



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:39 PM UTC

PDB ID : 3TLV / pdb_00003tlv
Title : The GLIC pentameric Ligand-Gated Ion Channel Loop2-22' oxidized mutant in a locally-closed conformation (LC3 subtype)
Authors : Sauguet, L.; Nury, H.; Corringer, P.J.; Delarue, M.
Deposited on : 2011-08-30
Resolution : 2.90 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

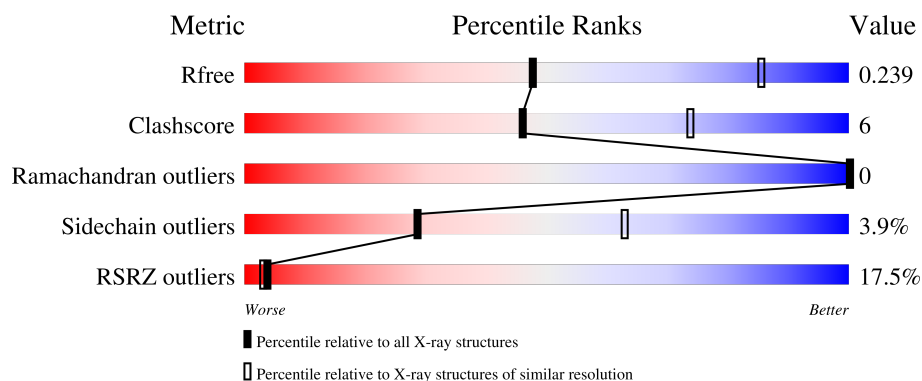
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	321	15% 80% 16% ..
1	B	321	18% 83% 13% ..
1	C	321	12% 80% 15% ..
1	D	321	21% 76% 20% ..
1	E	321	19% 78% 19% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12722 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 Glr4197 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2520	1658	403	454	5			
1	B	311	Total	C	N	O	S	0	0	0
			2520	1658	403	454	5			
1	C	311	Total	C	N	O	S	0	0	0
			2520	1658	403	454	5			
1	D	311	Total	C	N	O	S	0	0	0
			2520	1658	403	454	5			
1	E	311	Total	C	N	O	S	0	0	0
			2520	1658	403	454	5			

There are 40 discrepancies between the modelled and reference sequences:

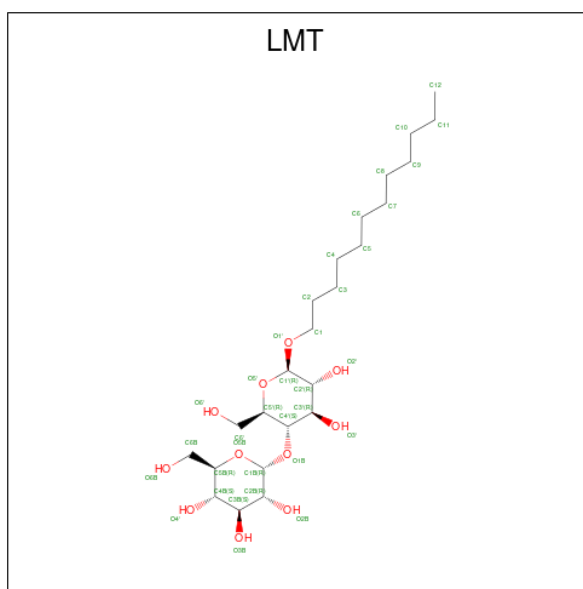
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q7NDN8
A	-2	SER	-	expression tag	UNP Q7NDN8
A	-1	ALA	-	expression tag	UNP Q7NDN8
A	0	ALA	-	expression tag	UNP Q7NDN8
A	1	ALA	-	expression tag	UNP Q7NDN8
A	27	SER	CYS	engineered mutation	UNP Q7NDN8
A	33	CYS	LYS	engineered mutation	UNP Q7NDN8
A	246	CYS	LEU	engineered mutation	UNP Q7NDN8
B	-3	GLY	-	expression tag	UNP Q7NDN8
B	-2	SER	-	expression tag	UNP Q7NDN8
B	-1	ALA	-	expression tag	UNP Q7NDN8
B	0	ALA	-	expression tag	UNP Q7NDN8
B	1	ALA	-	expression tag	UNP Q7NDN8
B	27	SER	CYS	engineered mutation	UNP Q7NDN8
B	33	CYS	LYS	engineered mutation	UNP Q7NDN8
B	246	CYS	LEU	engineered mutation	UNP Q7NDN8
C	-3	GLY	-	expression tag	UNP Q7NDN8
C	-2	SER	-	expression tag	UNP Q7NDN8
C	-1	ALA	-	expression tag	UNP Q7NDN8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ALA	-	expression tag	UNP Q7NDN8
C	1	ALA	-	expression tag	UNP Q7NDN8
C	27	SER	CYS	engineered mutation	UNP Q7NDN8
C	33	CYS	LYS	engineered mutation	UNP Q7NDN8
C	246	CYS	LEU	engineered mutation	UNP Q7NDN8
D	-3	GLY	-	expression tag	UNP Q7NDN8
D	-2	SER	-	expression tag	UNP Q7NDN8
D	-1	ALA	-	expression tag	UNP Q7NDN8
D	0	ALA	-	expression tag	UNP Q7NDN8
D	1	ALA	-	expression tag	UNP Q7NDN8
D	27	SER	CYS	engineered mutation	UNP Q7NDN8
D	33	CYS	LYS	engineered mutation	UNP Q7NDN8
D	246	CYS	LEU	engineered mutation	UNP Q7NDN8
E	-3	GLY	-	expression tag	UNP Q7NDN8
E	-2	SER	-	expression tag	UNP Q7NDN8
E	-1	ALA	-	expression tag	UNP Q7NDN8
E	0	ALA	-	expression tag	UNP Q7NDN8
E	1	ALA	-	expression tag	UNP Q7NDN8
E	27	SER	CYS	engineered mutation	UNP Q7NDN8
E	33	CYS	LYS	engineered mutation	UNP Q7NDN8
E	246	CYS	LEU	engineered mutation	UNP Q7NDN8

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 12 12	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Cl 1	0	0
3	B	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0
3	D	1	Total 1	Cl 1	0	0
3	E	1	Total 1	Cl 1	0	0

