



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:48 PM UTC

PDB ID : 4PEL / pdb_00004pel
Title : S1C mutant of Penicillin G acylase from *Kluyvera citrophila*
Authors : Ramasamy, S.; Chand, D.; Varshney, N.K.; Brannigan, J.A.; Wilkinson, A.J.; Suresh, C.G.
Deposited on : 2014-04-24
Resolution : 2.80 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
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

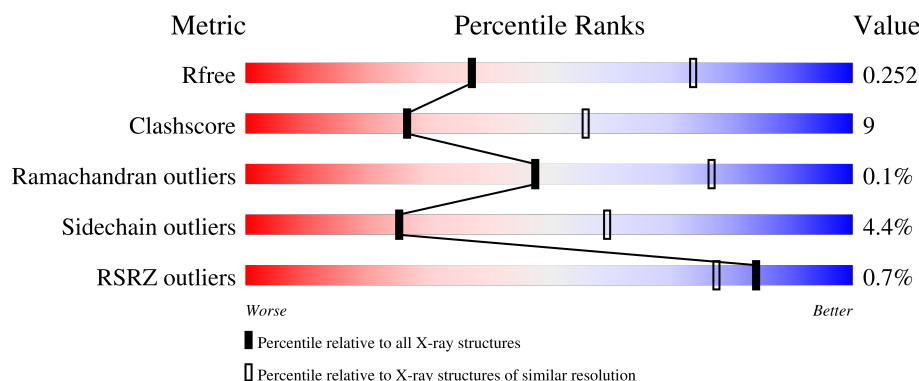
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	222	% 68% 15% • 13%
1	C	222	% 76% 11% • 13%
1	E	222	2% 76% 11% 13%
1	G	222	% 73% 14% 13%
2	B	565	% 79% 18% ••

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Mol	Chain	Length	Quality of chain
2	D	565	78% 19% ..
2	F	565	82% 16% ..
2	H	565	% 80% 16% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23734 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 Penicillin G acylase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1545	989	259	290	7			
1	C	194	Total	C	N	O	S	0	0	0
			1545	989	259	290	7			
1	E	194	Total	C	N	O	S	0	0	0
			1545	989	259	290	7			
1	G	194	Total	C	N	O	S	0	0	0
			1545	989	259	290	7			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	LEU	VAL	conflict	UNP P07941
A	168	LYS	ASN	conflict	UNP P07941
A	169	GLN	ASP	conflict	UNP P07941
A	170	GLN	GLU	conflict	UNP P07941
A	196	ALA	SER	conflict	UNP P07941
C	162	LEU	VAL	conflict	UNP P07941
C	168	LYS	ASN	conflict	UNP P07941
C	169	GLN	ASP	conflict	UNP P07941
C	170	GLN	GLU	conflict	UNP P07941
C	196	ALA	SER	conflict	UNP P07941
E	162	LEU	VAL	conflict	UNP P07941
E	168	LYS	ASN	conflict	UNP P07941
E	169	GLN	ASP	conflict	UNP P07941
E	170	GLN	GLU	conflict	UNP P07941
E	196	ALA	SER	conflict	UNP P07941
G	162	LEU	VAL	conflict	UNP P07941
G	168	LYS	ASN	conflict	UNP P07941
G	169	GLN	ASP	conflict	UNP P07941
G	170	GLN	GLU	conflict	UNP P07941
G	196	ALA	SER	conflict	UNP P07941

- Molecule 2 is a protein called Penicillin G acylase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	557	Total	C	N	O	S	0	0	0
			4379	2786	758	826	9			
2	D	557	Total	C	N	O	S	0	0	0
			4379	2786	758	826	9			
2	F	557	Total	C	N	O	S	0	0	0
			4379	2786	758	826	9			
2	H	557	Total	C	N	O	S	0	0	0
			4379	2786	758	826	9			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	CYS	SER	engineered mutation	UNP P07941
B	123	HIS	ASP	conflict	UNP P07941
B	132	ALA	ARG	conflict	UNP P07941
B	144	ASP	ALA	conflict	UNP P07941
B	211	GLY	-	insertion	UNP P07941
B	212	THR	ASP	conflict	UNP P07941
B	270	THR	ILE	conflict	UNP P07941
B	291	ARG	LEU	conflict	UNP P07941
B	295	ASN	-	insertion	UNP P07941
B	419	GLN	GLU	conflict	UNP P07941
B	526	ILE	LYS	conflict	UNP P07941
B	558	LEU	-	expression tag	UNP P07941
B	559	GLU	-	expression tag	UNP P07941
B	560	HIS	-	expression tag	UNP P07941
B	561	HIS	-	expression tag	UNP P07941
B	562	HIS	-	expression tag	UNP P07941
B	563	HIS	-	expression tag	UNP P07941
B	564	HIS	-	expression tag	UNP P07941
B	565	HIS	-	expression tag	UNP P07941
D	1	CYS	SER	engineered mutation	UNP P07941
D	123	HIS	ASP	conflict	UNP P07941
D	132	ALA	ARG	conflict	UNP P07941
D	144	ASP	ALA	conflict	UNP P07941
D	211	GLY	-	insertion	UNP P07941
D	212	THR	ASP	conflict	UNP P07941
D	270	THR	ILE	conflict	UNP P07941
D	291	ARG	LEU	conflict	UNP P07941
D	295	ASN	-	insertion	UNP P07941
D	419	GLN	GLU	conflict	UNP P07941
D	526	ILE	LYS	conflict	UNP P07941

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Chain	Residue	Modelled	Actual	Comment	Reference
D	558	LEU	-	expression tag	UNP P07941
D	559	GLU	-	expression tag	UNP P07941
D	560	HIS	-	expression tag	UNP P07941
D	561	HIS	-	expression tag	UNP P07941
D	562	HIS	-	expression tag	UNP P07941
D	563	HIS	-	expression tag	UNP P07941
D	564	HIS	-	expression tag	UNP P07941
D	565	HIS	-	expression tag	UNP P07941
F	1	CYS	SER	engineered mutation	UNP P07941
F	123	HIS	ASP	conflict	UNP P07941
F	132	ALA	ARG	conflict	UNP P07941
F	144	ASP	ALA	conflict	UNP P07941
F	211	GLY	-	insertion	UNP P07941
F	212	THR	ASP	conflict	UNP P07941
F	270	THR	ILE	conflict	UNP P07941
F	291	ARG	LEU	conflict	UNP P07941
F	295	ASN	-	insertion	UNP P07941
F	419	GLN	GLU	conflict	UNP P07941
F	526	ILE	LYS	conflict	UNP P07941
F	558	LEU	-	expression tag	UNP P07941
F	559	GLU	-	expression tag	UNP P07941
F	560	HIS	-	expression tag	UNP P07941
F	561	HIS	-	expression tag	UNP P07941
F	562	HIS	-	expression tag	UNP P07941
F	563	HIS	-	expression tag	UNP P07941
F	564	HIS	-	expression tag	UNP P07941
F	565	HIS	-	expression tag	UNP P07941
H	1	CYS	SER	engineered mutation	UNP P07941
H	123	HIS	ASP	conflict	UNP P07941
H	132	ALA	ARG	conflict	UNP P07941
H	144	ASP	ALA	conflict	UNP P07941
H	211	GLY	-	insertion	UNP P07941
H	212	THR	ASP	conflict	UNP P07941
H	270	THR	ILE	conflict	UNP P07941
H	291	ARG	LEU	conflict	UNP P07941
H	295	ASN	-	insertion	UNP P07941
H	419	GLN	GLU	conflict	UNP P07941
H	526	ILE	LYS	conflict	UNP P07941
H	558	LEU	-	expression tag	UNP P07941
H	559	GLU	-	expression tag	UNP P07941
H	560	HIS	-	expression tag	UNP P07941
H	561	HIS	-	expression tag	UNP P07941

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Chain	Residue	Modelled	Actual	Comment	Reference
H	562	HIS	-	expression tag	UNP P07941
H	563	HIS	-	expression tag	UNP P07941
H	564	HIS	-	expression tag	UNP P07941
H	565	HIS	-	expression tag	UNP P07941

