



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 01:56 AM UTC

PDB ID : 5XAY / pdb_00005xay
Title : Crystal structure of full length tytp, a tetr regulator from streptomyces fradiae
Authors : Ray, S.; Panjikar, S.; Anand, R.
Deposited on : 2017-03-15
Resolution : 2.58 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:

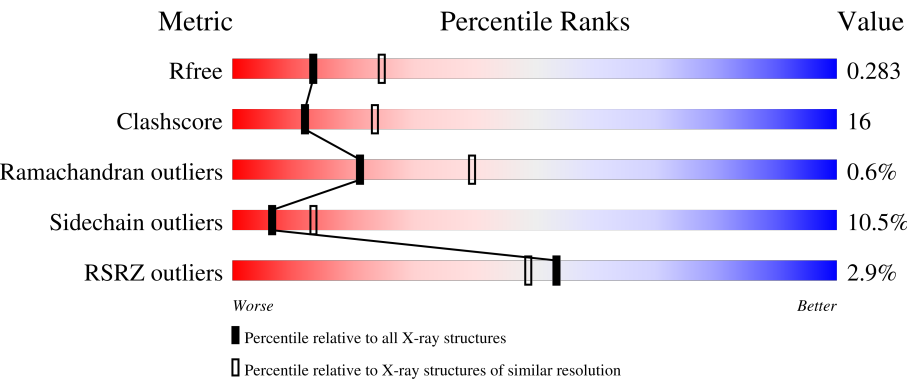
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	228	63% 29% • 6%
1	B	228	64% 26% • 6%
1	C	228	3% 66% 25% • • •
1	D	228	7% 49% 29% 7% • 14%
1	E	228	2% 57% 25% • • 14%

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Mol	Chain	Length	Quality of chain
1	F	228	2% 64% 18% 5% 13%
1	G	228	61% 24% 9% 6%
1	H	228	4% 55% 22% 7% 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12871 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 Gamma-butyrolactone receptor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	Se	0	1	0
			1666	1042	309	310	5			
1	B	215	Total	C	N	O	Se	0	1	0
			1666	1043	309	308	6			
1	C	219	Total	C	N	O	Se	0	1	0
			1691	1057	316	312	6			
1	D	197	Total	C	N	O	Se	0	1	0
			1529	961	282	281	5			
1	E	197	Total	C	N	O	Se	0	0	0
			1525	958	280	282	5			
1	F	199	Total	C	N	O	Se	0	0	0
			1533	962	282	284	5			
1	G	215	Total	C	N	O	Se	0	0	0
			1661	1039	309	308	5			
1	H	192	Total	C	N	O	Se	0	1	0
			1486	937	268	276	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	LEU	-	expression tag	UNP Q9XCC7
A	228	GLU	-	expression tag	UNP Q9XCC7
A	229	HIS	-	expression tag	UNP Q9XCC7
B	227	LEU	-	expression tag	UNP Q9XCC7
B	228	GLU	-	expression tag	UNP Q9XCC7
B	229	HIS	-	expression tag	UNP Q9XCC7
C	227	LEU	-	expression tag	UNP Q9XCC7
C	228	GLU	-	expression tag	UNP Q9XCC7
C	229	HIS	-	expression tag	UNP Q9XCC7
D	227	LEU	-	expression tag	UNP Q9XCC7
D	228	GLU	-	expression tag	UNP Q9XCC7
D	229	HIS	-	expression tag	UNP Q9XCC7
E	227	LEU	-	expression tag	UNP Q9XCC7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	228	GLU	-	expression tag	UNP Q9XCC7
E	229	HIS	-	expression tag	UNP Q9XCC7
F	227	LEU	-	expression tag	UNP Q9XCC7
F	228	GLU	-	expression tag	UNP Q9XCC7
F	229	HIS	-	expression tag	UNP Q9XCC7
G	227	LEU	-	expression tag	UNP Q9XCC7
G	228	GLU	-	expression tag	UNP Q9XCC7
G	229	HIS	-	expression tag	UNP Q9XCC7
H	227	LEU	-	expression tag	UNP Q9XCC7
H	228	GLU	-	expression tag	UNP Q9XCC7
H	229	HIS	-	expression tag	UNP Q9XCC7

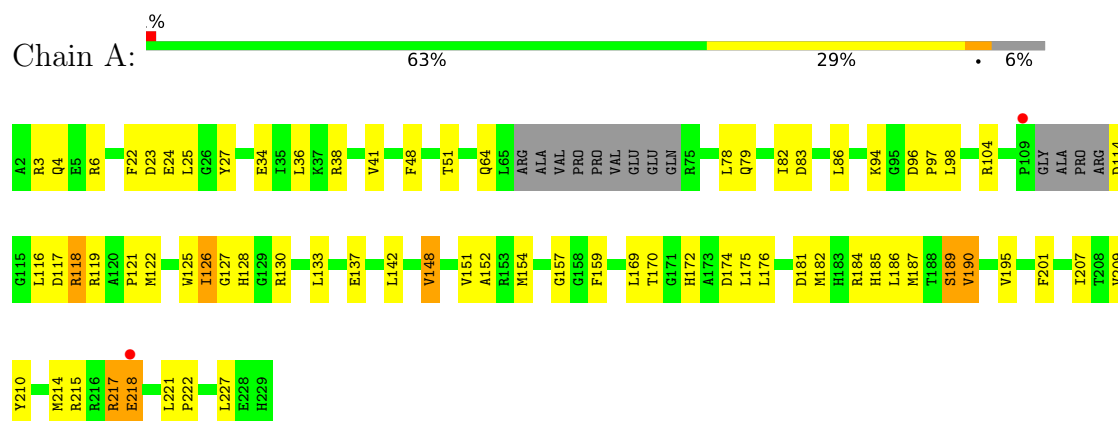
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	19	Total O 19 19	0	0
2	B	17	Total O 17 17	0	0
2	C	13	Total O 13 13	0	0
2	D	12	Total O 12 12	0	0
2	E	12	Total O 12 12	0	0
2	F	13	Total O 13 13	0	0
2	G	18	Total O 18 18	0	0
2	H	10	Total O 10 10	0	0

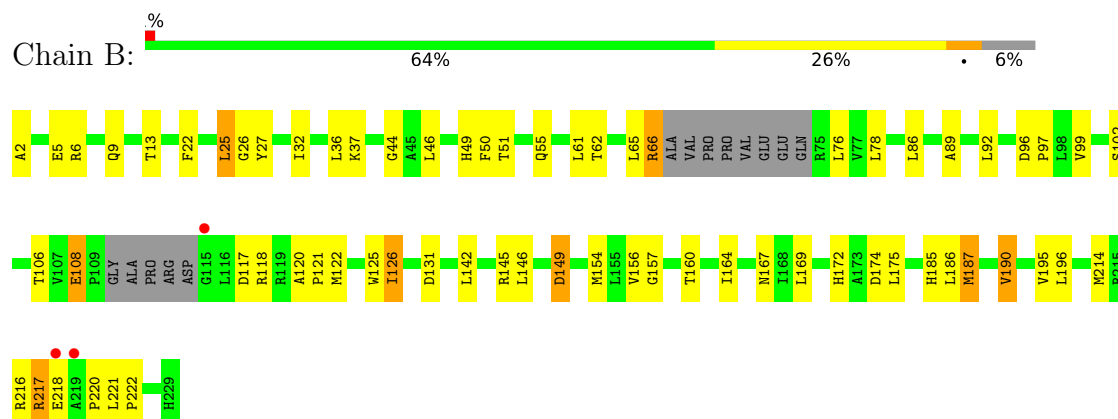
3 Residue-property plots

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.