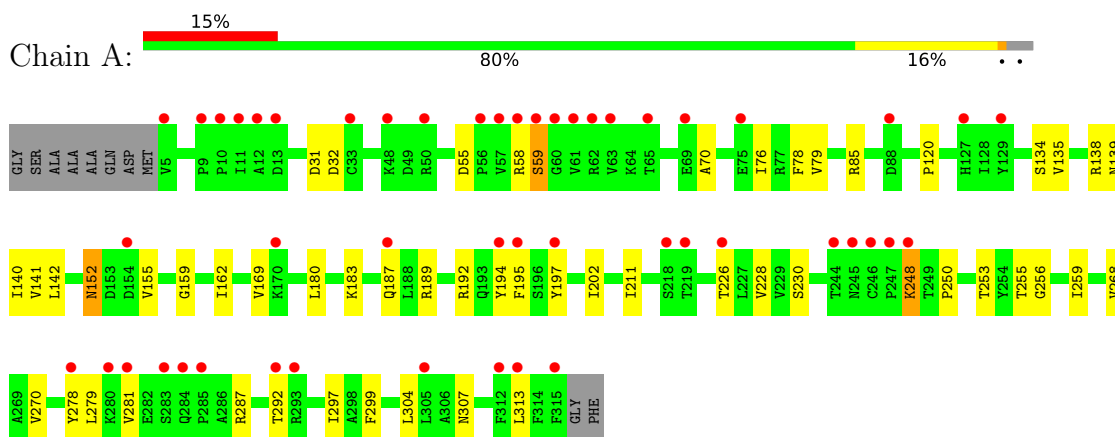
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total 22	O 22	0	0
4	B	26	Total 26	O 26	0	0
4	C	20	Total 20	O 20	0	0
4	D	17	Total 17	O 17	0	0
4	E	20	Total 20	O 20	0	0

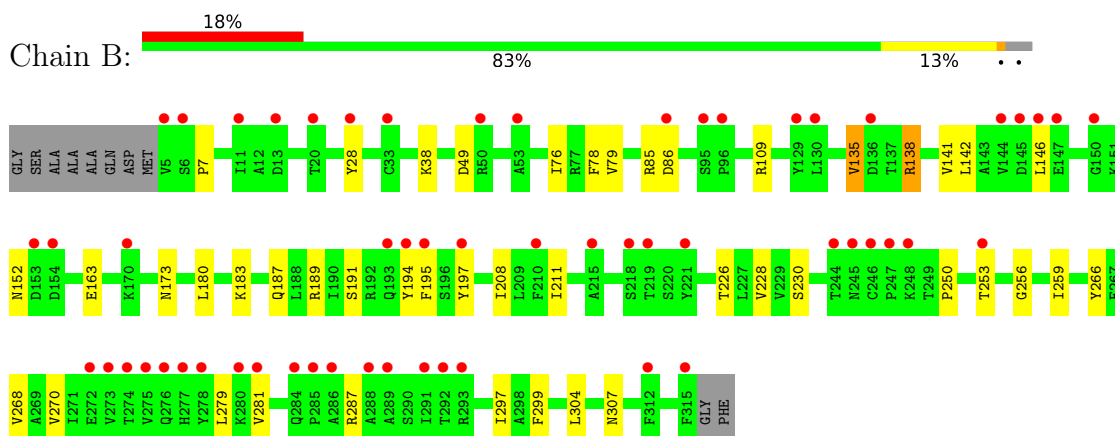
3 Residue-property plots [i](#)

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.

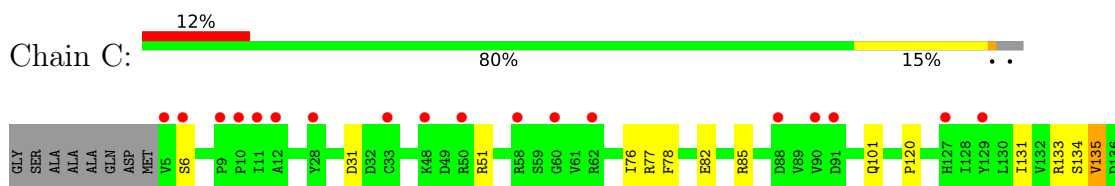
• Molecule 1: Glr4197 protein

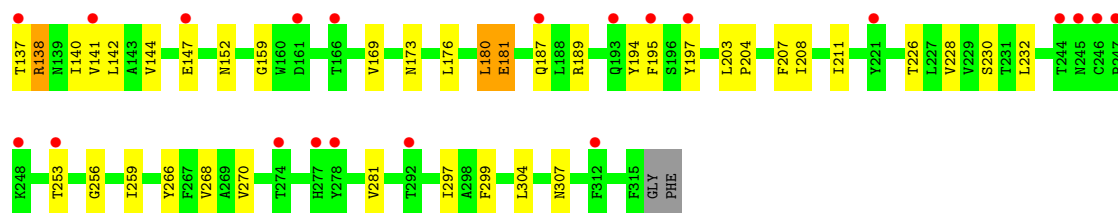


• Molecule 1: Glr4197 protein

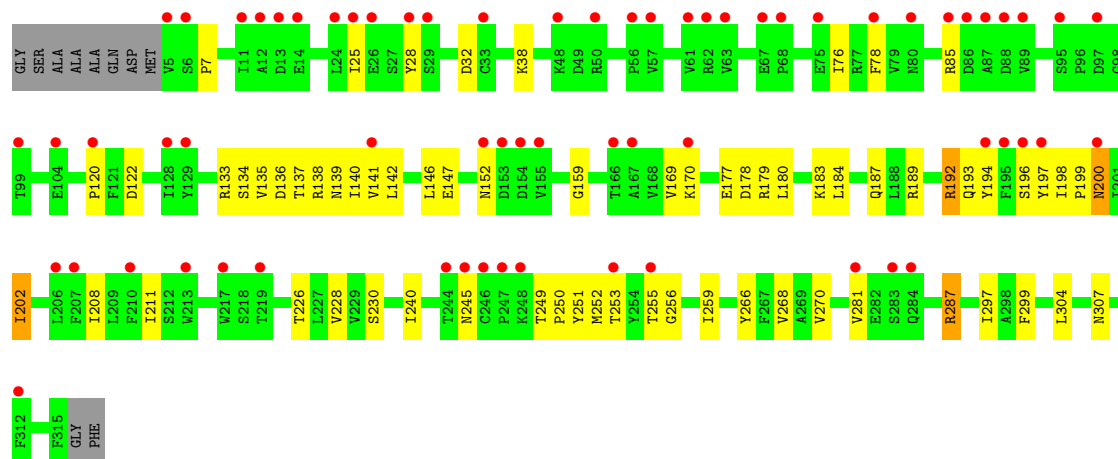
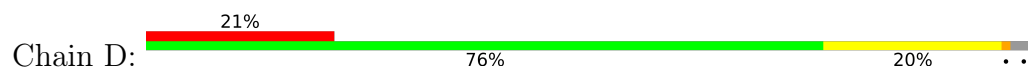