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	G	1	Total Ca 1 1	0	0

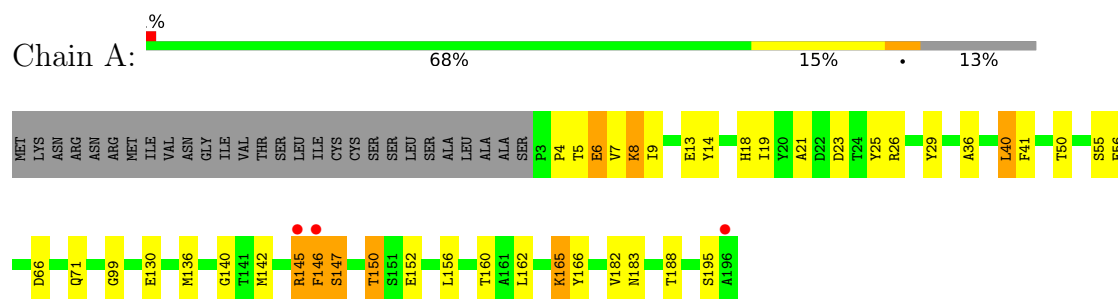
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total O 2 2	0	0
4	B	9	Total O 9 9	0	0
4	C	1	Total O 1 1	0	0
4	D	3	Total O 3 3	0	0
4	F	7	Total O 7 7	0	0
4	G	1	Total O 1 1	0	0
4	H	11	Total O 11 11	0	0

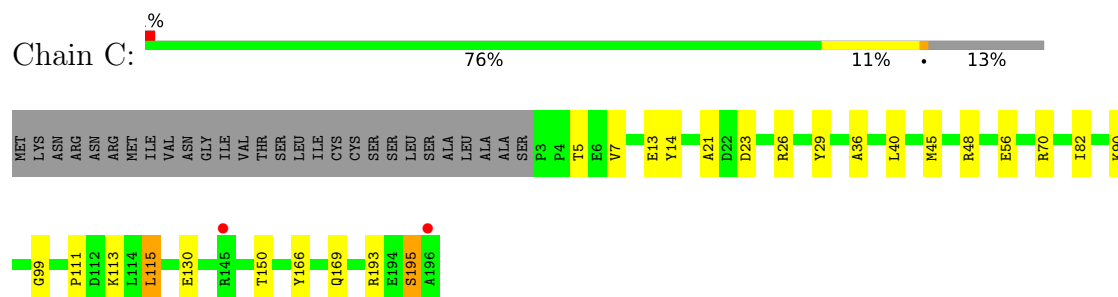
3 Residue-property plots [i](#)

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.

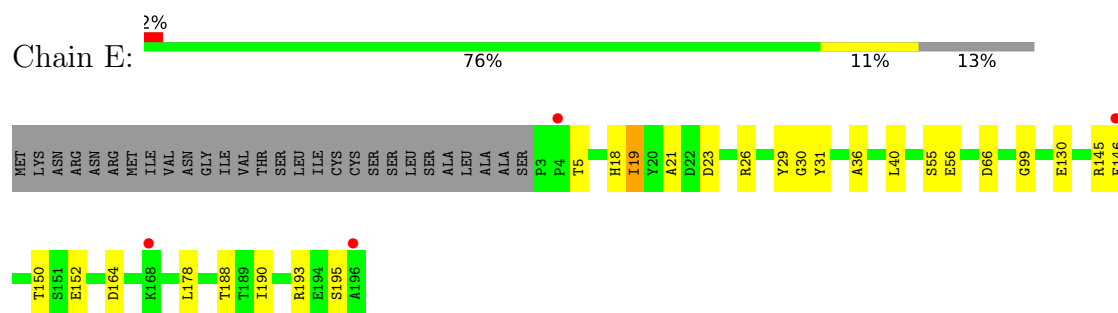
- Molecule 1: Penicillin G acylase subunit alpha



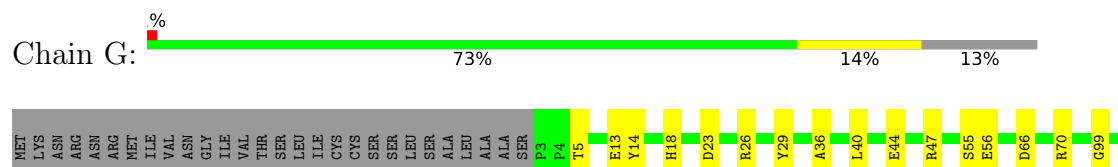
- Molecule 1: Penicillin G acylase subunit alpha



- Molecule 1: Penicillin G acylase subunit alpha



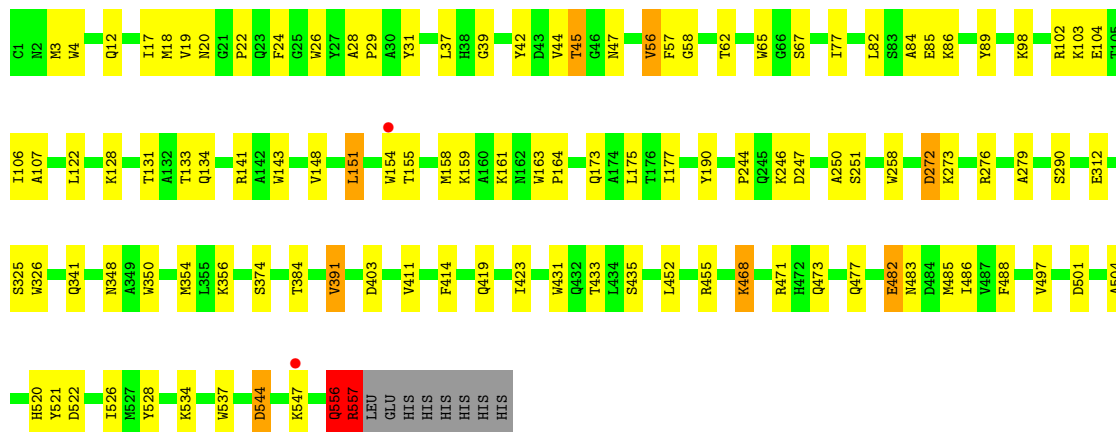
- Molecule 1: Penicillin G acylase subunit alpha





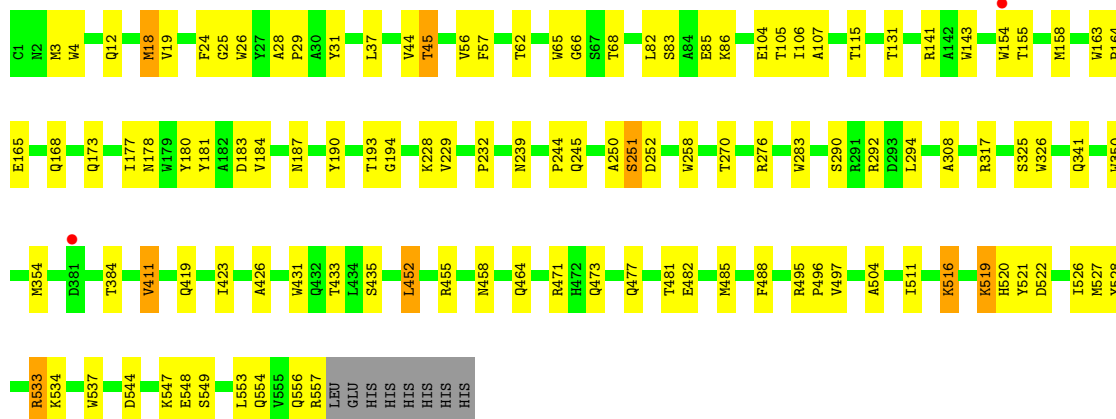
• Molecule 2: Penicillin G acylase subunit beta

Chain B: 79% 18% ..



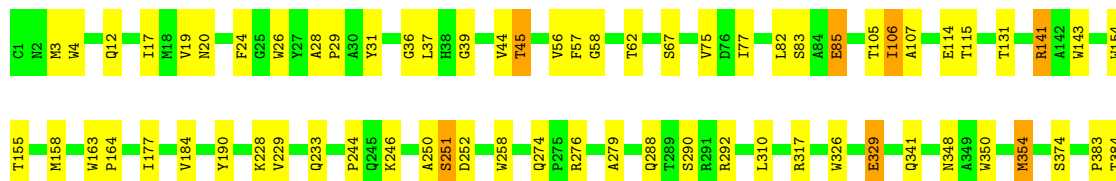
• Molecule 2: Penicillin G acylase subunit beta

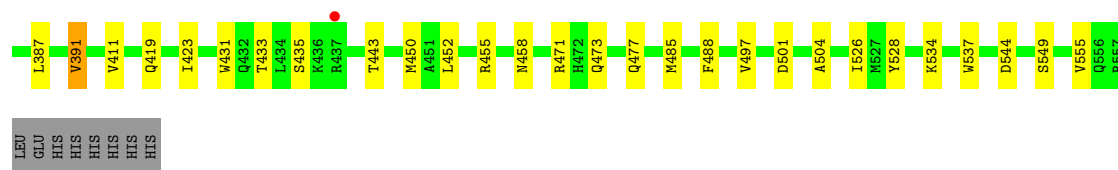
Chain D: 78% 19% ..



