



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2024 – 04:01 am BST

PDB ID : 2CB4
Title : Crystal structure of the catalytic domain of the mosquitocidal toxin from *Bacillus sphaericus*, mutant E197Q
Authors : Reinert, D.J.; Carpusca, I.; Aktories, K.; Schulz, G.E.
Deposited on : 2005-12-29
Resolution : 2.50 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

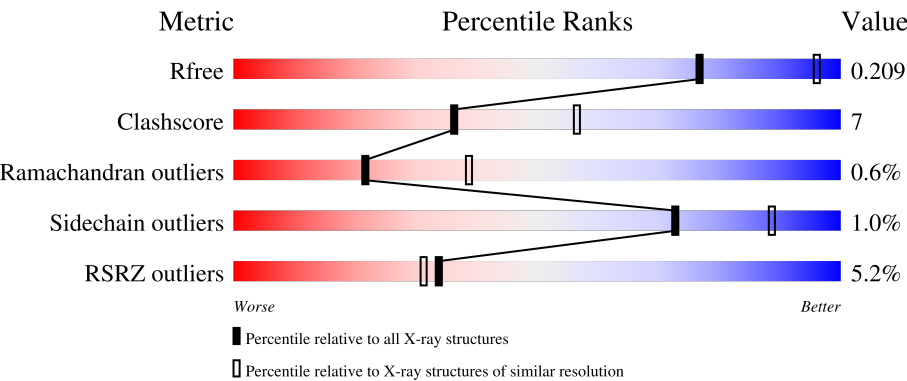
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.







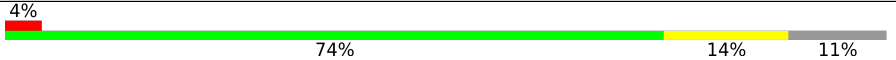
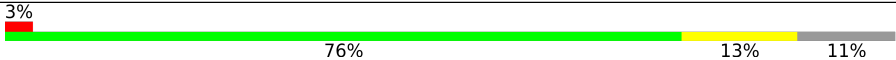
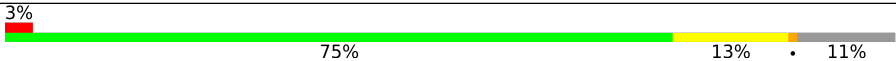
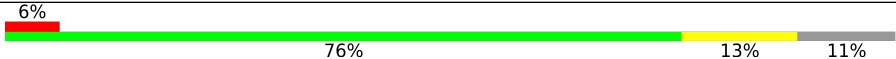
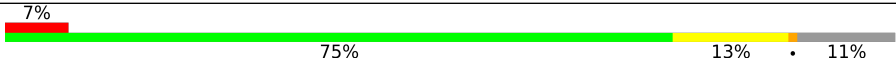
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	291	<div><div>5%</div><div><div></div><div>74%</div><div>14%</div><div>•</div><div>11%</div></div></div>
1	B	291	<div><div>3%</div><div><div></div><div>75%</div><div>13%</div><div></div><div>11%</div></div></div>
1	C	291	<div><div>6%</div><div><div></div><div>74%</div><div>14%</div><div>•</div><div>11%</div></div></div>
1	D	291	<div><div>4%</div><div><div></div><div>75%</div><div>13%</div><div>•</div><div>11%</div></div></div>
1	E	291	<div><div>4%</div><div><div></div><div>77%</div><div>12%</div><div></div><div>11%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	291	
1	G	291	
1	H	291	
1	I	291	
1	J	291	
1	K	291	
1	L	291	
1	M	291	
1	N	291	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30680 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 MOSQUITOCIDAL TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	B	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	C	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	D	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	E	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	F	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	G	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	H	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	I	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	J	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	K	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	L	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	M	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	N	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	GLN	GLU	engineered mutation	UNP Q03988

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Chain	Residue	Modelled	Actual	Comment	Reference
B	197	GLN	GLU	engineered mutation	UNP Q03988
C	197	GLN	GLU	engineered mutation	UNP Q03988
D	197	GLN	GLU	engineered mutation	UNP Q03988
E	197	GLN	GLU	engineered mutation	UNP Q03988
F	197	GLN	GLU	engineered mutation	UNP Q03988
G	197	GLN	GLU	engineered mutation	UNP Q03988
H	197	GLN	GLU	engineered mutation	UNP Q03988
I	197	GLN	GLU	engineered mutation	UNP Q03988
J	197	GLN	GLU	engineered mutation	UNP Q03988
K	197	GLN	GLU	engineered mutation	UNP Q03988
L	197	GLN	GLU	engineered mutation	UNP Q03988
M	197	GLN	GLU	engineered mutation	UNP Q03988
N	197	GLN	GLU	engineered mutation	UNP Q03988

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	93	Total O 93 93	0	0
2	B	108	Total O 108 108	0	0
2	C	120	Total O 120 120	0	0
2	D	114	Total O 114 114	0	0
2	E	82	Total O 82 82	0	0
2	F	81	Total O 81 81	0	0
2	G	96	Total O 96 96	0	0
2	H	86	Total O 86 86	0	0
2	I	109	Total O 109 109	0	0
2	J	112	Total O 112 112	0	0
2	K	80	Total O 80 80	0	0
2	L	92	Total O 92 92	0	0
2	M	93	Total O 93 93	0	0

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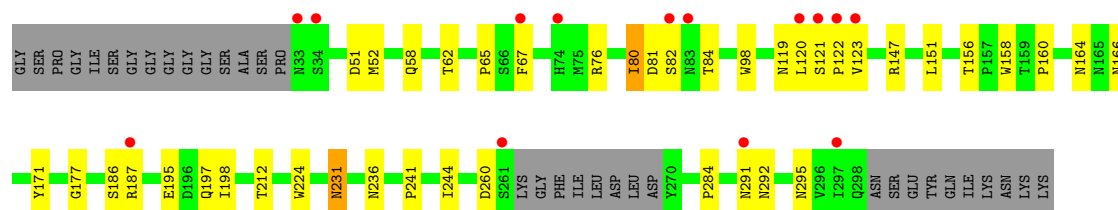
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	N	84	Total	O	0	0
			84	84		

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.

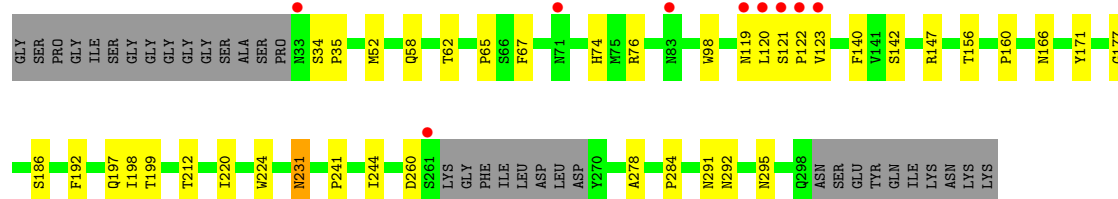
• Molecule 1: MOSQUITOCIDAL TOXIN

Chain A: 



