



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:58 PM UTC

PDB ID : 6AJF / pdb_00006ajf
Title : Crystal structure of mycolic acid transporter MmpL3 from Mycobacterium smegmatis
Authors : Zhang, B.; Li, J.; Yang, X.L.; Wu, L.J.; Yang, H.T.; Rao, Z.H.
Deposited on : 2018-08-27
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

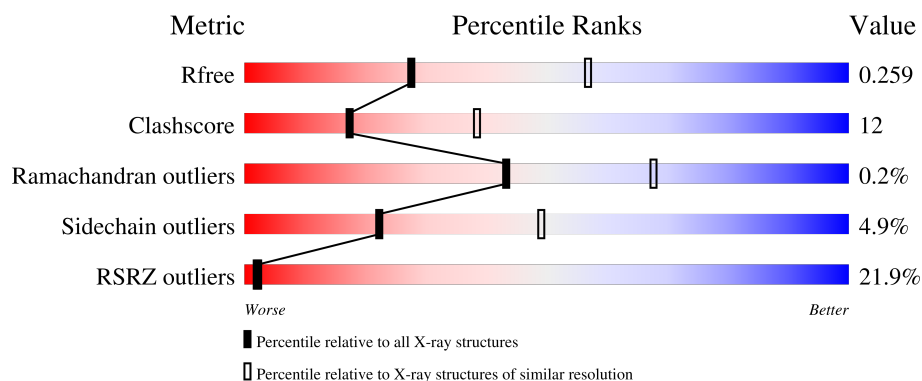
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	943	21% 74% 19% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7121 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 Drug exporters of the RND superfamily-like protein, Endolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	901	Total	C	N	O	S	0	0	0
			6955	4484	1182	1257	32			

There are 37 discrepancies between the modelled and reference sequences:

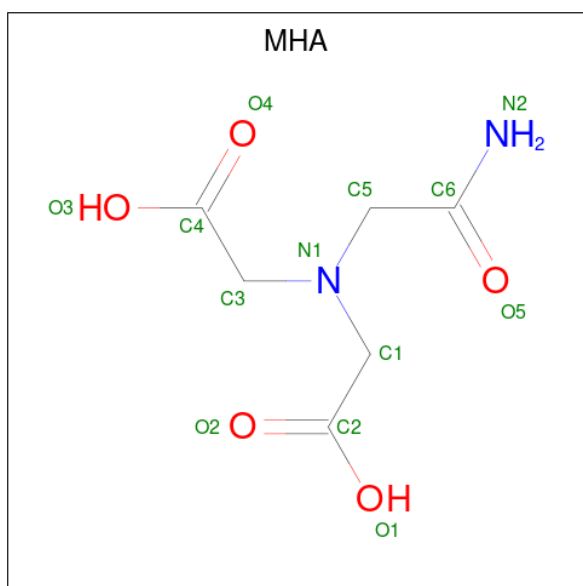
Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	expression tag	UNP I7G2R2
A	-11	PRO	-	expression tag	UNP I7G2R2
A	-10	GLU	-	expression tag	UNP I7G2R2
A	-9	VAL	-	expression tag	UNP I7G2R2
A	-8	VAL	-	expression tag	UNP I7G2R2
A	-7	GLY	-	expression tag	UNP I7G2R2
A	-6	SER	-	expression tag	UNP I7G2R2
A	-5	TYR	-	expression tag	UNP I7G2R2
A	-4	PHE	-	expression tag	UNP I7G2R2
A	-3	GLN	-	expression tag	UNP I7G2R2
A	-2	SER	-	expression tag	UNP I7G2R2
A	-1	ASN	-	expression tag	UNP I7G2R2
A	0	ALA	-	expression tag	UNP I7G2R2
A	749	GLU	-	linker	UNP I7G2R2
A	750	PHE	-	linker	UNP I7G2R2
A	803	THR	CYS	engineered mutation	UNP D9IEF7
A	846	ALA	CYS	engineered mutation	UNP D9IEF7
A	911	GLU	-	expression tag	UNP D9IEF7
A	912	PHE	-	expression tag	UNP D9IEF7
A	913	HIS	-	expression tag	UNP D9IEF7
A	914	LEU	-	expression tag	UNP D9IEF7
A	915	GLY	-	expression tag	UNP D9IEF7
A	916	GLY	-	expression tag	UNP D9IEF7
A	917	ILE	-	expression tag	UNP D9IEF7
A	918	LYS	-	expression tag	UNP D9IEF7
A	919	ALA	-	expression tag	UNP D9IEF7
A	920	PHE	-	expression tag	UNP D9IEF7

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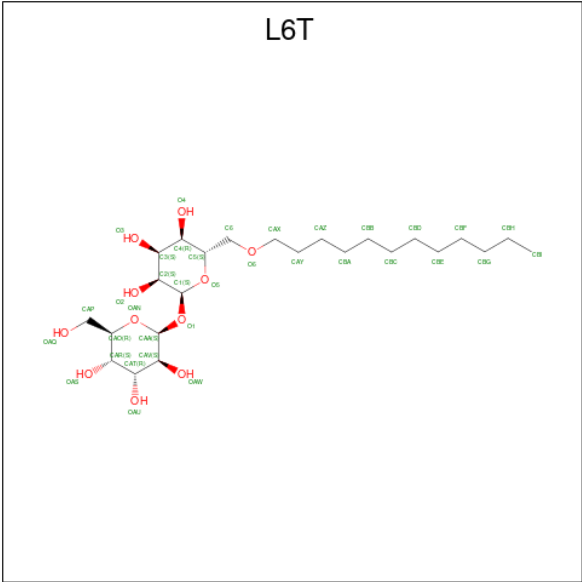
Chain	Residue	Modelled	Actual	Comment	Reference
A	921	HIS	-	expression tag	UNP D9IEF7
A	922	HIS	-	expression tag	UNP D9IEF7
A	923	HIS	-	expression tag	UNP D9IEF7
A	924	HIS	-	expression tag	UNP D9IEF7
A	925	HIS	-	expression tag	UNP D9IEF7
A	926	HIS	-	expression tag	UNP D9IEF7
A	927	HIS	-	expression tag	UNP D9IEF7
A	928	HIS	-	expression tag	UNP D9IEF7
A	929	HIS	-	expression tag	UNP D9IEF7
A	930	HIS	-	expression tag	UNP D9IEF7

- Molecule 2 is (CARBAMOYLMETHYL-CARBOXYMETHYL-AMINO)-ACETIC ACID (CCD ID: MHA) (formula: $C_6H_{10}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	6	2	5		
2	A	1	Total	C	N	O	0	0
			13	6	2	5		

- Molecule 3 is alpha-D-glucopyranosyl 6-O-dodecyl-alpha-D-glucopyranoside (CCD ID: L6T) (formula: $C_{24}H_{46}O_{11}$).