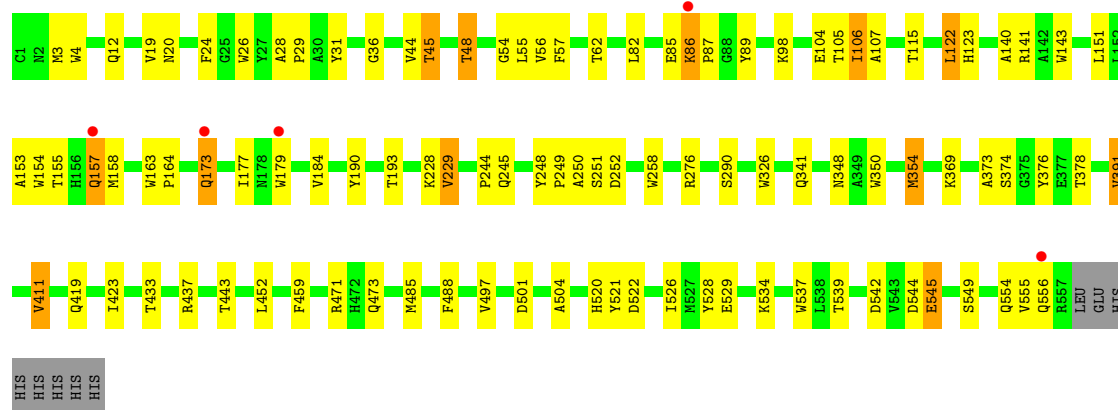
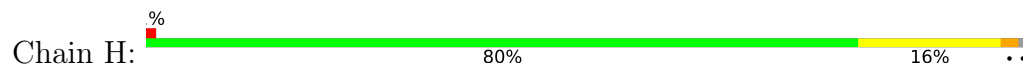
• Molecule 2: Penicillin G acylase subunit beta

Chain F: 82% 16% ..





- Molecule 2: Penicillin G acylase subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	96.26Å 96.26Å 100.21Å 69.27° 69.27° 76.77°	Depositor
Resolution (Å)	38.24 – 2.80 38.24 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.4 (38.24-2.80) 88.4 (38.24-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.214 , 0.251 0.216 , 0.252	Depositor DCC
R_{free} test set	3420 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 22.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.037 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23734	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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: CA

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	0.97	3/1584 (0.2%)	1.05	9/2146 (0.4%)
1	C	0.64	0/1584	0.92	0/2146
1	E	0.70	0/1584	0.96	1/2146 (0.0%)
1	G	0.69	0/1584	0.96	5/2146 (0.2%)
2	B	0.71	1/4507 (0.0%)	0.92	5/6147 (0.1%)
2	D	0.70	0/4507	0.90	1/6147 (0.0%)
2	F	0.69	0/4507	0.87	3/6147 (0.0%)
2	H	0.70	0/4507	0.90	6/6147 (0.1%)
All	All	0.71	4/24364 (0.0%)	0.92	30/33172 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	LYS	C-N	-20.77	1.07	1.33
1	A	9	ILE	C-N	-13.09	1.17	1.33
2	B	557	ARG	CA-C	7.81	1.69	1.52
1	A	19	ILE	C-N	6.17	1.41	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	LEU	N-CA-C	-13.62	92.56	110.53
2	H	48	THR	CB-CA-C	-10.35	95.84	109.92
1	G	145	ARG	CB-CA-C	-10.01	95.47	111.39
2	B	557	ARG	N-CA-C	8.92	135.97	111.00
2	H	545	GLU	N-CA-C	-7.83	98.21	109.96
2	F	391	VAL	CB-CA-C	-7.83	101.57	112.14
2	H	391	VAL	CB-CA-C	-7.55	102.14	112.04
2	B	391	VAL	CB-CA-C	-7.27	102.57	111.88
2	B	272	ASP	N-CA-C	-7.01	101.78	110.41
1	A	41	PHE	N-CA-CB	6.61	121.66	110.49
1	E	164	ASP	CB-CA-C	6.60	123.78	109.99
2	F	141	ARG	CB-CG-CD	6.53	126.33	111.30
1	A	183	ASN	CA-C-N	6.34	126.55	119.32
1	A	183	ASN	C-N-CA	6.34	126.55	119.32
1	A	146	PHE	N-CA-C	-6.30	99.42	109.76
2	B	556	GLN	N-CA-C	6.25	116.32	108.45
1	G	145	ARG	CA-CB-CG	5.60	125.30	114.10
2	H	48	THR	N-CA-C	5.38	115.05	108.11
1	A	165	LYS	N-CA-C	-5.38	100.94	109.76
2	B	58	GLY	N-CA-C	5.33	117.78	110.69
1	A	6	GLU	N-CA-C	5.23	118.75	109.96
1	A	18	HIS	CA-C-N	-5.23	115.84	123.06
1	A	18	HIS	C-N-CA	-5.23	115.84	123.06
2	H	229	VAL	CB-CA-C	-5.22	104.54	111.80
1	G	149	SER	N-CA-C	5.17	117.05	108.20
2	F	58	GLY	N-CA-C	5.15	117.53	110.69
2	H	157	GLN	CB-CA-C	-5.13	100.50	110.46
1	G	183	ASN	CA-C-N	5.10	126.22	119.84
1	G	183	ASN	C-N-CA	5.10	126.22	119.84
2	D	533	ARG	CB-CA-C	-5.02	99.70	111.09

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	LYS	Mainchain
2	B	556	GLN	Mainchain

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	1545	0	1506	36	0
1	C	1545	0	1507	32	0
1	E	1545	0	1507	24	0
1	G	1545	0	1507	53	1
2	B	4379	0	4198	85	1
2	D	4379	0	4198	111	0
2	F	4379	0	4198	66	0
2	H	4379	0	4198	99	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	2	0	0	0	0
4	B	9	0	0	1	0
4	C	1	0	0	0	0
4	D	3	0	0	0	0
4	F	7	0	0	0	0
4	G	1	0	0	0	0
4	H	11	0	0	1	0
All	All	23734	0	22819	434	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 9.

