



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:44 PM EDT

PDB ID : 3UU3 / pdb_00003uu3
Title : The GLIC pentameric Ligand-Gated Ion Channel Loop2-20' oxidized mutant in a locally-closed conformation (LC1 subtype)
Authors : Sauguet, L.; Nury, H.; Corringer, P.J.; Delarue, M.
Deposited on : 2011-11-28
Resolution : 3.15 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

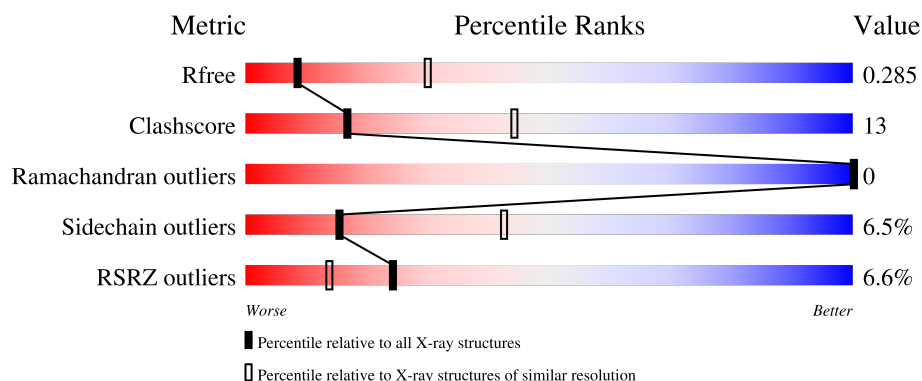
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	5% 65% 28% • 5%
1	B	321	6% 62% 30% • 5%
1	C	321	7% 61% 32% • 5%
1	D	321	8% 61% 31% • 5%
1	E	321	6% 59% 32% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12438 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	305	Total	C	N	O	S	0	0	0
			2480	1637	397	442	4			
1	B	305	Total	C	N	O	S	0	0	0
			2480	1637	397	442	4			
1	C	306	Total	C	N	O	S	0	0	0
			2486	1640	398	444	4			
1	D	306	Total	C	N	O	S	0	0	0
			2486	1640	398	444	4			
1	E	305	Total	C	N	O	S	0	0	0
			2480	1637	397	442	4			

There are 40 discrepancies between the modelled and reference sequences:

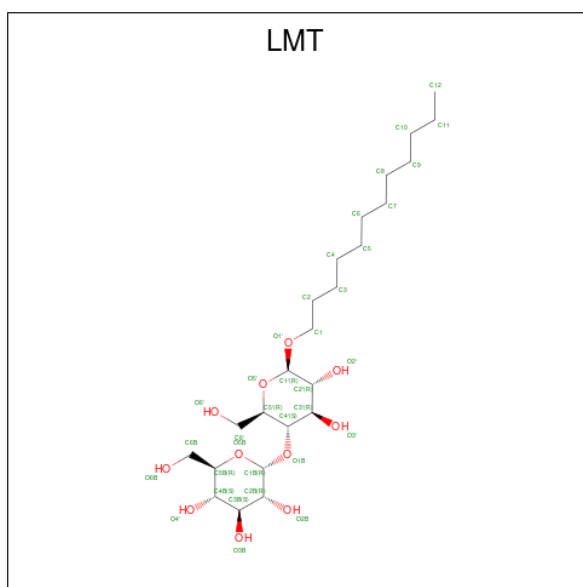
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q7NDN8
A	-2	SER	-	expression tag	UNP Q7NDN8
A	-1	ALA	-	expression tag	UNP Q7NDN8
A	0	ALA	-	expression tag	UNP Q7NDN8
A	1	ALA	-	expression tag	UNP Q7NDN8
A	27	SER	CYS	engineered mutation	UNP Q7NDN8
A	33	CYS	LYS	engineered mutation	UNP Q7NDN8
A	244	CYS	THR	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	244	CYS	THR	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

Continued on next page...

Continued from previous page...

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	244	CYS	THR	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	244	CYS	THR	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	244	CYS	THR	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	B	1	Total C 12 12	0	0

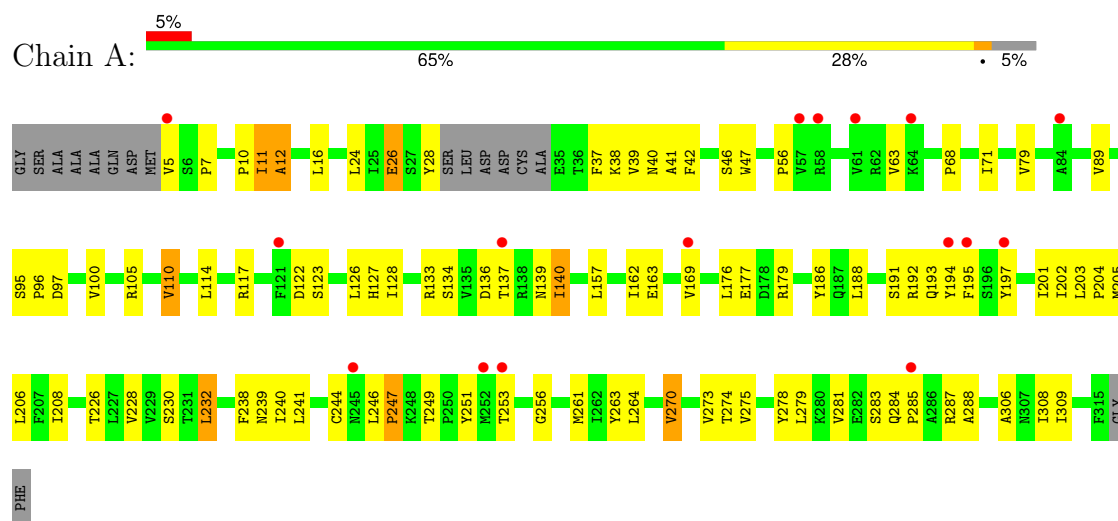
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	O 2	0	0
3	B	4	Total 4	O 4	0	0
3	C	4	Total 4	O 4	0	0
3	D	2	Total 2	O 2	0	0
3	E	2	Total 2	O 2	0	0

