



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 12:02 AM UTC

PDB ID : 5L24 / pdb_00005L24
Title : Structure of CNTnw N149L in the intermediate 2 state
Authors : Hirschi, M.; Johnson, Z.L.; Lee, S.-Y.
Deposited on : 2016-07-31
Resolution : 4.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 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

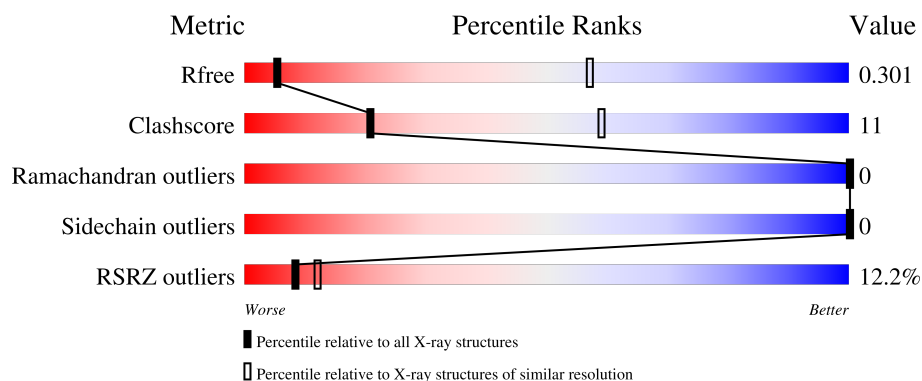
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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	10% 75% 22% .
1	B	431	11% 69% 26% 5%
1	C	431	14% 70% 22% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8741 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.

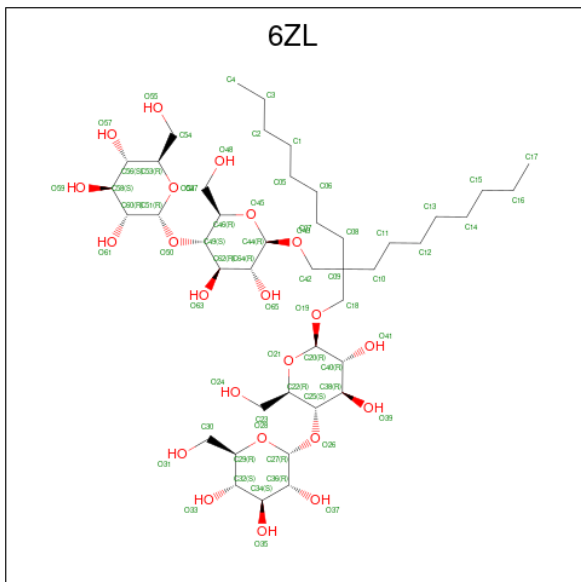
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3005	1972	485	533	15			
1	C	399	Total	C	N	O	S	0	0	0
			2745	1799	441	490	15			
1	B	408	Total	C	N	O	S	0	0	0
			2905	1908	468	515	14			

There are 21 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	LEU	ASN	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	LEU	ASN	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	LEU	ASN	engineered mutation	UNP G4CRQ5

- Molecule 2 is 2-[[[(4-O-alpha-D-glucopyranosyl)-beta-D-glucopyranosyl)oxy]methyl]-2-o

ctyldecyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (CCD ID: 6ZL) (formula: C₄₃H₈₀O₂₂).

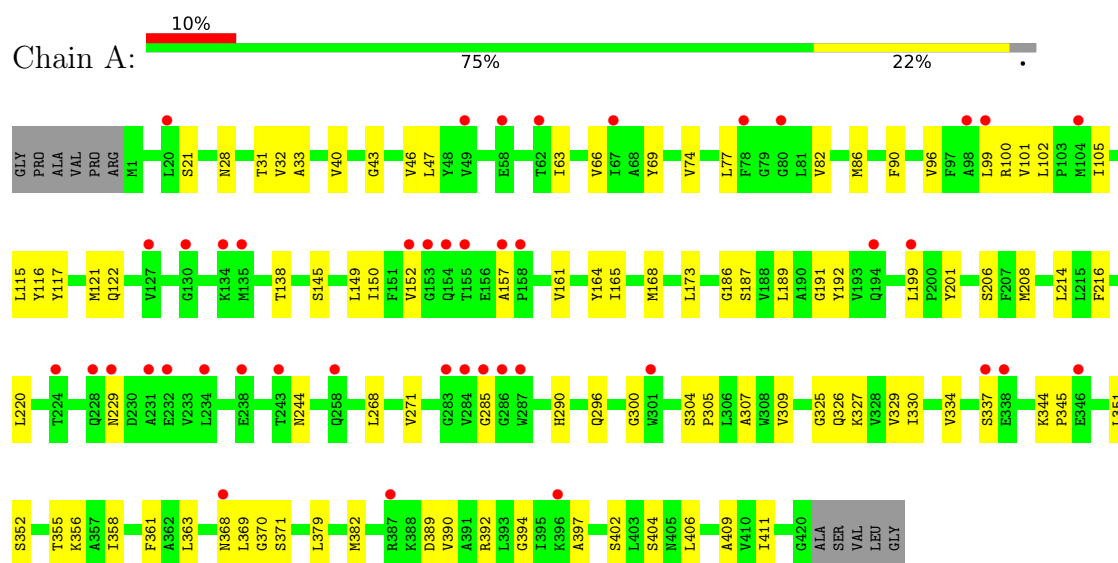


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 51	C 29	O 22	0	0
2	B	1	Total 35	C 24	O 11	0	0