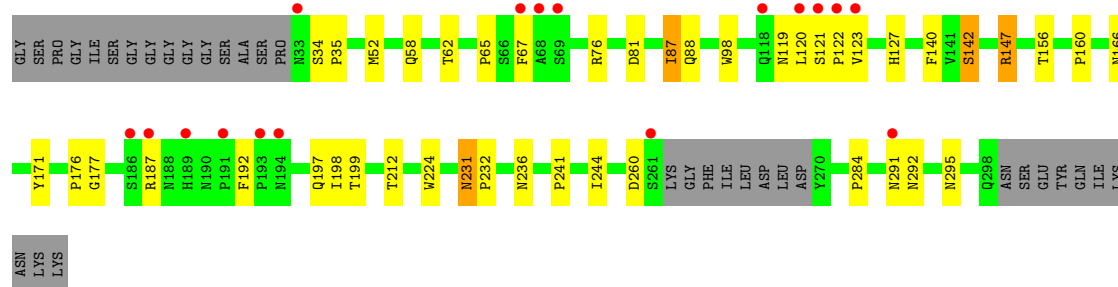
• Molecule 1: MOSQUITOCIDAL TOXIN

Chain B: 



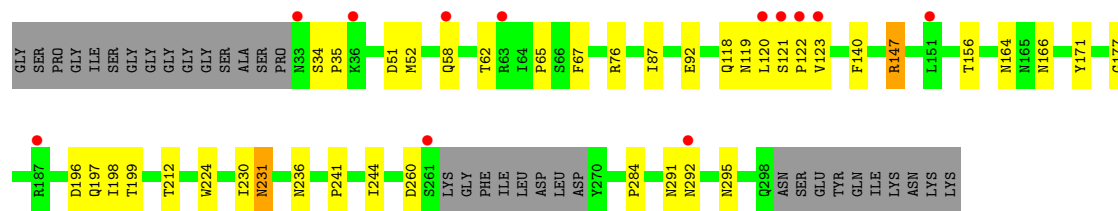
• Molecule 1: MOSQUITOCIDAL TOXIN

Chain C: 

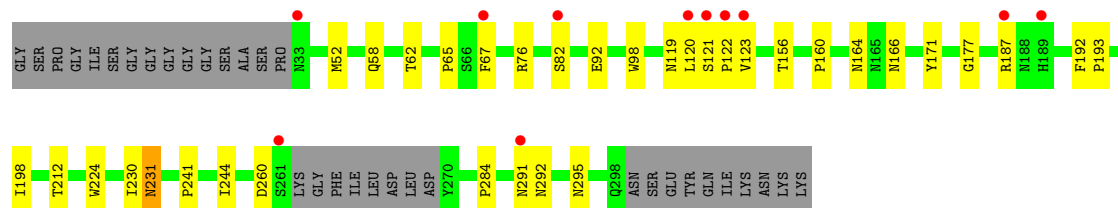
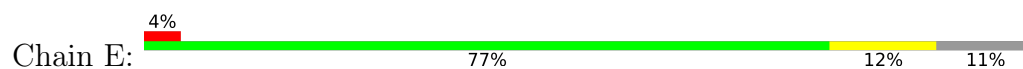


• Molecule 1: MOSQUITOCIDAL TOXIN

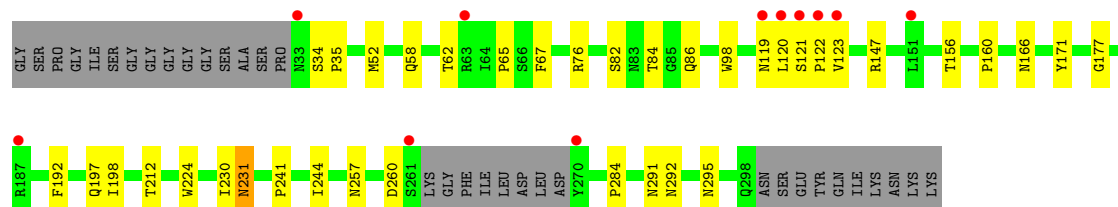
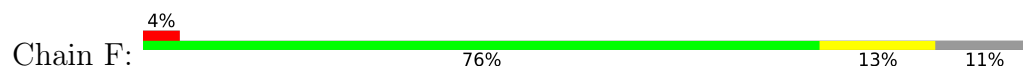
Chain D: 



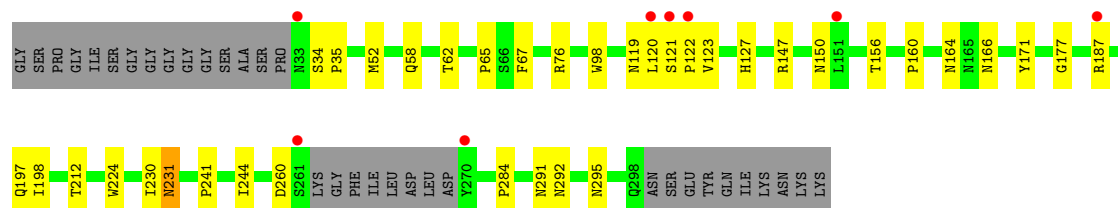
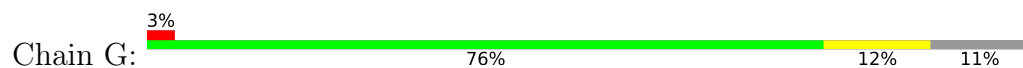
• Molecule 1: MOSQUITOCIDAL TOXIN



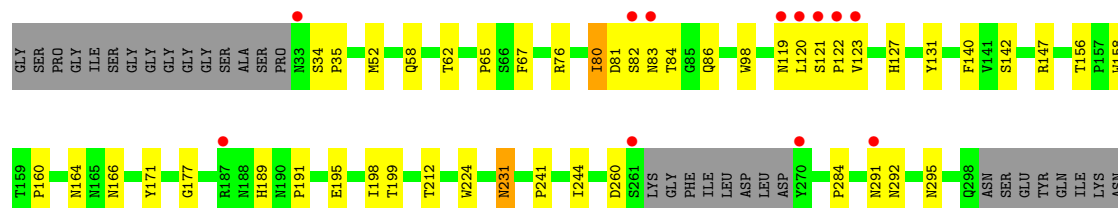
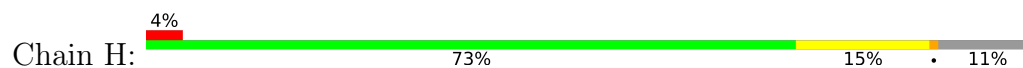
• Molecule 1: MOSQUITOCIDAL TOXIN



• Molecule 1: MOSQUITOCIDAL TOXIN



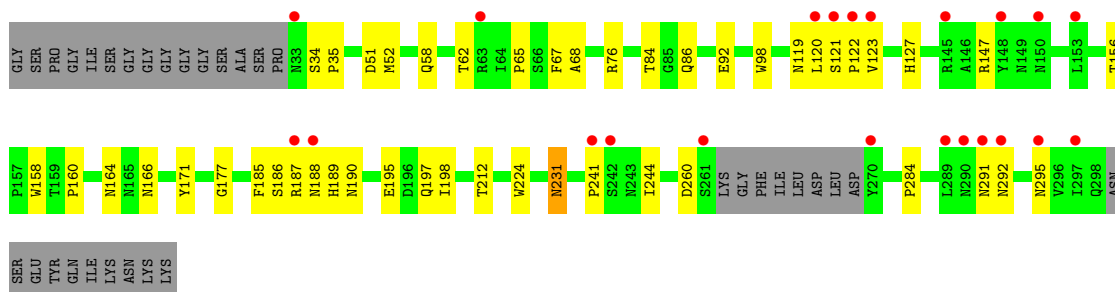
• Molecule 1: MOSQUITOCIDAL TOXIN




LYS
LYS

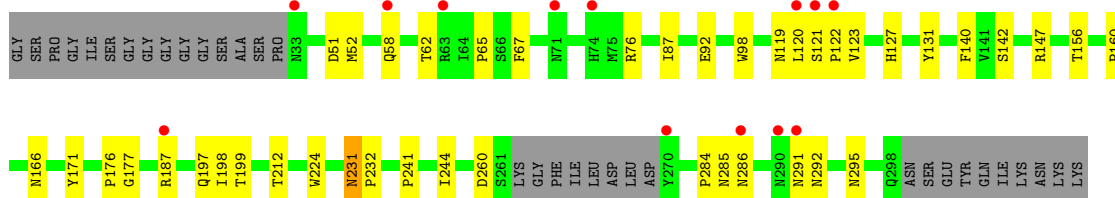
• Molecule 1: MOSQUITOCIDAL TOXIN

Chain I: 