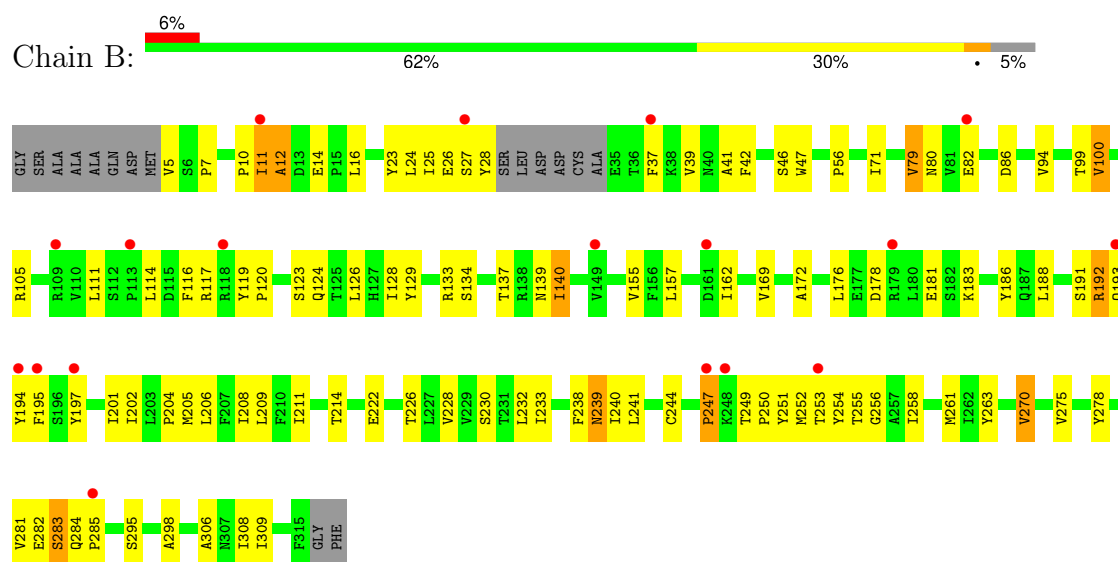
3 Residue-property plots [i](#)

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

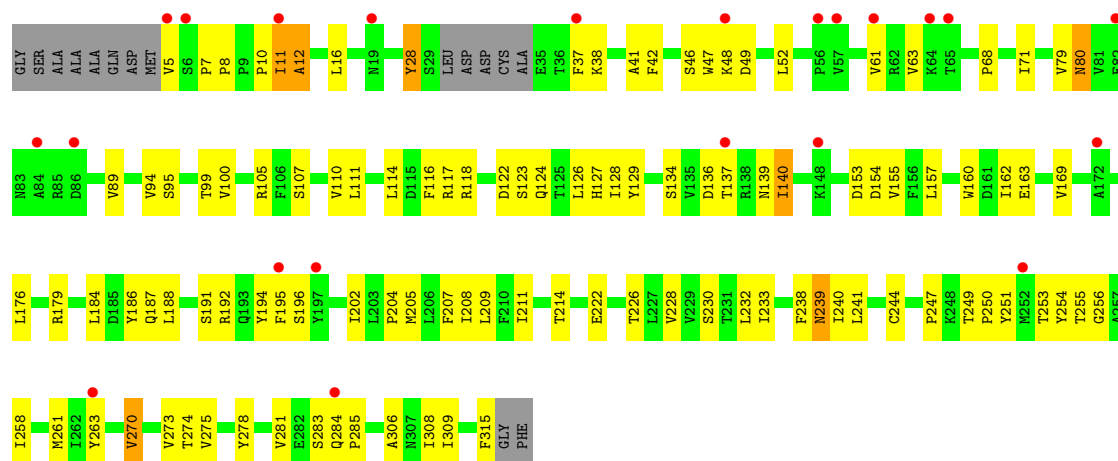


• Molecule 1: Glr4197 protein

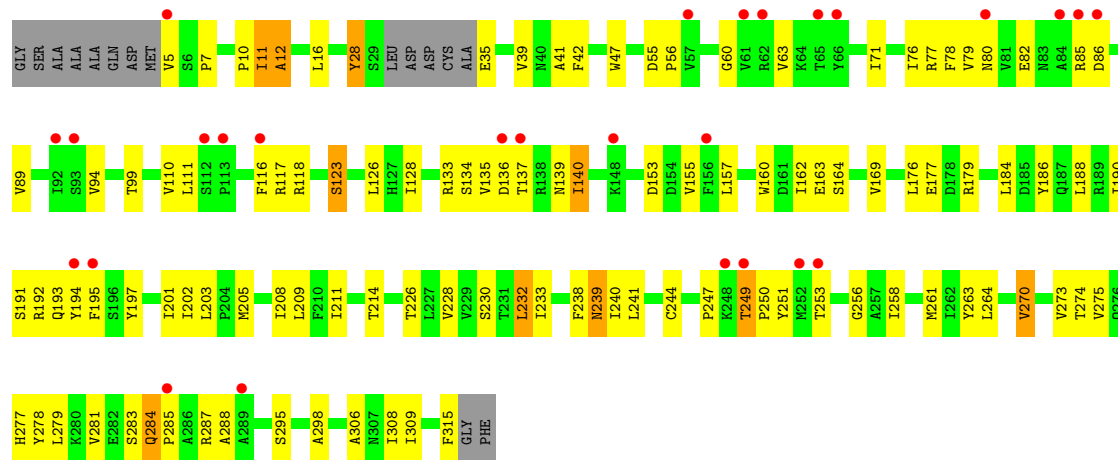


• Molecule 1: Glr4197 protein

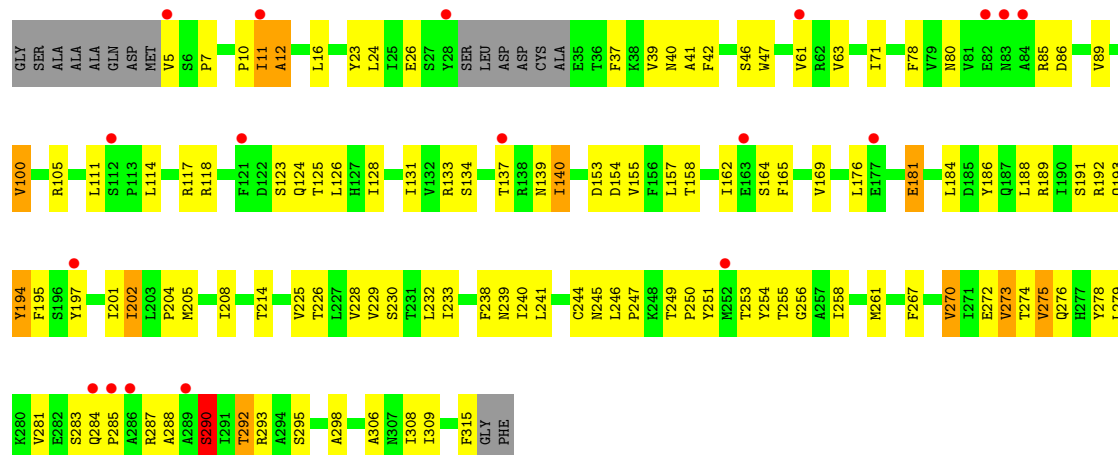




• Molecule 1: Glr4197 protein



• 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	181.62Å 134.23Å 160.05Å 90.00° 102.47° 90.00°	Depositor
Resolution (Å)	28.17 – 3.15 28.17 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.1 (28.17-3.15) 98.9 (28.17-3.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.248 , 0.272 0.259 , 0.285	Depositor DCC
R_{free} test set	3201 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	95.0	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 88.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12438	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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

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	0.84	1/2547 (0.0%)	1.34	19/3481 (0.5%)
1	B	0.86	0/2547	1.31	20/3481 (0.6%)
1	C	0.86	1/2553 (0.0%)	1.38	23/3489 (0.7%)
1	D	0.86	2/2553 (0.1%)	1.38	21/3489 (0.6%)
1	E	0.84	0/2547	1.33	23/3481 (0.7%)
All	All	0.85	4/12747 (0.0%)	1.35	106/17421 (0.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	193	GLN	CA-C	6.06	1.58	1.53
1	D	80	ASN	CA-C	5.12	1.59	1.53
1	C	239	ASN	CA-C	5.05	1.59	1.52
1	A	193	GLN	CA-C	5.04	1.58	1.53