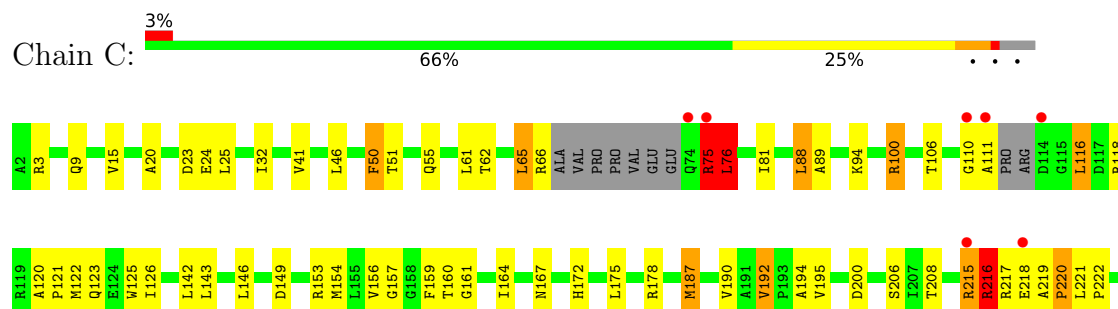
• Molecule 1: Gamma-butyrolactone receptor protein



• Molecule 1: Gamma-butyrolactone receptor protein

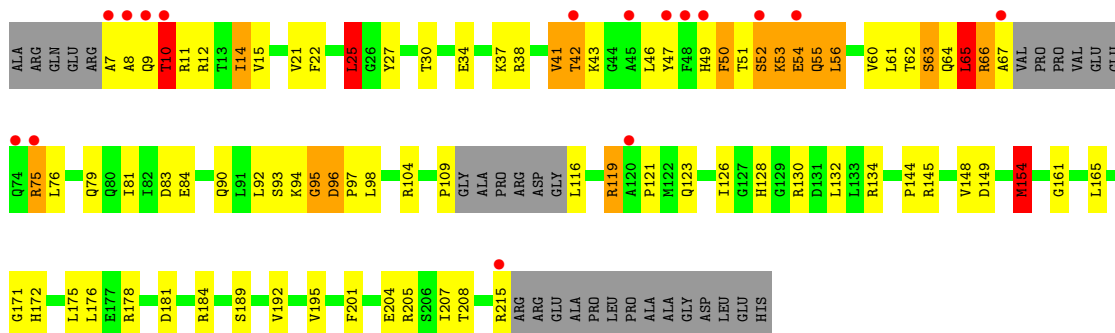


• Molecule 1: Gamma-butyrolactone receptor protein

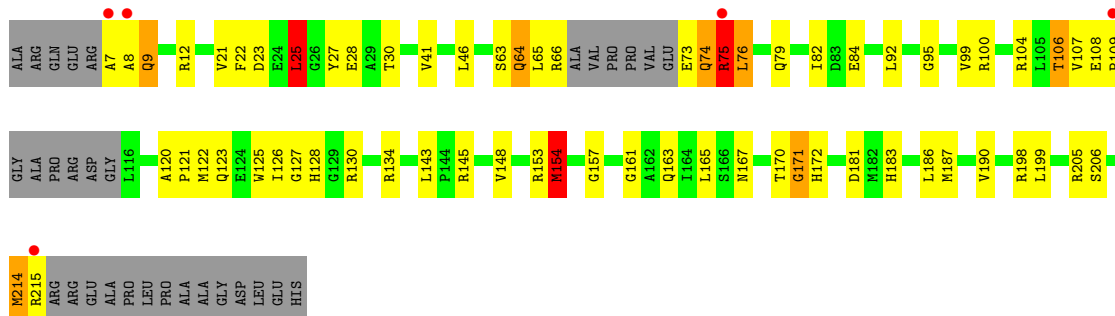




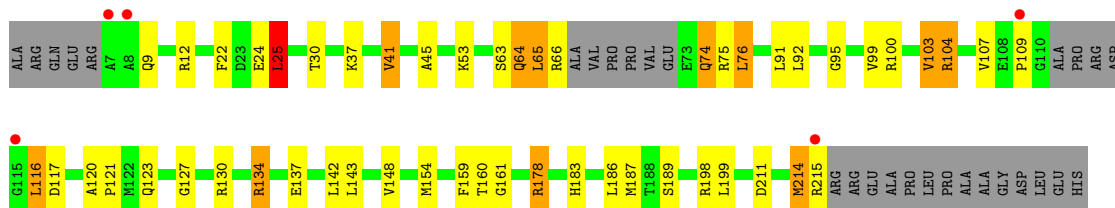
• Molecule 1: Gamma-butyrolactone receptor protein



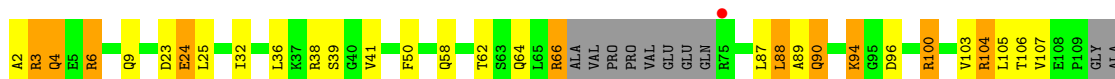
• Molecule 1: Gamma-butyrolactone receptor protein

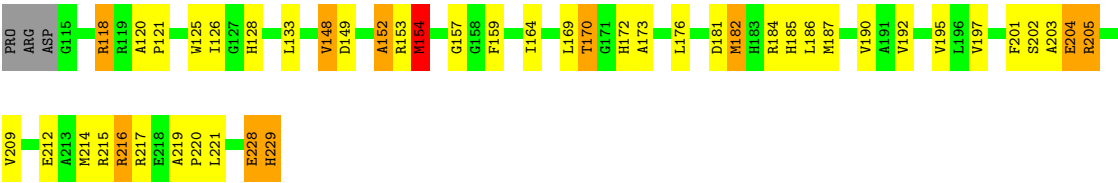


• Molecule 1: Gamma-butyrolactone receptor protein

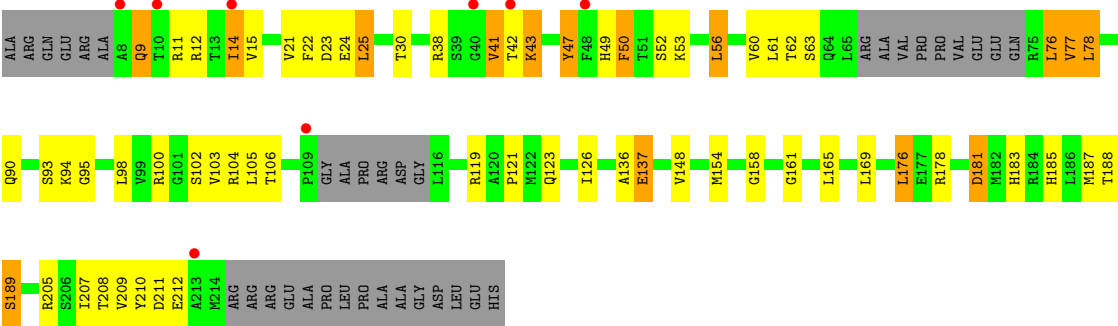


• Molecule 1: Gamma-butyrolactone receptor protein





• Molecule 1: Gamma-butyrolactone receptor protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.33Å 71.89Å 160.07Å 90.00° 102.54° 90.00°	Depositor
Resolution (Å)	19.92 – 2.58 19.92 – 2.58	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.92-2.58) 99.6 (19.92-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.227 , 0.284 0.228 , 0.283	Depositor DCC
R_{free} test set	994 reflections (1.40%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12871	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.46 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.0608e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.27	4/1684 (0.2%)	1.37	15/2268 (0.7%)
1	B	1.30	5/1684 (0.3%)	1.32	10/2267 (0.4%)
1	C	1.23	2/1709 (0.1%)	1.31	9/2300 (0.4%)
1	D	1.13	1/1544 (0.1%)	1.27	10/2078 (0.5%)
1	E	1.10	1/1537 (0.1%)	1.32	14/2069 (0.7%)
1	F	1.09	0/1545	1.29	10/2079 (0.5%)
1	G	1.34	4/1676 (0.2%)	1.37	16/2257 (0.7%)
1	H	1.10	2/1501 (0.1%)	1.24	5/2022 (0.2%)
All	All	1.20	19/12880 (0.1%)	1.31	89/17340 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	G	0	1
All	All	0	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	HIS	CG-ND1	-6.97	1.30	1.38
1	G	172	HIS	CG-ND1	-6.31	1.31	1.38
1	A	172	HIS	CD2-NE2	-6.28	1.30	1.37
1	G	229	HIS	CG-CD2	6.15	1.42	1.35
1	C	50	PHE	N-CA	5.96	1.53	1.46
1	B	49	HIS	CE1-NE2	5.85	1.38	1.32
1	E	76	LEU	C-O	-5.74	1.17	1.24
1	G	172	HIS	CD2-NE2	-5.71	1.31	1.37
1	B	117	ASP	C-O	-5.43	1.17	1.24
1	B	26	GLY	C-O	-5.40	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	49	HIS	CG-CD2	5.36	1.41	1.35
1	A	128	HIS	CG-CD2	5.33	1.41	1.35
1	H	78	LEU	C-O	-5.30	1.17	1.24
1	H	165	LEU	CA-C	-5.28	1.46	1.52
1	C	76	LEU	C-O	-5.24	1.17	1.23
1	B	126	ILE	CA-CB	-5.21	1.48	1.54
1	G	203	ALA	C-O	-5.07	1.17	1.24
1	A	127	GLY	C-O	-5.06	1.17	1.23
1	B	131	ASP	C-O	-5.02	1.18	1.24