• Molecule 1: Glr4197 protein

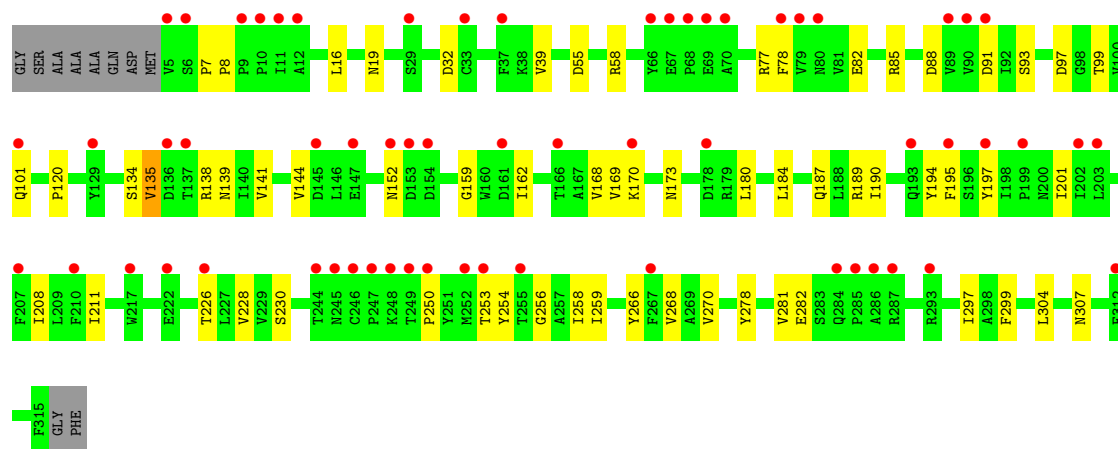
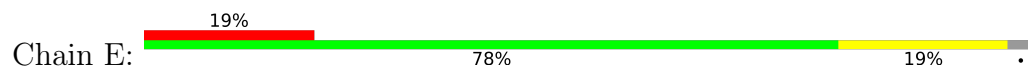




● Molecule 1: Glr4197 protein



● Molecule 1: Glr4197 protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	179.14Å 127.76Å 160.87Å 90.00° 101.55° 90.00°	Depositor
Resolution (Å)	49.23 – 2.90 49.23 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.23-2.90) 99.7 (49.23-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.91Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.1, BUSTER 2.11.1	Depositor
R, R_{free}	0.215 , 0.229 0.223 , 0.239	Depositor DCC
R_{free} test set	3933 reflections (2.79%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12722	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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: LMT, CL

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	0.81	1/2588 (0.0%)	1.26	6/3539 (0.2%)
1	B	0.83	0/2588	1.26	8/3539 (0.2%)
1	C	0.82	0/2588	1.25	5/3539 (0.1%)
1	D	0.82	0/2588	1.22	8/3539 (0.2%)
1	E	0.82	0/2588	1.29	11/3539 (0.3%)
All	All	0.82	1/12940 (0.0%)	1.26	38/17695 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	ILE	CA-CB	5.11	1.58	1.53

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	88	ASP	CA-CB-CG	7.99	120.59	112.60
1	B	195	PHE	N-CA-C	7.87	119.55	110.97
1	A	195	PHE	N-CA-C	7.58	119.23	110.97
1	E	195	PHE	N-CA-C	7.14	118.75	110.97
1	C	152	ASN	CA-CB-CG	6.85	119.45	112.60
1	D	245	ASN	CA-CB-CG	6.81	119.41	112.60
1	E	152	ASN	CA-CB-CG	6.73	119.33	112.60
1	A	152	ASN	CA-CB-CG	6.61	119.21	112.60
1	D	152	ASN	CA-CB-CG	6.59	119.19	112.60
1	D	202	ILE	N-CA-C	6.52	116.62	110.30
1	A	138	ARG	N-CA-C	6.51	119.04	108.76
1	C	169	VAL	N-CA-C	6.40	117.92	110.62
1	B	152	ASN	CA-CB-CG	6.32	118.92	112.60
1	B	86	ASP	CA-CB-CG	6.19	118.79	112.60
1	B	138	ARG	N-CA-C	6.11	118.41	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	ALA	N-CA-C	6.07	117.97	111.36
1	E	135	VAL	CA-C-N	6.06	128.65	120.65
1	E	135	VAL	C-N-CA	6.06	128.65	120.65
1	D	169	VAL	N-CA-C	5.91	117.36	110.62
1	D	138	ARG	N-CA-C	5.85	118.00	108.76
1	A	169	VAL	N-CA-C	5.73	117.15	110.62
1	C	228	VAL	N-CA-C	5.68	115.87	110.42
1	D	200	ASN	N-CA-C	5.68	117.55	111.36
1	A	228	VAL	N-CA-C	5.54	115.74	110.42
1	E	168	VAL	CA-C-N	5.50	128.28	120.53
1	E	168	VAL	C-N-CA	5.50	128.28	120.53
1	C	138	ARG	N-CA-C	5.45	117.37	108.76
1	B	228	VAL	N-CA-C	5.38	115.58	110.42
1	B	135	VAL	CA-C-N	5.29	128.15	120.79
1	B	135	VAL	C-N-CA	5.29	128.15	120.79
1	B	49	ASP	CA-CB-CG	5.26	117.86	112.60
1	E	91	ASP	N-CA-C	5.18	116.95	108.55
1	D	228	VAL	N-CA-C	5.15	115.36	110.42
1	E	82	GLU	CB-CG-CD	5.09	121.25	112.60
1	E	169	VAL	N-CA-C	5.03	116.36	110.62
1	C	82	GLU	CB-CG-CD	5.03	121.15	112.60
1	D	25	ILE	N-CA-C	-5.03	106.77	111.45
1	E	138	ARG	N-CA-C	5.00	116.68	109.07

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	2520	0	2529	33	0
1	B	2520	0	2529	24	0
1	C	2520	0	2529	29	0
1	D	2520	0	2529	46	0
1	E	2520	0	2529	29	0
2	A	12	0	23	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	22	0	0	0	0
4	B	26	0	0	1	0
4	C	20	0	0	3	0
4	D	17	0	0	0	0
4	E	20	0	0	2	0
All	All	12722	0	12668	147	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 6.

