



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:54 PM UTC

PDB ID : 4LMJ / pdb_00004lmj
Title : GLIC Liganded-closed-channel Conformation, Mutant T25'A
Authors : Grosman, C.; Gonzalez-Gutierrez, G.
Deposited on : 2013-07-10
Resolution : 3.44 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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

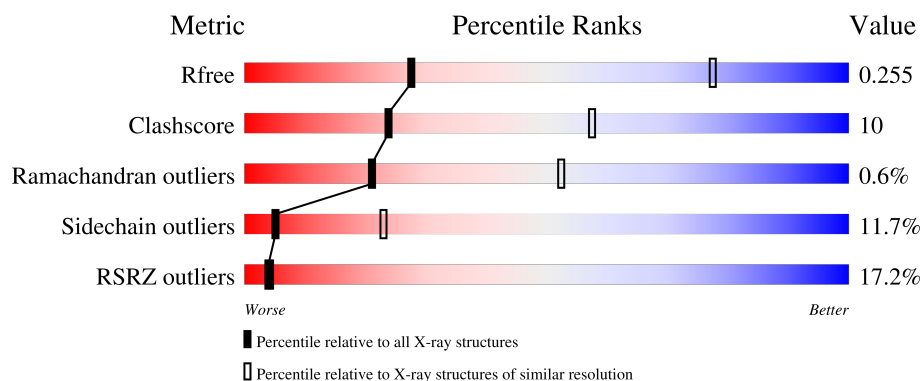
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.44 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	1736 (3.50-3.38)
Clashscore	190562	1808 (3.50-3.38)
Ramachandran outliers	187476	1776 (3.50-3.38)
Sidechain outliers	187428	1777 (3.50-3.38)
RSRZ outliers	180081	1736 (3.50-3.38)

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	318	15% 65% 29% • •
1	B	318	15% 68% 25% • •
1	C	318	18% 65% 28% • •
1	D	318	20% 65% 28% • •
1	E	318	15% 67% 26% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NA	C	401	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12617 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 Proton-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	310	Total	C	N	O	S	0	0	0
			2519	1661	403	451	4			
1	B	310	Total	C	N	O	S	0	0	0
			2519	1661	403	451	4			
1	C	310	Total	C	N	O	S	0	0	0
			2519	1661	403	451	4			
1	A	310	Total	C	N	O	S	0	0	0
			2519	1661	403	451	4			
1	D	310	Total	C	N	O	S	0	0	0
			2519	1661	403	451	4			

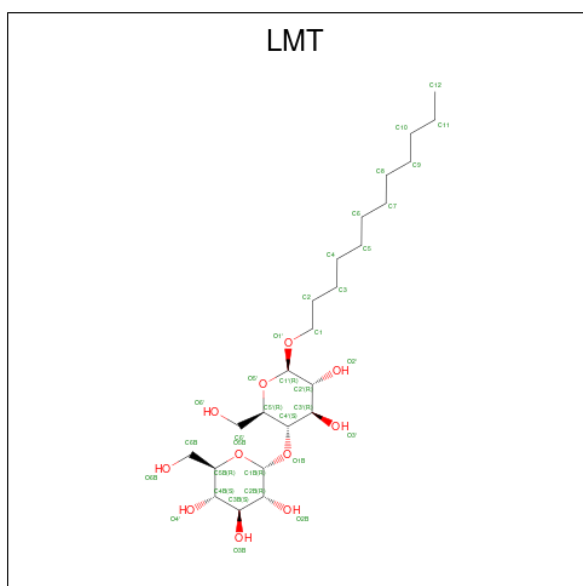
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLY	-	expression tag	UNP Q7NDN8
E	0	SER	-	expression tag	UNP Q7NDN8
E	248	ALA	THR	engineered mutation	UNP Q7NDN8
B	-1	GLY	-	expression tag	UNP Q7NDN8
B	0	SER	-	expression tag	UNP Q7NDN8
B	248	ALA	THR	engineered mutation	UNP Q7NDN8
C	-1	GLY	-	expression tag	UNP Q7NDN8
C	0	SER	-	expression tag	UNP Q7NDN8
C	248	ALA	THR	engineered mutation	UNP Q7NDN8
A	-1	GLY	-	expression tag	UNP Q7NDN8
A	0	SER	-	expression tag	UNP Q7NDN8
A	248	ALA	THR	engineered mutation	UNP Q7NDN8
D	-1	GLY	-	expression tag	UNP Q7NDN8
D	0	SER	-	expression tag	UNP Q7NDN8
D	248	ALA	THR	engineered mutation	UNP Q7NDN8

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

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

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C 12 12	0	0

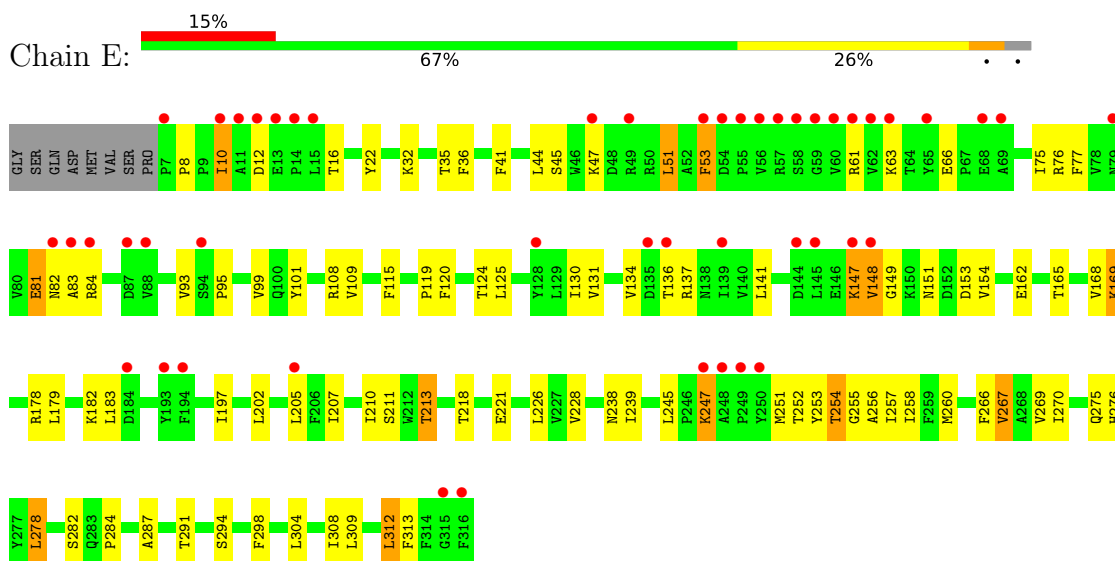
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Na 2 2	0	0
4	C	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0