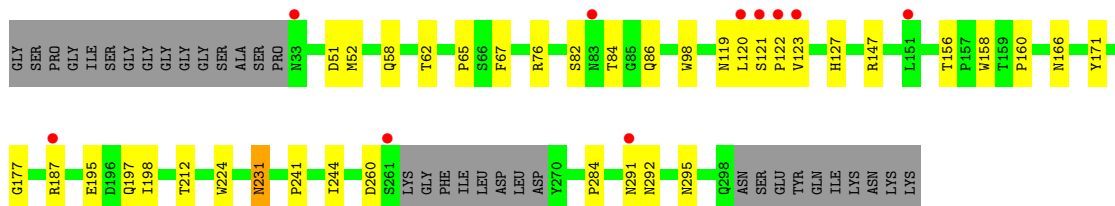
• Molecule 1: MOSQUITOCIDAL TOXIN

Chain J: 




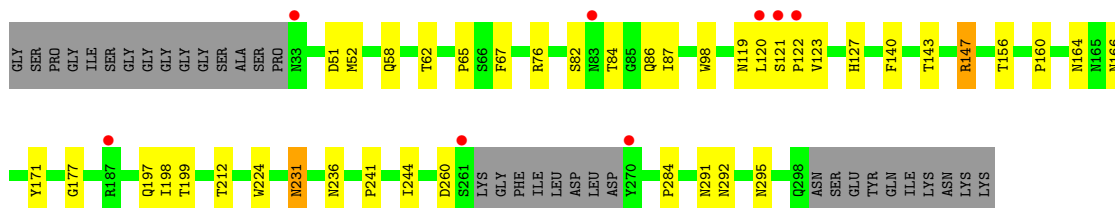
• Molecule 1: MOSQUITOCIDAL TOXIN

Chain K: 

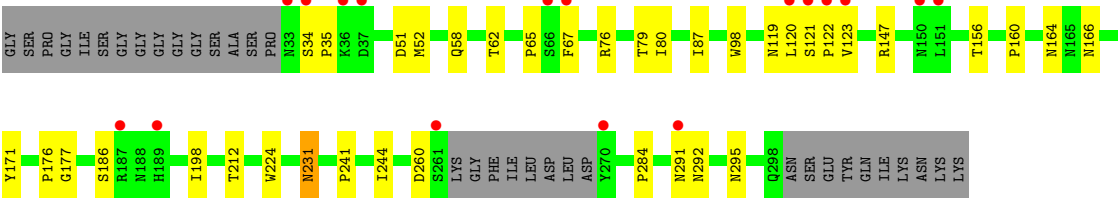
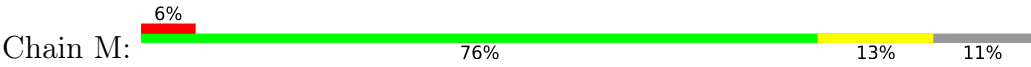


• Molecule 1: MOSQUITOCIDAL TOXIN

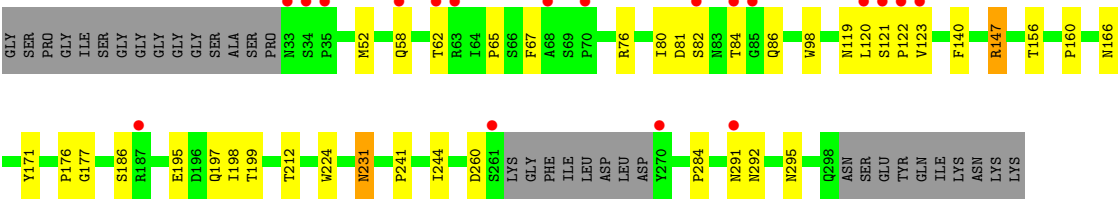
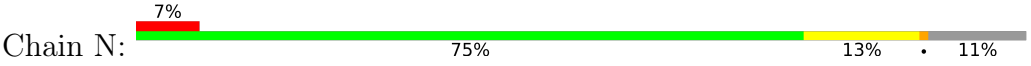
Chain L: 



• Molecule 1: MOSQUITOCIDAL TOXIN



• Molecule 1: MOSQUITOCIDAL TOXIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	123.71Å 143.27Å 135.81Å 90.00° 100.58° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 99.9 (50.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.57 (at 2.51Å)	Xtriage
Refinement program	TNT 5.6.1	Depositor
R, R_{free}	0.174 , 0.194 0.192 , 0.209	Depositor DCC
R_{free} test set	8035 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30680	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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 ⓘ

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	0.70	0/2149	0.82	2/2928 (0.1%)
1	B	0.71	0/2149	0.80	1/2928 (0.0%)
1	C	0.73	0/2149	0.84	3/2928 (0.1%)
1	D	0.69	0/2149	0.80	1/2928 (0.0%)
1	E	0.71	1/2149 (0.0%)	0.81	0/2928
1	F	0.69	1/2149 (0.0%)	0.83	1/2928 (0.0%)
1	G	0.72	0/2149	0.82	1/2928 (0.0%)
1	H	0.69	0/2149	0.81	1/2928 (0.0%)
1	I	0.70	0/2149	0.82	1/2928 (0.0%)
1	J	0.72	0/2149	0.83	1/2928 (0.0%)
1	K	0.69	0/2149	0.81	1/2928 (0.0%)
1	L	0.68	0/2149	0.81	1/2928 (0.0%)
1	M	0.70	0/2149	0.81	1/2928 (0.0%)
1	N	0.69	0/2149	0.81	1/2928 (0.0%)
All	All	0.70	2/30086 (0.0%)	0.82	16/40992 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	192	PHE	CE1-CZ	5.21	1.47	1.37
1	E	92	GLU	CG-CD	5.19	1.59	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	87	ILE	CG1-CB-CG2	-8.96	91.68	111.40
1	C	192	PHE	C-N-CD	-5.92	107.57	120.60
1	A	147	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	F	147	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	L	147	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	K	147	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	147	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	147	ARG	NE-CZ-NH1	5.05	122.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	GLN	CB-CA-C	-5.05	100.30	110.40
1	D	147	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	N	147	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	H	147	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	M	147	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	I	147	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	G	147	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	J	147	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	2095	0	1976	31	1
1	B	2095	0	1976	27	0
1	C	2095	0	1976	36	0
1	D	2095	0	1976	32	0
1	E	2095	0	1976	26	0
1	F	2095	0	1976	26	0
1	G	2095	0	1976	27	1
1	H	2095	0	1976	33	0
1	I	2095	0	1976	33	0
1	J	2095	0	1976	29	1
1	K	2095	0	1976	27	0
1	L	2095	0	1976	30	0
1	M	2095	0	1976	31	0
1	N	2095	0	1976	28	1
2	A	93	0	0	3	0
2	B	108	0	0	3	0
2	C	120	0	0	4	0
2	D	114	0	0	6	0
2	E	82	0	0	2	0
2	F	81	0	0	3	0
2	G	96	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	86	0	0	1	0
2	I	109	0	0	2	0
2	J	112	0	0	3	0
2	K	80	0	0	1	0
2	L	92	0	0	2	0
2	M	93	0	0	2	0
2	N	84	0	0	1	0
All	All	30680	0	27664	404	2

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 7.