All (147) 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:197:TYR:CE2	1:A:202:ILE:HD11	1.75	1.22
1:A:197:TYR:CD2	1:A:202:ILE:HD11	1.78	1.18
1:A:197:TYR:CD2	1:A:202:ILE:CD1	2.42	1.02
1:B:7:PRO:HG3	1:B:135:VAL:HG21	1.47	0.97
1:A:55:ASP:O	1:A:59:SER:OG	1.86	0.93
1:A:197:TYR:CE2	1:A:202:ILE:CD1	2.60	0.83
1:C:253:THR:HG23	1:C:256:GLY:H	1.44	0.82
1:B:253:THR:HG23	1:B:256:GLY:H	1.45	0.81
1:D:253:THR:HG23	1:D:256:GLY:H	1.46	0.80
1:A:253:THR:HG23	1:A:256:GLY:H	1.45	0.79
1:E:253:THR:HG23	1:E:256:GLY:H	1.46	0.79
1:C:211:ILE:HG23	1:D:270:VAL:HG11	1.71	0.72
1:C:208:ILE:HG22	1:C:266:TYR:OH	1.91	0.70
1:C:133:ARG:NH1	1:C:176:LEU:O	2.24	0.70
1:E:278:TYR:CE1	1:E:282:GLU:OE1	2.46	0.69
1:D:193:GLN:CG	1:D:193:GLN:O	2.39	0.69
1:E:55:ASP:OD2	1:E:58:ARG:HG3	1.92	0.68
1:D:197:TYR:CE2	1:D:202:ILE:HD11	2.27	0.68
1:A:197:TYR:CD2	1:A:202:ILE:HD12	2.29	0.67
1:C:147:GLU:HB3	4:C:326:HOH:O	1.93	0.67
1:D:193:GLN:O	1:D:193:GLN:HG2	1.95	0.66
1:C:207:PHE:O	1:C:211:ILE:HG13	1.97	0.64
1:A:32:ASP:OD1	1:A:192:ARG:NH2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:TYR:HE2	1:A:202:ILE:HD11	1.56	0.61
1:B:208:ILE:HG22	1:B:266:TYR:OH	2.00	0.61
1:D:122:ASP:OD1	1:D:192:ARG:NH1	2.33	0.59
1:C:131:ILE:HD11	1:C:181:GLU:HG2	1.85	0.58
1:C:195:PHE:HE1	1:D:252:MET:HB2	1.69	0.58
1:E:208:ILE:HG22	1:E:266:TYR:OH	2.03	0.57
1:B:211:ILE:HG23	1:C:270:VAL:HG11	1.85	0.57
1:D:194:TYR:CD2	1:D:197:TYR:HB2	2.41	0.56
1:A:197:TYR:HD2	1:A:202:ILE:CD1	2.14	0.56
1:A:253:THR:HG23	1:A:256:GLY:N	2.20	0.55
1:D:208:ILE:HG22	1:D:266:TYR:OH	2.06	0.55
1:A:270:VAL:HG11	1:E:211:ILE:HG23	1.89	0.55
1:C:253:THR:HG23	1:C:256:GLY:N	2.20	0.53
1:D:253:THR:HG23	1:D:256:GLY:N	2.21	0.53
1:E:253:THR:HG23	1:E:256:GLY:N	2.21	0.53
1:E:173:ASN:HB3	1:E:180:LEU:HD11	1.89	0.53
1:B:253:THR:HG23	1:B:256:GLY:N	2.21	0.53
2:A:318:LMT:H52	1:D:240:ILE:HG21	1.89	0.53
1:E:7:PRO:HG3	1:E:135:VAL:HG21	1.90	0.53
1:B:109:ARG:NH2	4:B:341:HOH:O	2.43	0.52
1:C:173:ASN:HB3	1:C:180:LEU:HD11	1.92	0.52
1:D:134:SER:HB3	1:D:139:ASN:HA	1.91	0.52
1:B:28:TYR:CE1	1:B:38:LYS:HB2	2.44	0.52
1:D:28:TYR:CE1	1:D:38:LYS:HB2	2.45	0.51
1:A:159:GLY:HA2	1:B:250:PRO:HB3	1.92	0.51
1:C:6:SER:O	1:C:51:ARG:NH2	2.45	0.50
1:E:187:GLN:OE1	1:E:189:ARG:NH2	2.45	0.50
1:D:198:ILE:HB	1:D:199:PRO:CD	2.42	0.50
1:B:279:LEU:HD13	1:B:287:ARG:HB3	1.94	0.50
1:D:120:PRO:HG3	1:D:197:TYR:CG	2.46	0.50
1:B:208:ILE:HG22	1:B:266:TYR:HH	1.77	0.49
1:D:196:SER:O	1:D:200:ASN:HB2	2.12	0.49
1:C:211:ILE:HD13	1:D:270:VAL:HG21	1.95	0.49
1:B:135:VAL:HG23	1:B:138:ARG:H	1.78	0.49
1:D:28:TYR:CE1	1:D:38:LYS:HD2	2.48	0.48
1:A:211:ILE:HG23	1:B:270:VAL:HG11	1.96	0.48
1:D:287:ARG:HH11	1:D:287:ARG:HA	1.79	0.48
1:A:134:SER:HB3	1:A:139:ASN:HA	1.96	0.48
1:B:173:ASN:HB3	1:B:180:LEU:HD11	1.96	0.48
1:C:77:ARG:NH1	4:C:321:HOH:O	2.46	0.47
1:A:78:PHE:CE2	1:A:85:ARG:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:VAL:HG23	1:C:137:THR:H	1.80	0.47
1:C:226:THR:O	1:C:230:SER:HB2	2.14	0.47
1:E:278:TYR:CZ	1:E:282:GLU:OE1	2.68	0.47
1:C:31:ASP:C	1:C:31:ASP:OD2	2.58	0.47
1:D:187:GLN:OE1	1:D:189:ARG:NH2	2.48	0.47
1:D:198:ILE:HB	1:D:199:PRO:HD3	1.96	0.47
1:D:211:ILE:HG23	1:E:270:VAL:HG11	1.96	0.47
1:A:226:THR:O	1:A:230:SER:HB2	2.15	0.47
1:E:77:ARG:NH1	4:E:333:HOH:O	2.47	0.47
1:C:134:SER:HA	1:C:140:ILE:HD12	1.97	0.46
1:B:78:PHE:CE2	1:B:85:ARG:HD3	2.50	0.46
1:A:187:GLN:OE1	1:A:189:ARG:NH2	2.49	0.46
1:C:187:GLN:OE1	1:C:189:ARG:NH2	2.48	0.46
1:D:28:TYR:CE1	1:D:38:LYS:CB	2.99	0.46
1:D:136:ASP:OD1	1:D:179:ARG:NH1	2.34	0.46
1:D:133:ARG:NH1	1:D:177:GLU:HB2	2.30	0.45
1:E:226:THR:O	1:E:230:SER:HB2	2.17	0.45