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	65	LEU	N-CA-C	-10.31	99.96	112.54
1	E	63	SER	N-CA-C	9.69	121.84	111.28
1	H	158	GLY	N-CA-C	-9.33	101.19	112.49
1	F	143	LEU	CA-C-N	-9.16	110.60	119.85
1	F	143	LEU	C-N-CA	-9.16	110.60	119.85
1	D	65	LEU	N-CA-C	-8.79	99.26	112.54
1	C	192	VAL	CA-C-N	-8.75	110.59	120.04
1	C	192	VAL	C-N-CA	-8.75	110.59	120.04
1	E	9	GLN	N-CA-C	-8.73	102.18	112.92
1	F	25	LEU	CA-C-N	-8.55	113.14	122.55
1	F	25	LEU	C-N-CA	-8.55	113.14	122.55
1	E	143	LEU	CA-C-N	-8.46	111.30	119.85
1	E	143	LEU	C-N-CA	-8.46	111.30	119.85
1	B	126	ILE	N-CA-C	8.43	119.21	110.36
1	D	55	GLN	N-CA-C	-8.19	101.62	111.69
1	G	152	ALA	N-CA-C	-7.65	103.02	111.36
1	A	170	THR	N-CA-C	-7.53	97.90	109.65
1	D	10	THR	N-CA-C	-7.39	104.50	113.97
1	H	62	THR	N-CA-C	7.36	122.10	113.20
1	B	142	LEU	N-CA-C	7.27	121.30	109.59
1	A	27	TYR	N-CA-C	7.13	119.72	111.02
1	G	25	LEU	CA-C-N	-7.12	111.78	122.04
1	G	25	LEU	C-N-CA	-7.12	111.78	122.04
1	G	170	THR	N-CA-C	-7.10	95.68	110.80
1	G	24	GLU	N-CA-C	7.03	118.60	111.07
1	C	75	ARG	N-CA-C	6.92	116.45	108.49
1	A	182	MSE	N-CA-C	-6.91	103.83	111.36
1	E	25	LEU	CA-C-N	-6.79	114.06	122.75
1	E	25	LEU	C-N-CA	-6.79	114.06	122.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	47	TYR	N-CA-C	6.75	121.74	112.90
1	B	76	LEU	N-CA-C	-6.75	99.60	110.32
1	E	126	ILE	N-CA-C	6.67	117.42	110.62
1	A	214	MSE	N-CA-C	-6.65	104.06	111.71
1	A	182	MSE	CG-SE-CE	6.55	113.33	98.92
1	A	217	ARG	N-CA-C	6.49	118.23	110.44
1	B	25	LEU	CA-C-N	-6.49	113.01	121.96
1	B	25	LEU	C-N-CA	-6.49	113.01	121.96
1	H	181	ASP	N-CA-C	-6.46	104.16	111.07
1	G	164	ILE	N-CA-C	6.44	117.12	110.36
1	E	154	MSE	CB-CA-C	6.21	123.06	110.38
1	C	76	LEU	N-CA-C	-6.18	100.43	110.20
1	B	169	LEU	N-CA-C	6.04	118.83	111.82
1	G	126	ILE	N-CA-C	6.03	116.21	110.42
1	B	187	MSE	N-CA-C	-5.92	104.83	111.28
1	A	64	GLN	N-CA-C	5.89	120.20	113.19
1	D	154	MSE	N-CA-C	-5.82	104.53	111.69
1	E	127	GLY	N-CA-C	-5.78	107.17	114.16
1	G	103	VAL	N-CA-CB	5.77	116.68	110.62
1	C	50	PHE	N-CA-C	5.72	118.81	108.69
1	F	127	GLY	N-CA-C	-5.71	105.72	113.37
1	A	215	ARG	N-CA-C	5.68	117.47	111.28
1	B	27	TYR	N-CA-C	-5.68	105.23	111.82
1	C	194	ALA	N-CA-C	-5.67	105.18	111.36
1	D	95	GLY	N-CA-C	5.65	123.03	114.61
1	A	48	PHE	N-CA-C	-5.64	105.21	111.36
1	G	6	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	E	154	MSE	CG-SE-CE	-5.57	86.67	98.92
1	C	187	MSE	N-CA-CB	5.56	118.29	110.12
1	F	104	ARG	N-CA-C	5.54	117.32	111.28
1	C	142	LEU	N-CA-C	5.53	118.83	109.76
1	G	205	ARG	CA-C-N	5.52	127.68	120.28
1	G	205	ARG	C-N-CA	5.52	127.68	120.28
1	F	117	ASP	N-CA-C	5.52	117.09	109.15
1	F	116	LEU	N-CA-C	-5.51	100.05	108.76
1	F	109	PRO	N-CA-C	-5.43	106.32	113.65
1	A	207	ILE	N-CA-C	5.42	116.05	110.36
1	D	119	ARG	N-CA-C	5.42	116.87	110.97
1	A	189	SER	N-CA-C	-5.33	106.16	113.30
1	D	25	LEU	CA-C-N	-5.32	116.69	122.55
1	D	25	LEU	C-N-CA	-5.32	116.69	122.55
1	G	228	GLU	N-CA-C	5.30	116.74	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	28	GLU	N-CA-C	5.29	117.74	111.33
1	G	182	MSE	N-CA-C	-5.29	105.51	111.28
1	G	154	MSE	CB-CA-C	-5.25	101.75	110.68
1	A	221	LEU	CA-C-N	-5.24	114.84	120.03
1	A	221	LEU	C-N-CA	-5.24	114.84	120.03
1	A	79	GLN	N-CA-C	-5.22	105.65	112.23
1	A	24	GLU	N-CA-C	5.20	116.75	111.14
1	E	190	VAL	CB-CA-C	-5.19	106.43	111.05
1	D	46	LEU	N-CA-C	5.16	116.71	111.14
1	E	27	TYR	CA-C-N	5.14	127.42	120.38
1	E	27	TYR	C-N-CA	5.14	127.42	120.38
1	G	182	MSE	CG-SE-CE	5.14	110.22	98.92
1	G	187	MSE	CA-CB-CG	-5.13	103.83	114.10
1	H	24	GLU	N-CA-C	5.13	116.56	111.07
1	C	15	VAL	N-CA-C	5.03	115.64	110.36
1	D	96	ASP	N-CA-C	-5.03	102.57	109.71
1	B	5	GLU	N-CA-C	-5.02	106.33	112.90
1	B	149	ASP	N-CA-CB	5.00	117.32	110.07

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	171	GLY	Peptide
1	G	106	THR	Peptide

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	1666	0	1705	58	0
1	B	1666	0	1710	51	1
1	C	1691	0	1733	54	1
1	D	1529	0	1581	83	0
1	E	1525	0	1571	51	0
1	F	1533	0	1577	34	0
1	G	1661	0	1701	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1486	0	1532	45	0
2	A	19	0	0	2	0
2	B	17	0	0	1	0
2	C	13	0	0	1	0
2	D	12	0	0	0	0
2	E	12	0	0	5	0
2	F	13	0	0	1	0
2	G	18	0	0	3	0
2	H	10	0	0	0	0
All	All	12871	0	13110	407	1

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 16.

