



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:40 PM UTC

PDB ID : 8QJ3 / pdb_00008qj3
Title : Receptor Sd-Amt1 (OFF-state)
Authors : Andrade, S.L.; Pflueger, T.; Gschell, M.
Deposited on : 2023-09-12
Resolution : 1.90 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

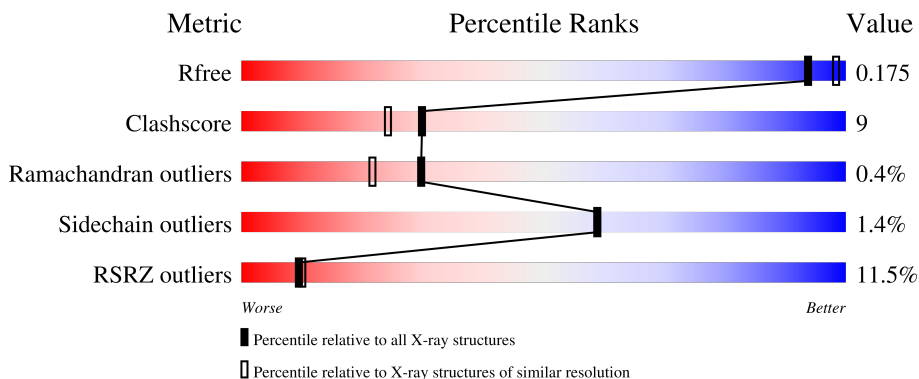
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	644	7% 54% 7% 38%
1	B	644	7% 53% 8% 38%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 6654 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.

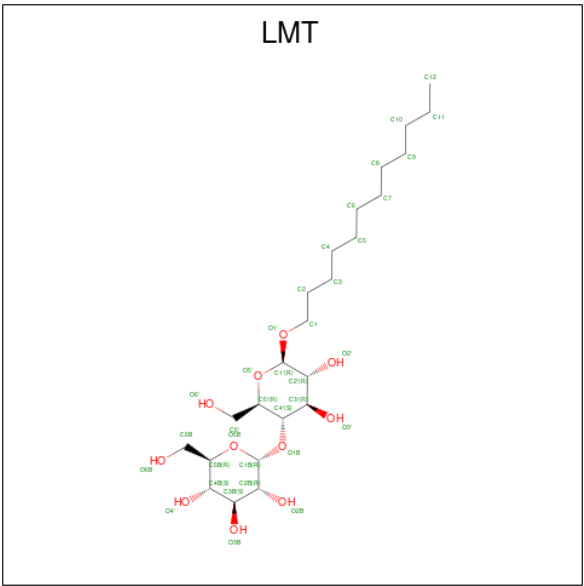
- Molecule 1 is a protein called Ammonium transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	9	0
			3096	2033	499	544	20			
1	B	400	Total	C	N	O	S	0	11	0
			3113	2044	502	546	21			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	189	Total	O	0	0
			189	189		
4	B	184	Total	O	0	0
			184	184		

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	114.76Å 114.76Å 278.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.97 – 1.90 48.97 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.97-1.90) 98.8 (48.97-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.162 , 0.184 0.174 , 0.175	Depositor DCC
R_{free} test set	5507 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.000 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.012 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.000 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.014 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.000 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6654	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7343e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CL, LMT