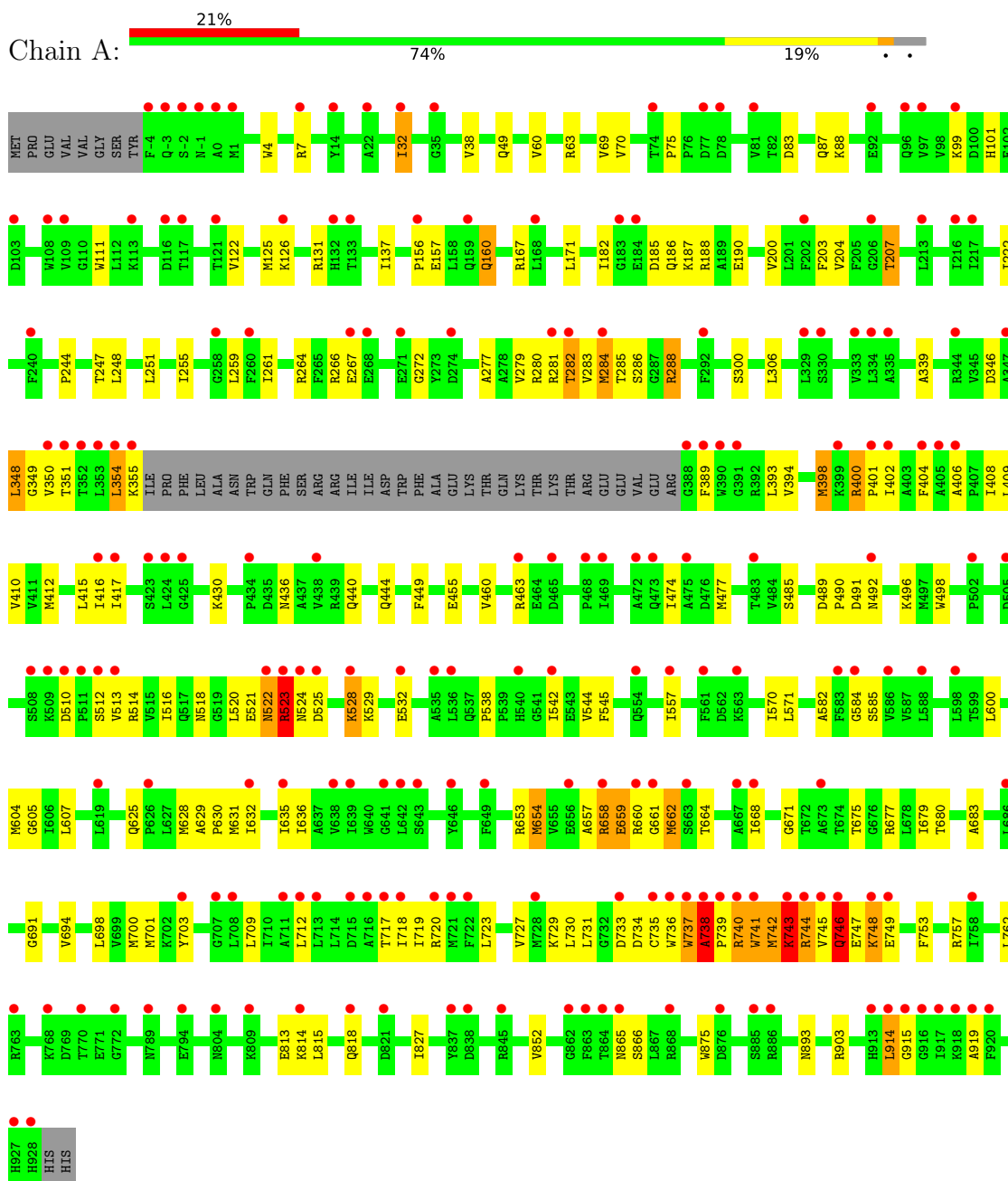


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		

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: Drug exporters of the RND superfamily-like protein, Endolysin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.32Å 138.34Å 139.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.24 – 2.70 41.24 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.24-2.70) 99.8 (41.24-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.223 , 0.249 0.243 , 0.259	Depositor DCC
R_{free} test set	2320 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	76.1	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7121	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: L6T, MHA

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	0.46	1/7099 (0.0%)	0.85	17/9643 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	VAL	C-O	-6.97	1.16	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	524	ASN	N-CA-C	-13.10	99.69	114.62
1	A	915	GLY	N-CA-C	8.17	126.22	111.02
1	A	738	ALA	CA-C-N	7.88	129.69	119.84
1	A	738	ALA	C-N-CA	7.88	129.69	119.84
1	A	417	ILE	CA-C-N	-7.54	112.08	120.45
1	A	417	ILE	C-N-CA	-7.54	112.08	120.45
1	A	523	ARG	N-CA-C	6.80	125.29	110.80
1	A	743	LYS	N-CA-C	-6.49	104.21	111.28
1	A	449	PHE	CA-C-N	6.03	125.64	119.56
1	A	449	PHE	C-N-CA	6.03	125.64	119.56
1	A	282	THR	CB-CA-C	-5.86	101.68	110.88
1	A	398	MET	N-CA-C	5.84	117.65	111.28
1	A	524	ASN	N-CA-CB	5.59	120.01	111.18
1	A	283	VAL	CA-C-O	-5.39	115.45	121.17
1	A	654	MET	N-CA-C	-5.28	105.53	111.28
1	A	746	GLN	N-CA-C	-5.24	103.23	110.35
1	A	485	SER	N-CA-C	5.09	116.68	111.03

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	6955	0	7120	177	0
2	A	26	0	16	4	0
3	A	140	0	0	2	0
All	All	7121	0	7136	178	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 12.

