.47
1:C:285:GLY:CA	1:C:291:GLY:HA3	2.45	0.46
1:C:205:ALA:HA	1:C:208:MET:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:LEU:O	1:C:410:VAL:HG23	2.14	0.46
1:A:66:VAL:HA	1:A:69:TYR:HD2	1.80	0.46
1:A:74:VAL:HG22	1:C:268:LEU:HD11	1.98	0.46
1:B:155:THR:HG22	1:B:375:LEU:HD23	1.98	0.46
1:B:300:GLY:O	1:B:304:SER:OG	2.24	0.46
1:C:216:PHE:HA	1:C:219:LEU:HD12	1.97	0.46
1:A:46:VAL:HB	1:A:56:LEU:HD22	1.98	0.46
1:C:138:THR:HG21	1:C:143:SER:HB2	1.98	0.46
1:C:3:VAL:HG12	1:C:414:LEU:HD11	1.97	0.46
1:B:161:VAL:O	1:B:165:ILE:HG13	2.15	0.45
1:C:188:VAL:HG13	1:C:189:LEU:N	2.31	0.45
1:A:376:VAL:HG22	1:A:390:VAL:HG12	1.97	0.45
1:C:159:LEU:HD21	1:C:259:ILE:HD13	1.98	0.45
1:C:341:LYS:HA	1:C:344:LYS:HE2	1.99	0.45
1:B:352:SER:HG	1:B:355:THR:HG1	1.64	0.45
1:B:229:ASN:OD1	1:B:229:ASN:N	2.50	0.45
1:C:49:VAL:HG12	1:C:51:GLN:H	1.82	0.45
1:B:133:GLN:O	1:B:137:GLY:HA2	2.16	0.45
1:B:372:ILE:HD12	1:C:244:ASN:HD21	1.81	0.45
1:C:125:ILE:HG12	1:C:144:MET:HG2	1.99	0.45
1:A:65:ASN:O	1:A:69:TYR:CD2	2.70	0.45
1:C:116:TYR:OH	1:C:160:VAL:O	2.18	0.45
1:C:112:MET:SD	1:C:160:VAL:HA	2.57	0.44
1:C:191:GLY:O	1:C:195:MET:HG3	2.18	0.44
1:B:46:VAL:HG23	1:B:47:LEU:HG	1.99	0.44
1:C:277:ILE:O	1:C:280:ILE:HB	2.18	0.44
1:B:163:PRO:HB2	1:B:231:ALA:HB1	1.98	0.44
1:A:67:ILE:HG23	1:A:104:MET:HE2	1.99	0.43
1:C:60:SER:HA	1:C:151:PHE:HD1	1.82	0.43
1:C:12:VAL:HG11	1:C:309:VAL:HG11	1.99	0.43
1:C:82:VAL:HA	1:C:100:ARG:NH2	2.34	0.43
1:A:372:ILE:HD12	1:B:244:ASN:HD21	1.83	0.43
1:C:15:ALA:O	1:C:19:LEU:HG	2.19	0.43
1:C:94:GLY:O	1:C:96:VAL:HG23	2.19	0.43
1:C:203:ILE:HD13	1:C:203:ILE:HA	1.86	0.43
1:B:104:MET:HG3	1:B:194:GLN:HG3	2.01	0.42
1:A:145:SER:HB2	1:A:161:VAL:HG11	2.01	0.42