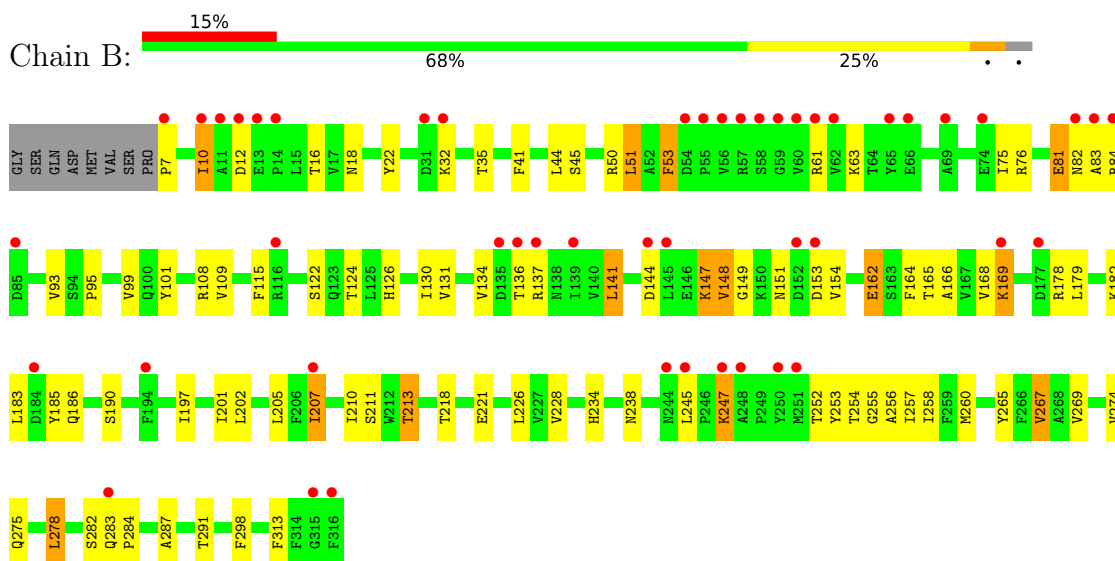
3 Residue-property plots [i](#)

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.

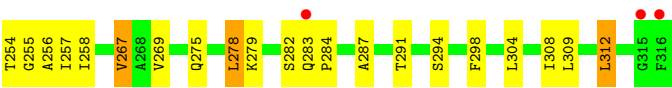
- Molecule 1: Proton-gated ion channel



- Molecule 1: Proton-gated ion channel



- Molecule 1: Proton-gated ion channel



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.12Å 134.32Å 159.89Å 90.00° 101.96° 90.00°	Depositor
Resolution (Å)	49.04 – 3.44 49.04 – 3.44	Depositor EDS
% Data completeness (in resolution range)	79.7 (49.04-3.44) 79.7 (49.04-3.44)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.227 , 0.255 0.228 , 0.255	Depositor DCC
R_{free} test set	1815 reflections (3.07%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 24.3	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	0.83	EDS
Total number of atoms	12617	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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: CL, NA, 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	0.71	1/2587 (0.0%)	1.05	10/3532 (0.3%)
1	B	0.70	1/2587 (0.0%)	1.04	11/3532 (0.3%)
1	C	0.69	0/2587	1.04	6/3532 (0.2%)
1	D	0.67	0/2587	1.05	11/3532 (0.3%)
1	E	0.70	2/2587 (0.1%)	1.05	9/3532 (0.3%)
All	All	0.69	4/12935 (0.0%)	1.05	47/17660 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	197	ILE	CA-CB	-7.05	1.50	1.54
1	A	8	PRO	CA-C	6.78	1.55	1.51
1	B	197	ILE	CA-CB	-5.57	1.51	1.54
1	E	8	PRO	CA-C	5.03	1.54	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	VAL	N-CA-C	6.81	117.60	110.72
1	B	256	ALA	N-CA-C	-6.63	103.32	111.40
1	E	256	ALA	N-CA-C	-6.25	103.78	111.40
1	A	256	ALA	N-CA-C	-6.23	103.80	111.40
1	C	143	VAL	N-CA-C	5.92	115.88	106.88
1	A	10	ILE	N-CA-C	5.91	116.99	108.48
1	E	202	LEU	CA-C-N	-5.90	112.79	119.28
1	E	202	LEU	C-N-CA	-5.90	112.79	119.28
1	B	7	PRO	CA-C-N	5.89	123.90	119.66
1	B	7	PRO	C-N-CA	5.89	123.90	119.66
1	D	256	ALA	N-CA-C	-5.84	104.27	111.40
1	A	8	PRO	N-CA-C	5.82	116.06	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	7	PRO	CA-C-N	5.72	123.84	119.66
1	D	7	PRO	C-N-CA	5.72	123.84	119.66
1	A	54	ASP	CA-C-N	5.67	125.34	119.05
1	A	54	ASP	C-N-CA	5.67	125.34	119.05
1	E	276	HIS	N-CA-C	5.60	117.46	111.36
1	D	283	GLN	CA-C-N	5.57	125.41	119.28
1	D	283	GLN	C-N-CA	5.57	125.41	119.28
1	C	276	HIS	N-CA-C	5.56	117.42	111.36
1	A	143	VAL	N-CA-C	5.56	115.33	106.88
1	C	256	ALA	N-CA-C	-5.47	104.73	111.40
1	D	202	LEU	CA-C-N	-5.37	113.09	119.05
1	D	202	LEU	C-N-CA	-5.37	113.09	119.05
1	C	202	LEU	CA-C-N	-5.36	113.10	119.05
1	C	202	LEU	C-N-CA	-5.36	113.10	119.05
1	E	10	ILE	N-CA-C	5.33	115.58	108.11
1	E	228	VAL	N-CA-C	5.32	116.09	110.72
1	B	283	GLN	CA-C-N	5.26	125.07	119.28
1	B	283	GLN	C-N-CA	5.26	125.07	119.28
1	D	200	ILE	N-CA-C	5.25	115.77	111.62
1	B	202	LEU	CA-C-N	-5.24	113.23	119.05
1	B	202	LEU	C-N-CA	-5.24	113.23	119.05
1	C	8	PRO	O-C-N	5.21	123.71	121.31
1	E	254	THR	N-CA-C	-5.17	102.73	110.23
1	D	162	GLU	N-CA-C	5.14	116.69	111.14
1	A	202	LEU	CA-C-N	-5.10	113.39	119.05
1	A	202	LEU	C-N-CA	-5.10	113.39	119.05
1	B	201	ILE	N-CA-C	5.08	115.30	110.53
1	B	162	GLU	N-CA-C	5.06	116.60	111.14
1	D	201	ILE	N-CA-C	5.05	115.28	110.53
1	A	292	ARG	CB-CG-CD	5.05	122.91	111.30
1	B	228	VAL	N-CA-C	5.04	115.81	110.72
1	B	144	ASP	N-CA-C	5.03	117.49	111.71
1	E	66	GLU	CA-C-N	5.01	124.79	119.28
1	E	66	GLU	C-N-CA	5.01	124.79	119.28
1	D	10	ILE	N-CA-C	5.01	115.69	108.48