All (404) 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:F:241:PRO:HB2	1:F:244:ILE:HD12	1.48	0.96
1:C:241:PRO:HB2	1:C:244:ILE:HD12	1.48	0.96
1:J:241:PRO:HB2	1:J:244:ILE:HD12	1.48	0.96
1:L:241:PRO:HB2	1:L:244:ILE:HD12	1.48	0.96
1:B:241:PRO:HB2	1:B:244:ILE:HD12	1.48	0.96
1:C:87:ILE:HD11	1:C:176:PRO:HD3	1.48	0.95
1:I:241:PRO:HB2	1:I:244:ILE:HD12	1.48	0.95
1:H:241:PRO:HB2	1:H:244:ILE:HD12	1.48	0.95
1:A:241:PRO:HB2	1:A:244:ILE:HD12	1.48	0.94
1:N:241:PRO:HB2	1:N:244:ILE:HD12	1.48	0.94
1:M:241:PRO:HB2	1:M:244:ILE:HD12	1.48	0.93
1:E:241:PRO:HB2	1:E:244:ILE:HD12	1.48	0.93
1:D:241:PRO:HB2	1:D:244:ILE:HD12	1.48	0.93
1:G:241:PRO:HB2	1:G:244:ILE:HD12	1.48	0.92
1:K:241:PRO:HB2	1:K:244:ILE:HD12	1.48	0.92
1:D:76:ARG:HD2	1:D:198:ILE:HG21	1.52	0.91
1:E:244:ILE:HD11	1:E:292:ASN:ND2	1.90	0.86
1:J:76:ARG:HD2	1:J:198:ILE:HG21	1.57	0.86
1:B:76:ARG:HD2	1:B:198:ILE:HG21	1.60	0.83
1:D:76:ARG:HD2	1:D:198:ILE:CG2	2.08	0.83
1:N:244:ILE:HD11	1:N:292:ASN:HD22	1.40	0.83
1:I:292:ASN:HB3	2:I:2075:HOH:O	1.79	0.81
1:A:76:ARG:HD2	1:A:198:ILE:HG21	1.63	0.79
1:B:76:ARG:HD2	1:B:198:ILE:CG2	2.12	0.79
1:C:244:ILE:HD11	1:C:292:ASN:HD22	1.47	0.79
1:H:76:ARG:HD2	1:H:198:ILE:CG2	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ILE:HD11	1:C:292:ASN:ND2	1.99	0.78
1:F:244:ILE:HD11	1:F:292:ASN:HD22	1.48	0.78
1:M:76:ARG:HD2	1:M:198:ILE:HG21	1.66	0.77
1:M:76:ARG:HD2	1:M:198:ILE:CG2	2.15	0.77
1:E:244:ILE:HD11	1:E:292:ASN:HD22	1.50	0.75
1:F:244:ILE:HD11	1:F:292:ASN:ND2	2.01	0.75
1:M:244:ILE:HD11	1:M:292:ASN:HD22	1.50	0.75
1:A:76:ARG:HD2	1:A:198:ILE:CG2	2.16	0.74
1:H:84:THR:HB	1:H:86:GLN:HG2	1.69	0.73
1:A:292:ASN:OD1	1:H:292:ASN:HB2	1.89	0.73
1:M:87:ILE:CD1	1:M:176:PRO:HD3	2.18	0.73
1:N:244:ILE:HD11	1:N:292:ASN:ND2	2.03	0.73
1:J:76:ARG:HD2	1:J:198:ILE:CG2	2.20	0.72
1:G:76:ARG:HD2	1:G:198:ILE:CG2	2.21	0.71
1:H:76:ARG:HD2	1:H:198:ILE:HG21	1.71	0.71
1:F:292:ASN:HB3	2:F:2056:HOH:O	1.91	0.70
1:C:156:THR:HG21	1:C:284:PRO:HG2	1.74	0.70
1:K:76:ARG:HD2	1:K:198:ILE:CG2	2.21	0.70
1:A:156:THR:HG21	1:A:284:PRO:HG2	1.74	0.70
1:H:81:ASP:OD1	1:H:83:ASN:HB2	1.90	0.70
1:J:244:ILE:HD11	1:J:292:ASN:HD22	1.57	0.70
1:M:156:THR:HG21	1:M:284:PRO:HG2	1.74	0.70
1:G:76:ARG:HD2	1:G:198:ILE:HG21	1.75	0.69
1:L:156:THR:HG21	1:L:284:PRO:HG2	1.74	0.69
1:H:156:THR:HG21	1:H:284:PRO:HG2	1.74	0.69
1:J:156:THR:HG21	1:J:284:PRO:HG2	1.74	0.69
1:K:156:THR:HG21	1:K:284:PRO:HG2	1.74	0.69
1:F:156:THR:HG21	1:F:284:PRO:HG2	1.74	0.69
1:N:156:THR:HG21	1:N:284:PRO:HG2	1.74	0.69
1:N:76:ARG:HD2	1:N:198:ILE:HG21	1.75	0.69
1:I:156:THR:HG21	1:I:284:PRO:HG2	1.74	0.68
1:B:156:THR:HG21	1:B:284:PRO:HG2	1.74	0.68
1:G:156:THR:HG21	1:G:284:PRO:HG2	1.74	0.68
1:G:244:ILE:HD11	1:G:292:ASN:HD22	1.58	0.68
1:E:156:THR:HG21	1:E:284:PRO:HG2	1.74	0.68
1:A:236:ASN:HB2	2:A:2066:HOH:O	1.93	0.68
1:I:76:ARG:HD2	1:I:198:ILE:CG2	2.24	0.67
1:K:76:ARG:HD2	1:K:198:ILE:HG21	1.77	0.67
1:C:87:ILE:HG12	2:C:2022:HOH:O	1.94	0.67
1:J:244:ILE:HD11	1:J:292:ASN:ND2	2.09	0.67
1:D:156:THR:HG21	1:D:284:PRO:HG2	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:244:ILE:HD11	1:G:292:ASN:ND2	2.10	0.67
1:N:76:ARG:HD2	1:N:198:ILE:CG2	2.25	0.66
2:J:2034:HOH:O	1:K:51:ASP:HB2	1.94	0.66
1:D:292:ASN:HB3	2:D:2111:HOH:O	1.94	0.66
1:C:87:ILE:HD11	1:C:176:PRO:CD	2.24	0.66
1:L:76:ARG:HD2	1:L:198:ILE:CG2	2.26	0.65
1:M:244:ILE:HD11	1:M:292:ASN:ND2	2.11	0.65
1:D:244:ILE:HD11	1:D:292:ASN:ND2	2.12	0.64
1:F:76:ARG:HD2	1:F:198:ILE:HG21	1.78	0.64
1:F:76:ARG:HD2	1:F:198:ILE:CG2	2.28	0.64
1:M:87:ILE:HD12	1:M:176:PRO:HD3	1.79	0.64
1:G:164:ASN:HB2	2:G:2042:HOH:O	1.96	0.63
1:E:76:ARG:HD2	1:E:198:ILE:CG2	2.27	0.63
1:H:244:ILE:HD11	1:H:292:ASN:ND2	2.14	0.63
1:L:244:ILE:HD11	1:L:292:ASN:HD22	1.64	0.63
1:C:81:ASP:HB2	1:C:88:GLN:OE1	1.99	0.62
1:A:292:ASN:HB2	1:H:292:ASN:OD1	1.98	0.62
1:L:76:ARG:HD2	1:L:198:ILE:HG21	1.82	0.62
1:I:76:ARG:HD2	1:I:198:ILE:HG21	1.81	0.61
1:H:76:ARG:HD2	1:H:198:ILE:HG23	1.82	0.61
1:C:236:ASN:HB2	2:C:2088:HOH:O	2.02	0.60
1:M:87:ILE:HD11	1:M:176:PRO:HD3	1.82	0.60
1:L:244:ILE:HD11	1:L:292:ASN:ND2	2.17	0.60
1:C:76:ARG:HD2	1:C:198:ILE:HG21	1.84	0.59
1:C:241:PRO:HB2	1:C:244:ILE:CD1	2.29	0.59
1:C:76:ARG:HD2	1:C:198:ILE:CG2	2.32	0.59
1:B:220:ILE:HD11	2:B:2107:HOH:O	2.02	0.59
1:B:241:PRO:HB2	1:B:244:ILE:CD1	2.29	0.59
1:E:76:ARG:HD2	1:E:198:ILE:HG21	1.84	0.58
1:L:241:PRO:HB2	1:L:244:ILE:CD1	2.29	0.58
1:H:241:PRO:HB2	1:H:244:ILE:CD1	2.29	0.58