1:C:46:VAL:HG21	1:C:204:ALA:HA	2.02	0.42
1:C:386:ARG:HD3	1:C:389:ASP:HB2	2.00	0.42
1:C:280:ILE:O	1:C:281:ILE:C	2.63	0.42
1:C:188:VAL:HG22	1:C:192:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:VAL:HG22	1:B:390:VAL:HG12	2.01	0.42
1:C:197:VAL:HG21	1:C:336:TYR:CD1	2.55	0.42
1:A:149:SER:O	1:A:183:SER:OG	2.30	0.41
1:A:49:VAL:HA	1:A:50:PRO:HD3	1.81	0.41
1:A:412:ALA:O	1:A:416:THR:OG1	2.27	0.41
1:B:272:ALA:HB1	1:C:70:GLY:HA2	2.03	0.41
1:C:297:ALA:O	1:C:301:TRP:N	2.51	0.41
1:C:361:PHE:CD2	1:C:412:ALA:HB2	2.56	0.41
1:A:158:PRO:C	1:A:160:VAL:H	2.29	0.41
1:C:277:ILE:O	1:C:281:ILE:HG13	2.21	0.41
1:C:356:LYS:O	1:C:360:SER:OG	2.35	0.41
1:A:403:LEU:HD23	1:A:406:LEU:HD12	2.03	0.40
1:C:267:LEU:HD21	1:C:374:VAL:HG23	2.02	0.40
1:B:45:LEU:O	1:B:52:GLY:HA3	2.22	0.40
1:B:268:LEU:HD22	1:C:106:VAL:HB	2.02	0.40
1:C:188:VAL:CG1	1:C:189:LEU:N	2.84	0.40
1:A:150:ILE:HD11	1:A:210:ALA:HB2	2.03	0.40
1:B:406:LEU:O	1:B:410:VAL:HG23	2.22	0.40
1:C:16:ILE:HA	1:C:19:LEU:HD12	2.04	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	420/431 (97%)	402 (96%)	18 (4%)	0	100	100
1	B	418/431 (97%)	406 (97%)	12 (3%)	0	100	100
1	C	402/431 (93%)	362 (90%)	39 (10%)	1 (0%)	43	74
All	All	1240/1293 (96%)	1170 (94%)	69 (6%)	1 (0%)	48	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	316	GLU

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	300/321 (94%)	300 (100%)	0	100	100
1	B	300/321 (94%)	299 (100%)	1 (0%)	86	83
1	C	283/321 (88%)	279 (99%)	4 (1%)	59	72
All	All	883/963 (92%)	878 (99%)	5 (1%)	78	80

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	221	VAL
1	C	23	ASP
1	C	54	ASP
1	C	312	VAL