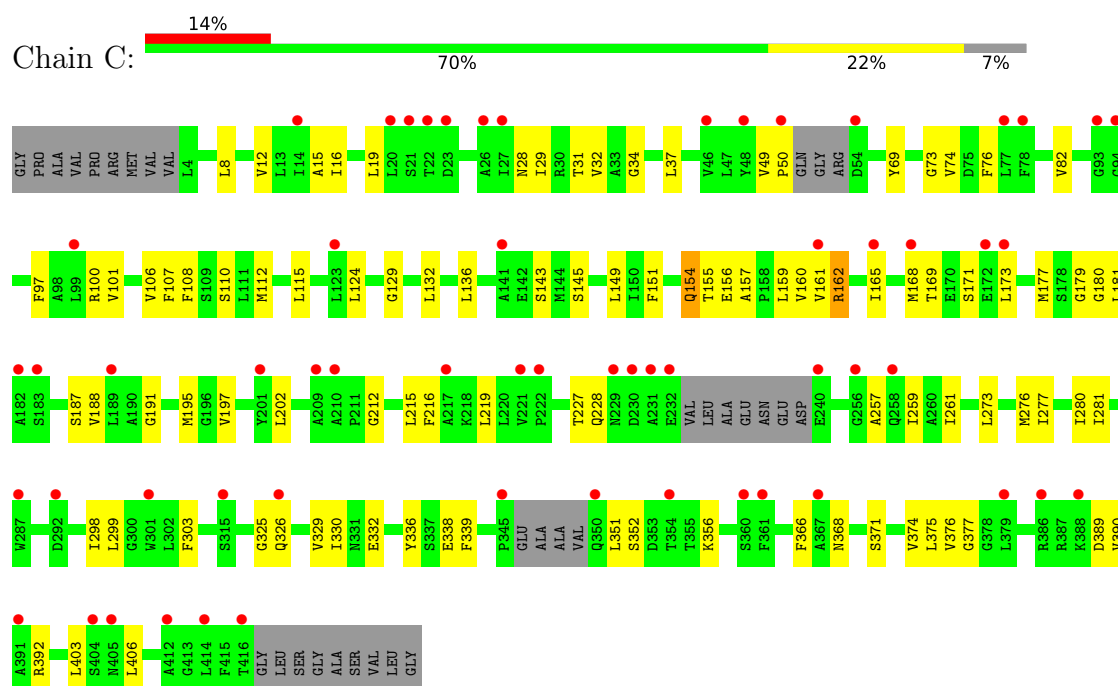
3 Residue-property plots [i](#)

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: Nucleoside permease

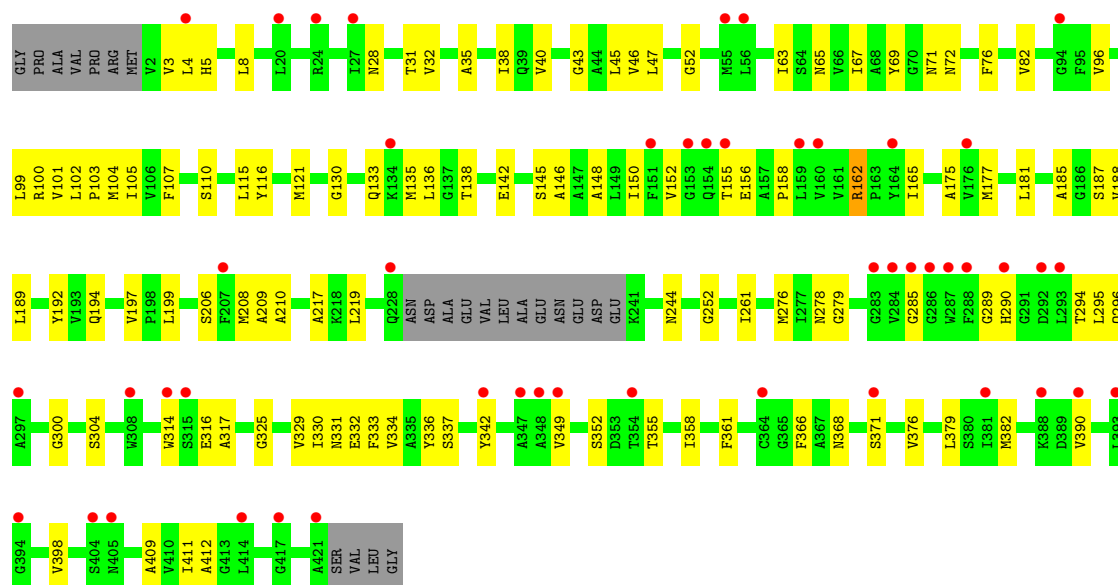


• Molecule 1: Nucleoside permease



● Molecule 1: Nucleoside permease

Chain B:  11% 69% 26% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	116.16Å 116.16Å 274.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.64 – 4.10 36.64 – 4.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (36.64-4.10) 98.6 (36.64-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 4.13Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.271 , 0.298 0.280 , 0.301	Depositor DCC
R_{free} test set	1141 reflections (6.94%)	wwPDB-VP
Wilson B-factor (Å ²)	82.2	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.069 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	8741	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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	0.71	0/3058	0.87	3/4159 (0.1%)
1	B	0.67	0/2955	0.86	3/4019 (0.1%)
1	C	0.62	0/2788	0.89	3/3798 (0.1%)
All	All	0.67	0/8801	0.87	9/11976 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	162	ARG	CA-C-N	-6.76	111.48	118.85
1	C	162	ARG	C-N-CA	-6.76	111.48	118.85
1	B	162	ARG	CA-C-N	-6.68	112.82	119.56
1	B	162	ARG	C-N-CA	-6.68	112.82	119.56
1	C	154	GLN	N-CA-C	5.69	117.56	111.36
1	A	229	ASN	CB-CA-C	-5.67	110.06	116.63
1	B	101	VAL	N-CA-C	5.65	115.78	110.30
1	A	157	ALA	CA-C-N	5.32	124.50	118.97
1	A	157	ALA	C-N-CA	5.32	124.50	118.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3005	0	3105	58	0
1	B	2905	0	3007	77	0
1	C	2745	0	2738	66	0
2	B	86	0	0	1	0
All	All	8741	0	8850	195	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 11.