All (407) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:MSE:HE1	1:B:217:ARG:NH1	1.40	1.37
1:A:122:MSE:HE2	2:A:318:HOH:O	1.17	1.28
1:E:171:GLY:C	2:E:301:HOH:O	1.89	1.14
1:D:65:LEU:HD22	1:D:65:LEU:O	1.46	1.14
1:H:9:GLN:HE21	1:H:9:GLN:HA	0.96	1.11
1:E:171:GLY:CA	2:E:301:HOH:O	1.96	1.09
1:D:54:GLU:OE1	1:D:116:LEU:HD12	1.56	1.06
1:B:214:MSE:CE	1:B:217:ARG:NH1	2.20	1.04
1:B:78:LEU:HD13	1:B:187:MSE:CE	1.87	1.04
1:C:122[A]:MSE:HE1	1:C:156:VAL:HG11	1.39	1.02
1:A:3:ARG:HH12	1:A:4:GLN:NE2	1.57	1.00
1:H:9:GLN:HA	1:H:9:GLN:NE2	1.77	0.97
1:E:171:GLY:HA2	2:E:301:HOH:O	1.56	0.96
1:F:9:GLN:HG2	1:F:12:ARG:HH12	1.29	0.96
1:H:9:GLN:HE21	1:H:9:GLN:CA	1.80	0.94
1:B:149:ASP:HB2	2:B:316:HOH:O	1.66	0.93
1:C:154:MSE:HE2	1:E:181:ASP:HB3	1.47	0.93
1:A:154:MSE:HE2	1:H:181:ASP:HB3	1.51	0.93
1:D:53:LYS:NZ	1:D:53:LYS:CB	2.33	0.92
1:G:176:LEU:HG	1:G:176:LEU:O	1.70	0.92
1:D:66:ARG:O	1:D:67:ALA:HB3	1.68	0.91
1:A:94:LYS:HG3	1:A:210:TYR:OH	1.70	0.91
1:G:58:GLN:O	1:G:62:THR:HG22	1.70	0.91
1:D:53:LYS:NZ	1:D:53:LYS:HB3	1.84	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:ALA:N	1:E:8:ALA:HA	1.87	0.89
1:A:3:ARG:NH1	1:A:4:GLN:HE21	1.69	0.89
1:C:23:ASP:OD1	1:C:100:ARG:NH1	2.06	0.89
1:B:122[B]:MSE:HE1	1:B:156:VAL:HG11	1.55	0.87
1:B:78:LEU:HD13	1:B:187:MSE:HE1	1.57	0.86
1:D:27:TYR:CE1	1:D:53:LYS:HD3	2.09	0.86
1:E:183:HIS:NE2	1:E:187:MSE:HE2	1.90	0.86
1:D:181:ASP:HB3	1:G:154:MSE:HE2	1.56	0.85
1:D:53:LYS:CB	1:D:53:LYS:HZ2	1.88	0.85
1:B:214:MSE:HE2	1:B:214:MSE:HA	1.61	0.83
1:A:3:ARG:HH12	1:A:4:GLN:HE21	0.87	0.82
1:D:51:THR:O	1:D:52:SER:HB3	1.79	0.81
1:A:78:LEU:HD13	1:A:187:MSE:HE1	1.63	0.81
1:E:214:MSE:HE2	1:E:214:MSE:HA	1.61	0.81
1:C:65:LEU:O	1:C:66:ARG:CG	2.30	0.80
1:D:51:THR:O	1:D:52:SER:CB	2.30	0.80
1:C:65:LEU:O	1:C:66:ARG:CB	2.29	0.80
1:C:216:ARG:O	1:C:216:ARG:HG3	1.78	0.80
1:F:214:MSE:HA	1:F:214:MSE:HE2	1.64	0.80
1:A:3:ARG:NH1	1:A:4:GLN:HG3	1.96	0.79
1:C:216:ARG:O	1:C:216:ARG:CG	2.30	0.79
1:C:65:LEU:O	1:C:66:ARG:HG3	1.83	0.78
1:D:53:LYS:HB3	1:D:53:LYS:HZ3	1.47	0.78
1:D:66:ARG:O	1:D:67:ALA:CB	2.30	0.78
1:B:214:MSE:HE1	1:B:217:ARG:CZ	2.13	0.78
1:A:34:GLU:OE2	1:A:38[B]:ARG:NH1	2.15	0.78
1:D:130:ARG:HD2	1:D:134:ARG:NH2	1.98	0.78
1:F:63:SER:O	1:F:64:GLN:HB3	1.84	0.77
1:B:61:LEU:HA	1:B:102:SER:HB2	1.66	0.77
1:C:149:ASP:HB2	2:C:306:HOH:O	1.84	0.77
1:C:118:ARG:O	1:C:121:PRO:HD2	1.84	0.76
1:F:63:SER:O	1:F:64:GLN:CB	2.32	0.76
1:A:6:ARG:NH2	1:G:50:PHE:O	2.18	0.76
1:D:65:LEU:O	1:D:65:LEU:CD2	2.30	0.76
1:D:154:MSE:HE3	1:G:181:ASP:HB3	1.67	0.75
1:A:3:ARG:NH1	1:A:4:GLN:NE2	2.30	0.75
1:A:218:GLU:O	1:A:218:GLU:CD	2.30	0.75
1:E:74:GLN:O	1:E:75:ARG:C	2.30	0.75
1:H:77:VAL:HG22	1:H:136:ALA:HB2	1.69	0.75
1:B:214:MSE:HE1	1:B:217:ARG:HH12	1.51	0.74
1:B:2:ALA:O	1:B:6:ARG:HG3	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:ILE:HD11	1:D:41:VAL:HG11	1.70	0.73
1:G:3:ARG:HG2	1:G:3:ARG:HH11	1.53	0.73
1:G:64:GLN:HE22	1:G:217:ARG:HH22	1.36	0.73
1:F:183:HIS:NE2	1:F:187:MSE:HE2	2.04	0.72
1:G:170:THR:HB	1:G:173:ALA:HB3	1.71	0.72
1:F:9:GLN:HG2	1:F:12:ARG:NH1	2.03	0.71
1:F:99:VAL:O	1:F:103:VAL:HG12	1.90	0.71
1:G:184:ARG:HA	1:G:201:PHE:CE2	2.26	0.70
1:A:78:LEU:HD13	1:A:187:MSE:CE	2.20	0.70
1:D:52:SER:O	1:D:53:LYS:C	2.34	0.70
1:F:41:VAL:HG13	1:F:45:ALA:HB3	1.72	0.70
1:C:215:ARG:O	1:C:216:ARG:CB	2.37	0.69
1:E:154:MSE:HE3	1:E:186:LEU:HD22	1.72	0.69
1:B:51:THR:H	1:B:55:GLN:NE2	1.90	0.69
1:C:118:ARG:C	1:C:121:PRO:HD2	2.18	0.69
1:D:63:SER:O	1:D:66:ARG:HB2	1.93	0.68
1:D:56:LEU:O	1:D:60:VAL:HG23	1.94	0.68
1:B:78:LEU:HD13	1:B:187:MSE:HE2	1.74	0.68
1:F:75:ARG:HG2	1:F:75:ARG:HH11	1.59	0.67
1:D:207:ILE:HG21	1:E:134:ARG:HD3	1.77	0.67
1:B:46:LEU:C	1:B:46:LEU:HD23	2.18	0.67
1:C:65:LEU:O	1:C:66:ARG:HB2	1.93	0.67
1:D:154:MSE:HE2	1:G:181:ASP:C	2.20	0.67
1:C:215:ARG:O	1:C:216:ARG:HB3	1.96	0.66
1:F:95:GLY:HA2	1:F:100:ARG:HD2	1.77	0.66
1:H:95:GLY:HA2	1:H:100:ARG:HD2	1.77	0.66
1:G:4:GLN:HG2	2:G:316:HOH:O	1.94	0.66
1:E:170:THR:O	2:E:301:HOH:O	2.12	0.66
1:D:95:GLY:O	1:D:96:ASP:C	2.31	0.65
1:A:3:ARG:HH11	1:A:4:GLN:HG3	1.62	0.65
1:D:53:LYS:HZ2	1:D:53:LYS:HB2	1.60	0.65
1:E:74:GLN:O	1:E:76:LEU:N	2.30	0.65
1:D:130:ARG:NH1	1:D:149:ASP:OD1	2.30	0.64
1:E:9:GLN:HB2	1:E:12:ARG:NH1	2.12	0.64
1:C:23:ASP:CG	1:C:100:ARG:HH11	2.05	0.64
1:B:214:MSE:CE	1:B:217:ARG:HH11	2.11	0.63
1:G:64:GLN:HE22	1:G:217:ARG:NH2	1.95	0.63
1:C:110:GLY:O	1:C:111:ALA:C	2.42	0.63
1:H:14:ILE:HD11	1:H:41:VAL:HG11	1.80	0.62
1:D:53:LYS:O	1:D:56:LEU:N	2.33	0.62
1:H:61:LEU:HD13	1:H:121:PRO:HG3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:GLY:HA2	1:E:100:ARG:HD2	1.82	0.62
1:E:21:VAL:HG12	1:E:30:THR:HG23	1.81	0.61
1:D:154:MSE:CE	1:G:181:ASP:HB3	2.30	0.61
1:D:54:GLU:OE1	1:D:116:LEU:CD1	2.40	0.61
1:F:25:LEU:HD23	1:F:25:LEU:N	2.15	0.61
1:B:118:ARG:O	1:B:121:PRO:HD2	2.00	0.60
1:C:23:ASP:CG	1:C:100:ARG:NH1	2.59	0.60
1:E:21:VAL:CG1	1:E:30:THR:HG23	2.31	0.60
1:G:62:THR:HG21	2:G:314:HOH:O	2.01	0.60
1:G:64:GLN:NE2	1:G:217:ARG:HH22	1.98	0.60
1:D:154:MSE:HE2	1:G:182:MSE:HA	1.84	0.60
1:B:120:ALA:HB3	1:B:121:PRO:HD3	1.84	0.60
1:C:217:ARG:HD2	1:C:218:GLU:N	2.17	0.60
1:B:50:PHE:O	1:G:6:ARG:NH2	2.30	0.60
1:A:157:GLY:O	1:H:161:GLY:HA3	2.03	0.59
1:A:218:GLU:CD	1:A:218:GLU:C	2.70	0.59
1:E:172:HIS:N	2:E:301:HOH:O	2.23	0.59
1:D:192:VAL:HG22	1:D:195:VAL:HB	1.85	0.59
1:E:74:GLN:C	1:E:76:LEU:N	2.59	0.58
1:D:21:VAL:HG12	1:D:30:THR:HG23	1.83	0.58
1:G:2:ALA:O	1:G:6:ARG:HG3	2.02	0.58
1:B:106:THR:O	1:B:118:ARG:NH1	2.36	0.58
1:C:126:ILE:HD13	1:C:153:ARG:HD2	1.85	0.58
1:E:75:ARG:HH11	1:E:75:ARG:HB2	1.69	0.58
1:D:64:GLN:O	1:D:64:GLN:HG3	2.04	0.58
1:A:184:ARG:HA	1:A:201:PHE:CE2	2.39	0.57
1:A:154:MSE:HE1	1:H:185:HIS:ND1	2.19	0.57
1:D:53:LYS:HB3	1:D:53:LYS:HZ2	1.56	0.57
1:H:14:ILE:HG21	1:H:50:PHE:HE2	1.68	0.57
1:G:228:GLU:O	1:G:229:HIS:C	2.48	0.57