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	0.77	0/3170	1.14	9/4312 (0.2%)
1	B	0.80	2/3187 (0.1%)	1.15	8/4333 (0.2%)
All	All	0.78	2/6357 (0.0%)	1.14	17/8645 (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	2
1	B	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	ASP	CG-OD2	7.77	1.40	1.25
1	B	114	MET	CB-CG	5.51	1.69	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	289	ASP	CA-CB-CG	9.95	122.55	112.60
1	B	119	TYR	N-CA-CB	8.71	122.64	110.01
1	A	119	TYR	N-CA-CB	6.67	119.89	109.94
1	B	266	PHE	CA-CB-CG	6.62	120.42	113.80
1	A	264	ILE	N-CA-C	-6.57	104.08	110.72
1	B	119	TYR	CB-CA-C	-6.46	100.74	110.88
1	A	202	ASP	CA-C-N	-6.40	113.26	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	ASP	C-N-CA	-6.40	113.26	122.67
1	B	396	ASN	CB-CA-C	-6.26	100.53	110.86
1	B	142	ARG	N-CA-CB	-6.13	103.30	110.35
1	A	266	PHE	CA-CB-CG	5.89	119.69	113.80
1	A	396	ASN	CB-CA-C	-5.76	101.76	110.92
1	A	349	ARG	CG-CD-NE	-5.69	99.48	112.00
1	A	264	ILE	CA-C-N	-5.27	113.22	120.28
1	A	264	ILE	C-N-CA	-5.27	113.22	120.28
1	B	255	CYS	CB-CA-C	-5.25	101.93	110.85
1	B	41	VAL	CG1-CB-CG2	5.19	122.21	110.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ARG	Sidechain
1	A	376	ARG	Sidechain
1	B	115	ARG	Sidechain
1	B	349	ARG	Sidechain

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	3096	0	3104	53	0
1	B	3113	0	3125	54	0
2	A	1	0	0	0	0
2	B	1	0	0	1	0
3	B	70	0	92	2	0
4	A	189	0	0	19	0
4	B	184	0	0	21	0
All	All	6654	0	6321	108	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 9.