All (178) 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:A:738:ALA:HB3	1:A:739:PRO:CD	1.47	1.36
1:A:738:ALA:CB	1:A:739:PRO:HD3	1.45	1.34
1:A:738:ALA:CB	1:A:739:PRO:CD	2.05	1.28
1:A:659:GLU:OE2	1:A:737:TRP:CH2	1.92	1.23
1:A:738:ALA:HB3	1:A:739:PRO:HD2	1.19	1.15
1:A:738:ALA:HB1	1:A:739:PRO:HD3	1.19	1.13
1:A:740:ARG:HG3	1:A:743:LYS:HB2	1.27	1.09
1:A:659:GLU:OE2	1:A:737:TRP:HH2	1.29	0.99
1:A:740:ARG:HG3	1:A:743:LYS:CB	1.92	0.99
1:A:584:GLY:HA2	1:A:744:ARG:NH1	1.79	0.96
1:A:288:ARG:NH1	1:A:582:ALA:O	1.98	0.95
1:A:584:GLY:HA2	1:A:744:ARG:HH11	1.30	0.92
1:A:740:ARG:HE	1:A:740:ARG:HA	1.37	0.90
1:A:489:ASP:OD1	1:A:492:ASN:HA	1.70	0.90
1:A:261:ILE:HD13	1:A:286:SER:HB3	1.53	0.88
1:A:740:ARG:CG	1:A:743:LYS:HB2	2.05	0.87
1:A:740:ARG:HG3	1:A:743:LYS:CG	2.08	0.84
1:A:919:ALA:HB3	2:A:1001:MHA:HN22	1.42	0.83
1:A:658:ARG:HG2	1:A:658:ARG:HH11	1.46	0.81
1:A:4:TRP:HA	1:A:7:ARG:HE	1.46	0.79
1:A:522:ASN:O	1:A:522:ASN:ND2	2.16	0.79
1:A:272:GLY:HA3	1:A:903:ARG:HG3	1.65	0.79
1:A:740:ARG:HA	1:A:740:ARG:NE	1.96	0.79
1:A:740:ARG:HG3	1:A:743:LYS:HG2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:ASP:HB3	1:A:528:LYS:HD2	1.65	0.76
1:A:277:ALA:O	1:A:281:ARG:HG3	1.86	0.76
1:A:628:MET:HE3	1:A:630:PRO:HG2	1.68	0.76
1:A:741:TRP:CD1	1:A:742:MET:N	2.54	0.75
1:A:49:GLN:HE21	1:A:545:PHE:HA	1.51	0.75
1:A:528:LYS:HD3	1:A:529:LYS:HE2	1.69	0.75
1:A:489:ASP:CG	1:A:492:ASN:HA	2.12	0.74
1:A:741:TRP:HD1	1:A:742:MET:N	1.85	0.73
1:A:474:ILE:HD11	1:A:514:ARG:HD3	1.71	0.72
1:A:63:ARG:NH2	3:A:1003:L6T:OAW	2.23	0.71
1:A:280:ARG:O	1:A:284:MET:HG3	1.91	0.70
1:A:654:MET:HE2	1:A:668:ILE:O	1.92	0.69
1:A:203:PHE:O	1:A:677:ARG:NH2	2.26	0.69
1:A:740:ARG:O	1:A:743:LYS:HB2	1.93	0.69
1:A:733:ASP:HA	1:A:736:TRP:HD1	1.58	0.68
1:A:745:VAL:HG22	1:A:746:GLN:O	1.93	0.68
1:A:248:LEU:HD22	1:A:701:MET:HE1	1.76	0.67
1:A:525:ASP:CG	1:A:528:LYS:NZ	2.53	0.66
1:A:207:THR:HG21	1:A:346:ASP:HA	1.78	0.65
1:A:400:ARG:HG2	1:A:400:ARG:HH11	1.63	0.63
1:A:737:TRP:CD1	1:A:737:TRP:H	2.14	0.62
1:A:400:ARG:HH11	1:A:400:ARG:CG	2.12	0.62
1:A:266:ARG:NH1	1:A:346:ASP:OD2	2.32	0.62
1:A:261:ILE:HD13	1:A:286:SER:CB	2.30	0.61
1:A:866:SER:H	2:A:1002:MHA:HN21	1.48	0.61
1:A:204:VAL:HG11	1:A:259:LEU:HD21	1.82	0.61
1:A:288:ARG:HH12	1:A:582:ALA:C	2.09	0.60
1:A:49:GLN:NE2	1:A:544:VAL:O	2.35	0.60
1:A:455:GLU:OE2	1:A:523:ARG:NE	2.35	0.60
1:A:733:ASP:HA	1:A:736:TRP:CD1	2.37	0.60
1:A:631:MET:HE3	1:A:700:MET:HB3	1.83	0.59
1:A:523:ARG:HG2	1:A:523:ARG:HH21	1.67	0.59
1:A:523:ARG:HG2	1:A:523:ARG:NH2	2.18	0.59
1:A:525:ASP:CG	1:A:528:LYS:HZ3	2.09	0.59
1:A:600:LEU:HD11	1:A:636:ILE:HD13	1.85	0.59
1:A:659:GLU:CD	1:A:737:TRP:HH2	2.08	0.58
1:A:460:VAL:HB	1:A:545:PHE:HB2	1.84	0.58
1:A:398:MET:O	1:A:729:LYS:HD3	2.03	0.58
1:A:914:LEU:HG	1:A:914:LEU:O	2.04	0.58
1:A:658:ARG:NH1	1:A:662:MET:O	2.37	0.58
1:A:744:ARG:HA	1:A:744:ARG:HE	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:HIS:NE2	1:A:157:GLU:OE1	2.37	0.57
1:A:741:TRP:HE1	1:A:742:MET:HE2	1.69	0.57
1:A:737:TRP:CD1	1:A:737:TRP:N	2.73	0.57
1:A:747:GLU:HA	1:A:747:GLU:OE2	2.03	0.57
1:A:740:ARG:O	1:A:743:LYS:CB	2.53	0.56
1:A:658:ARG:HG2	1:A:658:ARG:NH1	2.19	0.56
1:A:698:LEU:HD21	1:A:700:MET:HE2	1.88	0.56
1:A:538:PRO:HB3	1:A:544:VAL:HG23	1.88	0.56
1:A:657:ALA:O	1:A:660:ARG:HB3	2.06	0.55
1:A:893:ASN:N	2:A:1001:MHA:O1	2.39	0.55
1:A:628:MET:HG2	1:A:630:PRO:HD2	1.88	0.55
1:A:741:TRP:CD1	1:A:741:TRP:C	2.85	0.54
1:A:680:THR:HG23	1:A:720:ARG:HH12	1.72	0.54
1:A:354:LEU:C	1:A:355:LYS:HD3	2.33	0.54
1:A:404:PHE:O	1:A:408:ILE:HG12	2.09	0.53
1:A:584:GLY:CA	1:A:744:ARG:NH1	2.64	0.53
1:A:740:ARG:CG	1:A:743:LYS:HG2	2.37	0.53
1:A:349:GLY:O	1:A:350:VAL:C	2.50	0.53
1:A:156:PRO:O	1:A:160:GLN:NE2	2.42	0.53
1:A:875:TRP:HB3	1:A:903:ARG:HA	1.89	0.53
1:A:261:ILE:CD1	1:A:286:SER:HB3	2.35	0.53
1:A:683:ALA:HB1	1:A:712:LEU:HD21	1.91	0.52
1:A:743:LYS:HB3	1:A:744:ARG:HD2	1.91	0.52
1:A:185:ASP:OD1	1:A:188:ARG:NH1	2.42	0.52
1:A:628:MET:HE2	1:A:631:MET:HG2	1.91	0.52