All (195) 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:358:ILE:HG23	1:B:409:ALA:HB1	1.74	0.69
1:B:82:VAL:O	1:B:100:ARG:NH2	2.24	0.69
1:C:106:VAL:HG22	1:C:257:ALA:HA	1.74	0.68
1:C:368:ASN:OD1	1:C:371:SER:N	2.25	0.67
1:A:327:LYS:HD3	1:A:363:LEU:HA	1.77	0.67
1:B:278:ASN:OD1	1:B:295:LEU:N	2.26	0.66
1:B:63:ILE:HD11	1:B:199:LEU:HD11	1.78	0.66
1:C:160:VAL:HG23	1:C:161:VAL:HG13	1.78	0.65
1:A:43:GLY:HA2	1:A:208:MET:HE2	1.78	0.65
1:A:82:VAL:O	1:A:100:ARG:NH2	2.29	0.65
1:B:329:VAL:HG23	1:B:330:ILE:HG12	1.78	0.65
1:B:105:ILE:HG23	1:B:187:SER:HB2	1.80	0.64
1:B:71:ASN:HD21	1:B:194:GLN:NE2	1.96	0.64
1:A:105:ILE:HG23	1:A:187:SER:HB2	1.79	0.63
1:C:112:MET:HE2	1:C:156:GLU:HB3	1.81	0.63
1:C:403:LEU:HD23	1:C:406:LEU:HD12	1.80	0.62
1:B:138:THR:OG1	1:B:142:GLU:OE2	2.16	0.62
1:A:86:MET:O	1:A:90:PHE:N	2.32	0.62
1:B:32:VAL:HG11	1:B:219:LEU:HD21	1.81	0.61
1:B:35:ALA:HB2	1:B:136:LEU:HD21	1.83	0.61
1:B:285:GLY:O	1:B:289:GLY:N	2.33	0.61
1:A:173:LEU:HD21	1:A:390:VAL:HG22	1.83	0.59
1:C:159:LEU:O	1:C:162:ARG:NH2	2.37	0.58
1:B:368:ASN:OD1	1:B:371:SER:N	2.28	0.58
1:B:285:GLY:O	1:B:290:HIS:N	2.27	0.58
1:B:107:PHE:O	1:B:110:SER:OG	2.17	0.58
1:A:63:ILE:HD11	1:A:199:LEU:HD11	1.86	0.57
1:A:138:THR:HG21	1:A:214:LEU:HD13	1.85	0.57
1:C:15:ALA:O	1:C:19:LEU:HG	2.04	0.57
1:B:189:LEU:HA	1:B:192:TYR:CD2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LEU:HD22	1:C:180:GLY:HA2	1.85	0.57
1:C:82:VAL:O	1:C:100:ARG:NH2	2.37	0.57
1:A:201:TYR:HD1	1:A:361:PHE:CE2	2.22	0.57
1:C:366:PHE:CD1	1:C:366:PHE:O	2.57	0.56
1:B:379:LEU:HD12	1:B:382:MET:HE3	1.87	0.56
1:B:96:VAL:HG11	1:B:99:LEU:HD13	1.88	0.56
1:A:329:VAL:HG23	1:A:330:ILE:HG12	1.88	0.56
1:C:154:GLN:O	1:C:375:LEU:HD21	2.06	0.56
1:B:361:PHE:CE2	1:B:412:ALA:HB2	2.41	0.55
1:A:74:VAL:O	1:A:77:LEU:N	2.39	0.55
1:B:185:ALA:H	1:B:366:PHE:HZ	1.54	0.55
1:B:361:PHE:CD2	1:B:412:ALA:HB2	2.41	0.55
1:C:16:ILE:HA	1:C:19:LEU:HD12	1.89	0.55
1:B:46:VAL:HG23	1:B:47:LEU:HG	1.89	0.55
1:B:67:ILE:HG23	1:B:104:MET:HE2	1.88	0.54
1:C:273:LEU:O	1:C:276:MET:HB3	2.08	0.54
1:B:316:GLU:CD	1:B:352:SER:H	2.15	0.54
1:A:334:VAL:O	1:A:337:SER:OG	2.13	0.54
1:C:155:THR:HB	1:C:259:ILE:HG21	1.90	0.54
1:A:369:LEU:O	1:B:244:ASN:ND2	2.22	0.53
1:A:368:ASN:OD1	1:A:371:SER:N	2.34	0.53
1:C:124:LEU:HB3	1:C:151:PHE:HE2	1.73	0.53
1:B:28:ASN:ND2	1:B:31:THR:OG1	2.41	0.53
1:B:316:GLU:OE1	1:B:355:THR:OG1	2.26	0.53
1:C:161:VAL:HG23	1:C:165:ILE:HD11	1.90	0.52
1:A:189:LEU:HA	1:A:192:TYR:CD2	2.45	0.52
1:C:281:ILE:HD13	1:C:298:ILE:HD12	1.91	0.52
1:C:351:LEU:HD11	1:C:356:LYS:HA	1.92	0.51
1:C:129:GLY:HA2	1:C:143:SER:HB3	1.93	0.51
1:A:96:VAL:HB	1:A:99:LEU:HB2	1.92	0.51
1:C:216:PHE:HA	1:C:219:LEU:HD12	1.93	0.51
1:A:296:GLN:OE1	1:A:296:GLN:N	2.38	0.51
1:B:158:PRO:HB3	1:B:382:MET:SD	2.50	0.51
1:C:376:VAL:HG22	1:C:390:VAL:HG12	1.94	0.50
1:C:277:ILE:HA	1:C:280:ILE:HD12	1.92	0.50
1:C:389:ASP:HA	1:C:392:ARG:NH1	2.27	0.50
1:B:142:GLU:O	1:B:145:SER:OG	2.16	0.50
1:B:314:TRP:O	1:B:317:ALA:N	2.43	0.50
1:A:66:VAL:HA	1:A:69:TYR:CD2	2.47	0.49
1:A:150:ILE:HG23	1:A:206:SER:HB3	1.94	0.49