1:E:241:PRO:HB2	1:E:244:ILE:CD1	2.29	0.57
1:J:241:PRO:HB2	1:J:244:ILE:CD1	2.29	0.57
1:I:244:ILE:HD11	1:I:292:ASN:ND2	2.20	0.57
1:K:241:PRO:HB2	1:K:244:ILE:CD1	2.29	0.56
1:A:292:ASN:HB3	2:A:2059:HOH:O	2.03	0.56
1:C:142:SER:OG	1:C:197:GLN:OE1	2.23	0.56
1:I:58:GLN:O	1:I:62:THR:HG23	2.06	0.56
1:I:92:GLU:H	1:I:92:GLU:CD	2.09	0.56
1:A:58:GLN:O	1:A:62:THR:HG23	2.06	0.56
1:L:58:GLN:O	1:L:62:THR:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:GLN:O	1:B:62:THR:HG23	2.06	0.56
1:C:127:HIS:HE1	1:D:51:ASP:OD2	1.88	0.56
1:N:58:GLN:O	1:N:62:THR:HG23	2.06	0.56
1:K:58:GLN:O	1:K:62:THR:HG23	2.06	0.56
1:M:58:GLN:O	1:M:62:THR:HG23	2.06	0.56
1:I:241:PRO:HB2	1:I:244:ILE:CD1	2.29	0.55
1:E:58:GLN:O	1:E:62:THR:HG23	2.06	0.55
1:L:127:HIS:HE1	1:M:51:ASP:OD2	1.89	0.55
1:G:58:GLN:O	1:G:62:THR:HG23	2.06	0.55
1:H:58:GLN:O	1:H:62:THR:HG23	2.06	0.55
1:J:58:GLN:O	1:J:62:THR:HG23	2.06	0.55
1:K:244:ILE:HD11	1:K:292:ASN:ND2	2.22	0.55
1:F:58:GLN:O	1:F:62:THR:HG23	2.06	0.55
1:A:241:PRO:HB2	1:A:244:ILE:CD1	2.29	0.55
1:D:58:GLN:O	1:D:62:THR:HG23	2.06	0.55
1:C:58:GLN:O	1:C:62:THR:HG23	2.06	0.55
1:E:292:ASN:HB2	1:K:292:ASN:OD1	2.07	0.55
1:F:84:THR:HB	1:F:86:GLN:HG3	1.89	0.55
1:C:187:ARG:HG2	1:C:187:ARG:HH11	1.71	0.55
1:D:92:GLU:HB2	2:D:2019:HOH:O	2.07	0.54
1:J:131:TYR:HH	1:J:142:SER:HG	1.49	0.54
1:M:241:PRO:HB2	1:M:244:ILE:CD1	2.29	0.54
1:A:81:ASP:HB3	1:A:84:THR:OG1	2.07	0.54
1:G:241:PRO:HB2	1:G:244:ILE:CD1	2.29	0.54
1:N:84:THR:HB	1:N:86:GLN:HG3	1.89	0.53
1:D:241:PRO:HB2	1:D:244:ILE:CD1	2.29	0.53
1:N:241:PRO:HB2	1:N:244:ILE:CD1	2.29	0.53
1:M:76:ARG:HD2	1:M:198:ILE:HG23	1.90	0.53
1:K:84:THR:OG1	1:K:86:GLN:HB2	2.09	0.53
1:I:244:ILE:HD11	1:I:292:ASN:HD22	1.73	0.52
1:E:164:ASN:HB2	2:E:2040:HOH:O	2.08	0.52
1:I:186:SER:O	1:I:189:HIS:N	2.39	0.52
1:L:164:ASN:HB2	2:L:2040:HOH:O	2.10	0.52
1:I:84:THR:OG1	1:I:86:GLN:HB2	2.09	0.52
1:L:84:THR:OG1	1:L:86:GLN:HB2	2.10	0.52
1:B:142:SER:OG	1:B:197:GLN:OE1	2.27	0.52
1:A:241:PRO:CB	1:A:292:ASN:HD21	2.23	0.52
1:G:76:ARG:HD2	1:G:198:ILE:HG23	1.91	0.51
1:K:76:ARG:HD2	1:K:198:ILE:HG23	1.90	0.51
1:H:164:ASN:HB2	2:H:2041:HOH:O	2.11	0.51
1:I:76:ARG:HD2	1:I:198:ILE:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:ARG:HD2	1:E:198:ILE:HG23	1.93	0.51
1:F:241:PRO:HB2	1:F:244:ILE:CD1	2.29	0.51
1:C:52:MSE:HA	2:C:2005:HOH:O	2.10	0.51
1:N:292:ASN:HB3	2:N:2052:HOH:O	2.12	0.50
1:H:189:HIS:O	1:H:191:PRO:HD3	2.11	0.50
1:M:80:ILE:HD11	1:M:176:PRO:HB3	1.94	0.50
1:B:231:ASN:C	1:B:231:ASN:HD22	2.16	0.49
1:C:76:ARG:HD3	1:C:177:GLY:O	2.13	0.49
1:L:231:ASN:C	1:L:231:ASN:HD22	2.16	0.49
1:C:232:PRO:HG3	2:C:2085:HOH:O	2.12	0.49
1:F:76:ARG:HD3	1:F:177:GLY:O	2.13	0.49
1:H:76:ARG:HD3	1:H:177:GLY:O	2.13	0.49
1:B:76:ARG:HD3	1:B:177:GLY:O	2.13	0.49
1:D:231:ASN:C	1:D:231:ASN:HD22	2.16	0.49
1:A:241:PRO:CB	1:A:292:ASN:ND2	2.75	0.49
1:E:76:ARG:HD3	1:E:177:GLY:O	2.13	0.49
1:I:185:PHE:HB2	1:I:190:ASN:HB2	1.94	0.49
1:L:76:ARG:HD3	1:L:177:GLY:O	2.13	0.49
1:A:231:ASN:C	1:A:231:ASN:HD22	2.16	0.49
1:F:231:ASN:C	1:F:231:ASN:HD22	2.16	0.49
1:J:285:ASN:HB2	2:J:2105:HOH:O	2.13	0.49
1:J:231:ASN:HD22	1:J:231:ASN:C	2.16	0.49
1:K:231:ASN:C	1:K:231:ASN:HD22	2.16	0.49
1:L:76:ARG:HD2	1:L:198:ILE:HG23	1.94	0.49
1:N:76:ARG:HD3	1:N:177:GLY:O	2.13	0.49
1:D:76:ARG:HD3	1:D:177:GLY:O	2.13	0.49
1:I:76:ARG:HD3	1:I:177:GLY:O	2.13	0.49
1:M:76:ARG:HD3	1:M:177:GLY:O	2.13	0.49
1:H:231:ASN:HD22	1:H:231:ASN:C	2.16	0.48
1:H:291:ASN:HD21	1:H:295:ASN:HD21	1.61	0.48
1:K:177:GLY:HA2	2:K:2004:HOH:O	2.12	0.48
1:M:231:ASN:C	1:M:231:ASN:HD22	2.16	0.48
1:I:68:ALA:HA	1:I:189:HIS:CB	2.42	0.48
1:I:231:ASN:C	1:I:231:ASN:HD22	2.16	0.48
1:G:76:ARG:HD3	1:G:177:GLY:O	2.13	0.48
1:G:197:GLN:NE2	2:G:2055:HOH:O	2.46	0.48
1:J:76:ARG:HD3	1:J:177:GLY:O	2.13	0.48
1:K:76:ARG:HD3	1:K:177:GLY:O	2.13	0.48
1:K:291:ASN:HD21	1:K:295:ASN:HD21	1.61	0.48
1:A:76:ARG:HD3	1:A:177:GLY:O	2.13	0.48
1:C:291:ASN:HD21	1:C:295:ASN:HD21	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:291:ASN:HD21	1:G:295:ASN:HD21	1.61	0.48
1:K:195:GLU:HG2	1:K:197:GLN:HG3	1.96	0.48
1:D:236:ASN:HB2	2:D:2078:HOH:O	2.13	0.48
1:J:197:GLN:O	1:J:198:ILE:HD13	2.14	0.48
1:N:231:ASN:C	1:N:231:ASN:HD22	2.16	0.48
1:F:291:ASN:HD21	1:F:295:ASN:HD21	1.61	0.48
1:N:291:ASN:HD21	1:N:295:ASN:HD21	1.61	0.48
1:A:241:PRO:HB3	1:A:292:ASN:HD21	1.78	0.48
1:B:76:ARG:HD2	1:B:198:ILE:HG23	1.91	0.48
1:C:231:ASN:HD22	1:C:231:ASN:C	2.16	0.48
1:F:257:ASN:ND2	2:F:2070:HOH:O	2.46	0.48