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	PRO	N-CA-C	8.52	124.42	111.14
1	A	12	ALA	N-CA-C	-8.04	97.80	108.34
1	D	12	ALA	N-CA-C	-7.83	98.09	108.34
1	C	12	ALA	N-CA-C	-7.79	98.13	108.34
1	D	28	TYR	N-CA-C	7.72	118.07	107.73
1	E	12	ALA	N-CA-C	-7.70	98.25	108.34
1	B	195	PHE	N-CA-C	7.61	121.49	111.75
1	B	12	ALA	N-CA-C	-7.60	98.39	108.34
1	B	194	TYR	N-CA-C	7.60	120.44	111.71
1	A	195	PHE	N-CA-C	7.54	121.40	111.75
1	D	249	THR	N-CA-C	7.54	118.84	109.57
1	D	195	PHE	N-CA-C	7.53	121.39	111.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	195	PHE	N-CA-C	7.49	121.33	111.75
1	A	194	TYR	N-CA-C	7.44	120.26	111.71
1	E	154	ASP	CA-CB-CG	7.26	119.86	112.60
1	C	37	PHE	N-CA-C	7.24	121.00	108.76
1	D	194	TYR	N-CA-C	7.13	119.91	111.71
1	C	110	VAL	N-CA-CB	6.86	118.63	110.95
1	C	194	TYR	N-CA-C	6.80	119.53	111.71
1	A	97	ASP	CA-CB-CG	6.75	119.35	112.60
1	D	192	ARG	N-CA-C	6.64	119.29	110.53
1	D	247	PRO	N-CA-C	6.63	121.75	111.21
1	E	194	TYR	N-CA-C	6.53	119.22	111.71
1	D	41	ALA	N-CA-C	6.48	117.68	108.74
1	A	37	PHE	N-CA-C	6.48	120.06	109.24
1	B	12	ALA	CA-C-N	6.48	133.04	120.99
1	B	12	ALA	C-N-CA	6.48	133.04	120.99
1	B	37	PHE	N-CA-C	6.38	119.90	109.24
1	C	61	VAL	CA-C-N	6.36	128.71	120.44
1	C	61	VAL	C-N-CA	6.36	128.71	120.44
1	E	247	PRO	N-CA-C	6.36	121.06	111.14
1	D	12	ALA	CA-C-N	6.28	132.66	120.99
1	D	12	ALA	C-N-CA	6.28	132.66	120.99
1	E	41	ALA	N-CA-C	6.19	117.28	108.74
1	C	12	ALA	CA-C-N	6.18	132.49	120.99
1	C	12	ALA	C-N-CA	6.18	132.49	120.99
1	E	37	PHE	N-CA-C	6.02	119.29	109.24
1	C	247	PRO	N-CA-C	6.01	120.66	111.11
1	C	11	ILE	CB-CA-C	6.00	119.88	112.02
1	B	11	ILE	CA-C-N	5.91	132.08	122.39
1	B	11	ILE	C-N-CA	5.91	132.08	122.39
1	A	247	PRO	N-CA-C	5.90	120.58	111.21
1	D	11	ILE	CB-CA-C	5.83	120.02	112.14
1	E	11	ILE	CB-CA-C	5.82	119.99	112.14
1	D	110	VAL	N-CA-CB	5.77	117.23	110.82
1	E	292	THR	N-CA-C	-5.71	105.06	111.28
1	B	41	ALA	N-CA-C	5.69	116.59	108.74
1	C	41	ALA	N-CA-C	5.69	116.59	108.74
1	A	11	ILE	CA-C-N	5.68	131.70	122.39
1	A	11	ILE	C-N-CA	5.68	131.70	122.39
1	D	42	PHE	CA-CB-CG	5.65	119.45	113.80
1	D	11	ILE	CA-C-N	5.63	131.62	122.39
1	D	11	ILE	C-N-CA	5.63	131.62	122.39
1	A	42	PHE	CA-CB-CG	5.62	119.42	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	202	ILE	N-CA-C	5.57	116.35	110.72
1	B	11	ILE	CB-CA-C	5.55	119.64	112.14
1	E	169	VAL	N-CA-C	5.55	116.95	110.62
1	E	11	ILE	CA-C-N	5.53	131.46	122.39
1	E	11	ILE	C-N-CA	5.53	131.46	122.39
1	E	12	ALA	CA-C-N	5.53	132.10	121.54
1	E	12	ALA	C-N-CA	5.53	132.10	121.54
1	C	11	ILE	CA-C-N	5.53	131.46	122.39
1	C	11	ILE	C-N-CA	5.53	131.46	122.39
1	D	28	TYR	CA-C-N	5.53	131.65	121.70
1	D	28	TYR	C-N-CA	5.53	131.65	121.70
1	D	169	VAL	N-CA-C	5.52	116.91	110.62
1	E	42	PHE	CA-CB-CG	5.51	119.31	113.80
1	E	290	SER	N-CA-C	5.45	116.90	111.07
1	A	169	VAL	N-CA-C	5.44	116.83	110.62
1	B	42	PHE	CA-CB-CG	5.42	119.22	113.80
1	B	169	VAL	N-CA-C	5.39	116.77	110.62
1	A	41	ALA	N-CA-C	5.39	116.18	108.74
1	E	89	VAL	N-CA-CB	5.38	116.39	110.53
1	B	79	VAL	CA-C-N	-5.37	114.83	122.77
1	B	79	VAL	C-N-CA	-5.37	114.83	122.77
1	C	202	ILE	N-CA-C	5.35	116.13	110.72
1	E	80	ASN	N-CA-C	5.35	117.88	108.56
1	A	202	ILE	N-CA-C	5.34	116.12	110.72
1	D	164	SER	N-CA-C	5.30	117.12	109.07
1	A	110	VAL	N-CA-CB	5.29	116.69	110.82
1	C	42	PHE	CA-CB-CG	5.29	119.09	113.80
1	C	154	ASP	CA-CB-CG	5.23	117.83	112.60
1	D	89	VAL	N-CA-CB	5.22	116.22	110.53
1	C	80	ASN	N-CA-C	5.21	117.44	109.62
1	C	28	TYR	N-CA-C	5.21	116.20	108.60
1	A	89	VAL	N-CA-CB	5.16	116.15	110.53
1	D	202	ILE	N-CA-C	5.14	115.91	110.72
1	E	164	SER	CA-C-N	5.13	129.62	121.72
1	E	164	SER	C-N-CA	5.13	129.62	121.72
1	C	169	VAL	N-CA-C	5.12	116.45	110.62
1	E	61	VAL	CA-C-N	5.11	127.54	120.29
1	E	61	VAL	C-N-CA	5.11	127.54	120.29
1	C	68	PRO	CA-C-N	5.10	127.12	120.28
1	C	68	PRO	C-N-CA	5.10	127.12	120.28
1	E	225	VAL	N-CA-C	-5.10	105.52	110.42
1	B	14	GLU	N-CA-C	5.10	116.93	109.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	ARG	N-CA-C	5.08	117.99	110.48
1	C	89	VAL	N-CA-CB	5.06	116.05	110.53
1	B	56	PRO	CA-C-N	5.05	126.92	120.56
1	B	56	PRO	C-N-CA	5.05	126.92	120.56
1	A	68	PRO	CA-C-N	5.04	127.03	120.28
1	A	68	PRO	C-N-CA	5.04	127.03	120.28
1	A	127	HIS	N-CA-C	5.02	117.16	109.07
1	A	26	GLU	CA-C-N	5.01	129.78	121.86
1	A	26	GLU	C-N-CA	5.01	129.78	121.86
1	B	202	ILE	N-CA-C	5.01	115.78	110.72

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	2480	0	2500	59	0
1	B	2480	0	2500	87	0
1	C	2486	0	2505	77	0
1	D	2486	0	2505	88	0
1	E	2480	0	2500	63	0
2	B	12	0	23	5	0
3	A	2	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
All	All	12438	0	12533	319	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 13.