1:C:161:VAL:O	1:C:165:ILE:HG13	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:LEU:HD11	1:B:103:PRO:HB3	1.94	0.49
1:B:96:VAL:HG12	1:B:99:LEU:H	1.77	0.49
1:A:46:VAL:HG23	1:A:47:LEU:HG	1.93	0.49
1:A:389:ASP:HA	1:A:392:ARG:NH1	2.28	0.49
1:C:28:ASN:OD1	1:C:31:THR:N	2.43	0.49
1:A:101:VAL:HG13	1:A:191:GLY:HA2	1.94	0.49
1:C:325:GLY:O	1:C:329:VAL:HG22	2.12	0.49
1:C:332:GLU:CD	1:C:366:PHE:HA	2.38	0.49
1:C:299:LEU:HD22	1:C:303:PHE:HE2	1.78	0.49
1:B:45:LEU:O	1:B:52:GLY:HA3	2.12	0.48
1:A:164:TYR:O	1:A:168:MET:HB2	2.13	0.48
1:C:169:THR:C	1:C:171:SER:H	2.21	0.48
1:C:49:VAL:HB	1:C:50:PRO:HD2	1.96	0.48
1:B:150:ILE:HG23	1:B:206:SER:HB3	1.95	0.48
1:B:376:VAL:HG22	1:B:390:VAL:HG12	1.95	0.48
1:C:132:LEU:O	1:C:136:LEU:HG	2.14	0.47
1:C:352:SER:O	1:C:356:LYS:N	2.43	0.47
1:A:358:ILE:HG23	1:A:409:ALA:HB1	1.94	0.47
1:A:96:VAL:HG11	1:A:99:LEU:HD13	1.96	0.47
1:A:300:GLY:O	1:A:304:SER:OG	2.27	0.47
1:B:294:THR:HB	1:B:296:GLN:OE1	2.15	0.47
1:A:352:SER:HG	1:A:355:THR:HG1	1.60	0.47
1:A:28:ASN:ND2	1:A:31:THR:OG1	2.48	0.47
1:A:161:VAL:HB	1:A:165:ILE:HG13	1.97	0.47
1:C:162:ARG:HA	1:C:165:ILE:HD12	1.97	0.47
1:B:155:THR:O	1:B:158:PRO:HD2	2.15	0.47
1:B:352:SER:HG	1:B:355:THR:HG1	1.62	0.47
1:C:69:TYR:CE2	1:B:276:MET:HA	2.50	0.47
1:B:332:GLU:H	1:B:332:GLU:CD	2.23	0.47
1:A:285:GLY:O	1:A:290:HIS:N	2.47	0.47
1:C:168:MET:O	1:C:169:THR:OG1	2.28	0.46
1:B:43:GLY:HA2	1:B:208:MET:HE2	1.97	0.46
1:C:112:MET:O	1:C:115:LEU:N	2.48	0.46
1:A:116:TYR:O	1:A:122:GLN:NE2	2.49	0.46
1:A:325:GLY:O	1:A:329:VAL:HG22	2.15	0.46
1:B:148:ALA:O	1:B:152:VAL:HG22	2.16	0.46
1:C:73:GLY:O	1:C:76:PHE:HB3	2.16	0.46
1:C:326:GLN:HE22	1:C:338:GLU:CD	2.24	0.46
1:B:300:GLY:O	1:B:304:SER:HB2	2.16	0.46
1:A:368:ASN:OD1	1:A:370:GLY:N	2.49	0.46
1:B:314:TRP:HA	1:B:317:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LEU:O	1:A:105:ILE:HB	2.16	0.45
1:A:116:TYR:HE2	1:A:152:VAL:HG21	1.81	0.45
1:C:374:VAL:O	1:C:377:GLY:N	2.49	0.45
1:B:175:ALA:HA	1:B:217:ALA:HB1	1.98	0.45
1:A:21:SER:OG	1:A:220:LEU:O	2.35	0.45
1:C:261:ILE:HD11	1:B:261:ILE:HD13	1.99	0.45
1:A:351:LEU:O	1:A:356:LYS:HE3	2.17	0.44
1:C:69:TYR:OH	1:B:279:GLY:HA3	2.17	0.44
1:C:74:VAL:HG12	1:C:82:VAL:HG21	1.97	0.44
1:A:117:TYR:OH	1:A:244:ASN:HA	2.18	0.44
1:C:177:MET:O	1:C:181:LEU:HG	2.18	0.44
1:A:394:GLY:O	1:A:397:ALA:HB3	2.16	0.44
1:A:402:SER:O	1:A:406:LEU:HG	2.17	0.44
1:B:146:ALA:HB1	1:B:210:ALA:HB1	1.98	0.44
1:C:108:PHE:HB2	1:C:156:GLU:OE2	2.17	0.44
1:B:181:LEU:HD13	1:B:398:VAL:HA	1.99	0.44
1:A:296:GLN:HG3	1:A:326:GLN:NE2	2.33	0.44
1:A:406:LEU:HA	1:A:406:LEU:HD23	1.78	0.44
1:A:186:GLY:O	1:A:189:LEU:HB3	2.17	0.44
1:A:379:LEU:HD12	1:A:382:MET:HE3	2.00	0.44
1:B:116:TYR:OH	1:B:156:GLU:O	2.26	0.44
1:C:197:VAL:HG13	1:C:202:LEU:HD11	2.00	0.44
1:C:329:VAL:HG23	1:C:330:ILE:H	1.83	0.44
1:B:177:MET:O	1:B:181:LEU:HG	2.18	0.44
1:B:65:ASN:OD1	2:B:502:6ZL:O55	2.35	0.43
1:A:150:ILE:HG12	1:A:206:SER:O	2.18	0.43
1:A:32:VAL:HG23	1:A:33:ALA:N	2.33	0.43
1:A:115:LEU:HB3	1:A:121:MET:HG2	2.00	0.43
1:C:173:LEU:HD21	1:C:390:VAL:HG22	2.01	0.43
1:C:29:ILE:HA	1:C:32:VAL:HG22	2.00	0.43
1:B:102:LEU:HB2	1:B:103:PRO:HD3	2.01	0.43