1:H:56:LEU:O	1:H:60:VAL:HG23	2.04	0.57
1:D:34:GLU:OE2	1:D:38:ARG:HD2	2.05	0.57
1:H:61:LEU:HD21	1:H:105:LEU:HB2	1.86	0.57
1:D:192:VAL:CG2	1:D:195:VAL:HB	2.35	0.56
1:E:65:LEU:HD11	1:E:125:TRP:HA	1.87	0.56
1:G:94:LYS:HD2	1:G:94:LYS:O	2.05	0.56
1:H:21:VAL:CG2	1:H:38:ARG:HD3	2.34	0.56
1:H:205:ARG:O	1:H:208:THR:HB	2.06	0.56
1:A:78:LEU:HB3	1:A:187:MSE:CE	2.35	0.56
1:D:161:GLY:HA3	1:G:157:GLY:O	2.05	0.56
1:F:214:MSE:HA	1:F:214:MSE:CE	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:MSE:CE	1:B:214:MSE:HA	2.30	0.56
1:D:205:ARG:O	1:D:208:THR:HB	2.06	0.56
1:H:14:ILE:HG22	1:H:15:VAL:N	2.21	0.55
1:A:78:LEU:CD1	1:A:187:MSE:HE1	2.36	0.55
1:C:9:GLN:HG2	1:C:221:LEU:O	2.06	0.55
1:G:3:ARG:HH11	1:G:3:ARG:CG	2.17	0.55
1:C:106:THR:O	1:C:118:ARG:NH1	2.39	0.55
1:D:11:ARG:O	1:D:11:ARG:CG	2.55	0.55
1:C:65:LEU:C	1:C:66:ARG:HG3	2.32	0.55
1:G:87:LEU:O	1:G:88:LEU:C	2.48	0.55
1:A:154:MSE:HE2	1:H:181:ASP:CB	2.29	0.54
1:D:126:ILE:CD1	1:G:169:LEU:HD11	2.37	0.54
1:F:160:THR:HA	2:F:304:HOH:O	2.05	0.54
1:D:192:VAL:HG23	1:D:195:VAL:H	1.72	0.54
1:G:58:GLN:O	1:G:62:THR:CG2	2.50	0.54
1:A:78:LEU:HB3	1:A:187:MSE:HE1	1.88	0.54
1:C:157:GLY:O	1:E:161:GLY:HA3	2.08	0.54
1:B:146:LEU:HD13	1:B:190:VAL:HG22	1.90	0.54
1:B:214:MSE:HE2	1:B:214:MSE:CA	2.35	0.54
1:E:171:GLY:O	1:E:172:HIS:HB2	2.08	0.54
1:B:108:GLU:O	1:B:118:ARG:NH1	2.41	0.53
1:C:187:MSE:HE2	1:C:187:MSE:HA	1.91	0.53
1:A:126:ILE:CD1	1:H:169:LEU:HD11	2.37	0.53
1:D:11:ARG:O	1:D:11:ARG:HG3	2.09	0.53
1:A:159:PHE:CD1	1:A:159:PHE:C	2.86	0.53
1:F:130:ARG:HG3	1:F:148:VAL:HG12	1.91	0.53
1:D:171:GLY:O	1:D:172:HIS:HB2	2.08	0.53
1:E:130:ARG:HG3	1:E:148:VAL:HG12	1.90	0.53
1:B:92:LEU:HB2	1:B:99:VAL:HG11	1.90	0.53
1:D:126:ILE:HD11	1:G:169:LEU:HD11	1.91	0.53
1:D:90:GLN:O	1:D:94:LYS:HG3	2.09	0.52
1:D:62:THR:O	1:D:66:ARG:HD2	2.09	0.52
1:E:46:LEU:C	1:E:46:LEU:HD23	2.34	0.52
1:H:77:VAL:CG2	1:H:136:ALA:HB2	2.39	0.52
1:D:10:THR:C	1:D:12:ARG:N	2.65	0.52
1:F:24:GLU:HB3	1:F:25:LEU:HD23	1.90	0.52
1:G:217:ARG:O	1:G:217:ARG:HG3	2.09	0.52
1:C:120:ALA:O	1:C:123:GLN:HB3	2.08	0.52
1:G:202:SER:HB2	1:G:204:GLU:HG2	1.91	0.52
1:H:61:LEU:CD1	1:H:121:PRO:HG3	2.39	0.52
1:D:21:VAL:CG2	1:D:38:ARG:HD3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:LEU:HD21	1:E:163:GLN:HG3	1.91	0.52
1:F:120:ALA:HB3	1:F:121:PRO:HD3	1.92	0.52
1:F:154:MSE:HE3	1:F:186:LEU:HD22	1.91	0.52
1:C:116:LEU:HG	1:C:118:ARG:HG3	1.90	0.52
1:D:47:TYR:HA	1:D:50:PHE:O	2.09	0.52
1:C:65:LEU:HD21	1:C:125:TRP:HA	1.92	0.52
1:D:27:TYR:CZ	1:D:53:LYS:HD3	2.45	0.52
1:C:88:LEU:HD13	1:C:159:PHE:CZ	2.45	0.51
1:D:7:ALA:O	1:D:8:ALA:HB3	2.09	0.51
1:D:21:VAL:CG1	1:D:30:THR:HG23	2.40	0.51
1:C:161:GLY:HA3	1:E:157:GLY:O	2.10	0.51
1:G:87:LEU:O	1:G:90:GLN:N	2.43	0.51
1:B:157:GLY:O	1:F:161:GLY:HA3	2.11	0.51
1:F:91:LEU:O	1:F:92:LEU:C	2.54	0.51
1:B:78:LEU:CD1	1:B:187:MSE:HE1	2.36	0.51
1:E:9:GLN:HB2	1:E:12:ARG:HH12	1.77	0.50
1:F:64:GLN:C	1:F:66:ARG:N	2.69	0.50
1:A:218:GLU:O	1:A:218:GLU:OE1	2.30	0.50
1:B:44:GLY:HA2	1:G:9:GLN:OE1	2.11	0.50
1:F:22:PHE:O	1:F:25:LEU:O	2.30	0.50
1:H:183:HIS:NE2	1:H:187:MSE:HE3	2.27	0.50
1:D:104:ARG:O	1:D:104:ARG:HG3	2.12	0.49
1:D:154:MSE:HE1	1:G:185:HIS:ND1	2.27	0.49
1:G:62:THR:CG2	1:G:66:ARG:HH22	2.25	0.49
1:A:22:PHE:O	1:A:23:ASP:C	2.55	0.49
1:E:84:GLU:OE1	1:E:128:HIS:HE1	1.94	0.49
1:G:149:ASP:OD2	1:G:153:ARG:NH1	2.45	0.49
1:H:90:GLN:O	1:H:94:LYS:HG2	2.11	0.49
1:B:145:ARG:HB2	1:B:145:ARG:NH1	2.28	0.49
1:D:154:MSE:HE2	1:G:182:MSE:CA	2.42	0.49
1:E:23:ASP:O	1:E:104:ARG:HD3	2.12	0.49
1:C:160:THR:O	1:C:164:ILE:HG13	2.12	0.49
1:E:106:THR:HG21	1:E:122:MSE:HE2	1.94	0.49
1:B:122[B]:MSE:HE3	1:B:125:TRP:HB3	1.95	0.49
1:D:10:THR:C	1:D:12:ARG:H	2.19	0.49
1:E:64:GLN:C	1:E:66:ARG:H	2.19	0.49
1:A:104:ARG:O	1:A:104:ARG:HG3	2.13	0.49
1:E:214:MSE:HA	1:E:214:MSE:CE	2.36	0.49
1:A:176:LEU:HD12	1:A:176:LEU:O	2.12	0.48
1:F:92:LEU:HD13	1:F:103:VAL:HG11	1.95	0.48
1:C:122[A]:MSE:CE	1:C:156:VAL:HG11	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:ARG:H	1:D:75:ARG:HG3	1.35	0.48
1:H:23:ASP:O	1:H:104:ARG:NH1	2.46	0.48
1:C:20:ALA:O	1:C:24:GLU:HG3	2.14	0.48
1:C:192:VAL:HG23	1:C:195:VAL:H	1.77	0.48
1:A:122:MSE:HE1	1:A:125:TRP:CE3	2.48	0.48
1:E:74:GLN:HE21	1:E:74:GLN:HB3	1.46	0.48
1:B:61:LEU:HD22	1:B:122[A]:MSE:HE3	1.95	0.48
1:C:122[A]:MSE:SE	1:E:165:LEU:HD22	2.63	0.48
1:A:133:LEU:HB3	1:A:148:VAL:HG22	1.96	0.48
1:D:144:PRO:O	1:D:145:ARG:HG2	2.13	0.48
1:F:75:ARG:HG2	1:F:75:ARG:NH1	2.26	0.48
1:A:82:ILE:CG2	1:A:86:LEU:HD11	2.44	0.48
1:B:154:MSE:HE3	1:B:186:LEU:HD22	1.96	0.48
1:G:90:GLN:HA	1:G:90:GLN:NE2	2.29	0.48
1:A:189:SER:OG	1:H:185:HIS:HD2	1.97	0.48
1:B:32:ILE:O	1:B:36:LEU:HG	2.14	0.48
1:D:61:LEU:HD13	1:D:121:PRO:HG3	1.96	0.48
1:H:30:THR:O	1:H:53:LYS:NZ	2.30	0.47
1:C:75:ARG:HG2	1:C:76:LEU:O	2.14	0.47
1:A:122:MSE:CE	2:A:318:HOH:O	2.05	0.47
1:A:154:MSE:CE	1:H:181:ASP:HB3	2.35	0.47
1:F:199:LEU:HD23	1:F:199:LEU:HA	1.66	0.47
1:A:114:ASP:OD1	1:A:114:ASP:C	2.56	0.47
1:G:62:THR:HG21	1:G:66:ARG:HH22	1.78	0.47
1:H:90:GLN:NE2	1:H:176:LEU:HD11	2.29	0.47
1:D:43:LYS:O	1:D:47:TYR:CD2	2.68	0.47
1:A:117:ASP:OD1	1:A:119:ARG:HB3	2.15	0.47
1:G:88:LEU:HD23	1:G:159:PHE:CZ	2.50	0.46
1:A:94:LYS:HG3	1:A:210:TYR:HH	1.74	0.46
1:B:66:ARG:HB2	1:B:66:ARG:CZ	2.46	0.46
1:D:79:GLN:NE2	1:D:83:ASP:OD1	2.49	0.46
1:D:154:MSE:CE	1:G:181:ASP:C	2.87	0.46
1:G:216:ARG:HA	1:G:216:ARG:NH1	2.31	0.46
1:G:229:HIS:C	1:G:229:HIS:CD2	2.93	0.46
1:H:22:PHE:O	1:H:25:LEU:O	2.33	0.46
1:A:118:ARG:C	1:A:121:PRO:HD2	2.41	0.46
1:A:118:ARG:O	1:A:121:PRO:HD2	2.16	0.46
1:A:185:HIS:CD2	1:H:189:SER:HB2	2.50	0.46
1:G:3:ARG:CG	1:G:3:ARG:NH1	2.79	0.46
1:G:133:LEU:HB3	1:G:148:VAL:HG22	1.97	0.46
1:B:118:ARG:C	1:B:121:PRO:HD2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:ILE:HG22	1:D:15:VAL:N	2.29	0.45
1:A:3:ARG:NH1	1:A:4:GLN:CG	2.72	0.45
1:G:39:SER:HB2	1:G:41:VAL:HG23	1.98	0.45