1:G:292:ASN:HB3	2:G:2061:HOH:O	2.14	0.47
1:H:131:TYR:OH	1:H:142:SER:OG	2.28	0.47
1:I:291:ASN:HD21	1:I:295:ASN:HD21	1.62	0.47
1:L:87:ILE:N	1:L:87:ILE:HD13	2.28	0.47
1:L:291:ASN:HD21	1:L:295:ASN:HD21	1.61	0.47
1:A:51:ASP:OD2	1:G:127:HIS:HE1	1.96	0.47
1:B:244:ILE:HD11	1:B:292:ASN:ND2	2.29	0.47
1:H:127:HIS:HE1	1:I:51:ASP:OD2	1.97	0.47
1:G:231:ASN:C	1:G:231:ASN:HD22	2.16	0.47
1:E:231:ASN:C	1:E:231:ASN:HD22	2.16	0.47
1:J:291:ASN:HD21	1:J:295:ASN:HD21	1.61	0.47
1:K:127:HIS:HE1	1:L:51:ASP:OD2	1.97	0.47
1:C:140:PHE:HB3	1:C:199:THR:CG2	2.44	0.47
1:H:52:MSE:SE	1:H:120:LEU:HD21	2.65	0.47
1:N:52:MSE:SE	1:N:120:LEU:HD21	2.65	0.47
1:D:52:MSE:SE	1:D:120:LEU:HD21	2.65	0.47
2:F:2055:HOH:O	1:J:292:ASN:HB3	2.14	0.47
1:M:164:ASN:HB2	2:M:2042:HOH:O	2.15	0.47
1:E:291:ASN:HD21	1:E:295:ASN:HD21	1.61	0.47
1:I:241:PRO:CB	1:I:292:ASN:ND2	2.78	0.47
1:K:52:MSE:SE	1:K:120:LEU:HD21	2.65	0.47
1:A:291:ASN:HD21	1:A:295:ASN:HD21	1.61	0.46
1:C:171:TYR:CD1	1:C:212:THR:HB	2.51	0.46
1:J:52:MSE:SE	1:J:120:LEU:HD21	2.65	0.46
1:J:127:HIS:HE1	1:K:51:ASP:OD2	1.98	0.46
1:J:171:TYR:CD1	1:J:212:THR:HB	2.51	0.46
1:B:291:ASN:HD21	1:B:295:ASN:HD21	1.61	0.46
1:B:292:ASN:HB3	2:B:2075:HOH:O	2.15	0.46
1:M:291:ASN:HD21	1:M:295:ASN:HD21	1.62	0.46
1:E:171:TYR:CD1	1:E:212:THR:HB	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:52:MSE:SE	1:M:120:LEU:HD21	2.65	0.46
1:A:164:ASN:HB2	2:A:2040:HOH:O	2.14	0.46
1:I:164:ASN:HB2	2:I:2053:HOH:O	2.16	0.46
1:N:171:TYR:CD1	1:N:212:THR:HB	2.50	0.46
1:A:171:TYR:CD1	1:A:212:THR:HB	2.50	0.46
1:E:52:MSE:SE	1:E:120:LEU:HD21	2.65	0.46
1:F:171:TYR:CD1	1:F:212:THR:HB	2.51	0.46
1:G:52:MSE:SE	1:G:120:LEU:HD21	2.65	0.46
1:I:52:MSE:SE	1:I:120:LEU:HD21	2.65	0.46
1:K:171:TYR:CD1	1:K:212:THR:HB	2.51	0.46
1:L:52:MSE:SE	1:L:120:LEU:HD21	2.65	0.46
1:D:291:ASN:HD21	1:D:295:ASN:HD21	1.61	0.46
1:I:171:TYR:CD1	1:I:212:THR:HB	2.51	0.46
1:B:192:PHE:CG	1:B:278:ALA:HB3	2.51	0.46
1:F:52:MSE:SE	1:F:120:LEU:HD21	2.65	0.46
1:H:171:TYR:CD1	1:H:212:THR:HB	2.51	0.46
1:M:171:TYR:CD1	1:M:212:THR:HB	2.51	0.46
1:A:52:MSE:SE	1:A:120:LEU:HD21	2.65	0.46
1:C:52:MSE:SE	1:C:120:LEU:HD21	2.65	0.46
1:D:171:TYR:CD1	1:D:212:THR:HB	2.51	0.46
1:L:171:TYR:CD1	1:L:212:THR:HB	2.51	0.46
1:A:76:ARG:HD2	1:A:198:ILE:HG23	1.95	0.46
1:D:87:ILE:N	1:D:87:ILE:HD13	2.30	0.46
1:B:52:MSE:SE	1:B:120:LEU:HD21	2.65	0.45
1:E:292:ASN:HB3	2:E:2055:HOH:O	2.16	0.45
1:A:80:ILE:O	1:A:80:ILE:HG22	2.12	0.45
1:B:171:TYR:CD1	1:B:212:THR:HB	2.51	0.45
1:D:76:ARG:HD2	1:D:198:ILE:HG23	1.92	0.45
1:D:65:PRO:HB3	1:D:67:PHE:CE1	2.52	0.45
1:N:140:PHE:HB3	1:N:199:THR:CG2	2.46	0.45
1:C:34:SER:HA	1:C:35:PRO:HD3	1.87	0.45
1:G:171:TYR:CD1	1:G:212:THR:HB	2.51	0.45
1:I:65:PRO:HB3	1:I:67:PHE:CE1	2.52	0.45
1:K:65:PRO:HB3	1:K:67:PHE:CE1	2.52	0.45
1:N:76:ARG:HD2	1:N:198:ILE:HG23	1.98	0.45
1:B:65:PRO:HB3	1:B:67:PHE:CE1	2.52	0.45
1:C:87:ILE:HD13	1:C:87:ILE:HA	1.81	0.45
1:G:65:PRO:HB3	1:G:67:PHE:CE1	2.52	0.45
1:M:65:PRO:HB3	1:M:67:PHE:CE1	2.52	0.45
1:N:80:ILE:CG2	1:N:81:ASP:N	2.80	0.45
1:C:65:PRO:HB3	1:C:67:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:65:PRO:HB3	1:N:67:PHE:CE1	2.52	0.45
1:N:80:ILE:HG22	1:N:81:ASP:N	2.32	0.45
1:A:65:PRO:HB3	1:A:67:PHE:CE1	2.52	0.44
1:B:74:HIS:HB2	2:B:2006:HOH:O	2.18	0.44
1:H:65:PRO:HB3	1:H:67:PHE:CE1	2.52	0.44
1:A:241:PRO:HG2	1:A:292:ASN:HD22	1.82	0.44
1:C:127:HIS:CE1	1:D:51:ASP:OD2	2.69	0.44
1:L:65:PRO:HB3	1:L:67:PHE:CE1	2.52	0.44
1:B:34:SER:HA	1:B:35:PRO:HD3	1.87	0.44
1:C:212:THR:HG22	1:C:224:TRP:HB2	2.00	0.44
1:I:186:SER:O	1:I:188:ASN:N	2.50	0.44
1:K:158:TRP:CD1	1:K:195:GLU:HA	2.53	0.44
1:B:212:THR:HG22	1:B:224:TRP:HB2	2.00	0.44
1:I:212:THR:HG22	1:I:224:TRP:HB2	2.00	0.44
1:J:87:ILE:HD12	1:J:176:PRO:HD3	2.00	0.44
1:F:65:PRO:HB3	1:F:67:PHE:CE1	2.52	0.44
1:K:121:SER:HB3	1:K:122:PRO:HD2	2.00	0.44
1:N:212:THR:HG22	1:N:224:TRP:HB2	2.00	0.44
1:E:65:PRO:HB3	1:E:67:PHE:CE1	2.52	0.44
1:F:121:SER:HB3	1:F:122:PRO:HD2	2.00	0.44
1:E:212:THR:HG22	1:E:224:TRP:HB2	2.00	0.43
1:H:140:PHE:HB3	1:H:199:THR:CG2	2.47	0.43
1:J:121:SER:HB3	1:J:122:PRO:HD2	2.00	0.43
1:D:121:SER:HB3	1:D:122:PRO:HD2	2.00	0.43
1:M:121:SER:HB3	1:M:122:PRO:HD2	2.00	0.43
1:B:121:SER:HB3	1:B:122:PRO:HD2	2.00	0.43
1:M:212:THR:HG22	1:M:224:TRP:HB2	2.00	0.43
1:J:65:PRO:HB3	1:J:67:PHE:CE1	2.52	0.43
1:L:121:SER:HB3	1:L:122:PRO:HD2	2.00	0.43
1:D:166:ASN:HB3	1:D:260:ASP:OD1	2.19	0.43
1:G:121:SER:HB3	1:G:122:PRO:HD2	2.00	0.43