1:C:197:VAL:HB	1:C:336:TYR:OH	2.18	0.43
1:B:334:VAL:O	1:B:337:SER:OG	2.28	0.43
1:A:96:VAL:HG12	1:A:99:LEU:H	1.84	0.43
1:B:188:VAL:HG21	1:B:366:PHE:HE1	1.84	0.43
1:B:192:TYR:OH	1:B:332:GLU:HG3	2.18	0.43
1:C:149:LEU:HD13	1:C:179:GLY:C	2.43	0.43
1:C:336:TYR:O	1:C:339:PHE:HB3	2.19	0.43
1:B:162:ARG:HA	1:B:165:ILE:HD12	1.99	0.43
1:A:216:PHE:CE2	1:A:404:SER:HA	2.54	0.42
1:C:107:PHE:O	1:C:110:SER:OG	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:LEU:HA	1:C:406:LEU:HD12	2.01	0.42
1:B:332:GLU:HG2	1:B:333:PHE:N	2.34	0.42
1:A:271:VAL:HG21	1:B:76:PHE:CD2	2.54	0.42
1:C:368:ASN:H	1:C:371:SER:HB3	1.85	0.42
1:B:102:LEU:O	1:B:105:ILE:HB	2.19	0.42
1:B:325:GLY:O	1:B:329:VAL:HG22	2.19	0.42
1:A:305:PRO:O	1:A:309:VAL:HG23	2.20	0.42
1:B:40:VAL:HA	1:B:411:ILE:HD13	2.01	0.42
1:B:110:SER:HA	1:B:252:GLY:HA3	2.01	0.42
1:B:342:TYR:CE1	1:B:349:VAL:HG11	2.55	0.42
1:A:82:VAL:HB	1:A:100:ARG:NH1	2.34	0.42
1:B:197:VAL:HG21	1:B:336:TYR:CD1	2.55	0.42
1:A:352:SER:OG	1:A:355:THR:OG1	2.30	0.42
1:C:187:SER:OG	1:C:188:VAL:N	2.53	0.42
1:B:115:LEU:HB3	1:B:121:MET:HG2	2.00	0.42
1:A:40:VAL:HA	1:A:411:ILE:HD13	2.02	0.42
1:B:3:VAL:HG23	1:B:4:LEU:N	2.35	0.41
1:B:155:THR:OG1	1:B:156:GLU:OE1	2.37	0.41
1:C:329:VAL:HG23	1:C:330:ILE:N	2.35	0.41
1:B:38:ILE:HD11	1:B:135:MET:SD	2.61	0.41
1:B:342:TYR:HE1	1:B:349:VAL:HG11	1.85	0.41
1:C:212:GLY:O	1:C:215:LEU:HB3	2.20	0.41
1:A:304:SER:O	1:A:307:ALA:HB3	2.21	0.41
1:C:34:GLY:O	1:C:37:LEU:HB3	2.20	0.41
1:C:145:SER:O	1:C:149:LEU:HG	2.20	0.41
1:C:191:GLY:O	1:C:195:MET:HG2	2.21	0.41
1:C:227:THR:OG1	1:C:228:GLN:N	2.53	0.41
1:B:330:ILE:HG22	1:B:331:ASN:OD1	2.21	0.41
1:C:31:THR:HG23	1:C:136:LEU:HB2	2.03	0.41
1:B:69:TYR:HA	1:B:72:ASN:OD1	2.20	0.41
1:B:130:GLY:HA2	1:B:133:GLN:HG2	2.02	0.41
1:C:8:LEU:O	1:C:12:VAL:HG23	2.20	0.40
1:C:97:PHE:CE1	1:C:101:VAL:HG21	2.56	0.40
1:C:169:THR:O	1:C:171:SER:N	2.54	0.40
1:B:316:GLU:OE2	1:B:352:SER:N	2.54	0.40
1:A:145:SER:O	1:A:149:LEU:HG	2.21	0.40
1:C:157:ALA:O	1:C:160:VAL:HG22	2.21	0.40
1:B:115:LEU:HA	1:B:115:LEU:HD23	1.90	0.40
1:B:206:SER:O	1:B:209:ALA:N	2.54	0.40
1:A:344:LYS:HA	1:A:345:PRO:HD3	1.83	0.40
1:B:5:HIS:O	1:B:8:LEU:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LEU:HD23	1:B:181:LEU:HA	1.88	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	418/431 (97%)	394 (94%)	24 (6%)	0	100	100
1	B	404/431 (94%)	381 (94%)	23 (6%)	0	100	100
1	C	391/431 (91%)	364 (93%)	27 (7%)	0	100	100
All	All	1213/1293 (94%)	1139 (94%)	74 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	297/322 (92%)	297 (100%)	0	100	100
1	B	288/322 (89%)	288 (100%)	0	100	100
1	C	255/322 (79%)	255 (100%)	0	100	100
All	All	840/966 (87%)	840 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	194	GLN
1	A	326	GLN
1	A	405	ASN
1	C	71	ASN
1	C	154	GLN
1	C	326	GLN
1	B	28	ASN
1	B	194	GLN
1	B	405	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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	6ZL	B	501	-	54,54,68	0.63	1 (1%)	76,78,94	1.10	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	6ZL	B	502	-	36,36,68	0.57	0	50,50,94	0.83	1 (2%)