1:C:159:GLY:HA2	1:D:250:PRO:HB3	1.98	0.45
1:A:120:PRO:HG3	1:A:197:TYR:CD2	2.51	0.45
1:D:197:TYR:HE2	1:D:202:ILE:HD11	1.76	0.45
1:B:28:TYR:CE1	1:B:38:LYS:CB	3.00	0.45
1:B:226:THR:O	1:B:230:SER:HB2	2.17	0.45
1:D:78:PHE:CE2	1:D:85:ARG:HD3	2.52	0.45
1:D:226:THR:O	1:D:230:SER:HB2	2.17	0.45
1:E:78:PHE:CE2	1:E:85:ARG:HD3	2.52	0.45
1:B:187:GLN:OE1	1:B:189:ARG:NH2	2.49	0.45
1:B:79:VAL:HG21	1:B:183:LYS:HD2	1.99	0.44
1:D:197:TYR:OH	1:D:255:THR:HG23	2.17	0.44
1:A:79:VAL:HG21	1:A:183:LYS:HD2	1.99	0.44
1:C:194:TYR:HA	1:C:197:TYR:CD2	2.53	0.44
1:E:8:PRO:HG2	1:E:16:LEU:HD13	2.00	0.44
1:E:162:ILE:HG13	1:E:190:ILE:HG22	2.00	0.44
1:A:135:VAL:HG22	1:A:140:ILE:HD11	2.00	0.44
1:D:28:TYR:HE1	1:D:38:LYS:HD2	1.83	0.44
1:A:31:ASP:OD2	1:A:31:ASP:C	2.61	0.43
1:A:197:TYR:HD2	1:A:202:ILE:HD11	1.60	0.43
1:D:120:PRO:HG3	1:D:197:TYR:CD2	2.53	0.43
1:A:279:LEU:HD13	1:A:287:ARG:HB3	2.00	0.43
1:C:78:PHE:CE2	1:C:85:ARG:HD3	2.52	0.43
1:D:183:LYS:HG3	1:D:184:LEU:N	2.33	0.43
1:E:194:TYR:HA	1:E:197:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:ARG:HH11	1:D:177:GLU:HB2	1.84	0.43
1:C:120:PRO:O	1:C:194:TYR:HB3	2.19	0.43
1:E:97:ASP:OD2	1:E:99:THR:OG1	2.32	0.43
1:E:120:PRO:O	1:E:194:TYR:HB3	2.19	0.43
1:B:28:TYR:CE1	1:B:38:LYS:HD2	2.54	0.42
1:B:208:ILE:HG12	1:C:232:LEU:HD21	2.01	0.42
1:D:122:ASP:CG	1:D:192:ARG:NH1	2.76	0.42
1:E:134:SER:HB3	1:E:139:ASN:HA	2.00	0.42
1:A:248:LYS:HD3	1:E:201:ILE:HD11	2.01	0.42
1:C:203:LEU:HD23	1:C:203:LEU:HA	1.81	0.42
1:B:76:ILE:HD12	1:B:142:LEU:HD21	2.01	0.42
1:C:268:VAL:HG12	1:C:299:PHE:CZ	2.55	0.42
1:C:76:ILE:HD12	1:C:142:LEU:HD21	2.01	0.42
1:C:138:ARG:HB2	4:C:324:HOH:O	2.20	0.41
1:E:254:TYR:CZ	1:E:258:ILE:HD11	2.54	0.41
1:B:194:TYR:HA	1:B:197:TYR:CD2	2.56	0.41
1:D:249:THR:HG21	1:D:251:TYR:CE1	2.55	0.41
1:B:163:GLU:OE2	1:B:191:SER:OG	2.37	0.41
1:A:76:ILE:HD12	1:A:142:LEU:HD21	2.02	0.41
1:D:76:ILE:HD12	1:D:142:LEU:HD21	2.03	0.41
1:B:268:VAL:HG12	1:B:299:PHE:CZ	2.56	0.41
1:D:122:ASP:CG	1:D:192:ARG:HH11	2.24	0.41
1:D:122:ASP:OD2	1:D:192:ARG:NH1	2.54	0.41
1:D:193:GLN:O	1:D:193:GLN:HG3	2.20	0.41
1:A:268:VAL:HG12	1:A:299:PHE:CZ	2.56	0.41
1:A:120:PRO:O	1:A:194:TYR:HB3	2.21	0.41
1:A:197:TYR:OH	1:A:255:THR:CG2	2.69	0.41
1:A:250:PRO:HB3	1:E:159:GLY:HA2	2.03	0.41
1:E:32:ASP:OD2	4:E:338:HOH:O	2.22	0.41
1:E:268:VAL:HG12	1:E:299:PHE:CZ	2.56	0.41
1:A:152:ASN:HB3	1:A:155:VAL:HG23	2.03	0.41
1:D:268:VAL:HG12	1:D:299:PHE:CZ	2.56	0.41
1:E:144:VAL:HG22	1:E:184:LEU:HD13	2.03	0.41
1:D:120:PRO:HG3	1:D:197:TYR:CD1	2.57	0.40
1:D:159:GLY:HA2	1:E:250:PRO:HB3	2.03	0.40
1:E:282:GLU:O	1:E:282:GLU:HG2	2.21	0.40
1:A:278:TYR:HA	1:A:281:VAL:HG12	2.03	0.40
1:A:270:VAL:HG11	1:E:211:ILE:HG12	2.02	0.40
1:C:203:LEU:HB2	1:C:204:PRO:HD3	2.03	0.40
1:D:135:VAL:HG22	1:D:140:ILE:HD11	2.04	0.40
1:D:32:ASP:OD1	1:D:192:ARG:NH2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:PRO:HG2	1:D:137:THR:OG1	2.22	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	309/321 (96%)	298 (96%)	11 (4%)	0	100	100
1	B	309/321 (96%)	299 (97%)	10 (3%)	0	100	100
1	C	309/321 (96%)	302 (98%)	7 (2%)	0	100	100
1	D	309/321 (96%)	302 (98%)	7 (2%)	0	100	100
1	E	309/321 (96%)	299 (97%)	10 (3%)	0	100	100
All	All	1545/1605 (96%)	1500 (97%)	45 (3%)	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	280/285 (98%)	269 (96%)	11 (4%)	28	63
1	B	280/285 (98%)	273 (98%)	7 (2%)	42	74
1	C	280/285 (98%)	269 (96%)	11 (4%)	28	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	280/285 (98%)	267 (95%)	13 (5%)	24	57
1	E	280/285 (98%)	268 (96%)	12 (4%)	26	60
All	All	1400/1425 (98%)	1346 (96%)	54 (4%)	28	63