All (434) 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:G:107:VAL:HG13	1:G:114:LEU:O	1.12	1.28
1:A:145:ARG:HG2	1:A:146:PHE:N	1.55	1.18
1:G:107:VAL:HA	1:G:114:LEU:HB3	1.18	1.17
1:G:107:VAL:CG1	1:G:114:LEU:O	1.93	1.16
1:G:106:LYS:O	1:G:114:LEU:HD12	1.44	1.16
2:D:354:MET:HE1	2:D:423:ILE:HA	1.17	1.12
2:D:354:MET:CE	2:D:423:ILE:HA	1.84	1.07
1:G:106:LYS:O	1:G:114:LEU:CD1	2.01	1.06
2:D:25:GLY:O	2:D:481:THR:CG2	2.02	1.06
2:D:25:GLY:O	2:D:481:THR:HG22	1.58	1.03
1:C:14:TYR:CG	2:D:534:LYS:HE3	1.94	1.03
2:B:47:ASN:OD1	2:B:482:GLU:OE1	1.80	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LEU:O	1:A:165:LYS:O	1.78	0.98
1:G:106:LYS:C	1:G:114:LEU:HD13	1.88	0.98
2:D:308:ALA:O	2:D:317:ARG:NH2	1.97	0.96
1:E:26:ARG:NH1	2:F:555:VAL:O	1.98	0.96
2:B:556:GLN:HG2	2:B:557:ARG:N	1.80	0.95
2:D:354:MET:HE2	2:D:426:ALA:HB3	1.48	0.95
2:B:556:GLN:HG2	2:B:557:ARG:H	1.32	0.92
2:H:48:THR:CG2	2:H:55:LEU:HA	1.98	0.92
2:F:141:ARG:HD2	2:F:143:TRP:CZ2	2.05	0.91
2:D:354:MET:HE1	2:D:423:ILE:CA	2.02	0.90
2:D:173:GLN:HB3	2:D:193:THR:HG21	1.51	0.90
2:F:383:PRO:HG3	2:F:450:MET:HE3	1.52	0.90
2:B:556:GLN:CG	2:B:557:ARG:H	1.84	0.90
1:A:145:ARG:HG2	1:A:146:PHE:H	1.18	0.89
1:A:50:THR:HG23	1:A:140:GLY:HA3	1.54	0.89
1:A:145:ARG:CG	1:A:146:PHE:N	2.36	0.88
1:A:23:ASP:OD1	1:A:26:ARG:HD3	1.73	0.86
2:D:354:MET:HE2	2:D:426:ALA:CB	2.05	0.86
1:G:107:VAL:HG13	1:G:114:LEU:C	2.00	0.85
1:G:106:LYS:C	1:G:114:LEU:CD1	2.47	0.85
1:A:5:THR:C	1:A:26:ARG:HH12	1.84	0.85
1:C:14:TYR:CD2	2:D:534:LYS:HE3	2.12	0.84
1:C:45:MET:HA	1:C:45:MET:HE2	1.57	0.84
2:B:151:LEU:HD12	2:B:151:LEU:O	1.80	0.82
2:D:25:GLY:O	2:D:481:THR:HG21	1.80	0.82
2:H:154:TRP:CZ3	2:H:179:TRP:CH2	2.68	0.82
1:G:110:SER:O	1:G:114:LEU:HB2	1.80	0.81
1:A:23:ASP:CG	1:A:26:ARG:HD3	2.05	0.80
2:F:383:PRO:CG	2:F:450:MET:CE	2.59	0.80
2:D:556:GLN:HG3	2:D:557:ARG:H	1.43	0.80
2:D:3:MET:HE1	2:D:18:MET:HE3	1.66	0.78
2:H:542:ASP:O	2:H:545:GLU:O	2.02	0.78
2:F:383:PRO:HG3	2:F:450:MET:CE	2.14	0.77
2:D:68:THR:HG21	2:D:239:ASN:OD1	1.84	0.76
1:G:44:GLU:OE2	1:G:47:ARG:NH2	2.18	0.76
2:H:154:TRP:CE3	2:H:179:TRP:CH2	2.73	0.76
2:D:18:MET:HE1	2:D:65:TRP:C	2.09	0.76
1:A:50:THR:HG21	1:A:136:MET:O	1.84	0.76
2:D:68:THR:HG23	2:D:178:ASN:HD22	1.52	0.75
2:H:179:TRP:CD1	2:H:193:THR:HG21	2.22	0.75
2:B:279:ALA:O	2:B:485:MET:HE1	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:228:LYS:O	2:D:229:VAL:HG23	1.88	0.74
2:F:383:PRO:CG	2:F:450:MET:HE3	2.18	0.74
2:H:154:TRP:CZ3	2:H:179:TRP:CZ2	2.76	0.74
2:F:3:MET:HE3	2:F:20:ASN:CG	2.13	0.73
1:G:110:SER:HB2	1:G:114:LEU:HG	1.70	0.73
1:A:23:ASP:OD1	1:A:26:ARG:CD	2.37	0.72
2:D:68:THR:CG2	2:D:178:ASN:HB2	2.21	0.71
2:H:151:LEU:HD23	2:H:151:LEU:C	2.16	0.71
1:A:150:THR:HG22	1:A:152:GLU:HG3	1.72	0.71
2:D:68:THR:HG22	2:D:178:ASN:HB2	1.73	0.70
1:G:5:THR:HG23	2:H:556:GLN:HE21	1.57	0.70
2:D:556:GLN:CG	2:D:557:ARG:H	2.05	0.69
1:A:23:ASP:OD2	1:A:26:ARG:HD3	1.92	0.69
1:C:195:SER:HB2	2:D:245:GLN:HE21	1.56	0.69
2:D:183:ASP:OD2	2:D:187:ASN:ND2	2.25	0.69
2:B:482:GLU:HG3	2:B:483:ASN:N	2.05	0.69
2:F:279:ALA:O	2:F:485:MET:HE1	1.92	0.69
2:F:228:LYS:O	2:F:229:VAL:HG23	1.93	0.69
1:A:156:LEU:O	1:A:160:THR:HG23	1.93	0.69
2:H:48:THR:HG22	2:H:56:VAL:H	1.58	0.69
2:B:3:MET:HE3	2:B:20:ASN:CG	2.18	0.68
1:G:23:ASP:OD1	1:G:26:ARG:NH1	2.26	0.68
2:H:48:THR:HG23	2:H:55:LEU:HA	1.73	0.68
1:A:7:VAL:HG12	1:A:21:ALA:HB2	1.76	0.68
2:H:3:MET:HE3	2:H:20:ASN:CG	2.18	0.68
1:G:110:SER:HB2	1:G:114:LEU:CG	2.24	0.68
2:B:356:LYS:HD3	2:H:369:LYS:HG3	1.75	0.67
2:B:557:ARG:HH11	2:B:557:ARG:CG	2.07	0.67
2:D:250:ALA:HB2	2:D:258:TRP:CE3	2.30	0.67
2:F:19:VAL:HG22	2:F:485:MET:HG3	1.76	0.67
2:H:250:ALA:HB2	2:H:258:TRP:CE3	2.30	0.67
1:G:145:ARG:HD3	2:H:459:PHE:CZ	2.30	0.67
2:H:153:ALA:HB3	2:H:173:GLN:HG3	1.77	0.67
1:C:7:VAL:HG12	1:C:21:ALA:HB2	1.78	0.66
2:B:173:GLN:HE22	2:B:175:LEU:HB2	1.61	0.66
2:D:527:MET:HE1	2:D:534:LYS:HG3	1.76	0.66
1:G:107:VAL:HA	1:G:114:LEU:CB	2.11	0.66
1:G:23:ASP:OD1	1:G:26:ARG:HD2	1.96	0.65
1:A:50:THR:CG2	1:A:136:MET:O	2.44	0.65
1:C:150:THR:HG22	2:D:252:ASP:OD2	1.97	0.65
1:G:145:ARG:HD3	2:H:459:PHE:CE1	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:250:ALA:HB2	2:F:258:TRP:CE3	2.32	0.64
1:G:110:SER:O	1:G:114:LEU:N	2.30	0.64
2:B:250:ALA:HB2	2:B:258:TRP:CE3	2.32	0.64
1:A:145:ARG:NH1	2:B:31:TYR:OH	2.31	0.63
1:G:145:ARG:NE	1:G:146:PHE:CE2	2.66	0.63
2:B:455:ARG:HH22	2:H:437:ARG:HG3	1.63	0.63
2:D:292:ARG:O	2:D:294:LEU:HD12	1.97	0.63
2:F:24:PHE:CD2	2:F:31:TYR:CE2	2.86	0.63
2:H:24:PHE:CD2	2:H:31:TYR:CE2	2.87	0.63
2:D:24:PHE:CD2	2:D:31:TYR:CE2	2.87	0.63
1:A:150:THR:CG2	1:A:152:GLU:HG3	2.29	0.62
2:B:151:LEU:HD12	2:B:151:LEU:C	2.21	0.62
2:F:17:ILE:HG21	2:F:485:MET:HE2	1.81	0.62
2:B:18:MET:HE1	2:B:65:TRP:O	1.99	0.62
1:C:82:ILE:O	1:C:90:LYS:NZ	2.31	0.62
1:G:110:SER:C	1:G:114:LEU:HB2	2.24	0.62
1:G:56:GLU:HG3	2:H:107:ALA:HB3	1.81	0.62
1:G:145:ARG:HG2	2:H:459:PHE:CE1	2.35	0.61
2:H:179:TRP:CD1	2:H:193:THR:CG2	2.83	0.61
2:D:18:MET:HE1	2:D:66:GLY:N	2.15	0.61
2:H:539:THR:HG23	2:H:542:ASP:H	1.65	0.61
1:G:107:VAL:N	1:G:114:LEU:HD13	2.15	0.61
1:A:146:PHE:O	1:A:147:SER:CB	2.49	0.60
2:H:154:TRP:CE3	2:H:179:TRP:HH2	2.17	0.60
1:E:150:THR:HG22	2:F:252:ASP:OD2	2.02	0.60
1:G:145:ARG:CZ	1:G:146:PHE:CE2	2.84	0.60
2:F:383:PRO:HG2	2:F:450:MET:CE	2.30	0.60
1:G:145:ARG:NH1	2:H:31:TYR:OH	2.35	0.60
1:C:14:TYR:CG	2:D:534:LYS:CE	2.80	0.59
2:H:154:TRP:CE3	2:H:179:TRP:CZ2	2.90	0.59
1:C:14:TYR:CD2	2:D:534:LYS:CE	2.83	0.59
1:A:23:ASP:OD1	1:A:26:ARG:NE	2.35	0.59
1:C:26:ARG:HE	2:D:556:GLN:HE22	1.50	0.59
2:B:24:PHE:CD2	2:B:31:TYR:CE2	2.90	0.59
1:G:195:SER:HB3	2:H:245:GLN:HE21	1.68	0.59
2:B:557:ARG:HH11	2:B:557:ARG:HG2	1.68	0.58
2:D:173:GLN:HB3	2:D:193:THR:CG2	2.31	0.58
1:C:45:MET:HE1	1:C:48:ARG:HD2	1.84	0.58
1:E:56:GLU:HG3	2:F:107:ALA:HB3	1.86	0.58
1:C:111:PRO:HB3	1:C:115:LEU:HD23	1.86	0.58
2:B:19:VAL:HG22	2:B:485:MET:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LYS:O	1:A:166:TYR:HB2	2.04	0.57
2:H:48:THR:HG21	2:H:55:LEU:HA	1.84	0.57
1:G:107:VAL:CA	1:G:114:LEU:HB3	2.12	0.57
2:F:387:LEU:HD11	2:F:450:MET:HE1	1.84	0.57
2:B:56:VAL:HG23	2:B:57:PHE:CE1	2.39	0.57
2:D:3:MET:HG3	2:D:4:TRP:N	2.20	0.57
1:C:45:MET:HE2	1:C:45:MET:CA	2.32	0.57
2:D:3:MET:HE1	2:D:18:MET:HG3	1.87	0.56
2:B:272:ASP:O	2:B:273:LYS:HB3	2.02	0.56