1:A:731:LEU:HB2	1:A:735:CYS:HB3	1.92	0.52
1:A:69:VAL:HB	1:A:137:ILE:HB	1.91	0.52
1:A:182:ILE:HD12	1:A:244:PRO:HG3	1.92	0.52
1:A:727:VAL:O	1:A:731:LEU:HD12	2.10	0.52
1:A:658:ARG:HH11	1:A:658:ARG:CG	2.16	0.52
1:A:658:ARG:NH1	1:A:658:ARG:CG	2.73	0.52
1:A:584:GLY:CA	1:A:744:ARG:HH11	2.13	0.51
1:A:753:PHE:CD1	1:A:813:GLU:HG2	2.45	0.51
1:A:267:GLU:OE1	1:A:653:ARG:NH2	2.43	0.51
1:A:251:LEU:O	1:A:255:ILE:HG12	2.10	0.51
1:A:272:GLY:HA3	1:A:903:ARG:CG	2.36	0.51
1:A:348:LEU:N	1:A:348:LEU:HD13	2.26	0.51
1:A:744:ARG:HE	1:A:744:ARG:CA	2.24	0.51
1:A:75:PRO:O	1:A:131:ARG:NH2	2.43	0.49
1:A:264:ARG:HB3	1:A:282:THR:HG23	1.93	0.49
1:A:744:ARG:N	1:A:744:ARG:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:VAL:HG21	1:A:339:ALA:HB2	1.93	0.49
1:A:436:ASN:O	1:A:440:GLN:HG3	2.13	0.49
1:A:865:ASN:HB2	2:A:1002:MHA:HC51	1.95	0.49
1:A:744:ARG:CA	1:A:744:ARG:NE	2.74	0.49
1:A:827:ILE:HD11	1:A:852:VAL:HG21	1.95	0.49
1:A:306:LEU:HD11	1:A:570:ILE:HD12	1.94	0.48
1:A:389:PHE:O	1:A:393:LEU:N	2.42	0.48
1:A:122:VAL:HG13	1:A:125:MET:HE3	1.94	0.48
1:A:400:ARG:HA	1:A:400:ARG:HD2	1.37	0.48
1:A:525:ASP:CG	1:A:528:LYS:HZ2	2.22	0.48
1:A:741:TRP:HD1	1:A:742:MET:H	1.60	0.47
1:A:186:GLN:O	1:A:190:GLU:HG3	2.14	0.47
1:A:222:ILE:HD11	1:A:251:LEU:HB2	1.94	0.47
1:A:522:ASN:ND2	1:A:522:ASN:C	2.73	0.47
1:A:607:LEU:HB3	1:A:703:TYR:HE1	1.80	0.47
1:A:489:ASP:CG	1:A:492:ASN:CA	2.84	0.47
1:A:747:GLU:HG3	1:A:748:LYS:N	2.30	0.47
1:A:406:ALA:O	1:A:410:VAL:HG23	2.14	0.46
1:A:489:ASP:O	1:A:492:ASN:HB3	2.14	0.46
1:A:490:PRO:O	1:A:491:ASP:HB3	2.14	0.46
1:A:354:LEU:HB3	1:A:355:LYS:NZ	2.30	0.46
1:A:400:ARG:CG	1:A:400:ARG:NH1	2.73	0.46
1:A:394:VAL:O	1:A:398:MET:HG3	2.16	0.45
1:A:557:ILE:HG12	1:A:629:ALA:HB2	1.99	0.45
1:A:585:SER:HA	1:A:737:TRP:HA	1.99	0.45
1:A:658:ARG:O	1:A:661:GLY:N	2.49	0.45
1:A:463:ARG:HG2	1:A:542:ILE:HG22	1.98	0.45
1:A:520:LEU:HD12	1:A:520:LEU:HA	1.56	0.45
1:A:111:TRP:CE2	1:A:126:LYS:HD3	2.52	0.45
1:A:430:LYS:O	1:A:625:GLN:NE2	2.38	0.45
1:A:680:THR:HG22	1:A:720:ARG:HH22	1.82	0.44
1:A:498:TRP:H	1:A:518:ASN:HD22	1.66	0.44
1:A:207:THR:OG1	1:A:348:LEU:O	2.23	0.44
1:A:727:VAL:O	1:A:730:LEU:HB2	2.18	0.44
1:A:510:ASP:OD2	1:A:512:SER:HB3	2.17	0.44
1:A:731:LEU:HD12	1:A:731:LEU:H	1.82	0.44
1:A:753:PHE:O	1:A:757:ARG:N	2.50	0.44
1:A:814:LYS:O	1:A:818:GLN:HG3	2.17	0.44
1:A:489:ASP:OD2	1:A:492:ASN:HB2	2.18	0.44
1:A:523:ARG:HH21	1:A:523:ARG:CG	2.31	0.44
1:A:731:LEU:O	1:A:734:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ARG:NH1	1:A:582:ALA:HA	2.32	0.43
1:A:409:LEU:HD11	1:A:723:LEU:HD11	2.00	0.43
1:A:83:ASP:O	1:A:87:GLN:HG3	2.19	0.43
1:A:167:ARG:HH22	1:A:444:GLN:HG3	1.84	0.43
1:A:412:MET:HE1	1:A:719:ILE:HD11	2.00	0.43
1:A:528:LYS:O	1:A:532:GLU:HG3	2.19	0.43
1:A:632:ILE:HA	1:A:635:ILE:HG22	2.01	0.43
1:A:664:THR:OG1	1:A:733:ASP:OD1	2.30	0.43
1:A:32:ILE:H	1:A:32:ILE:HG13	1.64	0.43
1:A:660:ARG:O	1:A:660:ARG:HG3	2.19	0.43
1:A:717:THR:OG1	1:A:718:ILE:N	2.51	0.43
1:A:743:LYS:HA	1:A:743:LYS:HD3	1.69	0.43
1:A:477:MET:HG3	1:A:516:ILE:HD11	2.01	0.42
1:A:400:ARG:N	1:A:401:PRO:CD	2.82	0.42
1:A:412:MET:O	1:A:416:ILE:HG13	2.18	0.42
1:A:288:ARG:NH1	1:A:582:ALA:C	2.70	0.42
1:A:675:THR:HB	1:A:679:ILE:HG13	2.02	0.42
1:A:691:GLY:O	1:A:694:VAL:HG22	2.20	0.42
1:A:60:VAL:HG21	1:A:513:VAL:HB	2.01	0.42
1:A:222:ILE:HD13	1:A:247:THR:HG22	2.02	0.42
3:A:1006:L6T:CAO	3:A:1006:L6T:C2	2.98	0.42
1:A:400:ARG:N	1:A:401:PRO:HD3	2.35	0.41
1:A:757:ARG:HG3	1:A:762:LEU:HB2	2.03	0.41
1:A:200:VAL:O	1:A:204:VAL:HG23	2.21	0.41
1:A:709:LEU:HD23	1:A:709:LEU:HA	1.94	0.41
1:A:654:MET:HG2	1:A:671:GLY:HA3	2.01	0.41
1:A:743:LYS:CB	1:A:744:ARG:HD2	2.50	0.41
1:A:350:VAL:HG23	1:A:351:THR:HG23	2.04	0.40
1:A:415:LEU:O	1:A:605:GLY:HA3	2.21	0.40
1:A:653:ARG:HB3	1:A:671:GLY:HA2	2.03	0.40
1:A:300:SER:HA	1:A:571:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	897/943 (95%)	858 (96%)	37 (4%)	2 (0%)	43	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	738	ALA
1	A	523	ARG