1	C	381	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	39	GLN
1	A	65	ASN
1	A	326	GLN
1	A	405	ASN
1	B	39	GLN
1	B	244	ASN
1	B	258	GLN
1	B	326	GLN
1	C	72	ASN
1	C	154	GLN
1	C	194	GLN

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Mol	Chain	Res	Type
1	C	278	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	6ZL	A	501	-	55,55,68	0.68	2 (3%)	69,75,94	0.86	3 (4%)

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	6ZL	A	501	-	-	19/39/99/126	0/3/3/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	6ZL	O43-C44	2.03	1.43	1.40
2	A	501	6ZL	O19-C20	2.01	1.43	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	6ZL	C11-C10-C09	-2.53	109.53	117.19
2	A	501	6ZL	C07-C08-C09	-2.16	110.63	117.19
2	A	501	6ZL	C42-O43-C44	2.01	118.41	113.31

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	6ZL	C08-C09-C18-O19
2	A	501	6ZL	C10-C09-C18-O19
2	A	501	6ZL	O21-C20-O19-C18
2	A	501	6ZL	O45-C46-C47-O48
2	A	501	6ZL	C49-C46-C47-O48
2	A	501	6ZL	O45-C44-O43-C42
2	A	501	6ZL	C64-C44-O43-C42
2	A	501	6ZL	C06-C07-C08-C09
2	A	501	6ZL	C42-C09-C18-O19
2	A	501	6ZL	C05-C1-C2-C3
2	A	501	6ZL	C10-C11-C12-C13
2	A	501	6ZL	C1-C05-C06-C07
2	A	501	6ZL	C09-C10-C11-C12
2	A	501	6ZL	C25-C22-C23-O24
2	A	501	6ZL	C08-C09-C42-O43
2	A	501	6ZL	C10-C09-C42-O43
2	A	501	6ZL	O21-C22-C23-O24
2	A	501	6ZL	C09-C42-O43-C44
2	A	501	6ZL	C18-C09-C42-O43

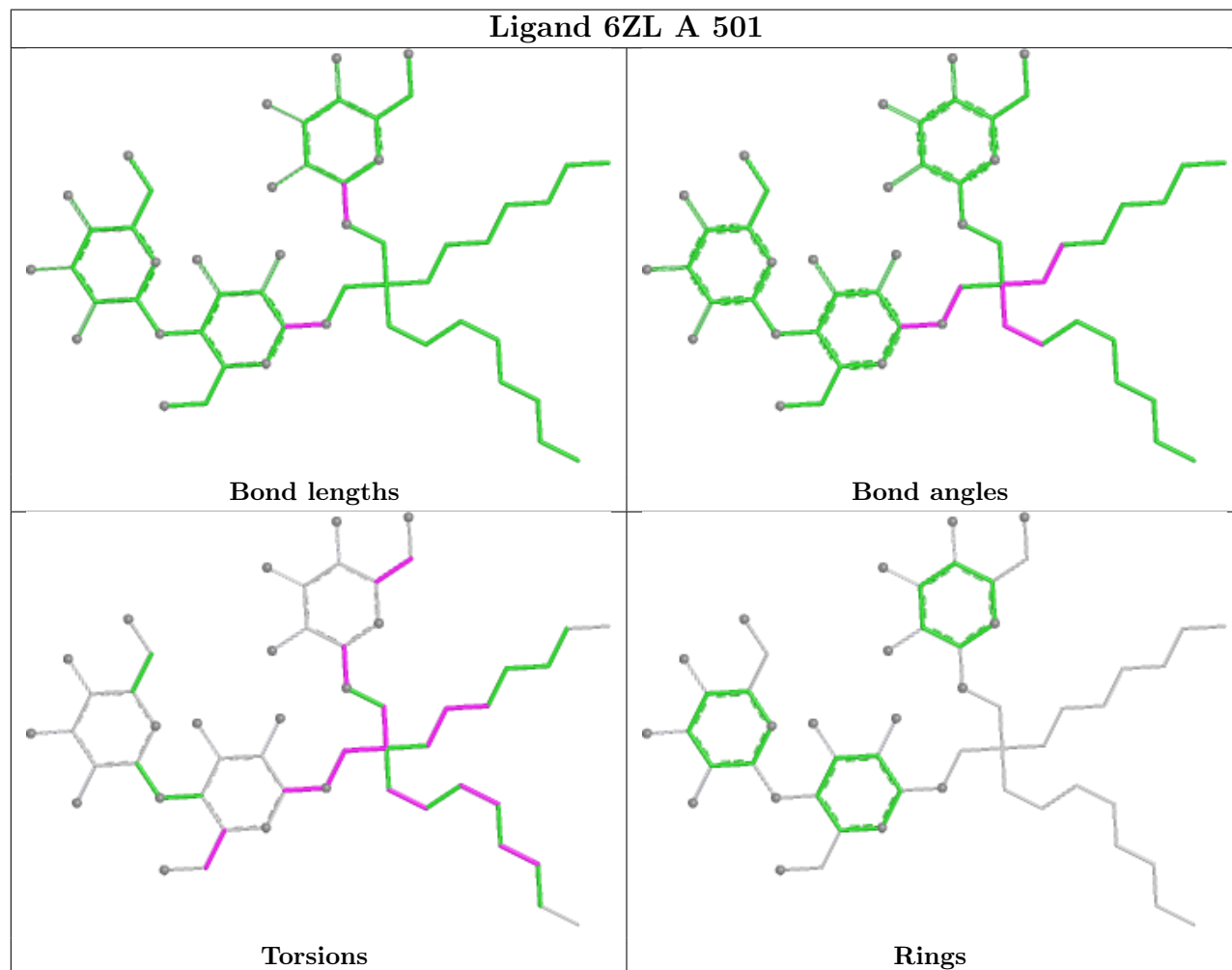
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	6ZL	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	422/431 (97%)	0.40	39 (9%) 14 10	27, 55, 88, 113	0
1	B	422/431 (97%)	0.79	61 (14%) 6 6	34, 75, 110, 133	0
1	C	406/431 (94%)	1.04	73 (17%) 3 4	35, 80, 113, 143	0