1:A:121:SER:HB3	1:A:122:PRO:HD2	2.00	0.43
1:J:166:ASN:HB3	1:J:260:ASP:OD1	2.19	0.43
1:A:212:THR:HG22	1:A:224:TRP:HB2	2.00	0.43
1:H:121:SER:HB3	1:H:122:PRO:HD2	2.00	0.43
1:L:236:ASN:HB2	2:L:2063:HOH:O	2.19	0.43
1:M:87:ILE:HD12	1:M:176:PRO:CD	2.48	0.43
1:N:121:SER:HB3	1:N:122:PRO:HD2	2.00	0.43
1:E:166:ASN:HB3	1:E:260:ASP:OD1	2.19	0.43
1:G:166:ASN:HB3	1:G:260:ASP:OD1	2.19	0.43
1:B:166:ASN:HB3	1:B:260:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:THR:HG22	1:D:224:TRP:HB2	2.00	0.43
1:K:212:THR:HG22	1:K:224:TRP:HB2	2.00	0.43
1:M:166:ASN:HB3	1:M:260:ASP:OD1	2.19	0.43
1:B:140:PHE:HB3	1:B:199:THR:CG2	2.49	0.43
1:D:230:ILE:HD12	1:D:230:ILE:HA	1.89	0.43
1:H:212:THR:HG22	1:H:224:TRP:HB2	2.00	0.43
1:L:212:THR:HG22	1:L:224:TRP:HB2	2.00	0.43
1:A:158:TRP:CD1	1:A:195:GLU:HA	2.54	0.42
1:H:166:ASN:HB3	1:H:260:ASP:OD1	2.19	0.42
1:I:127:HIS:HE1	1:J:51:ASP:OD2	2.02	0.42
1:N:80:ILE:HD11	1:N:176:PRO:HB3	1.99	0.42
1:N:166:ASN:HB3	1:N:260:ASP:OD1	2.19	0.42
1:A:166:ASN:HB3	1:A:260:ASP:OD1	2.19	0.42
1:C:121:SER:HB3	1:C:122:PRO:HD2	2.00	0.42
1:I:121:SER:HB3	1:I:122:PRO:HD2	2.00	0.42
1:J:52:MSE:HE2	1:J:52:MSE:HB3	1.78	0.42
1:C:166:ASN:HB3	1:C:260:ASP:OD1	2.19	0.42
1:E:121:SER:HB3	1:E:122:PRO:HD2	2.00	0.42
1:E:230:ILE:HD12	1:E:230:ILE:HA	1.89	0.42
1:F:76:ARG:HD2	1:F:198:ILE:HG23	2.01	0.42
1:F:212:THR:HG22	1:F:224:TRP:HB2	2.00	0.42
1:G:52:MSE:HE2	1:G:52:MSE:HB3	1.78	0.42
1:I:166:ASN:HB3	1:I:260:ASP:OD1	2.19	0.42
1:K:166:ASN:HB3	1:K:260:ASP:OD1	2.19	0.42
1:M:79:THR:C	1:M:80:ILE:HD12	2.40	0.42
1:N:195:GLU:HG2	1:N:197:GLN:HG3	2.01	0.42
1:H:52:MSE:HE2	1:H:52:MSE:HB3	1.78	0.42
1:H:80:ILE:O	1:H:80:ILE:HG22	2.18	0.42
1:D:76:ARG:CD	1:D:198:ILE:HG21	2.37	0.42
1:D:119:ASN:OD1	1:D:121:SER:HB2	2.20	0.42
1:F:230:ILE:HD12	1:F:230:ILE:HA	1.89	0.42
1:H:34:SER:HA	1:H:35:PRO:HD3	1.87	0.42
1:J:212:THR:HG22	1:J:224:TRP:HB2	2.00	0.42
1:N:119:ASN:OD1	1:N:121:SER:HB2	2.20	0.42
1:I:119:ASN:OD1	1:I:121:SER:HB2	2.20	0.42
1:M:34:SER:HA	1:M:35:PRO:HD3	1.87	0.42
1:D:140:PHE:HB3	1:D:199:THR:CG2	2.50	0.42
1:B:52:MSE:HE2	1:B:52:MSE:HB3	1.78	0.42
1:G:212:THR:HG22	1:G:224:TRP:HB2	2.00	0.42
1:J:119:ASN:OD1	1:J:121:SER:HB2	2.20	0.42
1:K:119:ASN:OD1	1:K:121:SER:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:166:ASN:HB3	1:L:260:ASP:OD1	2.19	0.42
1:M:292:ASN:HB3	2:M:2062:HOH:O	2.20	0.42
1:D:118:GLN:HB2	2:D:2033:HOH:O	2.20	0.41
1:L:127:HIS:CE1	1:M:51:ASP:OD2	2.71	0.41
1:M:119:ASN:OD1	1:M:121:SER:HB2	2.20	0.41
1:D:164:ASN:HB2	2:D:2051:HOH:O	2.20	0.41
1:D:177:GLY:HA2	2:D:2010:HOH:O	2.20	0.41
1:F:34:SER:HA	1:F:35:PRO:HD3	1.87	0.41
1:F:166:ASN:HB3	1:F:260:ASP:OD1	2.19	0.41
1:G:119:ASN:OD1	1:G:121:SER:HB2	2.20	0.41
1:L:143:THR:O	1:L:197:GLN:HA	2.20	0.41
1:C:119:ASN:OD1	1:C:121:SER:HB2	2.20	0.41
1:F:84:THR:CB	1:F:86:GLN:HG3	2.50	0.41
1:I:34:SER:HA	1:I:35:PRO:HD3	1.87	0.41
1:B:98:TRP:CD1	1:B:160:PRO:HD3	2.56	0.41
1:F:119:ASN:OD1	1:F:121:SER:HB2	2.20	0.41
1:H:98:TRP:CD1	1:H:160:PRO:HD3	2.56	0.41
1:M:98:TRP:CD1	1:M:160:PRO:HD3	2.56	0.41
1:B:119:ASN:OD1	1:B:121:SER:HB2	2.20	0.41
1:L:119:ASN:OD1	1:L:121:SER:HB2	2.20	0.41
1:D:34:SER:HA	1:D:35:PRO:HD3	1.87	0.41
1:E:192:PHE:HA	1:E:193:PRO:HD2	1.88	0.41
1:G:230:ILE:HD12	1:G:230:ILE:HA	1.89	0.41
1:J:140:PHE:HB3	1:J:199:THR:CG2	2.50	0.41
1:K:98:TRP:CD1	1:K:160:PRO:HD3	2.56	0.41
1:L:140:PHE:HB3	1:L:199:THR:CG2	2.50	0.41
1:N:98:TRP:CD1	1:N:160:PRO:HD3	2.56	0.41
1:C:76:ARG:HD2	1:C:198:ILE:HG23	2.03	0.41
1:C:98:TRP:CD1	1:C:160:PRO:HD3	2.56	0.41
1:E:119:ASN:OD1	1:E:121:SER:HB2	2.20	0.41
1:F:98:TRP:CD1	1:F:160:PRO:HD3	2.56	0.41
1:G:34:SER:HA	1:G:35:PRO:HD3	1.87	0.41
1:I:158:TRP:CD1	1:I:195:GLU:HA	2.55	0.41
1:E:98:TRP:CD1	1:E:160:PRO:HD3	2.56	0.41
1:H:119:ASN:OD1	1:H:121:SER:HB2	2.20	0.41
1:J:98:TRP:CD1	1:J:160:PRO:HD3	2.56	0.41
1:A:119:ASN:OD1	1:A:121:SER:HB2	2.20	0.40
1:G:98:TRP:CD1	1:G:160:PRO:HD3	2.56	0.40
1:L:98:TRP:CD1	1:L:160:PRO:HD3	2.56	0.40
1:C:147:ARG:HD3	1:C:156:THR:O	2.22	0.40
1:D:147:ARG:HD3	1:D:156:THR:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:158:TRP:CE2	1:H:195:GLU:HG3	2.55	0.40
1:J:232:PRO:HG3	2:J:2081:HOH:O	2.21	0.40
1:E:52:MSE:HE2	1:E:52:MSE:HB3	1.78	0.40
1:L:147:ARG:HD3	1:L:156:THR:O	2.22	0.40
1:N:147:ARG:HD3	1:N:156:THR:O	2.22	0.40
1:H:158:TRP:CD1	1:H:195:GLU:HA	2.57	0.40
1:I:98:TRP:CD1	1:I:160:PRO:HD3	2.56	0.40
1:A:98:TRP:CD1	1:A:160:PRO:HD3	2.56	0.40
1:C:52:MSE:HG3	1:C:52:MSE:O	2.22	0.40