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	B	501	-	-	17/28/108/126	0/4/4/4
2	6ZL	B	502	-	-	12/23/63/126	0/2/2/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	6ZL	O19-C20	2.16	1.43	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	6ZL	C42-O43-C44	3.36	120.99	113.80
2	B	501	6ZL	C20-O21-C22	2.60	118.80	113.72
2	B	501	6ZL	O43-C44-C64	2.44	111.98	108.27
2	B	501	6ZL	O52-C51-C60	-2.34	105.57	110.37
2	B	502	6ZL	C42-O43-C44	2.09	118.63	113.31
2	B	501	6ZL	C47-C46-C49	-2.05	107.62	113.38

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	6ZL	C42-C09-C18-O19
2	B	501	6ZL	C18-C09-C42-O43
2	B	501	6ZL	C09-C18-O19-C20
2	B	501	6ZL	O21-C20-O19-C18
2	B	501	6ZL	O28-C27-O26-C25
2	B	501	6ZL	C49-C46-C47-O48
2	B	501	6ZL	O28-C29-C30-O31
2	B	501	6ZL	C46-C49-O50-C51
2	B	501	6ZL	O45-C46-C47-O48
2	B	502	6ZL	O45-C46-C47-O48

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Mol	Chain	Res	Type	Atoms
2	B	501	6ZL	C32-C29-C30-O31
2	B	502	6ZL	C06-C05-C1-C2
2	B	501	6ZL	C08-C09-C18-O19
2	B	502	6ZL	C05-C1-C2-C3
2	B	502	6ZL	C49-C46-C47-O48
2	B	501	6ZL	C62-C49-O50-C51
2	B	501	6ZL	C64-C44-O43-C42
2	B	501	6ZL	C40-C20-O19-C18
2	B	502	6ZL	C18-C09-C42-O43
2	B	501	6ZL	C56-C53-C54-O55
2	B	501	6ZL	C08-C09-C42-O43
2	B	502	6ZL	C1-C05-C06-C07
2	B	502	6ZL	C10-C09-C42-O43
2	B	502	6ZL	C08-C09-C42-O43
2	B	502	6ZL	C46-C49-O50-C51
2	B	501	6ZL	C07-C08-C09-C42
2	B	502	6ZL	O52-C53-C54-O55
2	B	502	6ZL	C07-C08-C09-C10
2	B	502	6ZL	C62-C49-O50-C51

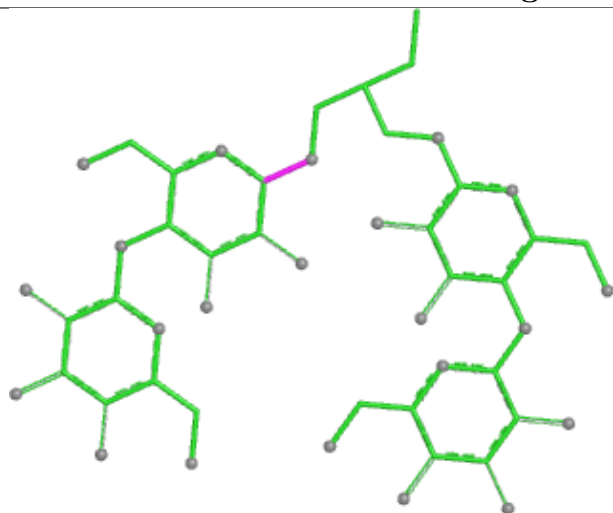
There are no ring outliers.

1 monomer is involved in 1 short contact:

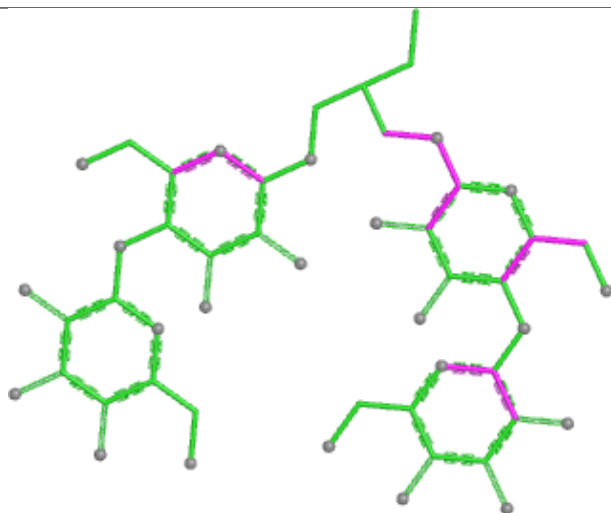
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	6ZL	1	0

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.