1:G:118:ARG:C	1:G:121:PRO:HD2	2.41	0.45
1:G:176:LEU:O	1:G:176:LEU:CG	2.53	0.45
1:H:43:LYS:O	1:H:47:TYR:CD2	2.69	0.45
1:A:130:ARG:HG2	1:A:148:VAL:CG1	2.47	0.45
1:B:167:ASN:HB2	1:B:172:HIS:NE2	2.31	0.45
1:D:41:VAL:HG13	1:D:42:THR:N	2.31	0.45
1:E:22:PHE:O	1:E:25:LEU:O	2.35	0.45
1:E:25:LEU:N	1:E:25:LEU:HD23	2.31	0.45
1:E:74:GLN:C	1:E:76:LEU:H	2.25	0.45
1:G:96:ASP:CG	1:G:217:ARG:HH11	2.24	0.45
1:B:62:THR:CG2	1:B:121:PRO:HB3	2.47	0.44
1:C:46:LEU:C	1:C:46:LEU:HD23	2.42	0.44
1:F:134:ARG:HH11	1:F:137:GLU:HB3	1.82	0.44
1:D:43:LYS:O	1:D:47:TYR:CE2	2.70	0.44
1:E:64:GLN:C	1:E:66:ARG:N	2.75	0.44
1:G:133:LEU:CB	1:G:148:VAL:HG22	2.47	0.44
1:A:98:LEU:HA	1:A:98:LEU:HD23	1.77	0.44
1:A:169:LEU:HD11	1:H:126:ILE:CD1	2.47	0.44
1:D:53:LYS:O	1:D:56:LEU:HB2	2.18	0.44
1:D:184[B]:ARG:HD3	1:D:201:PHE:CE1	2.52	0.44
1:F:178:ARG:HA	1:F:178:ARG:HD2	1.55	0.44
1:B:13:THR:HG21	1:B:222:PRO:HD3	1.99	0.44
1:B:62:THR:HB	1:B:65:LEU:HD12	2.00	0.44
1:G:90:GLN:HA	1:G:90:GLN:HE21	1.83	0.44
1:A:78:LEU:HD22	1:A:187:MSE:HE1	1.99	0.44
1:C:167:ASN:HB2	1:C:172:HIS:NE2	2.33	0.44
1:F:74:GLN:C	1:F:76:LEU:N	2.74	0.44
1:A:181:ASP:HB3	1:H:154:MSE:HE2	1.98	0.44
1:C:94:LYS:H	1:C:94:LYS:HG2	1.69	0.44
1:H:43:LYS:O	1:H:47:TYR:CE2	2.70	0.44
1:B:9:GLN:NE2	1:B:221:LEU:O	2.51	0.43
1:B:185:HIS:HD2	1:F:189:SER:OG	2.01	0.43
1:C:200:ASP:OD1	1:C:200:ASP:C	2.62	0.43
1:E:21:VAL:HG12	1:E:30:THR:CG2	2.47	0.43
1:G:23:ASP:OD2	1:G:100:ARG:HD3	2.17	0.43
1:A:142:LEU:HD22	1:A:190:VAL:HG13	2.00	0.43
1:D:95:GLY:O	1:D:97:PRO:N	2.51	0.43
1:A:82:ILE:O	1:A:83:ASP:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:120:ALA:HB3	1:G:121:PRO:HD3	2.01	0.43
1:G:133:LEU:HD12	1:G:152:ALA:HB2	2.01	0.43
1:A:174:ASP:O	1:A:175:LEU:C	2.61	0.43
1:D:178:ARG:HA	1:D:178:ARG:HD3	1.68	0.43
1:D:181:ASP:CB	1:G:154:MSE:HE2	2.38	0.43
1:F:134:ARG:HD2	1:F:134:ARG:HA	1.61	0.43
1:H:56:LEU:HD13	1:H:56:LEU:HA	1.77	0.43
1:C:62:THR:HG23	1:C:121:PRO:HB3	2.00	0.43
1:G:96:ASP:CG	1:G:217:ARG:NH1	2.77	0.43
1:G:219:ALA:HA	1:G:220:PRO:HD3	1.94	0.43
1:B:86:LEU:O	1:B:89:ALA:HB3	2.18	0.43
1:B:174:ASP:O	1:B:175:LEU:C	2.62	0.43
1:E:79:GLN:HA	1:E:82:ILE:HD12	2.00	0.43
1:C:23:ASP:OD2	1:C:100:ARG:NH1	2.52	0.43
1:C:120:ALA:N	1:C:121:PRO:CD	2.81	0.43
1:C:219:ALA:HA	1:C:220:PRO:HD3	1.84	0.43
1:E:73:GLU:HA	1:E:205:ARG:HH22	1.84	0.43
1:F:30:THR:O	1:F:53:LYS:HD2	2.19	0.43
1:B:160:THR:O	1:B:164:ILE:HD12	2.19	0.42
1:C:122[A]:MSE:CE	1:C:126:ILE:HG13	2.49	0.42
1:D:92:LEU:HB3	1:D:175:LEU:HD21	2.01	0.42
1:D:154:MSE:HE2	1:G:181:ASP:O	2.19	0.42
1:B:122[B]:MSE:HE2	1:B:126:ILE:HG13	2.01	0.42
1:C:61:LEU:HD22	1:C:122[B]:MSE:HE3	2.00	0.42
1:C:89:ALA:O	1:C:175:LEU:HD23	2.19	0.42
1:D:7:ALA:C	1:D:9:GLN:H	2.26	0.42
1:H:11:ARG:HB2	1:H:49:HIS:NE2	2.34	0.42
1:B:62:THR:HG23	1:B:121:PRO:HB3	2.00	0.42
1:D:76:LEU:HD23	1:D:76:LEU:HA	1.85	0.42
1:E:167:ASN:HB2	1:E:172:HIS:NE2	2.35	0.42
1:G:2:ALA:HB1	2:G:316:HOH:O	2.19	0.42
1:G:105:LEU:O	1:G:118:ARG:NH1	2.43	0.42
1:H:61:LEU:HA	1:H:102:SER:HB2	2.01	0.42
1:A:82:ILE:HG23	1:A:86:LEU:HD11	2.01	0.42
1:G:96:ASP:OD2	1:G:217:ARG:NH1	2.52	0.42
1:B:195:VAL:O	1:B:196:LEU:C	2.61	0.42
1:E:64:GLN:HG3	1:E:99:VAL:HG22	2.02	0.42
1:H:43:LYS:HD3	1:H:47:TYR:HE2	1.84	0.42
1:H:137:GLU:OE1	1:H:137:GLU:HA	2.18	0.42
1:A:151:VAL:O	1:A:152:ALA:C	2.62	0.42
1:F:211:ASP:HB3	1:F:215:ARG:HH22	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ASP:HA	1:B:97:PRO:HD3	1.89	0.42
1:C:50:PHE:HD1	1:C:55:GLN:HE21	1.68	0.42
1:E:108:GLU:HA	1:E:109:PRO:HD3	1.95	0.42
1:F:137:GLU:HB2	1:F:142:LEU:HD12	2.01	0.42
1:E:199:LEU:HD23	1:E:199:LEU:HA	1.74	0.41
1:G:170:THR:CB	1:G:173:ALA:HB3	2.45	0.41
1:C:122[A]:MSE:HE2	1:C:126:ILE:CG1	2.50	0.41
1:D:93:SER:HB3	1:D:175:LEU:HD23	2.02	0.41
1:F:159:PHE:CD1	1:F:159:PHE:C	2.99	0.41
1:G:24:GLU:CD	1:G:38:ARG:HH12	2.28	0.41
1:G:36:LEU:HA	1:G:36:LEU:HD23	1.55	0.41
1:H:61:LEU:HD21	1:H:105:LEU:CB	2.49	0.41
1:B:122[B]:MSE:CE	1:B:156:VAL:HG11	2.39	0.41
1:C:51:THR:H	1:C:55:GLN:NE2	2.18	0.41
1:C:154:MSE:CE	1:E:181:ASP:HB3	2.34	0.41
1:D:53:LYS:O	1:D:54:GLU:C	2.61	0.41
1:D:53:LYS:HA	1:D:56:LEU:HB2	2.02	0.41
1:G:94:LYS:HD2	1:G:94:LYS:C	2.46	0.41
1:H:188:THR:O	1:H:188:THR:HG22	2.20	0.41
1:A:222:PRO:HG2	1:A:227:LEU:CD2	2.51	0.41
1:D:41:VAL:CG1	1:D:42:THR:N	2.83	0.41
1:A:96:ASP:HA	1:A:97:PRO:HD3	1.92	0.41
1:D:84:GLU:OE1	1:D:128:HIS:HE1	2.03	0.41
1:D:109:PRO:HG3	1:G:104:ARG:NH1	2.36	0.41
1:A:36:LEU:HD23	1:A:36:LEU:HA	1.69	0.41
1:D:56:LEU:HA	1:D:56:LEU:HD13	1.81	0.41
1:G:125:TRP:O	1:G:128:HIS:HB3	2.21	0.41
1:A:122:MSE:HG3	1:H:169:LEU:HD21	2.03	0.41
1:A:186:LEU:HD23	1:A:186:LEU:HA	1.81	0.41
1:C:75:ARG:HB2	1:C:76:LEU:H	1.64	0.41
1:C:143:LEU:HD23	1:C:192:VAL:HG12	2.02	0.41
1:D:22:PHE:O	1:D:25:LEU:O	2.38	0.41
1:E:134:ARG:HD2	1:E:134:ARG:HA	1.90	0.41
1:G:32:ILE:O	1:G:36:LEU:HG	2.21	0.41
1:H:14:ILE:CG2	1:H:15:VAL:N	2.84	0.41
1:H:209:VAL:O	1:H:212:GLU:HB3	2.21	0.41
1:D:92:LEU:HD12	1:D:92:LEU:HA	1.78	0.41
1:F:74:GLN:O	1:F:75:ARG:C	2.64	0.41
1:B:145:ARG:HB2	1:B:145:ARG:HH11	1.85	0.40
1:G:186:LEU:HD23	1:G:186:LEU:HA	1.83	0.40
1:C:178:ARG:HA	1:C:178:ARG:HD3	1.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:178:ARG:HD3	1:H:178:ARG:HA	1.68	0.40
1:A:82:ILE:HG22	1:A:86:LEU:HD12	2.04	0.40
1:G:87:LEU:O	1:G:89:ALA:N	2.54	0.40
1:B:22:PHE:O	1:B:25:LEU:O	2.40	0.40
1:C:222:PRO:HG2	1:C:227:LEU:HD21	2.02	0.40
1:D:65:LEU:CD2	1:D:65:LEU:C	2.90	0.40
1:D:132:LEU:HD23	1:D:132:LEU:HA	1.96	0.40
1:E:145:ARG:HB2	1:E:145:ARG:NH1	2.36	0.40
1:A:78:LEU:CG	1:A:187:MSE:HE1	2.50	0.40
1:B:126:ILE:HG13	1:B:126:ILE:H	1.65	0.40
1:E:73:GLU:HA	1:E:205:ARG:NH2	2.35	0.40
1:E:104:ARG:O	1:E:104:ARG:HG3	2.20	0.40
1:E:120:ALA:N	1:E:121:PRO:HD2	2.36	0.40
1:H:210:TYR:O	1:H:211:ASP:C	2.65	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ARG:NH2	1:C:50:PHE:O[1_565]	2.16	0.04