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	2519	0	2535	50	0
1	B	2519	0	2535	51	0
1	C	2519	0	2535	61	0
1	D	2519	0	2535	54	0
1	E	2519	0	2535	54	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	E	12	0	23	1	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	12617	0	12698	256	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 10.

All (256) 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:E:255:GLY:HA2	1:E:258:ILE:HB	1.62	0.82
1:D:255:GLY:HA2	1:D:258:ILE:HB	1.62	0.80
1:A:255:GLY:HA2	1:A:258:ILE:HB	1.65	0.79
1:B:255:GLY:HA2	1:B:258:ILE:HB	1.64	0.78
1:C:255:GLY:HA2	1:C:258:ILE:HB	1.67	0.76
1:C:147:LYS:O	1:C:149:GLY:N	2.27	0.68
1:E:147:LYS:O	1:E:149:GLY:N	2.27	0.67
1:A:147:LYS:O	1:A:149:GLY:N	2.28	0.67
1:D:147:LYS:O	1:D:149:GLY:N	2.29	0.65
1:B:147:LYS:O	1:B:149:GLY:N	2.29	0.65
1:E:35:THR:OG1	1:E:108:ARG:NH2	2.30	0.64
1:B:35:THR:OG1	1:B:108:ARG:NH2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:THR:OG1	1:C:108:ARG:NH2	2.32	0.62
1:A:35:THR:OG1	1:A:108:ARG:NH2	2.33	0.61
1:D:130:ILE:HG22	1:D:182:LYS:HB2	1.83	0.60
1:B:234:HIS:C	1:B:234:HIS:HD1	2.09	0.60
1:E:137:ARG:HD2	1:E:179:LEU:HB3	1.83	0.60
1:D:137:ARG:HD2	1:D:179:LEU:HB3	1.82	0.59
1:D:35:THR:OG1	1:D:108:ARG:NH2	2.36	0.59
1:A:137:ARG:HD2	1:A:179:LEU:HB3	1.85	0.58
1:C:130:ILE:HG22	1:C:182:LYS:HB2	1.85	0.58
1:E:130:ILE:HG22	1:E:182:LYS:HB2	1.84	0.58
1:A:130:ILE:HG22	1:A:182:LYS:HB2	1.86	0.57
1:B:137:ARG:HD2	1:B:179:LEU:HB3	1.86	0.57
1:B:130:ILE:HG22	1:B:182:LYS:HB2	1.87	0.57
1:D:22:TYR:HA	1:D:149:GLY:HA2	1.87	0.57
1:C:234:HIS:C	1:C:234:HIS:HD1	2.13	0.56
1:D:32:LYS:HZ1	1:D:247:LYS:H	1.53	0.56
1:E:77:PHE:O	1:A:104:ARG:NH1	2.38	0.56
1:B:278:LEU:HB3	1:B:287:ALA:HB2	1.89	0.55
1:E:22:TYR:HA	1:E:149:GLY:HA2	1.89	0.54
1:C:22:TYR:HB3	1:C:41:PHE:HB2	1.89	0.54
1:A:53:PHE:CD1	1:A:95:PRO:HA	2.42	0.54
1:C:22:TYR:HA	1:C:149:GLY:HA2	1.89	0.54
1:B:22:TYR:HA	1:B:149:GLY:HA2	1.89	0.54
1:A:22:TYR:HA	1:A:149:GLY:HA2	1.91	0.53
1:B:22:TYR:HB3	1:B:41:PHE:HB2	1.91	0.53
1:C:137:ARG:HD2	1:C:179:LEU:HB3	1.90	0.53
1:E:213:THR:HG22	1:E:226:LEU:HD21	1.89	0.53
1:A:22:TYR:HB3	1:A:41:PHE:HB2	1.90	0.53
1:A:32:LYS:HZ1	1:A:247:LYS:H	1.57	0.52
1:B:267:VAL:HG23	1:B:298:PHE:CZ	2.45	0.52
1:A:51:LEU:HD13	1:A:93:VAL:HG11	1.90	0.52
1:A:53:PHE:HD1	1:A:95:PRO:HA	1.74	0.52
1:D:278:LEU:HB3	1:D:287:ALA:HB2	1.90	0.52
1:E:269:VAL:HG11	1:A:210:ILE:HG23	1.92	0.52
1:D:267:VAL:HG23	1:D:298:PHE:CZ	2.44	0.52
1:D:22:TYR:HB3	1:D:41:PHE:HB2	1.92	0.52
1:E:278:LEU:HB3	1:E:287:ALA:HB2	1.90	0.51
1:C:278:LEU:HB3	1:C:287:ALA:HB2	1.92	0.51
1:B:51:LEU:HD13	1:B:93:VAL:HG11	1.92	0.51
1:A:115:PHE:O	1:A:252:THR:HG23	2.11	0.51
1:B:234:HIS:C	1:B:234:HIS:ND1	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:VAL:HG23	1:A:298:PHE:CZ	2.46	0.51
1:B:115:PHE:O	1:B:252:THR:HG23	2.12	0.50
1:B:81:GLU:HB3	1:C:27:TYR:CZ	2.46	0.50
1:A:32:LYS:NZ	1:A:247:LYS:H	2.09	0.50
1:E:22:TYR:HB3	1:E:41:PHE:HB2	1.94	0.50
1:E:32:LYS:NZ	1:E:247:LYS:H	2.10	0.50
1:E:210:ILE:HG23	1:D:269:VAL:HG11	1.94	0.50
1:B:213:THR:HG22	1:B:226:LEU:HD21	1.94	0.50
1:D:51:LEU:HD13	1:D:93:VAL:HG11	1.93	0.50
1:E:267:VAL:HG23	1:E:298:PHE:CZ	2.46	0.50
1:B:32:LYS:HZ1	1:B:247:LYS:H	1.60	0.50
1:E:32:LYS:HZ1	1:E:247:LYS:H	1.60	0.49
1:E:53:PHE:CD1	1:E:95:PRO:HA	2.47	0.49
1:C:45:SER:HA	1:C:99:VAL:O	2.12	0.49
1:E:51:LEU:HD13	1:E:93:VAL:HG11	1.93	0.49
1:A:204:MET:HE1	1:A:258:ILE:HG12	1.94	0.49
1:E:45:SER:HA	1:E:99:VAL:O	2.13	0.49
1:B:234:HIS:HD2	1:B:265:TYR:CE1	2.31	0.49
1:A:278:LEU:HB3	1:A:287:ALA:HB2	1.95	0.49
1:D:32:LYS:NZ	1:D:247:LYS:H	2.10	0.49
1:B:82:ASN:HB2	1:B:108:ARG:HG2	1.94	0.48
1:B:53:PHE:CD1	1:B:95:PRO:HA	2.49	0.48
1:C:32:LYS:NZ	1:C:247:LYS:H	2.10	0.48
1:A:282:SER:C	1:A:284:PRO:HD3	2.38	0.48
1:C:78:VAL:HA	1:D:104:ARG:HH22	1.79	0.48
1:C:234:HIS:HD2	1:C:265:TYR:CE1	2.31	0.48
1:B:32:LYS:NZ	1:B:247:LYS:H	2.12	0.48
1:C:115:PHE:O	1:C:252:THR:HG23	2.14	0.48
1:A:7:PRO:O	1:A:50:ARG:NH2	2.47	0.48