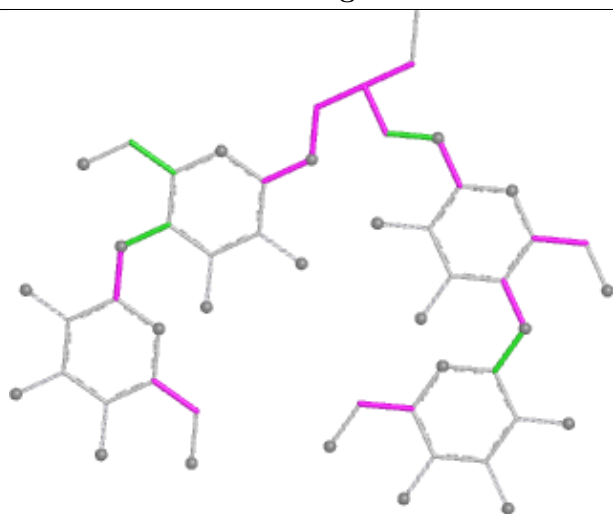
Ligand 6ZL B 501



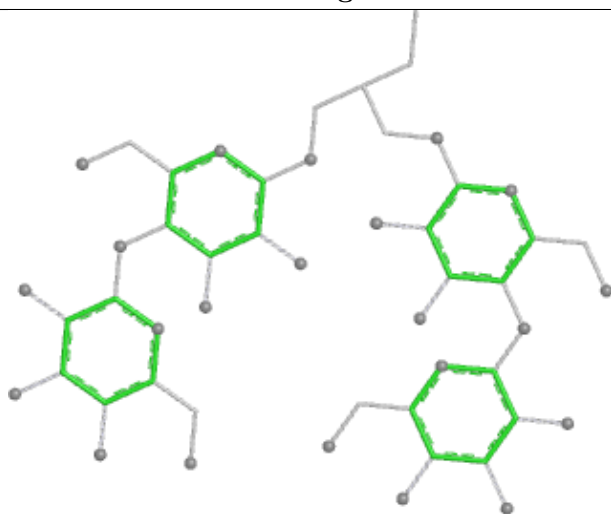
Bond lengths



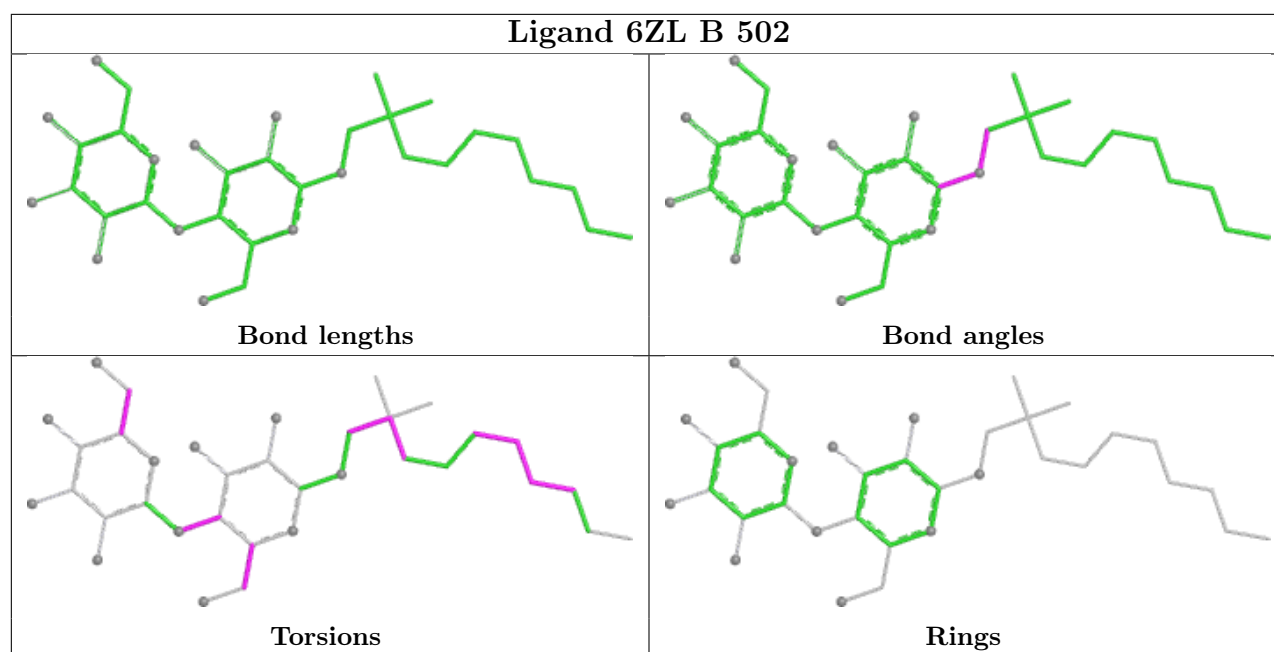
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	420/431 (97%)	0.77	43 (10%)	12 15	30, 59, 95, 113	0
1	B	408/431 (94%)	0.86	48 (11%)	9 12	35, 72, 104, 124	0
1	C	399/431 (92%)	1.07	59 (14%)	5 9	46, 90, 116, 131	0
All	All	1227/1293 (94%)	0.90	150 (12%)	8 12	30, 74, 110, 131	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	173	LEU	5.8
1	B	24	ARG	5.5
1	C	172	GLU	5.5
1	B	293	LEU	4.9
1	C	23	ASP	4.9
1	A	130	GLY	4.7
1	A	287	TRP	4.7
1	C	123	LEU	4.5
1	B	55	MET	4.4
1	B	154	GLN	4.4
1	C	20	LEU	4.2
1	C	412	ALA	4.0
1	B	290	HIS	3.8
1	B	286	GLY	3.7
1	C	21	SER	3.7
1	C	229	ASN	3.7
1	A	134	LYS	3.7
1	C	27	ILE	3.6
1	B	288	PHE	3.6
1	A	135	MET	3.6
1	B	287	TRP	3.6
1	C	360	SER	3.5
1	B	283	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	292	ASP	3.4
1	B	421	ALA	3.4
1	C	50	PRO	3.3
1	C	326	GLN	3.3
1	A	153	GLY	3.3
1	A	104	MET	3.3
1	A	232	GLU	3.3
1	C	350	GLN	3.3
1	A	231	ALA	3.2
1	C	99	LEU	3.2
1	A	152	VAL	3.2
1	B	308	TRP	3.2
1	A	154	GLN	3.2
1	C	405	ASN	3.2
1	A	78	PHE	3.1
1	A	229	ASN	3.1
1	C	232	GLU	3.1
1	B	155	THR	3.1
1	C	221	VAL	3.0
1	B	153	GLY	3.0
1	B	151	PHE	3.0
1	B	349	VAL	3.0
1	A	396	LYS	2.9
1	A	99	LEU	2.9
1	A	283	GLY	2.9
1	C	201	TYR	2.9
1	A	58	GLU	2.9
1	C	345	PRO	2.8
1	A	224	THR	2.8
1	B	390	VAL	2.8
1	C	54	ASP	2.8
1	C	77	LEU	2.8
1	C	161	VAL	2.8
1	B	228	GLN	2.8
1	C	93	GLY	2.7
1	B	284	VAL	2.7
1	B	417	GLY	2.7
1	A	387	ARG	2.7
1	B	56	LEU	2.7
1	B	27	ILE	2.7
1	A	127	VAL	2.7
1	A	234	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	67	ILE	2.6
1	B	371	SER	2.6
1	C	46	VAL	2.6
1	C	168	MET	2.6
1	B	292	ASP	2.6
1	B	134	LYS	2.6
1	C	182	ALA	2.6
1	B	314	TRP	2.6
1	C	240	GLU	2.6
1	A	284	VAL	2.6
1	C	354	THR	2.6
1	A	80	GLY	2.5
1	A	285	GLY	2.5
1	C	22	THR	2.5
1	C	379	LEU	2.5
1	C	287	TRP	2.5
1	B	348	ALA	2.5
1	C	48	TYR	2.5
1	C	361	PHE	2.5
1	C	367	ALA	2.5
1	B	347	ALA	2.5
1	A	62	THR	2.5
1	A	155	THR	2.5
1	C	26	ALA	2.5
1	B	20	LEU	2.4
1	A	258	GLN	2.4
1	B	94	GLY	2.4
1	B	159	LEU	2.4
1	A	368	ASN	2.4
1	A	338	GLU	2.4
1	A	301	TRP	2.4
1	B	354	THR	2.3
1	C	210	ALA	2.3
1	A	194	GLN	2.3
1	A	238	GLU	2.3
1	B	414	LEU	2.3
1	B	207	PHE	2.3
1	C	141	ALA	2.3
1	C	231	ALA	2.3
1	B	393	LEU	2.3
1	C	78	PHE	2.3
1	B	394	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	98	ALA	2.2
1	A	49	VAL	2.2
1	A	337	SER	2.2
1	A	199	LEU	2.2
1	B	315	SER	2.2
1	C	94	GLY	2.2
1	A	243	THR	2.2
1	C	416	THR	2.2
1	A	228	GLN	2.2
1	C	414	LEU	2.2
1	B	342	TYR	2.2
1	C	222	PRO	2.2
1	B	381	ILE	2.2
1	C	258	GLN	2.2
1	C	14	ILE	2.2
1	C	388	LYS	2.2
1	B	388	LYS	2.2
1	B	404	SER	2.2
1	C	217	ALA	2.1
1	B	160	VAL	2.1
1	A	346	GLU	2.1
1	C	189	LEU	2.1
1	C	386	ARG	2.1
1	B	164	TYR	2.1
1	B	285	GLY	2.1
1	A	158	PRO	2.1
1	C	256	GLY	2.1
1	B	4	LEU	2.1
1	B	405	ASN	2.1
1	A	157	ALA	2.1
1	C	165	ILE	2.1
1	B	297	ALA	2.1
1	C	183	SER	2.1
1	C	230	ASP	2.1
1	C	391	ALA	2.1
1	C	301	TRP	2.1
1	A	20	LEU	2.0
1	B	176	VAL	2.0
1	B	364	CYS	2.0
1	C	315	SER	2.0
1	A	286	GLY	2.0
1	C	209	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	404	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](#)