All (319) 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:C:10:PRO:HB2	1:C:12:ALA:O	1.57	1.05
1:E:10:PRO:HB2	1:E:12:ALA:O	1.57	1.05
1:D:10:PRO:HB2	1:D:12:ALA:O	1.58	1.04
1:A:10:PRO:HB2	1:A:12:ALA:O	1.57	1.02
1:B:10:PRO:HB2	1:B:12:ALA:O	1.59	1.02
1:D:135:VAL:HA	1:D:179:ARG:HH12	1.29	0.97
1:B:283:SER:C	1:B:285:PRO:HD3	1.92	0.94
1:A:253:THR:HG23	1:A:256:GLY:H	1.34	0.93
1:D:283:SER:C	1:D:285:PRO:HD3	1.96	0.91
1:A:240:ILE:HG13	1:E:241:LEU:HD23	1.54	0.89
1:D:136:ASP:CG	1:D:179:ARG:NH2	2.32	0.87
1:B:117:ARG:HG3	1:B:251:TYR:CE1	2.09	0.86
1:B:253:THR:HG23	1:B:256:GLY:H	1.38	0.86
1:D:76:ILE:O	1:D:85:ARG:NH2	2.09	0.86
1:B:25:ILE:HG22	1:B:26:GLU:HG2	1.58	0.83
1:A:26:GLU:HB2	1:A:40:ASN:HB3	1.60	0.83
1:B:205:MET:HE3	1:B:238:PHE:HD1	1.44	0.83
1:D:205:MET:HE3	1:D:238:PHE:HD1	1.45	0.82
1:E:205:MET:HE3	1:E:238:PHE:HD1	1.44	0.82
1:C:205:MET:HE3	1:C:238:PHE:HD1	1.45	0.81
1:D:78:PHE:CD2	1:D:85:ARG:HD3	2.15	0.81
1:A:205:MET:HE3	1:A:238:PHE:HD1	1.45	0.81
1:B:26:GLU:OE2	1:C:80:ASN:HA	1.81	0.81
1:B:116:PHE:N	1:B:251:TYR:OH	2.13	0.80
1:C:122:ASP:OD1	1:C:192:ARG:NH1	2.16	0.78
1:C:283:SER:C	1:C:285:PRO:HD3	2.10	0.77
1:B:278:TYR:O	1:B:281:VAL:HG12	1.85	0.76
1:C:241:LEU:HD23	1:D:240:ILE:HG13	1.68	0.76
1:E:283:SER:C	1:E:285:PRO:HD3	2.11	0.76
1:C:48:LYS:HG2	1:C:99:THR:OG1	1.86	0.75
1:D:135:VAL:HA	1:D:179:ARG:NH1	2.00	0.75
1:B:117:ARG:HG3	1:B:251:TYR:HE1	1.51	0.74
1:B:284:GLN:N	1:B:285:PRO:HD3	2.01	0.74
1:D:78:PHE:CE2	1:D:85:ARG:NH1	2.54	0.74
1:B:241:LEU:HD23	1:C:240:ILE:HG13	1.67	0.74
1:A:122:ASP:OD1	1:A:192:ARG:NH1	2.20	0.74
1:C:111:LEU:HD23	1:C:111:LEU:O	1.89	0.73
1:B:24:LEU:HD22	1:B:39:VAL:HG21	1.70	0.73
1:D:241:LEU:HD23	1:E:240:ILE:HG13	1.72	0.72
1:A:283:SER:C	1:A:285:PRO:HD3	2.15	0.72
1:E:245:ASN:O	1:E:246:LEU:HD23	1.91	0.71
1:E:284:GLN:N	1:E:285:PRO:HD3	2.05	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:GLN:N	1:C:285:PRO:HD3	2.06	0.70
1:D:78:PHE:HD2	1:D:85:ARG:HD3	1.53	0.70
1:D:162:ILE:HA	1:D:190:ILE:HG22	1.74	0.69
1:D:278:TYR:O	1:D:281:VAL:HG12	1.92	0.69
1:A:241:LEU:HD23	1:B:240:ILE:HG13	1.75	0.69
1:C:116:PHE:N	1:C:251:TYR:OH	2.26	0.68
1:D:116:PHE:HB2	1:D:249:THR:HG21	1.73	0.68
1:B:26:GLU:OE2	1:C:80:ASN:CA	2.42	0.67
1:D:78:PHE:HE2	1:D:85:ARG:HH11	1.41	0.67
1:D:126:LEU:HB2	1:D:188:LEU:HB3	1.77	0.67
1:B:111:LEU:O	1:B:111:LEU:HD23	1.95	0.67
1:C:278:TYR:O	1:C:281:VAL:HG12	1.94	0.67
1:B:117:ARG:HG3	1:B:251:TYR:CD1	2.28	0.67
1:A:24:LEU:HD22	1:A:39:VAL:HG21	1.77	0.66
1:A:176:LEU:HD11	1:E:23:TYR:CE2	2.30	0.66
1:E:278:TYR:O	1:E:281:VAL:HG12	1.97	0.65
1:B:214:THR:HB	1:C:274:THR:HG21	1.79	0.65
1:D:136:ASP:OD1	1:D:179:ARG:NH2	2.28	0.65
1:D:176:LEU:HD23	1:D:177:GLU:HG3	1.79	0.65
1:C:214:THR:HB	1:D:274:THR:HG21	1.77	0.65
1:E:287:ARG:HA	1:E:290:SER:OG	1.97	0.64
1:B:172:ALA:HB3	1:B:183:LYS:HB3	1.78	0.64
1:A:117:ARG:HG3	1:A:251:TYR:HE1	1.62	0.64
1:A:284:GLN:N	1:A:285:PRO:HD3	2.13	0.64
1:D:176:LEU:CD2	1:D:177:GLU:HG3	2.29	0.63
1:C:28:TYR:CG	1:D:111:LEU:HD11	2.34	0.62
1:D:55:ASP:OD1	1:D:56:PRO:HD2	2.00	0.62
1:B:23:TYR:CE2	1:C:176:LEU:HD21	2.35	0.62
1:C:114:LEU:HD23	1:C:124:GLN:HG3	1.82	0.61
1:E:46:SER:HA	1:E:100:VAL:O	2.01	0.61
1:C:28:TYR:CD2	1:D:111:LEU:HD11	2.35	0.61
1:A:284:GLN:HE22	1:A:287:ARG:HH21	1.50	0.60
2:B:318:LMT:H121	1:D:233:ILE:HG21	1.82	0.60
1:E:111:LEU:O	1:E:111:LEU:HD23	2.00	0.60
1:B:25:ILE:HG22	1:B:26:GLU:CG	2.30	0.60
1:D:157:LEU:HD23	1:D:190:ILE:HD13	1.84	0.59
1:D:116:PHE:HD2	1:D:249:THR:CG2	2.15	0.59
1:A:279:LEU:HD12	1:A:288:ALA:HA	1.84	0.59
1:B:28:TYR:CE2	1:C:111:LEU:HD11	2.37	0.59
1:D:136:ASP:CG	1:D:179:ARG:HH22	2.06	0.59
1:D:78:PHE:CE2	1:D:85:ARG:HD3	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:TYR:CZ	1:B:258:ILE:HD11	2.37	0.58
1:C:196:SER:HB3	1:D:250:PRO:O	2.04	0.58
1:A:253:THR:HG23	1:A:256:GLY:N	2.12	0.58
1:A:274:THR:HG21	1:E:214:THR:HB	1.85	0.58
1:B:253:THR:HG23	1:B:256:GLY:N	2.16	0.58
1:B:28:TYR:CD2	1:C:111:LEU:HD11	2.39	0.57
1:D:28:TYR:CD2	1:E:111:LEU:HD11	2.38	0.57
1:B:27:SER:OG	1:B:155:VAL:HG13	2.03	0.57
1:C:8:PRO:HB3	1:C:49:ASP:OD2	2.04	0.57
1:D:111:LEU:HD23	1:D:111:LEU:O	2.05	0.56
1:D:157:LEU:CD2	1:D:190:ILE:HD13	2.36	0.56
1:D:35:GLU:OE1	1:D:160:TRP:HZ2	1.89	0.56
1:B:25:ILE:HD13	1:B:105:ARG:CZ	2.36	0.56
1:A:208:ILE:HG12	1:B:232:LEU:HD21	1.89	0.55
1:D:28:TYR:CG	1:E:111:LEU:HD11	2.42	0.55
1:D:117:ARG:HG3	1:D:251:TYR:CD1	2.42	0.55
1:B:114:LEU:HD23	1:B:124:GLN:HG3	1.88	0.55
1:E:226:THR:O	1:E:230:SER:HB2	2.07	0.55
1:B:117:ARG:CG	1:B:251:TYR:CD1	2.91	0.54
1:C:254:TYR:CZ	1:C:258:ILE:HD11	2.43	0.54
1:D:253:THR:HG23	1:D:256:GLY:HA3	1.89	0.54
1:C:208:ILE:HG12	1:D:232:LEU:HD21	1.89	0.54
1:A:79:VAL:HA	1:E:105:ARG:HH22	1.73	0.54
1:A:26:GLU:OE1	1:B:111:LEU:HD22	2.08	0.54
1:B:46:SER:HA	1:B:100:VAL:O	2.08	0.54
1:B:283:SER:CA	1:B:285:PRO:HD3	2.38	0.54
1:C:127:HIS:HB3	1:C:129:TYR:CE2	2.42	0.54
1:E:254:TYR:CZ	1:E:258:ILE:HD11	2.43	0.54