All (108) 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:107:SER:HB3	4:B:849:HOH:O	1.45	1.16
1:A:41:VAL:HB	4:A:816:HOH:O	1.49	1.10
1:B:41:VAL:HB	4:B:814:HOH:O	1.55	1.07
1:A:107:SER:HB3	4:A:823:HOH:O	1.51	1.07
1:B:39[B]:VAL:HG13	4:B:967:HOH:O	1.63	0.96
1:A:263[A]:SER:HA	4:A:862:HOH:O	1.66	0.95
1:B:48[B]:ASP:OD1	4:B:802:HOH:O	1.85	0.93
1:B:373[A]:MET:HE2	4:B:985:HOH:O	1.69	0.90
1:A:263[B]:SER:HA	4:A:862:HOH:O	1.71	0.90
1:B:373[A]:MET:CE	4:B:985:HOH:O	2.21	0.88
1:B:401:GLY:O	4:B:804:HOH:O	1.93	0.85
1:B:289:ASP:OD1	4:B:805:HOH:O	1.96	0.84
1:B:30:SER:HB3	4:B:944:HOH:O	1.79	0.82
1:B:44:LYS:NZ	1:B:107:SER:OG	2.13	0.81
1:A:44:LYS:HD2	1:A:119:TYR:CE1	2.16	0.81
1:A:48[A]:ASP:OD1	4:A:801:HOH:O	2.02	0.77
1:A:44:LYS:NZ	1:A:107:SER:OG	2.18	0.76
1:A:255:CYS:SG	4:A:862:HOH:O	2.29	0.73
1:A:200:PHE:CD1	1:A:262:LEU:HD22	2.23	0.72
1:A:115:ARG:HD2	4:A:815:HOH:O	1.88	0.72
3:B:702:LMT:O3B	4:B:803:HOH:O	1.93	0.70
1:A:389:ARG:NH2	4:A:802:HOH:O	2.10	0.69
1:A:71:GLY:O	4:A:803:HOH:O	2.11	0.68
1:B:257:TRP:O	1:B:259:GLN:NE2	2.28	0.66
1:A:30:SER:HB2	4:A:876:HOH:O	1.95	0.65
1:B:43:LEU:CD2	1:B:400:PHE:CE1	2.78	0.65
1:B:400:PHE:CD2	4:B:967:HOH:O	2.48	0.65
1:A:263[B]:SER:CA	4:A:862:HOH:O	2.37	0.65
1:A:200:PHE:HD1	1:A:262:LEU:HD22	1.63	0.64
1:B:71:GLY:O	4:B:807:HOH:O	2.15	0.63
1:A:114:MET:HE3	1:A:119:TYR:N	2.15	0.61
1:B:44:LYS:HZ3	1:B:107:SER:CB	2.14	0.60
1:B:29:GLU:OE1	1:B:44:LYS:NZ	2.34	0.59
1:B:43:LEU:HD22	1:B:400:PHE:CE1	2.37	0.59
1:A:41:VAL:CB	4:A:816:HOH:O	2.27	0.58
1:A:29:GLU:OE2	1:A:44:LYS:HE2	2.03	0.58
1:B:255:CYS:SG	1:B:263[A]:SER:HB2	2.44	0.58
1:A:44:LYS:HZ3	1:A:107:SER:CB	2.17	0.58
1:B:110:VAL:HG11	1:B:179:CYS:HB3	1.86	0.57
1:A:263[B]:SER:CB	4:A:862:HOH:O	2.53	0.57
1:A:263[B]:SER:O	1:A:263[B]:SER:OG	2.23	0.57
1:A:43:LEU:CD2	1:A:400:PHE:CE1	2.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228[B]:LYS:O	1:B:229[B]:ILE:HD13	2.06	0.56
1:B:104[A]:THR:HG23	4:B:809:HOH:O	2.06	0.56
1:A:104[A]:THR:HG23	4:A:807:HOH:O	2.05	0.56
1:B:400:PHE:CG	4:B:967:HOH:O	2.59	0.55
1:A:370:LEU:HB3	1:A:371:PRO:HD3	1.87	0.55
1:B:200:PHE:CD1	1:B:262:LEU:HD12	2.41	0.55
1:A:114:MET:HE3	1:A:118:GLY:C	2.32	0.55
1:A:41:VAL:CG2	4:A:816:HOH:O	2.55	0.54
1:B:43:LEU:HG	1:B:116:PHE:CE1	2.43	0.54
1:B:227:GLY:O	1:B:228[A]:LYS:HB3	2.08	0.52
1:B:4:SER:HB2	1:B:87:HIS:CE1	2.45	0.52
1:A:204:LEU:N	1:A:205:PRO:CD	2.74	0.51
1:A:44:LYS:NZ	1:A:107:SER:CB	2.74	0.51
1:A:341:GLN:HG2	1:A:341:GLN:O	2.11	0.50
1:A:131:TYR:HB3	1:A:132:PRO:HD3	1.92	0.50
1:A:29:GLU:OE1	1:A:44:LYS:NZ	2.45	0.50
1:A:262:LEU:HD23	1:A:265:ARG:HG3	1.94	0.50