1:G:107:VAL:HG22	1:G:114:LEU:O	2.05	0.56
1:A:25:TYR:CE1	2:B:557:ARG:HD2	2.40	0.56
2:D:556:GLN:OE1	2:D:556:GLN:HA	2.05	0.56
1:E:19:ILE:CD1	1:E:31:TYR:N	2.69	0.56
2:F:141:ARG:HD2	2:F:143:TRP:CH2	2.40	0.56
2:H:376:TYR:O	2:H:378:THR:HG23	2.05	0.56
1:G:145:ARG:NE	1:G:146:PHE:CD2	2.74	0.55
1:G:150:THR:HG22	2:H:252:ASP:OD2	2.06	0.55
2:D:85:GLU:O	2:D:86:LYS:HB2	2.06	0.55
1:A:142:MET:O	1:A:146:PHE:O	2.24	0.55
1:G:145:ARG:CG	2:H:459:PHE:CE1	2.90	0.55
1:G:23:ASP:OD1	1:G:26:ARG:CZ	2.55	0.55
2:H:26:TRP:CD2	2:H:452:LEU:HD11	2.42	0.55
2:B:56:VAL:HB	2:B:154:TRP:CZ3	2.42	0.54
2:D:163:TRP:HB3	2:D:164:PRO:HD3	1.90	0.54
2:H:48:THR:HG21	2:H:54:GLY:O	2.08	0.54
2:B:18:MET:HE2	2:B:486:ILE:HD13	1.89	0.54
1:E:19:ILE:HD13	1:E:30:GLY:C	2.33	0.54
2:H:373:ALA:HB1	4:H:708:HOH:O	2.07	0.54
2:D:190:TYR:OH	2:D:244:PRO:HB3	2.08	0.54
2:B:17:ILE:HG21	2:B:485:MET:HE2	1.89	0.54
2:B:47:ASN:CG	2:B:482:GLU:OE1	2.48	0.54
2:H:163:TRP:HB3	2:H:164:PRO:HD3	1.90	0.54
1:C:7:VAL:HG23	2:D:553:LEU:HB2	1.90	0.54
2:D:283:TRP:CZ2	2:D:533:ARG:HG2	2.43	0.53
2:F:163:TRP:HB3	2:F:164:PRO:HD3	1.90	0.53
1:A:56:GLU:HG3	2:B:107:ALA:HB3	1.89	0.53
2:F:3:MET:CE	2:F:20:ASN:CG	2.80	0.53
2:H:19:VAL:HG22	2:H:485:MET:HG3	1.91	0.53
2:B:190:TYR:OH	2:B:244:PRO:HB3	2.08	0.53
2:B:419:GLN:HB2	1:C:193:ARG:HH21	1.73	0.53
2:B:557:ARG:HG2	2:B:557:ARG:NH1	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:193:THR:HG22	2:D:194:GLY:N	2.22	0.53
2:B:163:TRP:HB3	2:B:164:PRO:HD3	1.91	0.53
2:F:17:ILE:CG2	2:F:485:MET:HE2	2.39	0.53
2:F:26:TRP:CD2	2:F:452:LEU:HD11	2.44	0.53
2:D:547:LYS:O	2:D:548:GLU:HG3	2.09	0.53
2:F:190:TYR:OH	2:F:244:PRO:HB3	2.08	0.53
2:H:190:TYR:OH	2:H:244:PRO:HB3	2.08	0.53
2:B:26:TRP:CD2	2:B:452:LEU:HD11	2.44	0.53
2:D:516:LYS:O	2:D:516:LYS:HG2	2.08	0.53
2:H:179:TRP:HD1	2:H:193:THR:CG2	2.21	0.53
2:F:310:LEU:O	2:F:317:ARG:HD2	2.09	0.53
1:G:5:THR:HG23	2:H:555:VAL:O	2.08	0.53
1:G:107:VAL:CG2	1:G:114:LEU:O	2.57	0.52
1:G:145:ARG:HG2	2:H:459:PHE:HE1	1.74	0.52
2:D:83:SER:HB3	2:D:85:GLU:O	2.09	0.52
2:D:354:MET:CE	2:D:426:ALA:HB3	2.29	0.52
1:E:19:ILE:HD12	1:E:31:TYR:N	2.25	0.52
1:G:107:VAL:CB	1:G:114:LEU:O	2.56	0.52
2:D:19:VAL:HG22	2:D:485:MET:HG3	1.90	0.52
2:F:45:THR:HG21	2:F:537:TRP:O	2.10	0.52
2:F:387:LEU:HD21	2:F:450:MET:HE1	1.91	0.52
2:F:3:MET:HG3	2:F:4:TRP:N	2.24	0.52
2:D:473:GLN:NE2	2:D:477:GLN:OE1	2.43	0.52
1:A:4:PRO:O	1:A:26:ARG:NH1	2.43	0.51
2:D:350:TRP:CZ2	2:D:354:MET:HE3	2.45	0.51
2:F:83:SER:HB3	2:F:85:GLU:O	2.10	0.51
1:C:5:THR:HG23	2:D:554:GLN:HG2	1.91	0.51
2:D:56:VAL:HG12	2:D:57:PHE:CE1	2.46	0.51
2:D:556:GLN:CG	2:D:557:ARG:N	2.73	0.51
2:F:431:TRP:O	2:F:435:SER:OG	2.25	0.51
2:D:68:THR:HG23	2:D:178:ASN:HB2	1.93	0.51
1:E:19:ILE:CD1	1:E:30:GLY:C	2.83	0.51
2:B:45:THR:HG21	2:B:537:TRP:O	2.11	0.51
2:D:283:TRP:CH2	2:D:533:ARG:HG2	2.46	0.51
2:F:383:PRO:HG2	2:F:450:MET:HE2	1.92	0.51
2:H:3:MET:HG3	2:H:4:TRP:N	2.26	0.51
2:H:173:GLN:NE2	2:H:179:TRP:CE2	2.79	0.51
2:H:45:THR:HG21	2:H:537:TRP:O	2.11	0.50
2:H:56:VAL:HG12	2:H:57:PHE:CE1	2.46	0.50
2:B:473:GLN:NE2	2:B:477:GLN:OE1	2.44	0.50
2:H:452:LEU:HB3	2:H:473:GLN:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:MET:HG3	2:B:4:TRP:N	2.26	0.50
2:B:471:ARG:NH2	2:B:521:TYR:CE2	2.79	0.50
2:D:431:TRP:O	2:D:435:SER:OG	2.23	0.50
1:E:21:ALA:O	2:F:39:GLY:HA3	2.12	0.50
2:F:3:MET:HE3	2:F:20:ASN:OD1	2.11	0.50
2:H:122:LEU:C	2:H:122:LEU:HD22	2.37	0.50
1:A:36:ALA:O	1:A:40:LEU:HB2	2.12	0.50
2:F:56:VAL:HG12	2:F:57:PHE:CE1	2.46	0.50
2:F:473:GLN:NE2	2:F:477:GLN:OE1	2.45	0.50
1:G:166:TYR:CE1	2:H:411:VAL:HG11	2.46	0.49
1:A:4:PRO:O	1:A:26:ARG:CZ	2.60	0.49
2:D:350:TRP:NE1	2:D:354:MET:HE3	2.27	0.49
2:H:3:MET:HE3	2:H:20:ASN:OD1	2.13	0.49
2:H:473:GLN:NE2	2:H:529:GLU:HB3	2.28	0.49
2:D:45:THR:HG21	2:D:537:TRP:O	2.12	0.49
2:D:350:TRP:CE2	2:D:354:MET:HE3	2.48	0.49
1:G:66:ASP:HB3	2:H:106:ILE:HD13	1.93	0.49
2:B:3:MET:HE3	2:B:20:ASN:OD1	2.12	0.49
2:H:56:VAL:HG13	2:H:154:TRP:CZ3	2.48	0.49
2:F:348:ASN:ND2	2:F:374:SER:OG	2.46	0.49
1:C:150:THR:HG22	2:D:252:ASP:CG	2.37	0.49
2:H:3:MET:CE	2:H:20:ASN:CG	2.86	0.48
2:H:86:LYS:HG2	2:H:89:TYR:CD1	2.48	0.48
2:H:173:GLN:NE2	2:H:179:TRP:NE1	2.61	0.48
2:H:350:TRP:O	2:H:354:MET:HB2	2.13	0.48
2:B:3:MET:CE	2:B:20:ASN:CG	2.86	0.48
1:G:141:THR:HB	1:G:145:ARG:CZ	2.44	0.48
2:B:326:TRP:CD1	2:B:341:GLN:HG3	2.48	0.48
2:B:102:ARG:NH1	2:B:104:GLU:OE2	2.46	0.48
2:B:348:ASN:ND2	2:B:374:SER:OG	2.46	0.48
1:A:55:SER:OG	1:A:66:ASP:OD2	2.32	0.48
2:B:452:LEU:HB3	2:B:473:GLN:HB3	1.95	0.48
2:B:455:ARG:HH22	2:H:437:ARG:CG	2.27	0.48
1:C:195:SER:HB2	2:D:245:GLN:NE2	2.24	0.48
1:E:36:ALA:O	1:E:40:LEU:HB2	2.13	0.48
2:D:471:ARG:NH2	2:D:521:TYR:CE2	2.82	0.48
2:B:89:TYR:CE2	2:B:98:LYS:HG2	2.49	0.48
2:B:431:TRP:O	2:B:435:SER:OG	2.24	0.48
2:F:62:THR:O	2:F:184:VAL:HG23	2.14	0.48
2:F:292:ARG:NH2	2:F:329:GLU:OE1	2.47	0.48
1:C:14:TYR:CB	2:D:534:LYS:HE3	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:ARG:NH1	2:F:233:GLN:HE22	2.12	0.47
2:H:154:TRP:CH2	2:H:179:TRP:CZ2	3.02	0.47
2:D:350:TRP:O	2:D:354:MET:HB2	2.14	0.47
2:H:85:GLU:O	2:H:87:PRO:HD3	2.14	0.47
2:B:89:TYR:CZ	2:B:98:LYS:HG2	2.49	0.47
2:D:62:THR:O	2:D:184:VAL:HG23	2.13	0.47
1:C:36:ALA:O	1:C:40:LEU:HB2	2.15	0.47
2:D:458:ASN:OD1	2:D:464:GLN:OE1	2.32	0.47
2:H:348:ASN:ND2	2:H:374:SER:OG	2.48	0.47
2:B:350:TRP:O	2:B:354:MET:HB2	2.14	0.47
1:C:23:ASP:C	1:C:23:ASP:OD2	2.58	0.47
2:D:56:VAL:HG13	2:D:154:TRP:CZ3	2.50	0.47
2:B:44:VAL:HG11	2:B:158:MET:HB3	1.97	0.47
2:H:326:TRP:CD1	2:H:341:GLN:HG3	2.50	0.47
2:H:473:GLN:HE22	2:H:528:TYR:HD2	1.62	0.47
1:C:56:GLU:HG3	2:D:107:ALA:HB3	1.97	0.47
2:D:44:VAL:HG11	2:D:158:MET:HB3	1.97	0.47
2:H:157:GLN:OE1	2:H:179:TRP:CZ3	2.68	0.47
2:F:501:ASP:OD1	2:F:534:LYS:HE3	2.15	0.47
1:C:195:SER:CB	2:D:245:GLN:HE21	2.24	0.47
1:G:36:ALA:O	1:G:40:LEU:HB2	2.14	0.47
2:H:62:THR:O	2:H:184:VAL:HG23	2.14	0.47
2:F:350:TRP:O	2:F:354:MET:HB2	2.14	0.46
2:H:44:VAL:HG11	2:H:158:MET:HB3	1.97	0.46
2:D:350:TRP:CZ2	2:D:354:MET:HG2	2.51	0.46
2:F:452:LEU:HB3	2:F:473:GLN:HB3	1.96	0.46
2:H:122:LEU:HD22	2:H:123:HIS:N	2.29	0.46
2:F:383:PRO:CG	2:F:450:MET:HE2	2.44	0.46
2:D:26:TRP:CE2	2:D:452:LEU:HD21	2.50	0.46
1:A:165:LYS:O	1:A:166:TYR:CB	2.63	0.46
2:B:62:THR:HG21	2:B:161:LYS:HG3	1.98	0.46
2:H:473:GLN:NE2	2:H:528:TYR:HD2	2.14	0.46
1:C:14:TYR:CB	2:D:534:LYS:CE	2.93	0.46