1:C:28:TYR:CE1	1:C:38:LYS:HD3	2.42	0.53
1:C:226:THR:O	1:C:230:SER:HB2	2.08	0.53
1:B:247:PRO:HB2	1:B:249:THR:HG22	1.88	0.53
1:C:46:SER:HA	1:C:100:VAL:O	2.08	0.53
1:D:226:THR:O	1:D:230:SER:HB2	2.09	0.53
1:C:48:LYS:HA	1:C:99:THR:HA	1.91	0.53
1:A:226:THR:O	1:A:230:SER:HB2	2.09	0.52
1:C:284:GLN:N	1:C:285:PRO:CD	2.73	0.52
1:A:63:VAL:HG22	1:A:95:SER:HA	1.92	0.52
1:E:197:TYR:CD1	1:E:201:ILE:HD13	2.45	0.52
1:B:23:TYR:CZ	1:C:176:LEU:HD11	2.45	0.51
1:B:79:VAL:HB	1:B:129:TYR:HB2	1.93	0.51
1:B:80:ASN:ND2	1:B:111:LEU:O	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:THR:O	1:B:230:SER:HB2	2.11	0.51
1:D:176:LEU:HD23	1:D:176:LEU:C	2.36	0.51
1:A:56:PRO:HD3	1:A:96:PRO:HB3	1.93	0.51
1:A:117:ARG:HG3	1:A:251:TYR:CE1	2.42	0.51
1:B:283:SER:HA	1:B:285:PRO:HD3	1.91	0.51
1:B:233:ILE:HG21	2:B:318:LMT:H111	1.93	0.50
1:C:253:THR:HB	1:C:256:GLY:H	1.76	0.50
1:C:52:LEU:HB3	1:C:94:VAL:HG11	1.93	0.50
1:A:28:TYR:CG	1:B:111:LEU:HD11	2.47	0.50
1:D:117:ARG:HG3	1:D:251:TYR:CE1	2.47	0.49
1:D:283:SER:CA	1:D:285:PRO:HD3	2.43	0.49
1:E:284:GLN:N	1:E:285:PRO:CD	2.73	0.49
1:D:157:LEU:HD23	1:D:190:ILE:CD1	2.41	0.49
1:D:283:SER:HA	1:D:285:PRO:HD3	1.94	0.49
1:D:16:LEU:HD11	1:D:47:TRP:HB2	1.94	0.49
1:A:176:LEU:HD23	1:A:177:GLU:HG3	1.94	0.48
1:A:278:TYR:O	1:A:281:VAL:HG12	2.13	0.48
1:B:119:TYR:HE1	1:B:192:ARG:CZ	2.26	0.48
1:B:16:LEU:HD11	1:B:47:TRP:HB2	1.96	0.48
1:B:26:GLU:OE2	1:C:79:VAL:C	2.56	0.48
1:C:117:ARG:HG3	1:C:251:TYR:CE1	2.48	0.48
1:B:117:ARG:CG	1:B:251:TYR:HD1	2.27	0.48
1:B:192:ARG:HG2	1:B:193:GLN:N	2.29	0.48
2:B:318:LMT:H112	1:C:233:ILE:HG21	1.95	0.48
1:C:306:ALA:HA	1:C:309:ILE:HD12	1.96	0.48
1:C:63:VAL:HG22	1:C:95:SER:HA	1.96	0.47
1:A:24:LEU:HD22	1:A:39:VAL:CG2	2.42	0.47
1:B:306:ALA:HA	1:B:309:ILE:HD12	1.96	0.47
1:D:208:ILE:HG12	1:E:232:LEU:HD21	1.96	0.47
1:E:7:PRO:HG2	1:E:137:THR:HG21	1.97	0.47
1:C:123:SER:HA	1:C:191:SER:HA	1.97	0.47
1:D:279:LEU:HB2	1:D:288:ALA:HB2	1.97	0.47
1:C:204:PRO:HB3	1:D:263:TYR:CD1	2.50	0.47
1:B:24:LEU:HD22	1:B:39:VAL:CG2	2.44	0.47
1:C:118:ARG:HD3	1:C:315:PHE:CE1	2.49	0.47
1:D:284:GLN:NE2	1:D:287:ARG:HE	2.12	0.47
1:E:114:LEU:HD23	1:E:124:GLN:HG3	1.96	0.47
1:A:279:LEU:HB2	1:A:288:ALA:HB2	1.96	0.47
1:A:306:ALA:HA	1:A:309:ILE:HD12	1.97	0.47
1:E:306:ALA:HA	1:E:309:ILE:HD12	1.97	0.47
1:D:284:GLN:OE1	1:D:287:ARG:NH2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:LEU:HD11	1:C:47:TRP:HB2	1.96	0.46
1:A:16:LEU:HD11	1:A:47:TRP:HB2	1.96	0.46
1:B:261:MET:HE2	1:B:261:MET:HB3	1.82	0.46
1:A:279:LEU:HD12	1:A:288:ALA:CA	2.45	0.46
2:B:318:LMT:H122	1:E:233:ILE:HG21	1.97	0.46
1:D:284:GLN:HE22	1:D:287:ARG:HE	1.63	0.46
1:A:249:THR:HG22	1:A:251:TYR:CE2	2.50	0.46
1:D:214:THR:HB	1:E:274:THR:HG21	1.97	0.46
1:E:24:LEU:HD21	1:E:165:PHE:CZ	2.50	0.46
1:E:253:THR:HB	1:E:256:GLY:H	1.81	0.46
1:A:46:SER:HA	1:A:100:VAL:O	2.16	0.46
1:A:123:SER:HA	1:A:191:SER:HA	1.97	0.46
1:A:134:SER:HB3	1:A:139:ASN:HA	1.98	0.46
1:D:134:SER:HB3	1:D:139:ASN:HA	1.98	0.46
1:E:123:SER:HA	1:E:191:SER:HA	1.97	0.46
1:E:279:LEU:HB2	1:E:288:ALA:HB2	1.98	0.46
1:E:192:ARG:HG2	1:E:193:GLN:N	2.30	0.46
1:A:228:VAL:CG1	1:A:270:VAL:HG23	2.47	0.45
1:B:228:VAL:CG1	1:B:270:VAL:HG23	2.46	0.45
1:B:283:SER:C	1:B:285:PRO:CD	2.78	0.45
1:C:134:SER:HB3	1:C:139:ASN:HA	1.97	0.45
1:B:133:ARG:NH1	1:B:176:LEU:O	2.47	0.45
1:B:284:GLN:N	1:B:285:PRO:CD	2.68	0.45
1:C:7:PRO:HG2	1:C:137:THR:HG21	1.98	0.45
1:D:133:ARG:CZ	1:D:179:ARG:HB2	2.45	0.45
1:E:16:LEU:HD11	1:E:47:TRP:HB2	1.98	0.45
1:A:126:LEU:HB2	1:A:188:LEU:HB3	1.99	0.45
1:B:23:TYR:CE1	1:C:176:LEU:HD11	2.51	0.45
1:D:205:MET:HE3	1:D:238:PHE:CD1	2.36	0.45
1:B:233:ILE:HG21	2:B:318:LMT:C11	2.47	0.45
1:C:134:SER:HA	1:C:140:ILE:HD12	1.98	0.45
1:D:56:PRO:O	1:D:60:GLY:N	2.44	0.45
1:D:157:LEU:HB2	1:D:162:ILE:HD11	1.99	0.45
1:B:117:ARG:HE	1:B:251:TYR:HD1	1.63	0.45
1:D:118:ARG:HD3	1:D:315:PHE:CE1	2.52	0.45
1:C:117:ARG:HG3	1:C:251:TYR:CD1	2.52	0.45
1:D:283:SER:C	1:D:285:PRO:CD	2.81	0.45
1:A:232:LEU:HD21	1:E:208:ILE:HG12	1.98	0.45
1:A:136:ASP:OD1	1:A:179:ARG:NH2	2.50	0.44
1:A:28:TYR:CD2	1:B:111:LEU:HD11	2.52	0.44
1:A:134:SER:HA	1:A:140:ILE:HD12	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:SER:HA	1:B:140:ILE:HD12	1.99	0.44
1:C:205:MET:HE3	1:C:238:PHE:CD1	2.37	0.44
1:D:306:ALA:HA	1:D:309:ILE:HD12	1.99	0.44
1:E:134:SER:HA	1:E:140:ILE:HD12	1.99	0.44
1:B:208:ILE:HG12	1:C:232:LEU:HD21	1.99	0.44
1:A:204:PRO:HB3	1:B:263:TYR:CD1	2.53	0.44
1:B:204:PRO:HB3	1:C:263:TYR:CD1	2.53	0.44
1:C:196:SER:CB	1:D:250:PRO:O	2.65	0.44
1:C:241:LEU:HD21	1:D:239:ASN:HD22	1.81	0.44
1:E:131:ILE:HG12	1:E:181:GLU:HG2	2.00	0.44
1:A:205:MET:HE3	1:A:238:PHE:CD1	2.37	0.44
1:D:116:PHE:CD2	1:D:249:THR:CG2	2.99	0.44
1:D:134:SER:O	1:D:179:ARG:NH1	2.51	0.44
1:E:24:LEU:HD22	1:E:39:VAL:HG21	2.00	0.44
1:E:118:ARG:HD3	1:E:315:PHE:CE1	2.51	0.44
1:E:228:VAL:CG1	1:E:270:VAL:HG23	2.48	0.44
1:B:123:SER:HA	1:B:191:SER:HA	1.99	0.44