All	All	1250/1293 (96%)	0.74	173 (13%) 6 6	27, 70, 108, 143	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	207	PHE	12.1
1	C	30	ARG	10.6
1	A	346	GLU	10.5
1	C	353	ASP	10.3
1	C	29	ILE	9.8
1	C	32	VAL	8.4
1	C	351	LEU	8.2
1	C	31	THR	8.1
1	C	99	LEU	7.6
1	C	78	PHE	7.4
1	C	126	LYS	7.3
1	B	230	ASP	7.3
1	C	352	SER	6.8
1	B	342	TYR	6.6
1	C	33	ALA	6.6
1	C	98	ALA	6.4
1	C	371	SER	5.9
1	C	103	PRO	5.6
1	B	33	ALA	5.6
1	C	122	GLN	5.5
1	C	218	LYS	5.5
1	B	228	GLN	5.4
1	C	119	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	45	LEU	5.3
1	C	134	LYS	5.1
1	C	118	ILE	5.0
1	B	231	ALA	5.0
1	C	77	LEU	5.0
1	C	34	GLY	5.0
1	C	350	GLN	4.8
1	B	141	ALA	4.8
1	C	54	ASP	4.8
1	C	50	PRO	4.6
1	A	194	GLN	4.6
1	C	354	THR	4.6
1	A	210	ALA	4.6
1	C	374	VAL	4.4
1	A	377	GLY	4.4
1	B	46	VAL	4.3
1	B	204	ALA	4.2
1	B	163	PRO	4.2
1	A	78	PHE	4.2
1	C	341	LYS	4.2
1	C	102	LEU	4.2
1	C	135	MET	4.1
1	A	232	GLU	4.1
1	C	123	LEU	4.0
1	A	211	PRO	3.9
1	B	206	SER	3.9
1	B	108	PHE	3.9
1	A	227	THR	3.9
1	C	365	GLY	3.9
1	B	164	TYR	3.8
1	B	42	LEU	3.8
1	B	350	GLN	3.8
1	C	79	GLY	3.8
1	B	151	PHE	3.8
1	C	97	PHE	3.8
1	B	310	ILE	3.7
1	B	423	VAL	3.7
1	A	157	ALA	3.6
1	C	240	GLU	3.6
1	A	376	VAL	3.6
1	B	235	ALA	3.6
1	C	143	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	379	LEU	3.6
1	A	208	MET	3.5
1	A	39	GLN	3.5
1	C	349	VAL	3.5
1	C	28	ASN	3.4
1	C	154	GLN	3.4
1	B	95	PHE	3.4
1	B	208	MET	3.3
1	A	209	ALA	3.3
1	A	196	GLY	3.3
1	B	186	GLY	3.3
1	A	33	ALA	3.2
1	A	348	ALA	3.2
1	B	345	PRO	3.2
1	B	29	ILE	3.2
1	A	404	SER	3.2
1	C	378	GLY	3.2
1	B	341	LYS	3.2
1	A	103	PRO	3.2
1	B	232	GLU	3.1
1	C	82	VAL	3.1
1	C	104	MET	3.1
1	A	35	ALA	3.1
1	C	75	ASP	3.1
1	C	310	ILE	3.1
1	B	243	THR	3.1
1	A	77	LEU	3.0