1:B:78:PHE:HB2	3:B:702:LMT:H6'2	1.93	0.50
1:B:204:LEU:N	1:B:205:PRO:CD	2.75	0.49
1:A:263[A]:SER:CA	4:A:862:HOH:O	2.41	0.49
1:A:264:ILE:O	1:A:265:ARG:C	2.54	0.49
1:A:44:LYS:HE3	1:A:45:ASN:ND2	2.28	0.48
1:B:228[A]:LYS:C	1:B:229[A]:ILE:HG13	2.39	0.48
1:B:264:ILE:O	1:B:268[A]:LEU:HD13	2.14	0.48
1:A:38:SER:HA	4:A:876:HOH:O	2.13	0.48
1:B:395:LEU:O	1:B:400:PHE:CD2	2.67	0.48
1:A:68:SER:OG	1:A:71:GLY:HA2	2.13	0.47
1:B:160:ILE:CG2	1:B:334:LEU:HD11	2.45	0.47
1:A:43:LEU:HG	1:A:116:PHE:CE1	2.48	0.47
1:B:39[B]:VAL:CG1	4:B:967:HOH:O	2.42	0.47
1:A:81[A]:SER:OG	4:A:804:HOH:O	2.12	0.47
1:B:81[A]:SER:OG	4:B:806:HOH:O	2.06	0.47
1:B:114:MET:HE3	1:B:119:TYR:N	2.30	0.47
1:A:110:VAL:HG11	1:A:179:CYS:HB3	1.96	0.46
1:B:226:TYR:O	1:B:228[A]:LYS:HD3	2.15	0.46
1:A:43:LEU:HD23	1:A:400:PHE:CE1	2.52	0.45
1:A:44:LYS:HD2	1:A:119:TYR:CZ	2.50	0.45
1:B:38:SER:HA	4:B:814:HOH:O	2.16	0.45
1:B:200:PHE:CD1	1:B:262:LEU:CD1	2.99	0.45
1:B:127:ALA:O	4:B:808:HOH:O	2.21	0.44
1:B:395:LEU:O	1:B:399:GLU:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ILE:O	1:A:268[A]:LEU:HD13	2.18	0.44
1:B:44:LYS:NZ	1:B:107:SER:CB	2.79	0.44
1:B:264:ILE:O	1:B:265:ARG:C	2.59	0.44
1:A:52[B]:CYS:SG	1:A:103:ALA:CB	3.06	0.43
1:B:40:ASN:ND2	2:B:703:CL:CL	2.88	0.43
1:B:227:GLY:O	1:B:228[B]:LYS:HB3	2.19	0.43
1:A:2:SER:HB3	1:A:5:PHE:CE1	2.54	0.43
1:A:4:SER:HB2	1:A:87:HIS:CE1	2.54	0.42
1:B:114:MET:HE3	1:B:119:TYR:HA	2.00	0.42
1:B:104[A]:THR:CG2	4:B:809:HOH:O	2.67	0.42
1:B:43:LEU:HD23	1:B:400:PHE:CZ	2.54	0.42
1:A:29:GLU:OE2	1:A:41:VAL:HG22	2.20	0.42
1:A:44:LYS:HE2	4:A:806:HOH:O	2.19	0.42
1:B:278:ILE:C	1:B:278:ILE:HD12	2.44	0.42
1:B:370:LEU:HB3	1:B:371:PRO:HD3	2.02	0.42
1:B:29:GLU:OE2	1:B:41:VAL:HG22	2.20	0.41
1:B:289:ASP:HA	4:B:805:HOH:O	2.20	0.41
1:A:52[A]:CYS:SG	1:A:99:CYS:SG	3.13	0.41
1:A:43:LEU:HD22	1:A:400:PHE:CE1	2.55	0.41
1:A:44:LYS:HZ3	1:A:107:SER:HB2	1.82	0.41
1:B:38:SER:HA	4:B:839:HOH:O	2.20	0.41
1:B:52[A]:CYS:SG	1:B:123:THR:HG23	2.61	0.41
1:A:2:SER:HB3	1:A:5:PHE:CZ	2.56	0.41
1:A:320:VAL:HB	1:A:321:PRO:HD3	2.03	0.41
1:B:320:VAL:HB	1:B:321:PRO:HD3	2.02	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	407/644 (63%)	386 (95%)	19 (5%)	2 (0%)	24 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	409/644 (64%)	393 (96%)	14 (3%)	2 (0%)	24	16
All	All	816/1288 (63%)	779 (96%)	33 (4%)	4 (0%)	30	16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	228	LYS
1	B	228[A]	LYS
1	B	228[B]	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	329/532 (62%)	324 (98%)	5 (2%)	57	56
1	B	331/532 (62%)	326 (98%)	5 (2%)	57	56
All	All	660/1064 (62%)	650 (98%)	10 (2%)	59	56