1:E:66:ASP:HB3	2:F:106:ILE:HD13	1.97	0.46
2:F:44:VAL:HG11	2:F:158:MET:HB3	1.98	0.46
2:B:468:LYS:HB2	2:B:468:LYS:HE2	1.53	0.45
1:G:145:ARG:NH1	2:H:459:PHE:CE2	2.83	0.45
2:D:519:LYS:HE3	2:D:520:HIS:CE1	2.51	0.45
2:F:12:GLN:HB2	2:F:276:ARG:HB3	1.98	0.45
2:F:279:ALA:C	2:F:485:MET:HE1	2.41	0.45
2:D:68:THR:CG2	2:D:180:TYR:OH	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:SER:OG	1:E:66:ASP:OD2	2.31	0.45
2:F:326:TRP:CD1	2:F:341:GLN:HG3	2.51	0.45
2:H:350:TRP:CZ2	2:H:354:MET:HG2	2.51	0.45
1:E:18:HIS:CD2	2:F:36:GLY:HA3	2.52	0.45
2:B:84:ALA:HB2	2:B:134:GLN:NE2	2.32	0.45
1:C:166:TYR:CE1	2:D:411:VAL:HG11	2.51	0.45
1:G:145:ARG:CD	2:H:459:PHE:CE1	2.99	0.45
2:B:384:THR:HG22	2:B:455:ARG:NH2	2.31	0.45
1:E:190:ILE:HG23	2:F:229:VAL:HG21	1.99	0.45
2:B:471:ARG:NH2	2:B:521:TYR:CZ	2.85	0.45
2:D:471:ARG:NH1	2:D:522:ASP:OD1	2.49	0.45
1:A:145:ARG:NH2	2:B:31:TYR:OH	2.50	0.45
2:B:414:PHE:CZ	2:B:419:GLN:HG2	2.52	0.45
2:B:471:ARG:NH1	2:B:522:ASP:OD1	2.50	0.45
2:D:504:ALA:HB2	2:D:528:TYR:HB2	1.99	0.45
2:B:12:GLN:HB2	2:B:276:ARG:HB3	1.98	0.45
2:B:501:ASP:OD1	2:B:534:LYS:HE3	2.17	0.45
1:C:150:THR:HA	2:D:252:ASP:OD1	2.17	0.45
2:D:165:GLU:O	2:D:168:GLN:HG2	2.17	0.45
2:B:356:LYS:HD3	2:H:369:LYS:CG	2.42	0.44
2:H:105:THR:HG23	2:H:115:THR:HG22	1.98	0.44
2:H:228:LYS:O	2:H:229:VAL:HG13	2.16	0.44
1:C:29:TYR:O	1:C:99:GLY:HA3	2.18	0.44
2:D:12:GLN:HB2	2:D:276:ARG:HB3	1.98	0.44
2:F:105:THR:HG23	2:F:115:THR:HG22	1.99	0.44
2:F:488:PHE:CD1	2:F:497:VAL:HG22	2.53	0.44
2:F:350:TRP:CZ2	2:F:354:MET:HG2	2.52	0.44
2:B:544:ASP:OD1	2:B:547:LYS:HE3	2.17	0.44
2:D:471:ARG:NH2	2:D:521:TYR:CZ	2.86	0.44
2:H:12:GLN:HB2	2:H:276:ARG:HB3	1.98	0.44
2:D:326:TRP:CD1	2:D:341:GLN:HG3	2.53	0.44
1:C:70:ARG:NH1	2:D:104:GLU:OE1	2.50	0.44
2:F:504:ALA:HB2	2:F:528:TYR:HB2	2.00	0.44
2:H:471:ARG:NH2	2:H:521:TYR:CE2	2.86	0.44
2:D:317:ARG:NH2	2:H:98:LYS:HE3	2.32	0.44
2:B:28:ALA:HA	2:B:29:PRO:C	2.42	0.43
1:E:5:THR:HA	1:E:26:ARG:NH1	2.33	0.43
1:G:114:LEU:HD23	1:G:114:LEU:HA	1.82	0.43
2:H:539:THR:CG2	2:H:542:ASP:H	2.31	0.43
1:A:182:VAL:HG11	2:B:247:ASP:HA	2.00	0.43
2:B:17:ILE:CG2	2:B:485:MET:HE2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:105:THR:HG23	2:D:115:THR:HG22	2.00	0.43
1:E:145:ARG:HD3	1:E:146:PHE:CE2	2.53	0.43
1:E:188:THR:HG21	2:F:246:LYS:N	2.34	0.43
1:G:5:THR:HG22	2:H:554:GLN:HA	2.00	0.43
2:D:173:GLN:OE1	2:D:193:THR:HG21	2.19	0.43
1:E:145:ARG:CZ	1:E:146:PHE:CZ	3.02	0.43
2:H:504:ALA:HB2	2:H:528:TYR:HB2	2.01	0.43
2:D:141:ARG:HD3	2:D:143:TRP:CH2	2.54	0.43
1:A:6:GLU:O	1:A:26:ARG:NH2	2.51	0.43
1:A:14:TYR:C	2:B:520:HIS:CD2	2.97	0.43
2:B:151:LEU:C	2:B:151:LEU:CD1	2.90	0.43
2:B:488:PHE:CD1	2:B:497:VAL:HG22	2.53	0.43
2:D:354:MET:HE3	2:D:423:ILE:HA	1.87	0.43
2:D:384:THR:HG22	2:D:455:ARG:NH2	2.33	0.43
2:D:3:MET:CG	2:D:4:TRP:N	2.82	0.43
2:D:488:PHE:CD1	2:D:497:VAL:HG22	2.54	0.43
2:D:516:LYS:O	2:D:516:LYS:CG	2.67	0.43
2:H:419:GLN:O	2:H:423:ILE:HG13	2.19	0.43
1:A:21:ALA:O	2:B:39:GLY:HA3	2.19	0.43
2:B:141:ARG:HD3	2:B:143:TRP:CH2	2.54	0.43
2:D:28:ALA:HA	2:D:29:PRO:C	2.42	0.43
2:D:68:THR:CG2	2:D:178:ASN:HD22	2.27	0.43
2:D:419:GLN:O	2:D:423:ILE:HG13	2.19	0.43
2:B:504:ALA:HB2	2:B:528:TYR:HB2	2.01	0.43
1:E:145:ARG:HG2	1:E:146:PHE:CD2	2.54	0.43
1:G:145:ARG:CD	2:H:459:PHE:CZ	3.01	0.43
2:B:272:ASP:O	2:B:273:LYS:CB	2.67	0.42
2:H:539:THR:HG22	2:H:542:ASP:HB2	2.01	0.42
2:F:419:GLN:O	2:F:423:ILE:HG13	2.20	0.42
2:B:18:MET:HE2	2:B:486:ILE:CD1	2.47	0.42
2:B:455:ARG:HH12	2:H:437:ARG:HA	1.84	0.42
1:C:150:THR:HG22	2:D:252:ASP:OD1	2.20	0.42
1:E:23:ASP:OD1	1:E:26:ARG:HG3	2.19	0.42
1:E:29:TYR:O	1:E:99:GLY:HA3	2.20	0.42
1:E:152:GLU:HB2	2:F:77:ILE:HG13	2.00	0.42
2:H:488:PHE:CD1	2:H:497:VAL:HG22	2.54	0.42
1:A:188:THR:HG21	2:B:246:LYS:N	2.34	0.42
2:B:419:GLN:O	2:B:423:ILE:HG13	2.19	0.42
2:D:18:MET:CE	2:D:65:TRP:C	2.88	0.42
2:D:163:TRP:HB3	2:D:164:PRO:CD	2.49	0.42
1:E:150:THR:HG22	2:F:252:ASP:CG	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:384:THR:HG22	2:F:455:ARG:NH2	2.35	0.42
2:H:522:ASP:OD1	2:H:522:ASP:C	2.62	0.42
1:C:195:SER:CB	2:D:245:GLN:NE2	2.82	0.42
2:F:28:ALA:HA	2:F:29:PRO:C	2.44	0.42
1:G:29:TYR:O	1:G:99:GLY:HA3	2.18	0.42
2:H:157:GLN:NE2	2:H:179:TRP:CZ3	2.85	0.42
2:B:557:ARG:CG	2:B:557:ARG:NH1	2.73	0.42
2:D:68:THR:HG22	2:D:178:ASN:CB	2.46	0.42
2:F:163:TRP:HB3	2:F:164:PRO:CD	2.49	0.42
2:H:471:ARG:NH2	2:H:521:TYR:CZ	2.88	0.42
2:D:229:VAL:HG11	2:D:232:PRO:HB3	2.01	0.42
2:F:458:ASN:OD1	2:F:458:ASN:C	2.62	0.42
2:H:122:LEU:C	2:H:122:LEU:CD2	2.93	0.42
2:B:356:LYS:HG2	2:H:369:LYS:HE3	2.00	0.42
1:G:23:ASP:OD1	1:G:26:ARG:CD	2.65	0.42
2:D:37:LEU:HB2	2:D:44:VAL:CG2	2.50	0.42
2:H:28:ALA:HA	2:H:29:PRO:C	2.44	0.42
1:A:152:GLU:HB2	2:B:77:ILE:HG13	2.02	0.41
1:E:150:THR:HG23	2:F:75:VAL:HB	2.01	0.41
2:F:288:GLN:HA	2:F:329:GLU:OE2	2.19	0.41
1:A:29:TYR:O	1:A:99:GLY:HA3	2.20	0.41
1:G:110:SER:HB2	1:G:114:LEU:CD1	2.50	0.41
2:D:26:TRP:CD2	2:D:452:LEU:HD21	2.55	0.41
2:D:183:ASP:CG	2:D:187:ASN:OD1	2.63	0.41
2:F:56:VAL:HG13	2:F:154:TRP:CZ3	2.55	0.41
1:G:18:HIS:CD2	2:H:36:GLY:HA3	2.56	0.41
2:H:141:ARG:HD3	2:H:143:TRP:CH2	2.55	0.41
2:H:3:MET:CG	2:H:4:TRP:N	2.83	0.41
2:H:539:THR:HG23	2:H:542:ASP:N	2.34	0.41
2:B:37:LEU:HB2	2:B:44:VAL:CG2	2.51	0.41
2:B:85:GLU:O	2:B:86:LYS:HG3	2.21	0.41
2:H:123:HIS:O	2:H:140:ALA:HA	2.21	0.41
2:B:42:TYR:CZ	2:B:159:LYS:HE3	2.55	0.41
2:B:163:TRP:HB3	2:B:164:PRO:CD	2.51	0.41
2:H:248:TYR:HA	2:H:249:PRO:HD3	1.99	0.41
2:B:3:MET:CG	2:B:4:TRP:N	2.83	0.41
2:D:181:TYR:HE1	2:D:187:ASN:OD1	2.04	0.41
2:D:350:TRP:NE1	2:D:354:MET:CE	2.83	0.40
2:F:37:LEU:HB2	2:F:44:VAL:CG2	2.51	0.40
1:G:14:TYR:C	2:H:520:HIS:CD2	3.00	0.40
1:G:146:PHE:CZ	2:H:24:PHE:HD1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:163:TRP:HB3	2:H:164:PRO:CD	2.51	0.40
2:F:288:GLN:O	2:F:329:GLU:OE2	2.38	0.40
1:G:70:ARG:NH1	2:H:104:GLU:OE1	2.53	0.40
2:H:501:ASP:OD1	2:H:534:LYS:HE3	2.21	0.40
2:B:312:GLU:HG2	2:B:312:GLU:O	2.21	0.40
1:C:14:TYR:C	2:D:520:HIS:CD2	3.00	0.40
2:D:283:TRP:CZ2	2:D:533:ARG:CG	3.04	0.40
2:D:495:ARG:HB3	2:D:496:PRO:HD2	2.04	0.40
2:B:22:PRO:HB2	2:B:24:PHE:CE2	2.57	0.40
2:B:455:ARG:NH1	4:B:707:HOH:O	2.37	0.40
1:C:14:TYR:CB	2:D:534:LYS:NZ	2.85	0.40
2:D:68:THR:HG21	2:D:180:TYR:OH	2.22	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)
2:B:103:LYS:NZ	1:G:108:ASN:O[1_565]	1.90	0.30