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	210/228 (92%)	201 (96%)	9 (4%)	0	100	100
1	B	210/228 (92%)	199 (95%)	10 (5%)	1 (0%)	24	44
1	C	214/228 (94%)	202 (94%)	10 (5%)	2 (1%)	14	29
1	D	192/228 (84%)	173 (90%)	18 (9%)	1 (0%)	24	44
1	E	191/228 (84%)	185 (97%)	5 (3%)	1 (0%)	24	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	193/228 (85%)	181 (94%)	11 (6%)	1 (0%)	24	44
1	G	209/228 (92%)	194 (93%)	14 (7%)	1 (0%)	24	44
1	H	187/228 (82%)	167 (89%)	18 (10%)	2 (1%)	11	24
All	All	1606/1824 (88%)	1502 (94%)	95 (6%)	9 (1%)	21	39

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	216	ARG
1	D	52	SER
1	F	64	GLN
1	G	88	LEU
1	B	220	PRO
1	E	75	ARG
1	H	63	SER
1	H	76	LEU
1	C	220	PRO

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	173/178 (97%)	160 (92%)	13 (8%)	12	26
1	B	173/178 (97%)	166 (96%)	7 (4%)	28	52
1	C	174/178 (98%)	157 (90%)	17 (10%)	7	16
1	D	160/178 (90%)	134 (84%)	26 (16%)	2	4
1	E	160/178 (90%)	146 (91%)	14 (9%)	9	20
1	F	160/178 (90%)	145 (91%)	15 (9%)	8	17
1	G	172/178 (97%)	149 (87%)	23 (13%)	4	7
1	H	157/178 (88%)	133 (85%)	24 (15%)	3	5
All	All	1329/1424 (93%)	1190 (90%)	139 (10%)	6	13