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	738/777 (95%)	702 (95%)	36 (5%)	22	49

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

Mol	Chain	Res	Type
1	A	32	ILE
1	A	38	VAL
1	A	70	VAL
1	A	88	LYS
1	A	99	LYS
1	A	160	GLN
1	A	171	LEU
1	A	187	LYS
1	A	207	THR
1	A	284	MET
1	A	285	THR
1	A	288	ARG
1	A	348	LEU
1	A	354	LEU
1	A	400	ARG
1	A	402	ILE
1	A	496	LYS

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Mol	Chain	Res	Type
1	A	521	GLU
1	A	522	ASN
1	A	523	ARG
1	A	528	LYS
1	A	604	MET
1	A	658	ARG
1	A	659	GLU
1	A	662	MET
1	A	737	TRP
1	A	740	ARG
1	A	741	TRP
1	A	742	MET
1	A	743	LYS
1	A	744	ARG
1	A	746	GLN
1	A	748	LYS
1	A	749	GLU
1	A	815	LEU
1	A	914	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	96	GLN
1	A	172	ASN
1	A	444	GLN
1	A	522	ASN
1	A	524	ASN
1	A	818	GLN
1	A	927	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	MHA	A	1002	-	12,12,12	1.35	1 (8%)	15,15,15	1.13	0
2	MHA	A	1001	-	12,12,12	1.43	1 (8%)	15,15,15	1.16	1 (6%)
3	L6T	A	1006	-	36,36,36	1.33	5 (13%)	47,47,47	1.22	4 (8%)
3	L6T	A	1005	-	36,36,36	1.37	5 (13%)	47,47,47	1.03	2 (4%)
3	L6T	A	1003	-	36,36,36	1.51	7 (19%)	47,47,47	1.25	8 (17%)
3	L6T	A	1004	-	36,36,36	1.36	6 (16%)	47,47,47	1.47	7 (14%)

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	MHA	A	1002	-	-	5/12/12/12	-
2	MHA	A	1001	-	-	3/12/12/12	-
3	L6T	A	1006	-	-	7/20/60/60	0/2/2/2
3	L6T	A	1005	-	-	8/20/60/60	0/2/2/2
3	L6T	A	1003	-	-	8/20/60/60	0/2/2/2
3	L6T	A	1004	-	-	10/20/60/60	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	L6T	CAP-CAO	-3.79	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1005	L6T	OAN-CAO	3.65	1.53	1.44
3	A	1003	L6T	CAV-CAT	-3.38	1.43	1.52
3	A	1006	L6T	OAN-CAO	3.33	1.52	1.44
3	A	1006	L6T	CAP-CAO	-3.22	1.41	1.51
3	A	1005	L6T	CAP-CAO	-3.20	1.41	1.51
3	A	1004	L6T	CAP-CAO	-3.17	1.41	1.51
3	A	1004	L6T	OAN-CAO	3.07	1.51	1.44
2	A	1001	MHA	C6-N2	2.99	1.42	1.32
3	A	1003	L6T	CAT-CAR	-2.98	1.44	1.52
3	A	1003	L6T	CAA-CAV	-2.86	1.44	1.52
2	A	1002	MHA	C6-N2	2.86	1.42	1.32
3	A	1003	L6T	OAN-CAO	2.83	1.51	1.44
3	A	1003	L6T	C3-C2	-2.71	1.45	1.52
3	A	1004	L6T	C3-C2	-2.48	1.45	1.52
3	A	1005	L6T	CAV-CAT	-2.47	1.45	1.52
3	A	1004	L6T	CAV-CAT	-2.46	1.46	1.52
3	A	1003	L6T	C4-C3	-2.43	1.46	1.52
3	A	1004	L6T	O5-C1	2.41	1.48	1.41
3	A	1005	L6T	CAA-CAV	-2.37	1.45	1.52
3	A	1004	L6T	C4-C3	-2.35	1.46	1.52
3	A	1006	L6T	O5-C1	2.35	1.47	1.41
3	A	1006	L6T	CAV-CAT	-2.25	1.46	1.52
3	A	1005	L6T	O5-C1	2.23	1.47	1.41
3	A	1006	L6T	OAW-CAV	2.04	1.48	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1004	L6T	OAN-CAO-CAR	-4.40	101.77	109.70
3	A	1005	L6T	CAT-CAR-CAO	3.67	116.89	110.23
3	A	1004	L6T	CAA-OAN-CAO	-3.45	106.97	113.72
3	A	1006	L6T	CAV-CAT-CAR	3.34	116.69	110.83
3	A	1006	L6T	CAT-CAR-CAO	3.16	115.96	110.23
3	A	1006	L6T	CAA-O1-C1	-3.15	108.68	114.33
3	A	1006	L6T	CAA-CAV-CAT	2.88	116.08	110.01
3	A	1004	L6T	O5-C1-C2	2.84	116.20	110.37
3	A	1004	L6T	O1-CAA-OAN	-2.75	103.45	110.69
3	A	1003	L6T	CAA-O1-C1	-2.68	109.52	114.33
3	A	1004	L6T	CAA-CAV-CAT	2.63	115.55	110.01
3	A	1004	L6T	OAN-CAA-CAV	2.47	115.45	110.37
3	A	1005	L6T	CAV-CAT-CAR	2.39	115.02	110.83
3	A	1003	L6T	C6-C5-C4	-2.35	107.14	112.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	L6T	OAS-CAR-CAT	-2.31	104.93	110.38
3	A	1003	L6T	CAP-CAO-CAR	-2.30	107.38	113.02
3	A	1004	L6T	CAP-CAO-CAR	-2.17	107.70	113.02
3	A	1003	L6T	O5-C5-C6	2.13	110.93	106.69
3	A	1003	L6T	O3-C3-C2	-2.09	105.46	110.38
3	A	1003	L6T	OAN-CAO-CAR	-2.05	106.01	109.70
2	A	1001	MHA	O3-C4-O4	-2.02	118.14	123.33
3	A	1003	L6T	OAU-CAT-CAR	-2.00	105.65	110.38