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	192/222 (86%)	184 (96%)	8 (4%)	0	100	100
1	C	192/222 (86%)	186 (97%)	6 (3%)	0	100	100
1	E	192/222 (86%)	187 (97%)	5 (3%)	0	100	100
1	G	192/222 (86%)	184 (96%)	8 (4%)	0	100	100
2	B	555/565 (98%)	537 (97%)	18 (3%)	0	100	100
2	D	555/565 (98%)	533 (96%)	21 (4%)	1 (0%)	43	72
2	F	555/565 (98%)	538 (97%)	16 (3%)	1 (0%)	43	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	555/565 (98%)	535 (96%)	19 (3%)	1 (0%)	43 72
All	All	2988/3148 (95%)	2884 (96%)	101 (3%)	3 (0%)	48 77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	251	SER
2	D	251	SER
2	F	251	SER

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	164/188 (87%)	157 (96%)	7 (4%)	26 60
1	C	164/188 (87%)	158 (96%)	6 (4%)	30 65
1	E	164/188 (87%)	160 (98%)	4 (2%)	43 77
1	G	164/188 (87%)	159 (97%)	5 (3%)	36 72
2	B	449/457 (98%)	424 (94%)	25 (6%)	19 50
2	D	449/457 (98%)	428 (95%)	21 (5%)	23 57
2	F	449/457 (98%)	427 (95%)	22 (5%)	22 55
2	H	449/457 (98%)	432 (96%)	17 (4%)	29 64
All	All	2452/2580 (95%)	2345 (96%)	107 (4%)	25 59