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LYS
1	A	218	TRP
1	A	228	LYS
1	A	262	LEU
1	A	341	GLN
1	B	73	VAL
1	B	147	GLU
1	B	218	TRP
1	B	228[A]	LYS
1	B	228[B]	LYS

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

Mol	Chain	Res	Type
1	A	32	ASN
1	A	45	ASN
1	B	45	ASN
1	B	222	ASN
1	B	341	GLN
1	B	347	ASN
1	B	352	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	LMT	B	702	-	36,36,36	0.48	0	47,47,47	0.69	0
3	LMT	B	701	-	36,36,36	0.52	0	47,47,47	1.17	4 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '–' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	B	702	-	-	13/21/61/61	0/2/2/2
3	LMT	B	701	-	-	13/21/61/61	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	LMT	C3B-C4B-C5B	4.17	117.78	110.23
3	B	701	LMT	C1'-O5'-C5'	3.64	120.84	113.72
3	B	701	LMT	O5B-C5B-C4B	2.77	114.70	109.70
3	B	701	LMT	C4B-C3B-C2B	2.20	114.69	110.83

There are no chirality outliers.

All (26) torsion outliers are listed below:

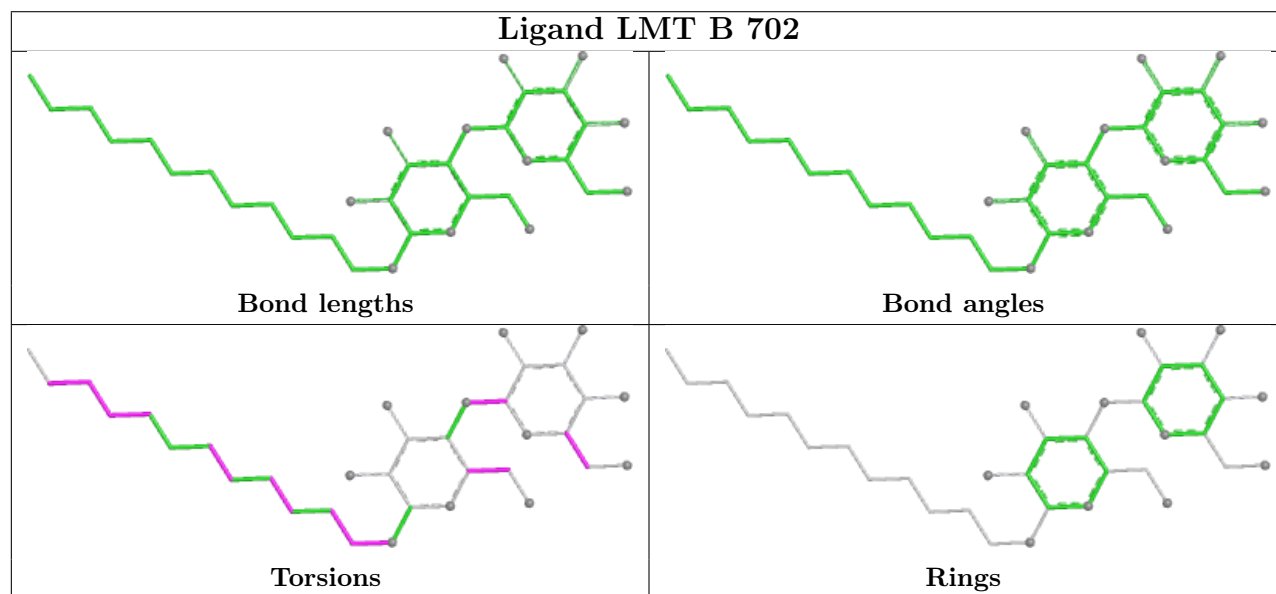
Mol	Chain	Res	Type	Atoms
3	B	701	LMT	C2'-C1'-O1'-C1
3	B	701	LMT	O5'-C1'-O1'-C1
3	B	701	LMT	C4B-C5B-C6B-O6B
3	B	701	LMT	C5'-C4'-O1B-C1B
3	B	701	LMT	O5B-C5B-C6B-O6B
3	B	701	LMT	O1'-C1-C2-C3
3	B	701	LMT	C3'-C4'-O1B-C1B
3	B	701	LMT	C4-C5-C6-C7
3	B	702	LMT	C2-C3-C4-C5
3	B	702	LMT	C4'-C5'-C6'-O6'
3	B	701	LMT	C2-C3-C4-C5
3	B	701	LMT	C6-C7-C8-C9
3	B	702	LMT	C4B-C5B-C6B-O6B
3	B	702	LMT	C11-C10-C9-C8
3	B	702	LMT	C7-C8-C9-C10
3	B	702	LMT	O5'-C5'-C6'-O6'
3	B	701	LMT	C5-C6-C7-C8
3	B	702	LMT	C2-C1-O1'-C1'
3	B	702	LMT	O5B-C5B-C6B-O6B
3	B	702	LMT	C9-C10-C11-C12
3	B	701	LMT	C9-C10-C11-C12
3	B	702	LMT	O1'-C1-C2-C3
3	B	701	LMT	C2-C1-O1'-C1'
3	B	702	LMT	C4-C5-C6-C7
3	B	702	LMT	O5B-C1B-O1B-C4'
3	B	702	LMT	C2B-C1B-O1B-C4'