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	MHA	N1-C5-C6-O5
2	A	1001	MHA	N1-C5-C6-N2
3	A	1005	L6T	CAV-CAA-O1-C1
3	A	1005	L6T	C4-C5-C6-O6
2	A	1002	MHA	N1-C1-C2-O1
2	A	1002	MHA	N1-C1-C2-O2
2	A	1002	MHA	N1-C3-C4-O3
2	A	1002	MHA	N1-C3-C4-O4
2	A	1002	MHA	C4-C3-N1-C5
3	A	1005	L6T	O5-C1-O1-CAA
3	A	1005	L6T	OAN-CAA-O1-C1
3	A	1006	L6T	O5-C1-O1-CAA
3	A	1003	L6T	CBA-CBB-CBC-CBD
3	A	1003	L6T	O6-CAX-CAY-CAZ
3	A	1004	L6T	C2-C1-O1-CAA
3	A	1005	L6T	C2-C1-O1-CAA
3	A	1006	L6T	C2-C1-O1-CAA
3	A	1004	L6T	O6-CAX-CAY-CAZ
3	A	1004	L6T	CAR-CAO-CAP-OAQ
3	A	1004	L6T	O5-C1-O1-CAA
3	A	1005	L6T	O5-C5-C6-O6
3	A	1003	L6T	CAZ-CBA-CBB-CBC
2	A	1001	MHA	C4-C3-N1-C5
3	A	1003	L6T	CBC-CBD-CBE-CBF
3	A	1004	L6T	CBD-CBE-CBF-CBG
3	A	1004	L6T	OAN-CAO-CAP-OAQ
3	A	1004	L6T	CAY-CAZ-CBA-CBB
3	A	1006	L6T	CBB-CBC-CBD-CBE
3	A	1003	L6T	CBB-CBC-CBD-CBE

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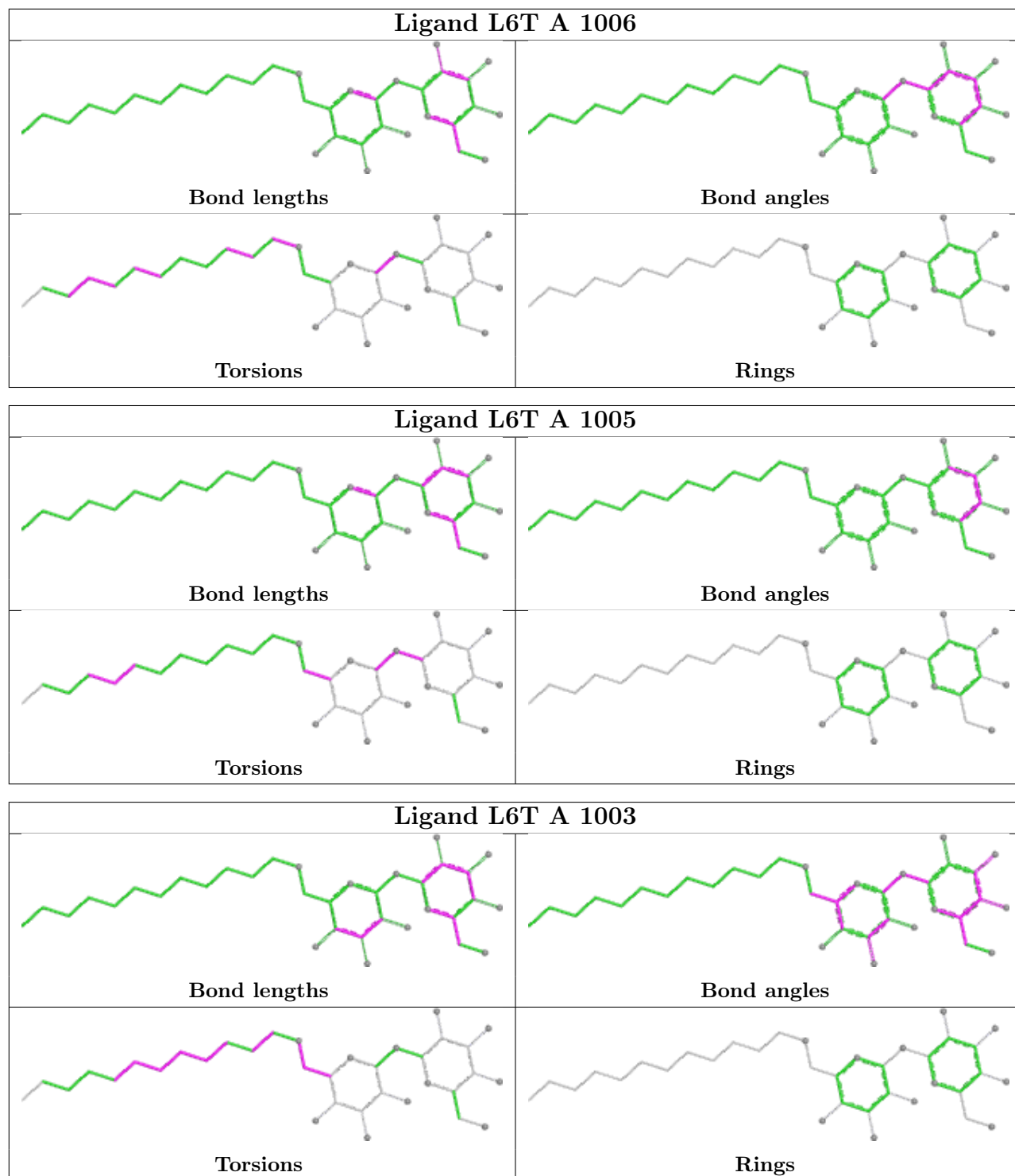
Mol	Chain	Res	Type	Atoms
3	A	1006	L6T	CAY-CAX-O6-C6
3	A	1004	L6T	CBF-CBG-CBH-CBI
3	A	1006	L6T	CAX-CAY-CAZ-CBA
3	A	1003	L6T	CAY-CAZ-CBA-CBB
3	A	1003	L6T	O5-C5-C6-O6
3	A	1006	L6T	CBD-CBE-CBF-CBG
3	A	1004	L6T	C4-C5-C6-O6
3	A	1003	L6T	C5-C6-O6-CAX
3	A	1006	L6T	CBE-CBF-CBG-CBH
3	A	1004	L6T	O5-C5-C6-O6
3	A	1005	L6T	CBD-CBE-CBF-CBG
3	A	1005	L6T	CBC-CBD-CBE-CBF