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	71	GLN
1	A	130	GLU
1	A	145	ARG
1	A	147	SER

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Mol	Chain	Res	Type
1	A	150	THR
1	A	195	SER
2	B	45	THR
2	B	56	VAL
2	B	67	SER
2	B	82	LEU
2	B	106	ILE
2	B	122	LEU
2	B	128	LYS
2	B	131	THR
2	B	133	THR
2	B	148	VAL
2	B	151	LEU
2	B	155	THR
2	B	177	ILE
2	B	251	SER
2	B	290	SER
2	B	325	SER
2	B	391	VAL
2	B	403	ASP
2	B	411	VAL
2	B	433	THR
2	B	468	LYS
2	B	482	GLU
2	B	526	ILE
2	B	544	ASP
2	B	557	ARG
1	C	13	GLU
1	C	113	LYS
1	C	115	LEU
1	C	130	GLU
1	C	169	GLN
1	C	195	SER
2	D	18	MET
2	D	45	THR
2	D	82	LEU
2	D	106	ILE
2	D	131	THR
2	D	155	THR
2	D	177	ILE
2	D	251	SER
2	D	270	THR

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Mol	Chain	Res	Type
2	D	290	SER
2	D	325	SER
2	D	411	VAL
2	D	433	THR
2	D	452	LEU
2	D	482	GLU
2	D	511	ILE
2	D	516	LYS
2	D	519	LYS
2	D	526	ILE
2	D	544	ASP
2	D	549	SER
1	E	19	ILE
1	E	130	GLU
1	E	178	LEU
1	E	195	SER
2	F	45	THR
2	F	67	SER
2	F	82	LEU
2	F	85	GLU
2	F	106	ILE
2	F	114	GLU
2	F	131	THR
2	F	155	THR
2	F	177	ILE
2	F	251	SER
2	F	274	GLN
2	F	290	SER
2	F	329	GLU
2	F	354	MET
2	F	391	VAL
2	F	411	VAL
2	F	433	THR
2	F	443	THR
2	F	471	ARG
2	F	526	ILE
2	F	544	ASP
2	F	549	SER
1	G	13	GLU
1	G	55	SER
1	G	113	LYS
1	G	130	GLU

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Mol	Chain	Res	Type
1	G	182	VAL
2	H	45	THR
2	H	82	LEU
2	H	86	LYS
2	H	106	ILE
2	H	122	LEU
2	H	155	THR
2	H	173	GLN
2	H	177	ILE
2	H	290	SER
2	H	354	MET
2	H	391	VAL
2	H	411	VAL
2	H	433	THR
2	H	443	THR
2	H	526	ILE
2	H	544	ASP
2	H	549	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
2	B	47	ASN
2	B	157	GLN
2	B	169	GLN
2	B	173	GLN
2	B	348	ASN
2	B	409	GLN
2	B	419	GLN
2	B	432	GLN
1	C	169	GLN
2	D	20	ASN
2	D	157	GLN
2	D	169	GLN
2	D	245	GLN
2	D	409	GLN
2	D	440	ASN
2	D	556	GLN
2	F	20	ASN
2	F	47	ASN
2	F	157	GLN

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Mol	Chain	Res	Type
2	F	169	GLN
2	F	233	GLN
2	F	274	GLN
2	F	348	ASN
2	F	380	GLN
2	F	409	GLN
2	F	440	ASN
2	F	494	ASN
1	G	169	GLN
2	H	20	ASN
2	H	47	ASN
2	H	169	GLN
2	H	203	HIS
2	H	245	GLN
2	H	348	ASN
2	H	401	GLN
2	H	440	ASN
2	H	473	GLN
2	H	556	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	9:ILE	C	10:VAL	N	1.17
1	A	8:LYS	C	9:ILE	N	1.07

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	194/222 (87%)	-0.05	3 (1%) 72 63	26, 47, 78, 114	0
1	C	194/222 (87%)	-0.11	2 (1%) 79 72	24, 54, 82, 98	0
1	E	194/222 (87%)	-0.23	4 (2%) 63 54	26, 43, 67, 98	0
1	G	194/222 (87%)	-0.15	3 (1%) 72 63	31, 47, 68, 93	0
2	B	557/565 (98%)	-0.19	2 (0%) 88 84	23, 45, 73, 113	0
2	D	557/565 (98%)	-0.08	2 (0%) 88 84	27, 50, 79, 103	0
2	F	557/565 (98%)	-0.29	1 (0%) 91 88	25, 44, 67, 93	0
2	H	557/565 (98%)	-0.21	5 (0%) 81 74	24, 45, 68, 101	0
All	All	3004/3148 (95%)	-0.18	22 (0%) 84 77	23, 46, 74, 114	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	196	ALA	5.0
2	H	173	GLN	4.7
1	A	145	ARG	4.4
1	E	4	PRO	3.8
1	G	114	LEU	3.5
1	A	196	ALA	3.5
2	H	556	GLN	3.3
1	C	196	ALA	3.1
2	H	179	TRP	2.9
1	E	196	ALA	2.8
1	G	145	ARG	2.7
2	D	154	TRP	2.6
1	C	145	ARG	2.6
1	A	146	PHE	2.6
2	B	547	LYS	2.3
2	H	86	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	381	ASP	2.2
1	E	168	LYS	2.2
2	F	437	ARG	2.1
2	H	157	GLN	2.1
1	E	146	PHE	2.1
2	B	154	TRP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	G	601	1/1	0.98	0.03	44,44,44,44	0
3	CA	C	601	1/1	1.00	0.02	34,34,34,34	0
3	CA	E	601	1/1	1.00	0.01	31,31,31,31	0
3	CA	A	601	1/1	1.00	0.01	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.