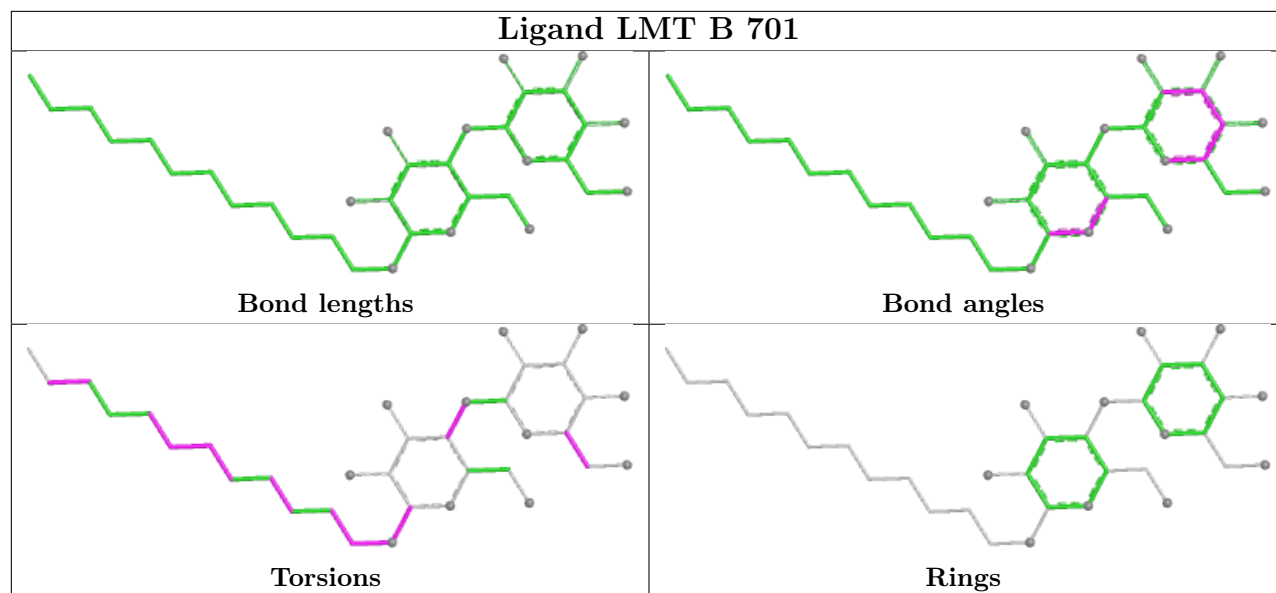
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	LMT	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	400/644 (62%)	0.34	47 (11%)	9 9	6, 22, 56, 98	9 (2%)
1	B	400/644 (62%)	0.25	45 (11%)	10 10	6, 20, 52, 102	11 (2%)
All	All	800/1288 (62%)	0.29	92 (11%)	9 10	6, 21, 55, 102	20 (2%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	TRP	8.2
1	A	262	LEU	8.2
1	B	262	LEU	7.9
1	A	344	ILE	7.2
1	B	257	TRP	6.6
1	A	264	ILE	6.4
1	B	193	LYS	6.3
1	A	69	ILE	6.2
1	A	261	LEU	6.1
1	B	397	PHE	6.1
1	B	69	ILE	5.9
1	A	148	THR	5.4
1	B	264	ILE	5.4
1	B	192	ASN	5.4
1	A	256	ILE	5.0
1	A	259	GLN	4.9
1	A	400	PHE	4.8
1	A	397	PHE	4.7
1	B	400	PHE	4.7
1	B	344	ILE	4.6
1	A	401	GLY	4.6
1	A	346	GLY	4.4
1	A	193	LYS	4.4
1	B	194	HIS	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	147	GLU	4.3
1	B	261	LEU	4.3
1	B	147	GLU	4.3
1	B	258	GLN	4.1
1	B	253	LEU	4.0
1	A	192	ASN	4.0
1	B	70	ASP	3.9
1	B	200	PHE	3.9
1	A	258	GLN	3.9
1	B	256	ILE	3.8
1	B	263[A]	SER	3.7
1	B	380	ARG	3.7
1	B	259	GLN	3.6
1	A	72	ILE	3.6
1	B	401	GLY	3.5
1	B	191	ASN	3.5
1	A	200	PHE	3.5
1	A	194	HIS	3.5
1	A	395	LEU	3.3
1	A	265	ARG	3.1
1	A	156	GLN	3.1
1	B	72	ILE	3.0
1	A	2	SER	2.9
1	B	398	GLY	2.9
1	B	2	SER	2.9
1	A	263[A]	SER	2.8
1	B	255	CYS	2.8
1	A	82	THR	2.7
1	B	195	GLY	2.7
1	A	253	LEU	2.7
1	B	76	ASN	2.7
1	A	377	LEU	2.6
1	B	75	ALA	2.6
1	A	3	GLU	2.6
1	A	73	VAL	2.6
1	A	41	VAL	2.6
1	A	191	ASN	2.5
1	B	265	ARG	2.5
1	B	41	VAL	2.5
1	A	310	LYS	2.5
1	B	228[A]	LYS	2.4
1	B	3	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	73	VAL	2.4
1	A	255	CYS	2.4
1	B	395	LEU	2.4
1	A	143	ILE	2.4
1	A	345	ALA	2.4
1	A	146	SER	2.4
1	B	197	ASN	2.3
1	A	380	ARG	2.3
1	A	119	TYR	2.3
1	A	71	GLY	2.3
1	A	43	LEU	2.2
1	B	231	ASP	2.2
1	A	68	SER	2.2
1	A	341	GLN	2.1
1	B	381	VAL	2.1
1	B	196	VAL	2.1
1	A	228	LYS	2.1
1	A	373	MET	2.1
1	B	341	GLN	2.1
1	A	260	SER	2.1
1	B	376	ARG	2.1
1	B	119	TYR	2.0
1	A	229[A]	ILE	2.0
1	B	106	ILE	2.0
1	B	150	THR	2.0
1	B	346	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](#)