1:C:228:VAL:CG1	1:C:270:VAL:HG23	2.48	0.44
1:D:133:ARG:NH1	1:D:177:GLU:HB2	2.33	0.44
1:B:26:GLU:OE2	1:C:80:ASN:HB3	2.18	0.44
1:B:222:GLU:OE1	1:C:222:GLU:OE2	2.36	0.44
1:D:123:SER:HA	1:D:191:SER:HA	1.99	0.44
1:E:275:VAL:HG12	1:E:276:GLN:N	2.33	0.44
1:A:228:VAL:HG11	1:A:270:VAL:HG23	1.99	0.43
1:B:157:LEU:HB2	1:B:162:ILE:HD11	2.00	0.43
1:E:134:SER:HB3	1:E:139:ASN:HA	2.00	0.43
1:B:249:THR:HA	1:B:250:PRO:HD3	1.87	0.43
1:B:228:VAL:HG11	1:B:270:VAL:HG23	1.99	0.43
1:D:176:LEU:HD23	1:D:177:GLU:N	2.34	0.43
1:E:157:LEU:HB2	1:E:162:ILE:HD11	2.01	0.43
1:E:78:PHE:HE2	1:E:85:ARG:HD3	1.84	0.43
1:A:133:ARG:NH1	1:A:176:LEU:O	2.51	0.43
1:A:197:TYR:CD1	1:A:201:ILE:HD13	2.54	0.43
1:D:136:ASP:OD2	1:D:179:ARG:NH2	2.32	0.43
1:A:157:LEU:HB2	1:A:162:ILE:HD11	2.00	0.43
1:B:7:PRO:HG2	1:B:137:THR:HG21	2.00	0.43
1:C:157:LEU:HB2	1:C:162:ILE:HD11	1.99	0.43
1:C:184:LEU:HD23	1:C:184:LEU:HA	1.92	0.43
1:C:228:VAL:HG11	1:C:270:VAL:HG23	2.01	0.43
1:E:26:GLU:HB2	1:E:40:ASN:HB3	2.00	0.43
1:E:125:THR:HG23	1:E:189:ARG:HG2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:LEU:HD23	1:E:184:LEU:HA	1.92	0.43
1:E:276:GLN:NE2	1:E:292:THR:OG1	2.52	0.43
1:C:105:ARG:HH22	1:D:79:VAL:HA	1.84	0.43
1:C:249:THR:HA	1:C:250:PRO:HD3	1.83	0.43
1:D:261:MET:HE2	1:D:261:MET:HB3	1.85	0.43
1:E:272:GLU:OE1	1:E:273:VAL:N	2.51	0.43
1:E:153:ASP:C	1:E:155:VAL:H	2.27	0.43
1:E:250:PRO:HD2	1:E:251:TYR:HD2	1.83	0.43
1:A:246:LEU:HA	1:A:247:PRO:HD3	1.84	0.42
1:C:136:ASP:OD1	1:C:179:ARG:NH2	2.52	0.42
1:E:261:MET:HE2	1:E:261:MET:HB3	1.85	0.42
1:B:134:SER:HB3	1:B:139:ASN:HA	2.00	0.42
1:D:230:SER:HB3	1:E:229:VAL:CG1	2.49	0.42
1:B:25:ILE:HG22	1:B:26:GLU:N	2.33	0.42
1:D:184:LEU:HD23	1:D:184:LEU:HA	1.93	0.42
1:E:249:THR:HA	1:E:250:PRO:HD3	1.81	0.42
1:B:23:TYR:CZ	1:C:176:LEU:CD1	3.03	0.42
1:B:105:ARG:HH22	1:C:79:VAL:HA	1.84	0.42
1:C:160:TRP:CZ2	1:C:192:ARG:NH2	2.88	0.42
1:A:7:PRO:HG2	1:A:137:THR:HG21	2.01	0.42
1:B:176:LEU:HD13	1:B:181:GLU:OE1	2.20	0.42
1:C:126:LEU:HB2	1:C:188:LEU:HB3	2.02	0.42
1:C:153:ASP:C	1:C:155:VAL:H	2.28	0.42
1:E:295:SER:HA	1:E:298:ALA:HB3	2.02	0.42
1:B:128:ILE:HB	1:B:186:TYR:HB2	2.01	0.42
1:B:206:LEU:HD23	1:B:206:LEU:HA	1.88	0.42
1:D:228:VAL:CG1	1:D:270:VAL:HG23	2.49	0.42
1:C:38:LYS:NZ	1:D:82:GLU:OE2	2.53	0.42
1:D:134:SER:HA	1:D:140:ILE:HD12	2.01	0.42
1:D:197:TYR:CD1	1:D:201:ILE:HD13	2.55	0.42
1:D:211:ILE:HG13	1:E:267:PHE:HD1	1.85	0.42
1:D:211:ILE:HG23	1:E:270:VAL:HG21	2.02	0.42
1:A:128:ILE:HB	1:A:186:TYR:HB2	2.02	0.42
1:A:261:MET:HE2	1:A:261:MET:HB3	1.88	0.42
1:B:126:LEU:HB2	1:B:188:LEU:HB3	2.01	0.42
1:D:203:LEU:HD23	1:D:203:LEU:HA	1.86	0.42
1:E:128:ILE:HB	1:E:186:TYR:HB2	2.01	0.41
1:E:205:MET:HE3	1:E:238:PHE:CD1	2.36	0.41
1:A:241:LEU:HD21	1:B:239:ASN:HD22	1.85	0.41
1:C:207:PHE:CE2	1:D:264:LEU:HA	2.55	0.41
1:D:128:ILE:HB	1:D:186:TYR:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:PHE:O	1:C:253:THR:HG23	2.20	0.41
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.86	0.41
1:C:127:HIS:HE1	1:C:187:GLN:HE21	1.67	0.41
1:C:261:MET:HE2	1:C:261:MET:HB3	1.82	0.41
1:B:26:GLU:OE2	1:C:80:ASN:CB	2.68	0.41
1:B:119:TYR:CD1	1:B:120:PRO:HA	2.56	0.41
1:D:7:PRO:HG2	1:D:137:THR:HG21	2.01	0.41
1:A:206:LEU:HD23	1:A:206:LEU:HA	1.89	0.41
1:A:284:GLN:N	1:A:285:PRO:CD	2.80	0.41
1:C:105:ARG:HH11	1:D:77:ARG:HE	1.68	0.41
1:E:117:ARG:CZ	1:E:251:TYR:CD1	3.03	0.41
1:E:126:LEU:HB2	1:E:188:LEU:HB3	2.03	0.41
1:B:295:SER:HA	1:B:298:ALA:HB3	2.03	0.41
1:C:211:ILE:HG23	1:D:270:VAL:HG21	2.03	0.41
1:A:38:LYS:NZ	1:B:82:GLU:OE1	2.51	0.41
1:D:249:THR:HA	1:D:250:PRO:HD3	1.81	0.41
1:A:105:ARG:HH22	1:B:79:VAL:HA	1.85	0.41
1:B:133:ARG:HA	1:B:181:GLU:HG2	2.03	0.41
1:B:133:ARG:HG3	1:B:181:GLU:CG	2.51	0.41
1:E:194:TYR:O	1:E:195:PHE:C	2.64	0.41
1:E:133:ARG:NH1	1:E:176:LEU:O	2.46	0.40
1:E:228:VAL:HG11	1:E:270:VAL:HG23	2.02	0.40
1:A:263:TYR:CD1	1:E:204:PRO:HB3	2.56	0.40
1:B:197:TYR:CD1	1:B:201:ILE:HD13	2.56	0.40
1:B:205:MET:HE3	1:B:238:PHE:CD1	2.36	0.40
1:D:153:ASP:C	1:D:155:VAL:H	2.29	0.40
1:D:228:VAL:HG11	1:D:270:VAL:HG23	2.04	0.40
1:D:295:SER:HA	1:D:298:ALA:HB3	2.03	0.40
1:A:249:THR:HB	1:A:251:TYR:CD2	2.57	0.40
1:B:211:ILE:HG23	1:C:270:VAL:HG21	2.03	0.40
1:C:128:ILE:HB	1:C:186:TYR:HB2	2.04	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	301/321 (94%)	282 (94%)	19 (6%)	0	100	100
1	B	301/321 (94%)	279 (93%)	22 (7%)	0	100	100
1	C	302/321 (94%)	283 (94%)	19 (6%)	0	100	100
1	D	302/321 (94%)	280 (93%)	22 (7%)	0	100	100
1	E	301/321 (94%)	275 (91%)	26 (9%)	0	100	100
All	All	1507/1605 (94%)	1399 (93%)	108 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	275/285 (96%)	260 (94%)	15 (6%)	19	47
1	B	275/285 (96%)	256 (93%)	19 (7%)	14	40
1	C	276/285 (97%)	262 (95%)	14 (5%)	21	50
1	D	276/285 (97%)	254 (92%)	22 (8%)	11	35
1	E	275/285 (96%)	256 (93%)	19 (7%)	14	40
All	All	1377/1425 (97%)	1288 (94%)	89 (6%)	15	42