1:C:53:PHE:CD1	1:C:95:PRO:HA	2.48	0.48
1:C:251:MET:HE1	1:D:198:PRO:HG2	1.95	0.48
1:D:210:ILE:O	1:D:213:THR:HB	2.14	0.48
1:C:82:ASN:HB2	1:C:108:ARG:HG2	1.96	0.47
1:E:115:PHE:O	1:E:252:THR:HG23	2.14	0.47
1:B:45:SER:HA	1:B:99:VAL:O	2.14	0.47
1:B:137:ARG:HA	1:B:137:ARG:HD3	1.44	0.47
1:D:53:PHE:CD1	1:D:95:PRO:HA	2.49	0.47
1:B:260:MET:HB3	1:B:260:MET:HE2	1.70	0.47
1:C:51:LEU:HD13	1:C:93:VAL:HG11	1.96	0.47
1:C:137:ARG:HA	1:C:137:ARG:HD3	1.47	0.47
1:B:269:VAL:HG11	1:C:210:ILE:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:HIS:C	1:C:234:HIS:ND1	2.73	0.47
1:A:45:SER:HA	1:A:99:VAL:O	2.14	0.47
1:B:151:ASN:ND2	1:B:153:ASP:HB2	2.30	0.47
1:B:210:ILE:O	1:B:213:THR:HB	2.14	0.47
1:E:82:ASN:HB2	1:E:108:ARG:HG2	1.96	0.47
1:E:253:TYR:HA	1:E:313:PHE:CE2	2.50	0.47
1:D:213:THR:HG22	1:D:226:LEU:HD21	1.95	0.47
1:D:151:ASN:O	1:D:154:VAL:HG22	2.15	0.47
1:E:183:LEU:HD23	1:E:183:LEU:HA	1.63	0.46
1:C:267:VAL:HG23	1:C:298:PHE:CZ	2.50	0.46
1:A:82:ASN:HB2	1:A:108:ARG:HG2	1.97	0.46
1:D:83:ALA:O	1:D:84:ARG:HG2	2.16	0.46
1:D:204:MET:HE1	1:D:258:ILE:HG12	1.97	0.46
1:D:82:ASN:HB2	1:D:108:ARG:HG2	1.96	0.46
1:E:76:ARG:HH12	1:E:130:ILE:HD11	1.80	0.46
1:B:126:HIS:CE1	1:B:186:GLN:HG2	2.49	0.46
1:C:75:ILE:HD13	1:C:131:VAL:HB	1.98	0.46
1:A:122:SER:OG	1:A:190:SER:HB3	2.15	0.46
1:D:53:PHE:HD1	1:D:95:PRO:HA	1.80	0.46
1:C:32:LYS:HZ1	1:C:247:LYS:H	1.62	0.46
1:C:210:ILE:O	1:C:213:THR:HB	2.16	0.46
1:A:210:ILE:O	1:A:213:THR:HB	2.16	0.46
1:D:115:PHE:O	1:D:252:THR:HG23	2.15	0.46
1:E:137:ARG:HD3	1:E:137:ARG:HA	1.48	0.46
1:C:151:ASN:O	1:C:154:VAL:HG22	2.16	0.46
1:E:83:ALA:O	1:E:84:ARG:HG2	2.15	0.46
1:B:221:GLU:OE2	1:C:221:GLU:HG3	2.16	0.46
1:E:81:GLU:HG3	1:E:108:ARG:HG3	1.98	0.46
1:E:266:PHE:O	1:E:270:ILE:HG12	2.16	0.46
1:C:309:LEU:HD12	1:C:309:LEU:HA	1.82	0.46
1:D:183:LEU:HD23	1:D:183:LEU:HA	1.62	0.46
1:A:166:ALA:HB2	1:A:185:TYR:CD2	2.51	0.46
1:D:282:SER:C	1:D:284:PRO:HD3	2.40	0.46
1:B:147:LYS:O	1:B:147:LYS:HG2	2.16	0.45
1:B:207:ILE:HD11	1:B:234:HIS:HA	1.98	0.45
1:D:75:ILE:HD13	1:D:131:VAL:HB	1.98	0.45
1:D:122:SER:OG	1:D:190:SER:HB3	2.16	0.45
1:E:205:LEU:HA	1:E:205:LEU:HD23	1.74	0.45
1:B:169:LYS:HE2	1:B:169:LYS:HB3	1.79	0.45
1:E:75:ILE:HD13	1:E:131:VAL:HB	1.97	0.45
1:E:251:MET:HE1	1:A:198:PRO:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ALA:O	1:A:84:ARG:HG2	2.16	0.45
1:E:53:PHE:HD1	1:E:95:PRO:HA	1.81	0.45
1:C:183:LEU:HA	1:C:183:LEU:HD23	1.61	0.45
1:D:166:ALA:HB2	1:D:185:TYR:CD2	2.52	0.45
1:B:53:PHE:CE2	1:B:63:LYS:HB2	2.52	0.45
1:B:205:LEU:HA	1:B:205:LEU:HD23	1.75	0.45
1:C:53:PHE:HD1	1:C:95:PRO:HA	1.80	0.45
1:C:278:LEU:HD12	1:C:278:LEU:HA	1.65	0.45
1:E:226:LEU:HD12	1:E:226:LEU:HA	1.71	0.45
1:E:282:SER:C	1:E:284:PRO:HD3	2.42	0.45
1:B:81:GLU:HB3	1:C:27:TYR:CE1	2.52	0.45
1:D:81:GLU:HG3	1:D:108:ARG:HG3	1.99	0.45
1:E:147:LYS:O	1:E:147:LYS:HG2	2.18	0.44
1:B:151:ASN:O	1:B:154:VAL:HG22	2.17	0.44
1:A:226:LEU:HD12	1:A:226:LEU:HA	1.82	0.44
1:D:45:SER:HA	1:D:99:VAL:O	2.18	0.44
1:D:304:LEU:O	1:D:308:ILE:HG12	2.17	0.44
1:B:53:PHE:HD1	1:B:95:PRO:HA	1.82	0.44
1:C:204:MET:HE1	1:C:258:ILE:HG12	1.98	0.44
1:C:213:THR:HG22	1:C:226:LEU:HD21	1.99	0.44
1:A:147:LYS:O	1:A:147:LYS:HG2	2.17	0.44
1:B:76:ARG:HH12	1:B:130:ILE:HD11	1.82	0.44
1:E:210:ILE:O	1:E:213:THR:HB	2.17	0.44
1:C:83:ALA:O	1:C:84:ARG:HG2	2.17	0.44
1:A:151:ASN:O	1:A:154:VAL:HG22	2.18	0.44
1:D:53:PHE:CE2	1:D:63:LYS:HB2	2.52	0.44
1:D:137:ARG:HA	1:D:137:ARG:HD3	1.43	0.44
1:B:75:ILE:HD13	1:B:131:VAL:HB	1.98	0.44
1:A:253:TYR:HA	1:A:313:PHE:CE2	2.52	0.44
1:E:81:GLU:HB3	1:A:27:TYR:CE1	2.53	0.44
1:B:282:SER:C	1:B:284:PRO:HD3	2.43	0.44
1:C:122:SER:OG	1:C:190:SER:HB3	2.18	0.44
1:A:183:LEU:HA	1:A:183:LEU:HD23	1.63	0.44
1:E:210:ILE:HG12	1:D:269:VAL:HG11	2.00	0.43
1:A:75:ILE:HD13	1:A:131:VAL:HB	2.00	0.43
1:B:44:LEU:HB2	1:B:101:TYR:HB3	2.00	0.43
1:C:226:LEU:HD12	1:C:226:LEU:HA	1.74	0.43
1:A:36:PHE:CD1	1:A:125:LEU:HD13	2.53	0.43