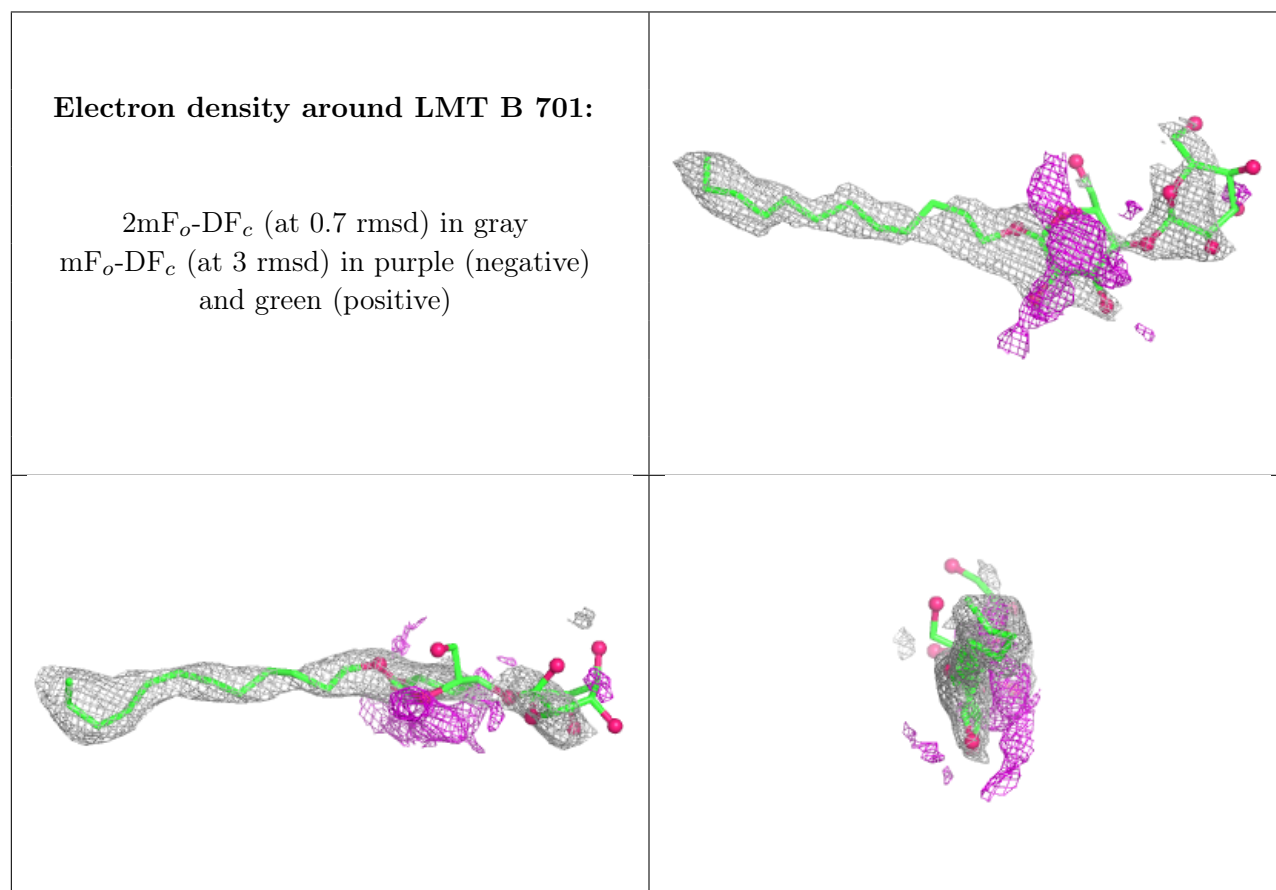
There are no oligosaccharides in this entry.