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	11	ILE
1	A	71	ILE
1	A	110	VAL
1	A	114	LEU
1	A	140	ILE
1	A	163	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	232	LEU
1	A	239	ASN
1	A	244	CYS
1	A	264	LEU
1	A	270	VAL
1	A	273	VAL
1	A	275	VAL
1	A	308	ILE
1	B	5	VAL
1	B	11	ILE
1	B	71	ILE
1	B	86	ASP
1	B	94	VAL
1	B	99	THR
1	B	100	VAL
1	B	140	ILE
1	B	178	ASP
1	B	209	LEU
1	B	239	ASN
1	B	244	CYS
1	B	252	MET
1	B	255	THR
1	B	270	VAL
1	B	275	VAL
1	B	282	GLU
1	B	283	SER
1	B	308	ILE
1	C	5	VAL
1	C	11	ILE
1	C	71	ILE
1	C	107	SER
1	C	140	ILE
1	C	163	GLU
1	C	209	LEU
1	C	239	ASN
1	C	244	CYS
1	C	255	THR
1	C	270	VAL
1	C	273	VAL
1	C	275	VAL
1	C	308	ILE
1	D	5	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	11	ILE
1	D	39	VAL
1	D	63	VAL
1	D	71	ILE
1	D	86	ASP
1	D	94	VAL
1	D	99	THR
1	D	123	SER
1	D	140	ILE
1	D	163	GLU
1	D	209	LEU
1	D	232	LEU
1	D	239	ASN
1	D	244	CYS
1	D	258	ILE
1	D	270	VAL
1	D	273	VAL
1	D	275	VAL
1	D	277	HIS
1	D	284	GLN
1	D	308	ILE
1	E	5	VAL
1	E	11	ILE
1	E	63	VAL
1	E	71	ILE
1	E	86	ASP
1	E	100	VAL
1	E	140	ILE
1	E	158	THR
1	E	181	GLU
1	E	202	ILE
1	E	239	ASN
1	E	244	CYS
1	E	255	THR
1	E	270	VAL
1	E	273	VAL
1	E	275	VAL
1	E	290	SER
1	E	293	ARG
1	E	308	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	187	GLN
1	A	200	ASN
1	A	284	GLN
1	B	83	ASN
1	B	200	ASN
1	B	276	GLN
1	B	277	HIS
1	C	83	ASN
1	C	187	GLN
1	C	200	ASN
1	C	284	GLN
1	D	187	GLN
1	D	200	ASN
1	D	239	ASN
1	D	277	HIS
1	E	83	ASN
1	E	200	ASN
1	E	239	ASN
1	E	276	GLN
1	E	277	HIS
1	E	284	GLN