1:C:53:PHE:CE2	1:C:63:LYS:HB2	2.53	0.43
1:D:309:LEU:HD12	1:D:309:LEU:HA	1.81	0.43
1:C:147:LYS:HE2	1:C:165:THR:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:LYS:HB3	1:C:169:LYS:HE2	1.81	0.43
1:A:119:PRO:HD2	1:A:120:PHE:CE1	2.53	0.43
1:B:166:ALA:HB2	1:B:185:TYR:CD2	2.53	0.43
1:C:7:PRO:O	1:C:50:ARG:NH2	2.51	0.43
1:A:137:ARG:HA	1:A:137:ARG:HD3	1.44	0.43
1:B:183:LEU:HA	1:B:183:LEU:HD23	1.61	0.43
1:C:76:ARG:HH12	1:C:130:ILE:HD11	1.84	0.43
1:C:304:LEU:O	1:C:308:ILE:HG12	2.19	0.43
1:E:36:PHE:CD1	1:E:125:LEU:HD13	2.54	0.43
1:E:119:PRO:HD2	1:E:120:PHE:CE1	2.54	0.43
1:C:47:LYS:HE3	1:C:47:LYS:HB2	1.70	0.43
1:C:282:SER:C	1:C:284:PRO:HD3	2.44	0.43
1:A:81:GLU:HG3	1:A:108:ARG:HG3	2.00	0.43
1:A:274:VAL:O	1:A:278:LEU:HB2	2.18	0.43
1:D:36:PHE:CD1	1:D:125:LEU:HD13	2.54	0.43
1:E:221:GLU:HG3	1:D:221:GLU:OE2	2.18	0.42
1:B:149:GLY:HA3	1:B:164:PHE:HD1	1.83	0.42
1:B:253:TYR:HA	1:B:313:PHE:CE2	2.54	0.42
1:A:53:PHE:CE2	1:A:63:LYS:HB2	2.53	0.42
1:B:83:ALA:O	1:B:84:ARG:HG2	2.20	0.42
1:D:76:ARG:HH12	1:D:130:ILE:HD11	1.84	0.42
1:C:81:GLU:HG3	1:C:108:ARG:HG3	2.00	0.42
1:E:151:ASN:ND2	1:E:153:ASP:HB2	2.34	0.42
1:D:205:LEU:HD23	1:D:205:LEU:HA	1.75	0.42
1:C:207:ILE:CD1	1:C:234:HIS:HA	2.49	0.42
1:A:54:ASP:HA	1:A:55:PRO:HD2	1.76	0.42
1:A:81:GLU:H	1:A:81:GLU:HG2	1.57	0.42
1:E:260:MET:HE2	1:E:260:MET:HB3	1.69	0.42
1:D:44:LEU:HB2	1:D:101:TYR:HB3	2.02	0.42
1:D:126:HIS:CE1	1:D:186:GLN:HG2	2.55	0.42
1:E:169:LYS:HB3	1:E:169:LYS:HE2	1.80	0.42
1:E:239:ILE:HG21	3:E:402:LMT:H82	2.02	0.42
1:C:119:PRO:HD2	1:C:120:PHE:CE1	2.55	0.42
1:C:207:ILE:HD11	1:C:234:HIS:HA	2.02	0.42
1:A:207:ILE:HD11	1:A:234:HIS:HA	2.01	0.42
1:D:54:ASP:HA	1:D:55:PRO:HD2	1.85	0.42
1:D:278:LEU:HD12	1:D:278:LEU:HA	1.71	0.42
1:E:278:LEU:HD12	1:E:278:LEU:HA	1.66	0.42
1:B:122:SER:OG	1:B:190:SER:HB3	2.19	0.42
1:D:169:LYS:HA	1:D:170:PRO:HD2	1.93	0.42
1:D:169:LYS:HE2	1:D:169:LYS:HB3	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:LYS:HE3	1:D:279:LYS:HB2	1.78	0.41
1:E:22:TYR:HA	1:E:149:GLY:CA	2.51	0.41
1:B:81:GLU:HG3	1:B:108:ARG:HG3	2.01	0.41
1:B:207:ILE:CD1	1:B:234:HIS:HA	2.50	0.41
1:E:151:ASN:O	1:E:154:VAL:HG22	2.20	0.41
1:C:15:LEU:HD11	1:C:46:TRP:HB2	2.02	0.41
1:C:279:LYS:HE3	1:C:279:LYS:HB2	1.83	0.41
1:E:44:LEU:HB2	1:E:101:TYR:HB3	2.02	0.41
1:C:253:TYR:HA	1:C:313:PHE:CE2	2.56	0.41
1:D:219:SER:HB3	1:D:222:ALA:HB3	2.02	0.41
1:C:44:LEU:HB2	1:C:101:TYR:HB3	2.03	0.41
1:D:151:ASN:ND2	1:D:153:ASP:HB2	2.35	0.41
1:C:54:ASP:HA	1:C:55:PRO:HD2	1.85	0.41
1:B:10:ILE:HD11	1:B:50:ARG:HD3	2.03	0.41
1:C:151:ASN:ND2	1:C:153:ASP:HB2	2.36	0.41
1:A:260:MET:HE2	1:A:260:MET:HB3	1.65	0.41
1:A:297:ALA:O	1:A:301:VAL:HG23	2.21	0.41
1:D:22:TYR:HA	1:D:149:GLY:CA	2.50	0.41
1:D:207:ILE:HD11	1:D:234:HIS:HA	2.03	0.41
1:D:222:ALA:O	1:D:226:LEU:HB2	2.20	0.41
1:D:312:LEU:HD12	1:D:312:LEU:HA	1.90	0.41
1:E:47:LYS:HE3	1:E:47:LYS:HB2	1.71	0.41
1:E:304:LEU:O	1:E:308:ILE:HG12	2.21	0.41
1:B:274:VAL:O	1:B:278:LEU:HB2	2.21	0.40
1:A:309:LEU:HD12	1:A:309:LEU:HA	1.83	0.40
1:E:53:PHE:CE2	1:E:63:LYS:HB2	2.57	0.40
1:D:47:LYS:HE3	1:D:47:LYS:HB2	1.70	0.40
1:B:18:ASN:HA	1:B:141:LEU:O	2.22	0.40
1:C:166:ALA:HB2	1:C:185:TYR:CD2	2.57	0.40
1:C:274:VAL:O	1:C:278:LEU:HB2	2.21	0.40
1:E:309:LEU:HD12	1:E:309:LEU:HA	1.79	0.40
1:A:222:ALA:O	1:A:226:LEU:HB2	2.21	0.40
1:E:221:GLU:OE2	1:A:221:GLU:HG3	2.22	0.40
1:E:312:LEU:HD12	1:E:312:LEU:HA	1.89	0.40
1:C:18:ASN:HA	1:C:141:LEU:O	2.22	0.40
1:C:147:LYS:O	1:C:147:LYS:HG2	2.22	0.40
1:C:260:MET:HE2	1:C:260:MET:HB3	1.68	0.40
1:A:283:GLN:N	1:A:284:PRO:HD3	2.36	0.40
1:A:304:LEU:O	1:A:308:ILE:HG12	2.21	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	308/318 (97%)	302 (98%)	4 (1%)	2 (1%)	21	52
1	B	308/318 (97%)	301 (98%)	5 (2%)	2 (1%)	21	52
1	C	308/318 (97%)	302 (98%)	4 (1%)	2 (1%)	21	52
1	D	308/318 (97%)	302 (98%)	4 (1%)	2 (1%)	21	52
1	E	308/318 (97%)	302 (98%)	4 (1%)	2 (1%)	21	52
All	All	1540/1590 (97%)	1509 (98%)	21 (1%)	10 (1%)	21	52