1	B	30	ARG	3.0
1	B	344	LYS	3.0
1	B	369	LEU	3.0
1	C	219	LEU	3.0
1	B	362	ALA	3.0
1	B	211	PRO	2.9
1	B	307	ALA	2.9
1	A	229	ASN	2.9
1	C	8	LEU	2.9
1	B	349	VAL	2.9
1	B	203	ILE	2.9
1	B	64	SER	2.8
1	C	155	THR	2.8
1	C	74	VAL	2.8
1	A	212	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	316	GLU	2.8
1	B	167	ARG	2.8
1	C	10	MET	2.7
1	C	411	ILE	2.7
1	B	385	LYS	2.7
1	C	306	LEU	2.7
1	B	406	LEU	2.7
1	B	160	VAL	2.6
1	B	409	ALA	2.6
1	C	337	SER	2.6
1	C	356	LYS	2.6
1	B	161	VAL	2.6
1	C	209	ALA	2.6
1	C	410	VAL	2.6
1	C	137	GLY	2.6
1	A	223	GLU	2.6
1	B	233	VAL	2.6
1	B	32	VAL	2.6
1	C	35	ALA	2.6
1	B	348	ALA	2.5
1	C	217	ALA	2.5
1	B	150	ILE	2.5
1	B	60	SER	2.5
1	C	375	LEU	2.5
1	A	184	VAL	2.5
1	B	346	GLU	2.4
1	C	293	LEU	2.4
1	B	16	ILE	2.4
1	C	315	SER	2.4
1	C	177	MET	2.4
1	A	378	GLY	2.4
1	B	293	LEU	2.4
1	A	5	HIS	2.4
1	B	358	ILE	2.4
1	B	61	LYS	2.4
1	C	387	ARG	2.3
1	C	206	SER	2.3
1	A	59	ALA	2.3
1	C	60	SER	2.3
1	B	240	GLU	2.3
1	C	9	GLY	2.3
1	C	164	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	213	GLY	2.3
1	A	76	PHE	2.2
1	B	244	ASN	2.2
1	B	306	LEU	2.2
1	A	310	ILE	2.2
1	A	99	LEU	2.2
1	C	309	VAL	2.2
1	B	154	GLN	2.2
1	C	197	VAL	2.1
1	B	338	GLU	2.1
1	B	25	LYS	2.1
1	C	182	ALA	2.1
1	A	14	ILE	2.1
1	A	104	MET	2.1
1	B	347	ALA	2.1
1	A	32	VAL	2.1
1	A	13	LEU	2.1
1	A	165	ILE	2.1
1	C	260	ALA	2.1
1	C	20	LEU	2.1
1	A	58	GLU	2.0
1	A	159	LEU	2.0
1	B	360	SER	2.0
1	C	7	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

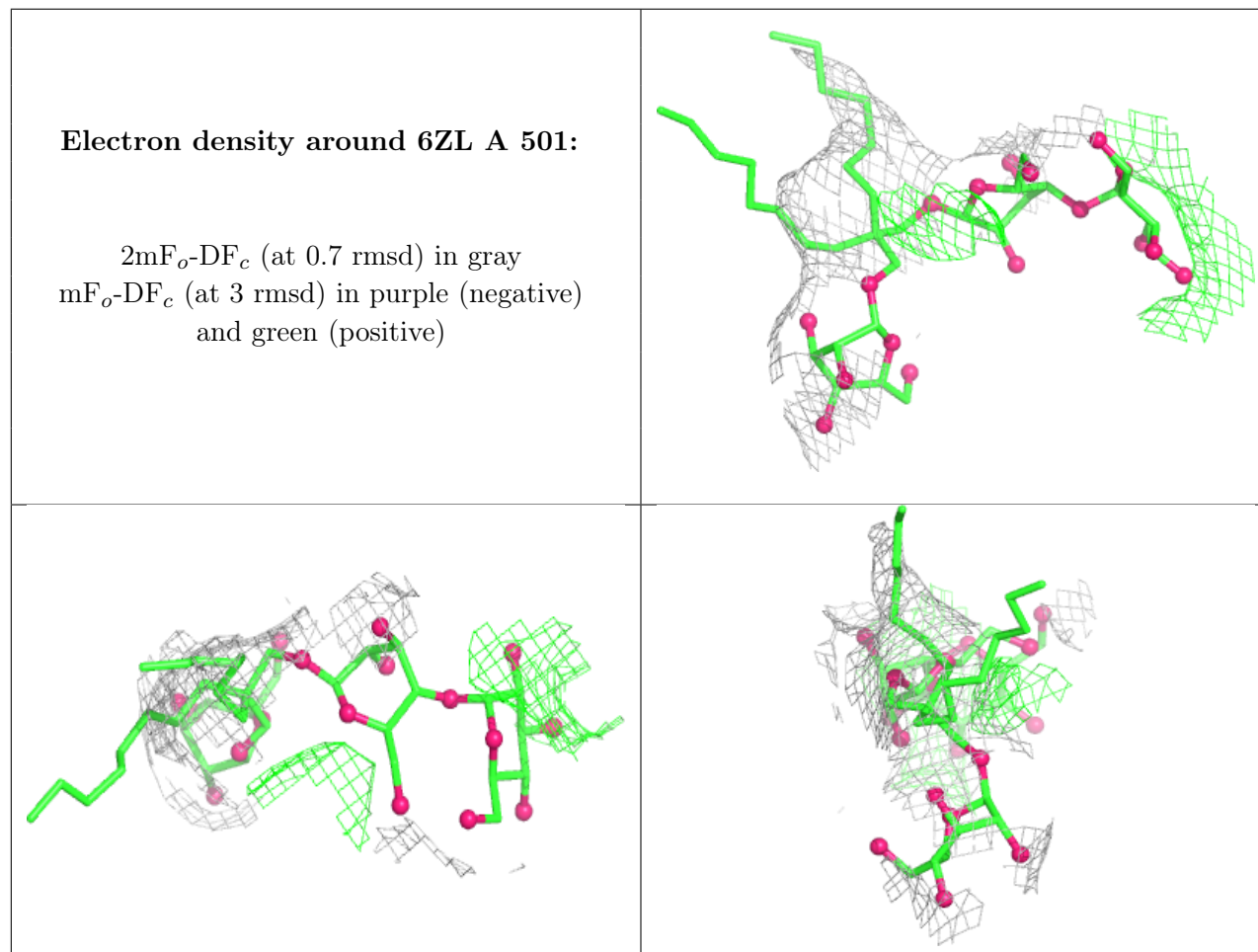
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
2	6ZL	A	501	53/65	0.84	0.15	35,94,120,130	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 ⓘ

There are no such residues in this entry.