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	LMT	B	318	-	11,11,36	0.66	0	10,10,47	0.77	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	B	318	-	-	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 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	318	LMT	5	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	305/321 (95%)	0.38	16 (5%)	33	19	78, 113, 176, 253	0
1	B	305/321 (95%)	0.40	18 (5%)	28	16	75, 111, 159, 206	0
1	C	306/321 (95%)	0.47	22 (7%)	21	12	79, 114, 181, 217	0
1	D	306/321 (95%)	0.53	27 (8%)	15	9	83, 120, 189, 233	0
1	E	305/321 (95%)	0.35	18 (5%)	28	16	73, 117, 178, 207	0
All	All	1527/1605 (95%)	0.42	101 (6%)	24	14	73, 115, 178, 253	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	65	THR	5.9
1	D	61	VAL	4.4
1	E	82	GLU	4.1
1	A	197	TYR	4.0
1	B	193	GLN	4.0
1	C	57	VAL	3.8
1	D	137	THR	3.6
1	B	195	PHE	3.6
1	A	121	PHE	3.4
1	A	245	ASN	3.3
1	C	37	PHE	3.2
1	D	92	ILE	3.2
1	E	28	TYR	3.2
1	C	11	ILE	3.2
1	B	11	ILE	3.1
1	A	84	ALA	3.1
1	D	194	TYR	3.0
1	C	84	ALA	3.0
1	C	65	THR	3.0
1	E	11	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	82	GLU	2.9
1	D	195	PHE	2.9
1	B	194	TYR	2.9
1	B	197	TYR	2.9
1	A	195	PHE	2.9
1	D	249	THR	2.9
1	B	285	PRO	2.8
1	D	5	VAL	2.8
1	A	64	LYS	2.8
1	C	284	GLN	2.8
1	B	253	THR	2.8
1	C	252	MET	2.7
1	A	5	VAL	2.7
1	C	61	VAL	2.7
1	D	57	VAL	2.7
1	B	179	ARG	2.7
1	C	64	LYS	2.7
1	D	148	LYS	2.7
1	D	136	ASP	2.7
1	C	19	ASN	2.7
1	E	285	PRO	2.7
1	E	286	ALA	2.7
1	E	121	PHE	2.7
1	E	5	VAL	2.7
1	B	247	PRO	2.6
1	D	253	THR	2.6
1	E	252	MET	2.6
1	D	85	ARG	2.6
1	C	82	GLU	2.6
1	C	172	ALA	2.6
1	E	289	ALA	2.6
1	C	197	TYR	2.6
1	D	112	SER	2.6
1	A	61	VAL	2.5
1	E	61	VAL	2.5
1	D	113	PRO	2.5
1	C	48	LYS	2.5
1	C	148	LYS	2.5
1	D	252	MET	2.5
1	A	285	PRO	2.5
1	B	161	ASP	2.5
1	E	112	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	56	PRO	2.4
1	D	289	ALA	2.4
1	D	156	PHE	2.4
1	D	93	SER	2.4
1	A	194	TYR	2.4
1	D	116	PHE	2.4
1	A	252	MET	2.3
1	C	6	SER	2.3
1	A	253	THR	2.3
1	B	109	ARG	2.3
1	C	137	THR	2.3
1	D	84	ALA	2.3
1	E	284	GLN	2.3
1	B	113	PRO	2.3
1	D	86	ASP	2.3
1	A	57	VAL	2.3
1	E	197	TYR	2.3
1	D	66	TYR	2.2
1	E	83	ASN	2.2
1	B	27	SER	2.2
1	E	163	GLU	2.2
1	E	177	GLU	2.2
1	D	285	PRO	2.2
1	E	84	ALA	2.2
1	A	137	THR	2.2
1	C	263	TYR	2.2
1	D	80	ASN	2.2
1	B	118	ARG	2.2
1	C	195	PHE	2.2
1	A	169	VAL	2.1
1	E	137	THR	2.1
1	C	5	VAL	2.1
1	C	86	ASP	2.1
1	D	248	LYS	2.1
1	B	149	VAL	2.1
1	A	58	ARG	2.1
1	B	37	PHE	2.1
1	B	248	LYS	2.1
1	D	62	ARG	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	B	318	12/35	0.87	0.32	91,96,97,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.