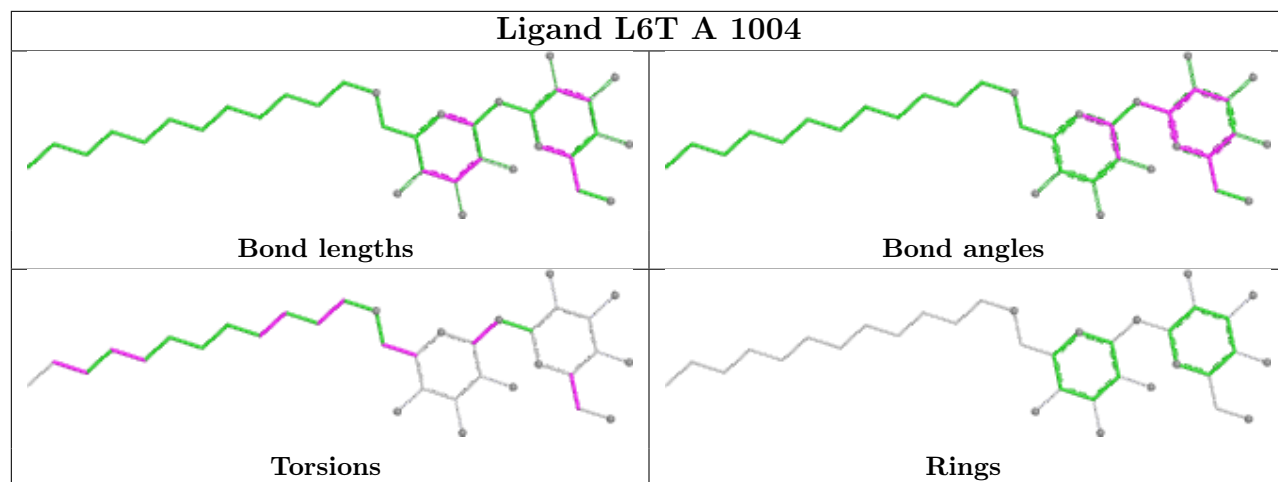
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	MHA	2	0
2	A	1001	MHA	2	0
3	A	1006	L6T	1	0
3	A	1003	L6T	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	901/943 (95%)	1.13	197 (21%) 2 2	51, 82, 140, 202	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	918	LYS	7.3
1	A	-4	PHE	6.7
1	A	-2	SER	6.7
1	A	206	GLY	6.5
1	A	737	TRP	6.1
1	A	78	ASP	6.0
1	A	716	ALA	6.0
1	A	919	ALA	5.9
1	A	424	LEU	5.9
1	A	818	GLN	5.5
1	A	389	PHE	5.3
1	A	509	LYS	5.3
1	A	914	LEU	5.3
1	A	388	GLY	5.2
1	A	525	ASP	5.1
1	A	789	ASN	5.1
1	A	350	VAL	5.0
1	A	738	ALA	5.0
1	A	920	PHE	4.9
1	A	355	LYS	4.8
1	A	472	ALA	4.6
1	A	184	GLU	4.5
1	A	511	PRO	4.4
1	A	281	ARG	4.4
1	A	96	GLN	4.4
1	A	524	ASN	4.4
1	A	399	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	741	TRP	4.2
1	A	717	THR	4.1
1	A	468	PRO	4.1
1	A	183	GLY	4.0
1	A	642	LEU	4.0
1	A	404	PHE	4.0
1	A	703	TYR	4.0
1	A	523	ARG	3.9
1	A	334	LEU	3.9
1	A	510	ASP	3.9
1	A	423	SER	3.9
1	A	390	TRP	3.9
1	A	351	THR	3.9
1	A	401	PRO	3.9
1	A	660	ARG	3.8
1	A	512	SER	3.7
1	A	838	ASP	3.7
1	A	868	ARG	3.7
1	A	646	TYR	3.6
1	A	739	PRO	3.6
1	A	744	ARG	3.6
1	A	865	ASN	3.6
1	A	168	LEU	3.6
1	A	528	LYS	3.6
1	A	1	MET	3.6
1	A	540	HIS	3.5
1	A	641	GLY	3.5
1	A	402	ILE	3.5
1	A	927	HIS	3.5
1	A	406	ALA	3.4
1	A	391	GLY	3.4
1	A	405	ALA	3.4
1	A	722	PHE	3.4
1	A	121	THR	3.4
1	A	639	ILE	3.3
1	A	728	MET	3.3
1	A	821	ASP	3.3
1	A	463	ARG	3.3
1	A	721	MET	3.3
1	A	768	LYS	3.3
1	A	438	VAL	3.3
1	A	656	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	713	LEU	3.3
1	A	632	ILE	3.3
1	A	330	SER	3.2
1	A	635	ILE	3.2
1	A	864	THR	3.2
1	A	733	ASP	3.1
1	A	92	GLU	3.1
1	A	535	ALA	3.1
1	A	353	LEU	3.1
1	A	748	LYS	3.0
1	A	673	ALA	3.0
1	A	505	ASP	3.0
1	A	772	GLY	3.0
1	A	271	GLU	2.9
1	A	7	ARG	2.9
1	A	103	ASP	2.9
1	A	770	THR	2.9
1	A	557	ILE	2.9
1	A	258	GLY	2.9
1	A	347	ALA	2.9
1	A	735	CYS	2.9
1	A	475	ALA	2.9
1	A	354	LEU	2.9
1	A	74	THR	2.9
1	A	626	PRO	2.8
1	A	736	TRP	2.8
1	A	804	ASN	2.8
1	A	417	ILE	2.8
1	A	862	GLY	2.8
1	A	513	VAL	2.8
1	A	267	GLU	2.8
1	A	663	SER	2.8
1	A	814	LYS	2.8
1	A	584	GLY	2.8
1	A	715	ASP	2.8
1	A	913	HIS	2.8
1	A	22	ALA	2.8
1	A	886	ARG	2.7
1	A	35	GLY	2.7
1	A	465	ASP	2.7
1	A	667	ALA	2.7
1	A	916	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	282	THR	2.7
1	A	260	PHE	2.6
1	A	649	PHE	2.6
1	A	863	PHE	2.6
1	A	335	ALA	2.6
1	A	718	ILE	2.6
1	A	845	ARG	2.6
1	A	-3	GLN	2.6
1	A	32	ILE	2.6
1	A	837	TYR	2.6
1	A	425	GLY	2.6
1	A	720	ARG	2.5
1	A	915	GLY	2.5
1	A	81	VAL	2.5
1	A	77	ASP	2.5
1	A	213	LEU	2.5
1	A	598	LEU	2.5
1	A	928	HIS	2.5
1	A	583	PHE	2.5
1	A	876	ASP	2.5
1	A	268	GLU	2.5
1	A	0	ALA	2.5
1	A	643	SER	2.5
1	A	99	LYS	2.4
1	A	794	GLU	2.4
1	A	159	GLN	2.4
1	A	116	ASP	2.4
1	A	156	PRO	2.4
1	A	745	VAL	2.4
1	A	740	ARG	2.4
1	A	483	THR	2.4
1	A	522	ASN	2.4
1	A	707	GLY	2.4
1	A	711	ALA	2.4
1	A	536	LEU	2.4
1	A	109	VAL	2.4
1	A	619	LEU	2.3
1	A	469	ILE	2.3
1	A	352	THR	2.3
1	A	274	ASP	2.3
1	A	108	TRP	2.3
1	A	502	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	492	ASN	2.3
1	A	14	TYR	2.3
1	A	284	MET	2.3
1	A	749	GLU	2.3
1	A	809	LYS	2.3
1	A	885	SER	2.3
1	A	473	GLN	2.3
1	A	333	VAL	2.3
1	A	586	VAL	2.2
1	A	917	ILE	2.2
1	A	133	THR	2.2
1	A	532	GLU	2.2
1	A	746	GLN	2.2
1	A	588	LEU	2.2
1	A	132	HIS	2.2
1	A	542	ILE	2.2
1	A	202	PHE	2.2
1	A	561	PHE	2.2
1	A	708	LEU	2.1
1	A	292	PHE	2.1
1	A	344	ARG	2.1
1	A	113	LYS	2.1
1	A	743	LYS	2.1
1	A	712	LEU	2.1
1	A	97	VAL	2.1
1	A	217	ILE	2.1
1	A	329	LEU	2.1
1	A	668	ILE	2.1
1	A	508	SER	2.1
1	A	117	THR	2.1
1	A	554	GLN	2.1
1	A	686	LEU	2.1
1	A	-1	ASN	2.1
1	A	658	ARG	2.0
1	A	763	ARG	2.0
1	A	126	LYS	2.0
1	A	434	PRO	2.0
1	A	216	ILE	2.0
1	A	758	ILE	2.0
1	A	638	VAL	2.0
1	A	240	PHE	2.0
1	A	563	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	416	ILE	2.0
1	A	661	GLY	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](#)