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	148	VAL
1	A	148	VAL
1	E	148	VAL
1	B	148	VAL
1	D	148	VAL
1	E	134	VAL
1	B	134	VAL
1	C	134	VAL
1	A	134	VAL
1	D	134	VAL

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	277/284 (98%)	243 (88%)	34 (12%)	4	21
1	B	277/284 (98%)	246 (89%)	31 (11%)	6	24
1	C	277/284 (98%)	246 (89%)	31 (11%)	6	24
1	D	277/284 (98%)	244 (88%)	33 (12%)	5	22
1	E	277/284 (98%)	244 (88%)	33 (12%)	5	22
All	All	1385/1420 (98%)	1223 (88%)	162 (12%)	5	23

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	10	ILE
1	E	12	ASP
1	E	16	THR
1	E	51	LEU
1	E	53	PHE
1	E	61	ARG
1	E	81	GLU
1	E	109	VAL
1	E	124	THR
1	E	136	THR
1	E	141	LEU
1	E	147	LYS
1	E	148	VAL
1	E	162	GLU
1	E	165	THR
1	E	168	VAL
1	E	169	LYS
1	E	178	ARG
1	E	207	ILE
1	E	211	SER
1	E	213	THR
1	E	218	THR
1	E	238	ASN
1	E	245	LEU
1	E	247	LYS
1	E	254	THR
1	E	257	ILE
1	E	267	VAL
1	E	275	GLN
1	E	278	LEU
1	E	291	THR

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Mol	Chain	Res	Type
1	E	294	SER
1	E	312	LEU
1	B	10	ILE
1	B	12	ASP
1	B	16	THR
1	B	51	LEU
1	B	53	PHE
1	B	61	ARG
1	B	81	GLU
1	B	109	VAL
1	B	124	THR
1	B	136	THR
1	B	141	LEU
1	B	147	LYS
1	B	148	VAL
1	B	162	GLU
1	B	165	THR
1	B	168	VAL
1	B	169	LYS
1	B	178	ARG
1	B	207	ILE
1	B	211	SER
1	B	213	THR
1	B	218	THR
1	B	238	ASN
1	B	245	LEU
1	B	247	LYS
1	B	254	THR
1	B	257	ILE
1	B	267	VAL
1	B	275	GLN
1	B	278	LEU
1	B	291	THR
1	C	10	ILE
1	C	12	ASP
1	C	16	THR
1	C	51	LEU
1	C	53	PHE
1	C	61	ARG
1	C	81	GLU
1	C	109	VAL
1	C	124	THR