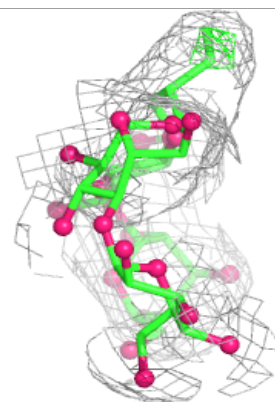
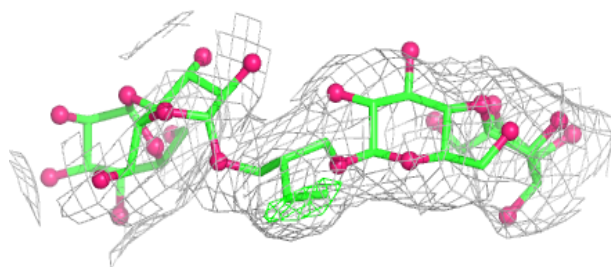
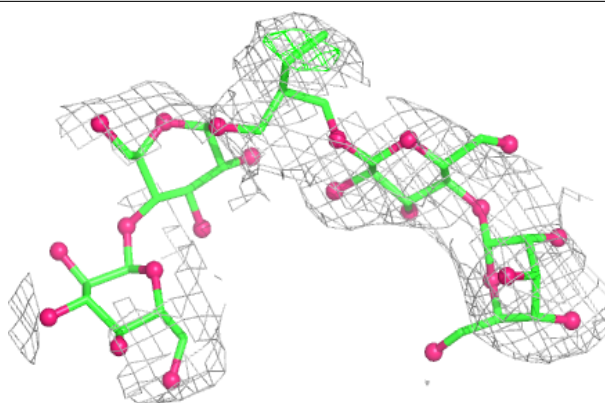
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	6ZL	B	501	51/65	0.70	0.23	72,109,149,152	0
2	6ZL	B	502	35/65	0.83	0.22	64,97,110,112	0

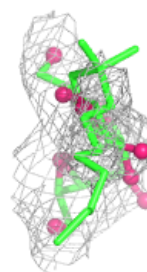
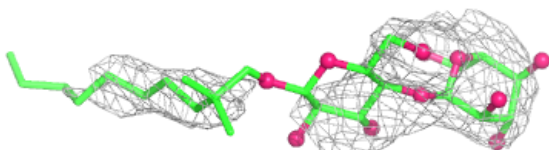
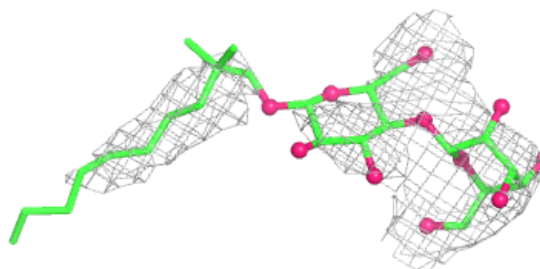
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6ZL 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 6ZL B 502:**

$2mF_o-DF_c$ (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.