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ARG
1	A	59	SER
1	A	141	VAL
1	A	180	LEU
1	A	248	LYS
1	A	259	ILE
1	A	292	THR
1	A	297	ILE
1	A	304	LEU
1	A	307	ASN
1	A	313	LEU
1	B	141	VAL
1	B	146	LEU
1	B	259	ILE
1	B	281	VAL
1	B	297	ILE
1	B	304	LEU
1	B	307	ASN
1	C	101	GLN
1	C	135	VAL
1	C	141	VAL
1	C	144	VAL
1	C	180	LEU
1	C	181	GLU
1	C	259	ILE
1	C	281	VAL
1	C	297	ILE
1	C	304	LEU
1	C	307	ASN
1	D	141	VAL
1	D	146	LEU
1	D	147	GLU
1	D	170	LYS
1	D	178	ASP

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Mol	Chain	Res	Type
1	D	180	LEU
1	D	192	ARG
1	D	259	ILE
1	D	281	VAL
1	D	287	ARG
1	D	297	ILE
1	D	304	LEU
1	D	307	ASN
1	E	19	ASN
1	E	39	VAL
1	E	93	SER
1	E	101	GLN
1	E	141	VAL
1	E	170	LYS
1	E	228	VAL
1	E	259	ILE
1	E	281	VAL
1	E	297	ILE
1	E	304	LEU
1	E	307	ASN

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

Mol	Chain	Res	Type
1	A	239	ASN
1	A	277	HIS
1	A	284	GLN
1	B	239	ASN
1	B	277	HIS
1	C	83	ASN
1	C	277	HIS
1	D	101	GLN
1	D	277	HIS
1	E	83	ASN
1	E	239	ASN
1	E	276	GLN
1	E	277	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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	$\# Z > 2$
2	LMT	A	318	-	11,11,36	0.58	0	10,10,47	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	A	318	-	-	3/9/9/61	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

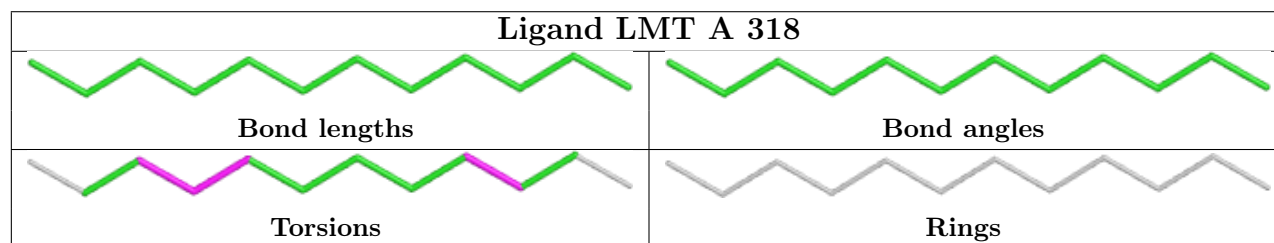
Mol	Chain	Res	Type	Atoms
2	A	318	LMT	C11-C10-C9-C8
2	A	318	LMT	C7-C8-C9-C10
2	A	318	LMT	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	318	LMT	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	311/321 (96%)	0.96	49 (15%) 5 4	53, 79, 115, 151	0
1	B	311/321 (96%)	1.05	57 (18%) 3 3	48, 74, 103, 124	0
1	C	311/321 (96%)	0.84	39 (12%) 8 7	48, 72, 101, 118	0
1	D	311/321 (96%)	1.18	66 (21%) 2 2	54, 76, 110, 141	0
1	E	311/321 (96%)	1.06	61 (19%) 3 2	47, 74, 105, 127	0
All	All	1555/1605 (96%)	1.02	272 (17%) 4 3	47, 75, 107, 151	0