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Mol	Chain	Res	Type
1	C	136	THR
1	C	141	LEU
1	C	147	LYS
1	C	148	VAL
1	C	162	GLU
1	C	165	THR
1	C	168	VAL
1	C	169	LYS
1	C	178	ARG
1	C	207	ILE
1	C	211	SER
1	C	213	THR
1	C	218	THR
1	C	238	ASN
1	C	245	LEU
1	C	247	LYS
1	C	254	THR
1	C	257	ILE
1	C	267	VAL
1	C	275	GLN
1	C	278	LEU
1	C	291	THR
1	A	10	ILE
1	A	12	ASP
1	A	16	THR
1	A	47	LYS
1	A	51	LEU
1	A	53	PHE
1	A	56	VAL
1	A	61	ARG
1	A	81	GLU
1	A	109	VAL
1	A	124	THR
1	A	136	THR
1	A	141	LEU
1	A	147	LYS
1	A	162	GLU
1	A	165	THR
1	A	168	VAL
1	A	169	LYS
1	A	178	ARG
1	A	207	ILE

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Mol	Chain	Res	Type
1	A	211	SER
1	A	213	THR
1	A	218	THR
1	A	238	ASN
1	A	245	LEU
1	A	247	LYS
1	A	254	THR
1	A	257	ILE
1	A	267	VAL
1	A	275	GLN
1	A	278	LEU
1	A	291	THR
1	A	294	SER
1	A	312	LEU
1	D	10	ILE
1	D	12	ASP
1	D	16	THR
1	D	51	LEU
1	D	53	PHE
1	D	61	ARG
1	D	81	GLU
1	D	109	VAL
1	D	124	THR
1	D	136	THR
1	D	141	LEU
1	D	147	LYS
1	D	148	VAL
1	D	162	GLU
1	D	165	THR
1	D	168	VAL
1	D	169	LYS
1	D	178	ARG
1	D	207	ILE
1	D	211	SER
1	D	213	THR
1	D	218	THR
1	D	238	ASN
1	D	245	LEU
1	D	247	LYS
1	D	254	THR
1	D	257	ILE
1	D	267	VAL

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Mol	Chain	Res	Type
1	D	275	GLN
1	D	278	LEU
1	D	291	THR
1	D	294	SER
1	D	312	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	18	ASN
1	E	244	ASN
1	B	18	ASN
1	C	18	ASN
1	A	234	HIS
1	D	18	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 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
3	LMT	E	402	-	11,11,36	0.11	0	10,10,47	0.63	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
3	LMT	E	402	-	-	0/9/9/61	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	402	LMT	1	0

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	310/318 (97%)	1.01	48 (15%) 5 5	33, 58, 97, 129	0
1	B	310/318 (97%)	1.07	48 (15%) 5 5	31, 62, 104, 128	0
1	C	310/318 (97%)	1.01	57 (18%) 3 4	33, 61, 108, 140	0
1	D	310/318 (97%)	1.21	65 (20%) 2 3	30, 65, 116, 150	0
1	E	310/318 (97%)	0.92	48 (15%) 5 5	31, 59, 105, 142	0
All	All	1550/1590 (97%)	1.04	266 (17%) 4 4	30, 61, 109, 150	0