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	41	VAL
1	A	51	THR
1	A	116	LEU
1	A	118	ARG
1	A	126	ILE
1	A	137	GLU
1	A	148	VAL
1	A	190	VAL
1	A	195	VAL
1	A	209	VAL
1	A	217	ARG
1	A	218	GLU
1	B	37	LYS
1	B	66	ARG
1	B	108	GLU
1	B	190	VAL
1	B	216	ARG
1	B	217	ARG
1	B	218	GLU
1	C	3	ARG
1	C	25	LEU
1	C	32	ILE
1	C	41	VAL
1	C	65	LEU
1	C	75	ARG
1	C	76	LEU
1	C	81	ILE
1	C	88	LEU
1	C	100	ARG
1	C	116	LEU
1	C	146	LEU
1	C	190	VAL
1	C	206	SER
1	C	208	THR
1	C	215	ARG
1	C	216	ARG
1	D	10	THR
1	D	14	ILE
1	D	25	LEU
1	D	37	LYS
1	D	41	VAL

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Mol	Chain	Res	Type
1	D	42	THR
1	D	50	PHE
1	D	53	LYS
1	D	54	GLU
1	D	55	GLN
1	D	56	LEU
1	D	63	SER
1	D	65	LEU
1	D	66	ARG
1	D	75	ARG
1	D	81	ILE
1	D	98	LEU
1	D	119	ARG
1	D	123	GLN
1	D	148	VAL
1	D	154	MSE
1	D	165	LEU
1	D	176	LEU
1	D	189	SER
1	D	204	GLU
1	D	215	ARG
1	E	25	LEU
1	E	41	VAL
1	E	64	GLN
1	E	74	GLN
1	E	75	ARG
1	E	106	THR
1	E	107	VAL
1	E	123	GLN
1	E	153	ARG
1	E	154	MSE
1	E	198	ARG
1	E	206	SER
1	E	214	MSE
1	E	215	ARG
1	F	25	LEU
1	F	37	LYS
1	F	41	VAL
1	F	65	LEU
1	F	74	GLN
1	F	76	LEU
1	F	103	VAL

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Mol	Chain	Res	Type
1	F	104	ARG
1	F	107	VAL
1	F	116	LEU
1	F	123	GLN
1	F	134	ARG
1	F	178	ARG
1	F	198	ARG
1	F	214	MSE
1	G	3	ARG
1	G	4	GLN
1	G	66	ARG
1	G	90	GLN
1	G	94	LYS
1	G	100	ARG
1	G	104	ARG
1	G	107	VAL
1	G	118	ARG
1	G	148	VAL
1	G	154	MSE
1	G	190	VAL
1	G	192	VAL
1	G	195	VAL
1	G	197	VAL
1	G	204	GLU
1	G	205	ARG
1	G	209	VAL
1	G	212	GLU
1	G	214	MSE
1	G	215	ARG
1	G	216	ARG
1	G	221	LEU
1	H	9	GLN
1	H	12	ARG
1	H	14	ILE
1	H	25	LEU
1	H	41	VAL
1	H	42	THR
1	H	43	LYS
1	H	50	PHE
1	H	52	SER
1	H	56	LEU
1	H	76	LEU

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Mol	Chain	Res	Type
1	H	77	VAL
1	H	78	LEU
1	H	93	SER
1	H	98	LEU
1	H	103	VAL
1	H	106	THR
1	H	119	ARG
1	H	123	GLN
1	H	137	GLU
1	H	148	VAL
1	H	176	LEU
1	H	189	SER
1	H	207	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	49	HIS
1	A	163	GLN
1	A	185	HIS
1	B	9	GLN
1	B	55	GLN
1	B	185	HIS
1	C	55	GLN
1	C	123	GLN
1	C	163	GLN
1	C	167	ASN
1	D	90	GLN
1	D	128	HIS
1	D	163	GLN
1	D	185	HIS
1	E	74	GLN
1	E	128	HIS
1	E	185	HIS
1	F	49	HIS
1	F	58	GLN
1	G	4	GLN
1	G	64	GLN
1	G	90	GLN
1	G	229	HIS
1	H	9	GLN

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Mol	Chain	Res	Type
1	H	163	GLN
1	H	185	HIS

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](#)

There are no ligands in this entry.

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	210/228 (92%)	-0.44	2 (0%) 79 77	13, 26, 51, 74	1 (0%)
1	B	210/228 (92%)	-0.45	3 (1%) 73 70	13, 25, 56, 93	0
1	C	214/228 (93%)	-0.37	7 (3%) 49 44	13, 25, 54, 84	0
1	D	192/228 (84%)	0.18	16 (8%) 17 14	12, 39, 85, 106	1 (0%)
1	E	192/228 (84%)	-0.36	5 (2%) 57 52	16, 31, 62, 85	0
1	F	194/228 (85%)	-0.31	5 (2%) 57 52	15, 32, 66, 84	0
1	G	210/228 (92%)	-0.43	1 (0%) 87 86	12, 27, 49, 79	0
1	H	187/228 (82%)	-0.01	8 (4%) 40 35	12, 39, 85, 103	1 (0%)
All	All	1609/1824 (88%)	-0.28	47 (2%) 53 49	12, 29, 69, 106	3 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	7	ALA	6.6
1	D	67	ALA	6.2
1	C	110	GLY	5.6
1	D	9	GLN	5.1
1	C	215	ARG	5.1
1	D	8	ALA	4.9
1	C	114	ASP	4.9
1	C	111	ALA	4.8
1	C	74	GLN	4.5
1	D	52	SER	4.4
1	B	115	GLY	4.3
1	F	7	ALA	4.1
1	D	75	ARG	3.9
1	E	8	ALA	3.8
1	E	7	ALA	3.7
1	H	8	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	H	48	PHE	3.6
1	D	10	THR	3.5
1	C	75	ARG	3.2
1	E	75	ARG	3.1
1	D	48	PHE	3.0
1	B	218	GLU	2.9
1	D	54	GLU	2.9
1	A	109	PRO	2.8
1	F	8	ALA	2.8
1	H	42	THR	2.7
1	D	42	THR	2.7
1	D	74	GLN	2.7
1	D	215	ARG	2.7
1	D	47	TYR	2.7
1	A	218	GLU	2.4
1	B	219	ALA	2.4
1	D	45	ALA	2.4
1	D	49	HIS	2.3
1	H	14	ILE	2.3
1	F	215	ARG	2.2
1	G	75	ARG	2.2
1	F	109	PRO	2.2
1	H	10	THR	2.1
1	F	115	GLY	2.1
1	H	40	GLY	2.1
1	C	218	GLU	2.1
1	H	109	PRO	2.1
1	E	215	ARG	2.1
1	D	120	ALA	2.0
1	H	213	ALA	2.0
1	E	109	PRO	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.