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	248	LYS	8.9
1	E	245	ASN	8.5
1	A	245	ASN	8.3
1	D	153	ASP	8.2
1	B	5	VAL	7.3
1	A	57	VAL	7.0
1	B	245	ASN	6.9
1	E	153	ASP	6.7
1	D	154	ASP	6.5
1	B	147	GLU	6.5
1	C	245	ASN	6.5
1	A	244	THR	6.3
1	E	248	LYS	6.2
1	C	5	VAL	6.0
1	E	244	THR	5.9
1	C	11	ILE	5.8
1	E	5	VAL	5.8
1	B	195	PHE	5.8
1	A	246	CYS	5.6
1	D	245	ASN	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	312	PHE	5.5
1	C	244	THR	5.4
1	E	195	PHE	5.4
1	E	11	ILE	5.4
1	A	195	PHE	5.1
1	E	253	THR	5.0
1	D	246	CYS	4.9
1	D	152	ASN	4.9
1	D	210	PHE	4.8
1	D	253	THR	4.7
1	D	11	ILE	4.7
1	A	5	VAL	4.7
1	A	61	VAL	4.7
1	B	246	CYS	4.6
1	C	62	ARG	4.6
1	E	68	PRO	4.6
1	E	247	PRO	4.6
1	E	67	GLU	4.6
1	D	5	VAL	4.5
1	D	244	THR	4.4
1	B	244	THR	4.4
1	C	33	CYS	4.4
1	A	56	PRO	4.4
1	C	246	CYS	4.3
1	E	255	THR	4.3
1	B	276	GLN	4.3
1	D	28	TYR	4.3
1	C	195	PHE	4.3
1	A	62	ARG	4.3
1	B	154	ASP	4.2
1	B	197	TYR	4.2
1	D	48	LYS	4.2
1	D	62	ARG	4.2
1	D	194	TYR	4.1
1	D	75	GLU	4.1
1	E	33	CYS	4.0
1	A	170	LYS	4.0
1	D	26	GLU	4.0
1	E	246	CYS	4.0
1	E	154	ASP	3.9
1	A	284	GLN	3.9
1	D	155	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	247	PRO	3.8
1	B	280	LYS	3.8
1	A	127	HIS	3.7
1	B	6	SER	3.7
1	D	97	ASP	3.7
1	A	65	THR	3.7
1	A	248	LYS	3.6
1	E	312	PHE	3.6
1	B	194	TYR	3.6
1	E	10	PRO	3.6
1	D	283	SER	3.6
1	D	78	PHE	3.6
1	A	13	ASP	3.6
1	B	292	THR	3.6
1	D	12	ALA	3.5
1	B	247	PRO	3.5
1	C	312	PHE	3.5
1	D	57	VAL	3.5
1	D	197	TYR	3.5
1	A	69	GLU	3.4
1	A	63	VAL	3.4
1	E	6	SER	3.4
1	A	50	ARG	3.4
1	A	33	CYS	3.4
1	C	9	PRO	3.4
1	D	170	LYS	3.4
1	C	166	THR	3.3
1	D	255	THR	3.3
1	A	11	ILE	3.3
1	B	210	PHE	3.3
1	D	89	VAL	3.3
1	C	129	TYR	3.3
1	A	12	ALA	3.3
1	A	154	ASP	3.3
1	D	50	ARG	3.3
1	A	60	GLY	3.3
1	D	213	TRP	3.3
1	C	10	PRO	3.2
1	E	9	PRO	3.2
1	E	252	MET	3.2
1	D	99	THR	3.2
1	D	61	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	193	GLN	3.2
1	C	147	GLU	3.2
1	E	147	GLU	3.2
1	C	193	GLN	3.1
1	C	247	PRO	3.1
1	B	248	LYS	3.1
1	A	283	SER	3.0
1	B	150	GLY	3.0
1	B	272	GLU	3.0
1	E	101	GLN	3.0
1	E	197	TYR	3.0
1	D	67	GLU	3.0
1	D	195	PHE	3.0
1	E	89	VAL	3.0
1	E	69	GLU	2.9
1	A	129	TYR	2.9
1	C	197	TYR	2.9
1	E	285	PRO	2.9
1	C	12	ALA	2.9
1	D	63	VAL	2.9
1	A	9	PRO	2.9
1	B	278	TYR	2.9
1	E	79	VAL	2.9
1	E	210	PHE	2.9
1	B	11	ILE	2.9
1	C	127	HIS	2.8
1	D	95	SER	2.8
1	E	226	THR	2.8
1	C	187	GLN	2.8
1	A	58	ARG	2.8
1	C	137	THR	2.8
1	C	50	ARG	2.8
1	B	129	TYR	2.8
1	C	88	ASP	2.8
1	D	166	THR	2.8
1	B	286	ALA	2.7
1	E	152	ASN	2.7
1	B	218	SER	2.7
1	A	187	GLN	2.7
1	A	219	THR	2.7
1	D	281	VAL	2.7
1	A	312	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	86	ASP	2.7
1	A	48	LYS	2.7
1	B	289	ALA	2.6
1	A	10	PRO	2.6
1	B	291	ILE	2.6
1	A	247	PRO	2.6
1	E	250	PRO	2.6
1	B	193	GLN	2.6
1	B	145	ASP	2.6
1	D	167	ALA	2.6
1	B	50	ARG	2.6
1	A	194	TYR	2.6
1	D	56	PRO	2.6
1	B	53	ALA	2.6
1	C	91	ASP	2.6
1	E	12	ALA	2.6
1	A	281	VAL	2.6
1	E	90	VAL	2.6
1	D	104	GLU	2.6
1	C	161	ASP	2.6
1	D	88	ASP	2.6
1	E	178	ASP	2.6
1	C	6	SER	2.5
1	A	280	LYS	2.5
1	C	90	VAL	2.5
1	E	287	ARG	2.5
1	A	218	SER	2.5
1	D	196	SER	2.5
1	B	170	LYS	2.5
1	B	130	LEU	2.4
1	D	24	LEU	2.4
1	E	91	ASP	2.4
1	E	203	LEU	2.4
1	D	29	SER	2.4
1	E	129	TYR	2.4
1	D	87	ALA	2.4
1	E	286	ALA	2.4
1	D	80	ASN	2.4
1	B	136	ASP	2.4
1	B	144	VAL	2.4
1	C	60	GLY	2.4
1	D	85	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	278	TYR	2.4
1	C	221	TYR	2.4
1	C	278	TYR	2.4
1	E	66	TYR	2.4
1	C	253	THR	2.4
1	C	274	THR	2.4
1	D	128	ILE	2.4
1	E	199	PRO	2.4
1	D	207	PHE	2.4
1	B	215	ALA	2.4
1	E	70	ALA	2.4
1	B	284	GLN	2.4
1	B	20	THR	2.4
1	B	28	TYR	2.4
1	D	68	PRO	2.4
1	A	315	PHE	2.3
1	B	153	ASP	2.3
1	E	145	ASP	2.3
1	C	248	LYS	2.3
1	A	88	ASP	2.3
1	D	33	CYS	2.3
1	E	166	THR	2.3
1	B	285	PRO	2.3
1	E	267	PHE	2.3
1	E	136	ASP	2.3
1	A	197	TYR	2.3
1	D	120	PRO	2.3
1	E	80	ASN	2.3
1	D	284	GLN	2.3
1	C	58	ARG	2.3
1	E	137	THR	2.3
1	D	141	VAL	2.3
1	E	37	PHE	2.2
1	E	222	GLU	2.2
1	D	206	LEU	2.2
1	E	170	LYS	2.2
1	B	13	ASP	2.2
1	A	285	PRO	2.2
1	B	219	THR	2.2
1	B	281	VAL	2.2
1	E	202	ILE	2.2
1	B	253	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	274	THR	2.2
1	B	221	TYR	2.2
1	C	28	TYR	2.2
1	C	48	LYS	2.2
1	E	161	ASP	2.2
1	D	217	TRP	2.2
1	D	219	THR	2.2
1	A	313	LEU	2.2
1	B	315	PHE	2.2
1	B	96	PRO	2.1
1	D	13	ASP	2.1
1	A	226	THR	2.1
1	A	292	THR	2.1
1	B	146	LEU	2.1
1	D	312	PHE	2.1
1	E	217	TRP	2.1
1	A	59	SER	2.1
1	A	293	ARG	2.1
1	D	25	ILE	2.1
1	B	277	HIS	2.1
1	C	141	VAL	2.1
1	C	292	THR	2.1
1	E	78	PHE	2.1
1	B	288	ALA	2.1
1	B	33	CYS	2.1
1	D	6	SER	2.1
1	E	29	SER	2.1
1	E	284	GLN	2.1
1	B	275	VAL	2.1
1	D	200	ASN	2.1
1	E	249	THR	2.1
1	B	293	ARG	2.1
1	E	293	ARG	2.1
1	D	14	GLU	2.1
1	D	129	TYR	2.1
1	C	277	HIS	2.1
1	E	207	PHE	2.1
1	B	86	ASP	2.1
1	B	95	SER	2.0
1	B	273	VAL	2.0
1	A	305	LEU	2.0
1	A	75	GLU	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](#)