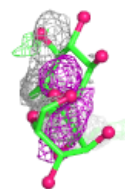
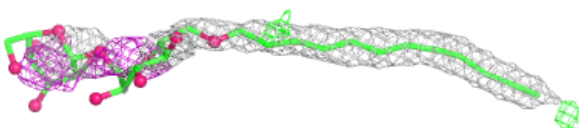
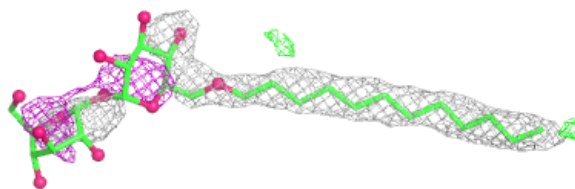
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	L6T	A	1005	35/35	0.72	0.22	53,144,160,163	0
3	L6T	A	1006	35/35	0.75	0.21	66,142,153,155	0
2	MHA	A	1002	13/13	0.77	0.18	126,135,143,144	0
2	MHA	A	1001	13/13	0.81	0.26	99,109,120,127	0
3	L6T	A	1004	35/35	0.83	0.17	78,124,140,145	0
3	L6T	A	1003	35/35	0.95	0.12	49,64,83,84	0

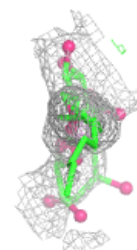
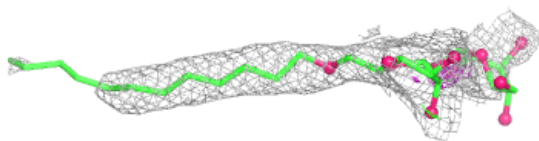
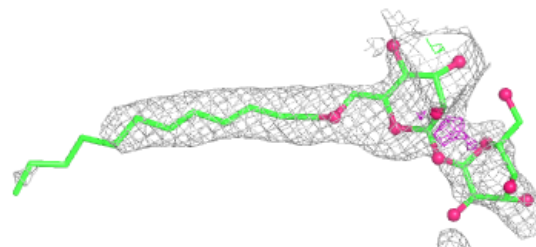
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around L6T A 1005:

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

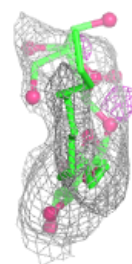
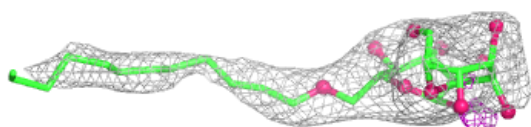
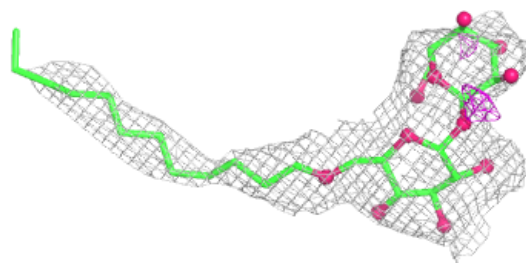
**Electron density around L6T A 1006:**

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

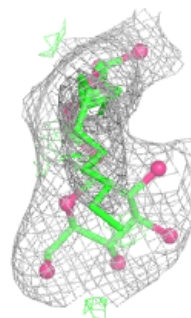
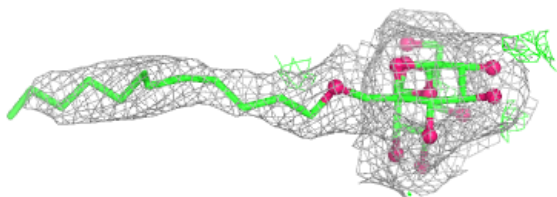
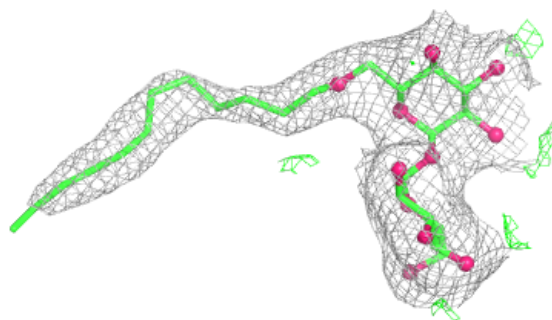


Electron density around L6T A 1004:

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

**Electron density around L6T A 1003:**

$2mF_o-DF_c$ (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.