All (266) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	59	GLY	11.6
1	D	59	GLY	10.9
1	D	60	VAL	9.7
1	D	194	PHE	8.8
1	A	59	GLY	8.6
1	B	60	VAL	8.1
1	D	58	SER	7.7
1	D	64	THR	7.7
1	C	148	VAL	7.6
1	D	55	PRO	7.2
1	C	152	ASP	7.1
1	D	144	ASP	6.9
1	D	65	TYR	6.5
1	D	11	ALA	6.4
1	A	316	PHE	6.1
1	B	316	PHE	5.8
1	B	58	SER	5.8
1	B	61	ARG	5.7
1	A	315	GLY	5.6
1	E	61	ARG	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	153	ASP	5.5
1	D	54	ASP	5.5
1	E	60	VAL	5.5
1	E	316	PHE	5.5
1	C	90	ASP	5.4
1	E	250	TYR	5.4
1	A	11	ALA	5.3
1	B	315	GLY	5.2
1	B	11	ALA	5.2
1	C	56	VAL	5.2
1	D	248	ALA	5.2
1	C	84	ARG	5.2
1	E	148	VAL	5.1
1	D	7	PRO	5.1
1	D	14	PRO	5.1
1	A	7	PRO	5.1
1	B	250	TYR	5.0
1	D	67	PRO	5.0
1	D	56	VAL	4.9
1	A	61	ARG	4.9
1	A	204	MET	4.9
1	D	250	TYR	4.8
1	A	56	VAL	4.8
1	B	12	ASP	4.8
1	B	144	ASP	4.8
1	C	251	MET	4.7
1	C	55	PRO	4.7
1	A	153	ASP	4.6
1	D	179	LEU	4.6
1	D	61	ARG	4.5
1	E	14	PRO	4.5
1	D	148	VAL	4.5
1	E	11	ALA	4.5
1	C	11	ALA	4.4
1	C	144	ASP	4.4
1	D	12	ASP	4.4
1	D	66	GLU	4.3
1	A	83	ALA	4.3
1	D	147	LYS	4.3
1	E	315	GLY	4.3
1	B	251	MET	4.3
1	C	248	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	82	ASN	4.3
1	E	83	ALA	4.2
1	C	13	GLU	4.2
1	A	60	VAL	4.1
1	E	87	ASP	4.1
1	B	14	PRO	4.1
1	D	13	GLU	4.0
1	D	198	PRO	4.0
1	C	315	GLY	4.0
1	E	55	PRO	4.0
1	E	84	ARG	4.0
1	C	250	TYR	4.0
1	B	82	ASN	3.9
1	E	82	ASN	3.9
1	B	56	VAL	3.8
1	B	13	GLU	3.8
1	C	91	ILE	3.8
1	E	248	ALA	3.8
1	A	12	ASP	3.8
1	E	56	VAL	3.8
1	A	84	ARG	3.8
1	E	63	LYS	3.7
1	D	82	ASN	3.7
1	C	7	PRO	3.7
1	C	87	ASP	3.6
1	C	65	TYR	3.6
1	E	94	SER	3.6
1	D	136	THR	3.6
1	E	184	ASP	3.6
1	B	55	PRO	3.5
1	C	83	ALA	3.5
1	A	250	TYR	3.5
1	C	12	ASP	3.5
1	C	149	GLY	3.5
1	D	84	ARG	3.5
1	C	58	SER	3.5
1	B	135	ASP	3.5
1	E	193	TYR	3.5
1	B	283	GLN	3.5
1	B	84	ARG	3.5
1	E	62	VAL	3.4
1	C	194	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	58	SER	3.4
1	D	193	TYR	3.4
1	D	137	ARG	3.4
1	E	58	SER	3.4
1	E	12	ASP	3.4
1	C	281	GLU	3.4
1	E	54	ASP	3.4
1	A	55	PRO	3.4
1	D	62	VAL	3.3
1	D	185	TYR	3.3
1	B	194	PHE	3.3
1	C	18	ASN	3.3
1	C	316	PHE	3.3
1	C	60	VAL	3.3
1	A	184	ASP	3.3
1	C	147	LYS	3.3
1	E	13	GLU	3.3
1	D	49	ARG	3.3
1	E	194	PHE	3.3
1	A	205	LEU	3.3
1	D	135	ASP	3.2
1	C	146	GLU	3.2
1	C	143	VAL	3.2
1	D	316	PHE	3.2
1	A	152	ASP	3.2
1	A	145	LEU	3.2
1	E	79	ASN	3.1
1	C	63	LYS	3.1
1	A	53	PHE	3.1
1	B	54	ASP	3.1
1	B	136	THR	3.1
1	C	136	THR	3.1
1	E	49	ARG	3.0
1	C	49	ARG	3.0
1	D	53	PHE	3.0
1	C	101	TYR	3.0
1	A	185	TYR	3.0
1	B	62	VAL	3.0
1	E	7	PRO	3.0
1	B	177	ASP	3.0
1	D	201	ILE	3.0
1	A	148	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	54	ASP	2.9
1	C	179	LEU	2.9
1	B	69	ALA	2.9
1	E	139	ILE	2.9
1	D	197	ILE	2.9
1	B	184	ASP	2.9
1	E	47	LYS	2.9
1	D	141	LEU	2.9
1	B	7	PRO	2.9
1	A	95	PRO	2.9
1	C	82	ASN	2.9
1	A	251	MET	2.9
1	D	184	ASP	2.8
1	E	68	GLU	2.8
1	E	205	LEU	2.8
1	B	65	TYR	2.8
1	D	10	ILE	2.8
1	C	153	ASP	2.8
1	C	14	PRO	2.8
1	E	59	GLY	2.8
1	C	10	ILE	2.8
1	C	86	ALA	2.8
1	D	90	ASP	2.8
1	D	47	LYS	2.8
1	B	85	ASP	2.7
1	C	64	THR	2.7
1	E	57	ARG	2.7
1	A	51	LEU	2.7
1	A	66	GLU	2.7
1	A	47	LYS	2.7
1	C	145	LEU	2.7
1	B	10	ILE	2.7
1	A	146	GLU	2.7
1	A	135	ASP	2.6
1	E	147	LYS	2.6
1	D	9	PRO	2.6
1	D	247	LYS	2.6
1	C	103	GLU	2.6
1	E	65	TYR	2.6
1	B	137	ARG	2.6
1	E	249	PRO	2.6
1	E	69	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	116	ARG	2.6
1	E	144	ASP	2.6
1	C	85	ASP	2.6
1	D	176	GLU	2.6
1	B	169	LYS	2.6
1	C	61	ARG	2.6
1	A	186	GLN	2.6
1	C	57	ARG	2.6
1	B	245	LEU	2.5
1	C	141	LEU	2.5
1	E	10	ILE	2.5
1	C	177	ASP	2.5
1	D	74	GLU	2.5
1	D	70	ILE	2.5
1	D	315	GLY	2.5
1	D	91	ILE	2.5
1	A	246	PRO	2.5
1	B	83	ALA	2.5
1	A	26	CYS	2.5
1	A	248	ALA	2.5
1	D	139	ILE	2.5
1	E	53	PHE	2.5
1	E	247	LYS	2.5
1	D	57	ARG	2.5
1	A	94	SER	2.4
1	E	135	ASP	2.4
1	B	32	LYS	2.4
1	B	57	ARG	2.4
1	B	116	ARG	2.4
1	C	47	LYS	2.4
1	A	57	ARG	2.4
1	C	100	GLN	2.4
1	A	192	GLN	2.4
1	B	66	GLU	2.4
1	D	145	LEU	2.4
1	E	128	TYR	2.4
1	B	248	ALA	2.3
1	D	175	LEU	2.3
1	D	221	GLU	2.3
1	B	31	ASP	2.3
1	B	139	ILE	2.3
1	A	245	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	63	LYS	2.3
1	E	88	VAL	2.3
1	D	95	PRO	2.3
1	A	259	PHE	2.3
1	D	283	GLN	2.3
1	D	93	VAL	2.3
1	B	74	GLU	2.2
1	C	151	ASN	2.2
1	A	10	ILE	2.2
1	A	49	ARG	2.2
1	B	207	ILE	2.2
1	E	136	THR	2.2
1	E	145	LEU	2.2
1	D	183	LEU	2.2
1	B	247	LYS	2.2
1	D	246	PRO	2.2
1	A	209	PHE	2.2
1	D	96	ASP	2.2
1	C	68	GLU	2.1
1	C	135	ASP	2.1
1	D	143	VAL	2.1
1	A	128	TYR	2.1
1	B	152	ASP	2.1
1	A	52	ALA	2.1
1	D	203	PRO	2.1
1	E	15	LEU	2.1
1	A	161	ILE	2.1
1	D	87	ASP	2.1
1	D	202	LEU	2.1
1	B	145	LEU	2.1
1	C	137	ARG	2.0
1	C	247	LYS	2.0
1	B	244	ASN	2.0
1	C	196	TYR	2.0
1	A	14	PRO	2.0
1	C	88	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
4	NA	C	401	1/1	0.57	0.52	63,63,63,63	0
4	NA	B	403	1/1	0.64	0.35	63,63,63,63	0
4	NA	D	401	1/1	0.73	0.39	50,50,50,50	0
4	NA	A	401	1/1	0.77	0.34	56,56,56,56	0
3	LMT	E	402	12/35	0.80	0.34	25,34,56,60	0
2	CL	E	401	1/1	0.87	0.11	67,67,67,67	0
4	NA	B	401	1/1	0.88	0.32	55,55,55,55	0
2	CL	B	402	1/1	0.92	0.09	66,66,66,66	0
2	CL	C	402	1/1	0.93	0.08	65,65,65,65	0
2	CL	D	402	1/1	0.93	0.10	63,63,63,63	0
2	CL	A	402	1/1	0.96	0.06	63,63,63,63	0

6.5 Other polymers ⓘ

There are no such residues in this entry.