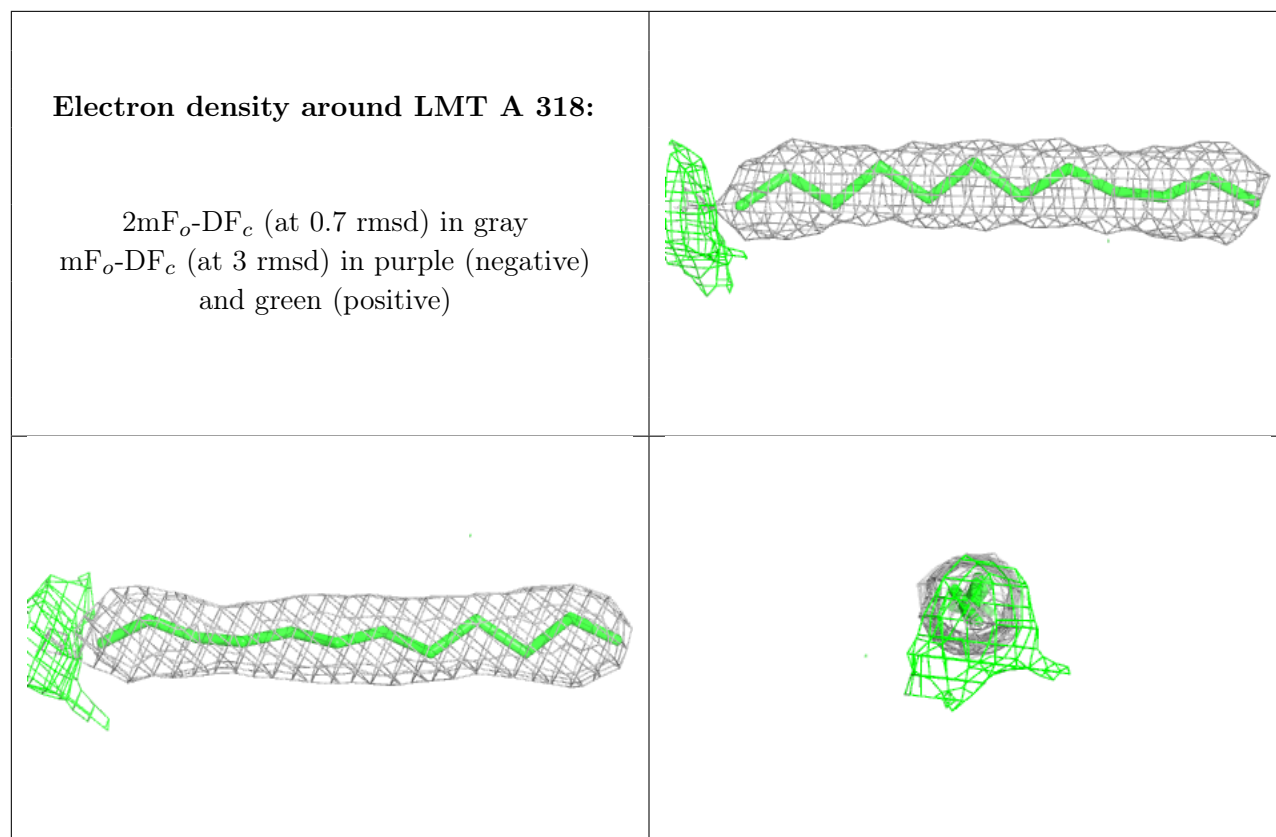
There are no oligosaccharides in this entry.

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	LMT	A	318	12/35	0.94	0.17	59,64,65,65	0
3	CL	B	318	1/1	0.97	0.10	62,62,62,62	0
3	CL	A	319	1/1	0.98	0.07	61,61,61,61	0
3	CL	C	318	1/1	0.98	0.06	58,58,58,58	0
3	CL	D	318	1/1	0.98	0.15	64,64,64,64	0
3	CL	E	318	1/1	0.99	0.17	64,64,64,64	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.