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.

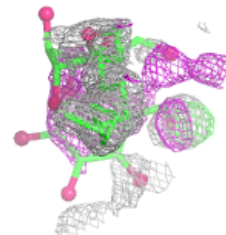
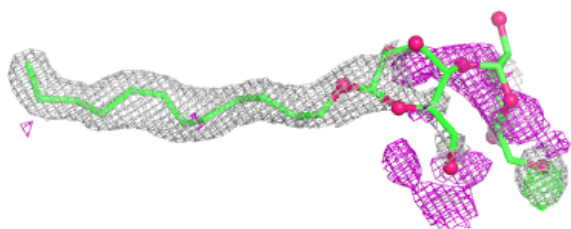
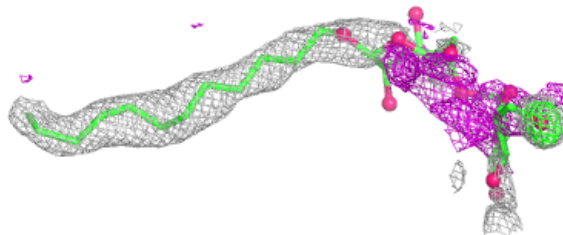
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LMT	B	701	35/35	0.66	0.26	63,79,108,112	0
3	LMT	B	702	35/35	0.69	0.28	50,90,121,131	0
2	CL	A	701	1/1	0.96	0.14	33,33,33,33	0
2	CL	B	703	1/1	0.97	0.11	34,34,34,34	0

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 LMT B 702:

$2mF_o-DF_c$ (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.