All (2) 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:G:150:ASN:N	1:J:286:ASN:ND2[2_557]	2.14	0.06
1:A:151:LEU:CD2	1:N:62:THR:CG2[2_556]	2.17	0.03

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	254/291 (87%)	240 (94%)	12 (5%)	2 (1%)	16	31
1	B	254/291 (87%)	241 (95%)	12 (5%)	1 (0%)	30	49
1	C	254/291 (87%)	239 (94%)	14 (6%)	1 (0%)	30	49
1	D	254/291 (87%)	239 (94%)	14 (6%)	1 (0%)	30	49
1	E	254/291 (87%)	240 (94%)	12 (5%)	2 (1%)	16	31
1	F	254/291 (87%)	240 (94%)	13 (5%)	1 (0%)	30	49
1	G	254/291 (87%)	241 (95%)	11 (4%)	2 (1%)	16	31
1	H	254/291 (87%)	241 (95%)	12 (5%)	1 (0%)	30	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	254/291 (87%)	240 (94%)	12 (5%)	2 (1%)	16	31
1	J	254/291 (87%)	240 (94%)	12 (5%)	2 (1%)	16	31
1	K	254/291 (87%)	240 (94%)	11 (4%)	3 (1%)	11	21
1	L	254/291 (87%)	241 (95%)	12 (5%)	1 (0%)	30	49
1	M	254/291 (87%)	241 (95%)	12 (5%)	1 (0%)	30	49
1	N	254/291 (87%)	240 (94%)	13 (5%)	1 (0%)	30	49
All	All	3556/4074 (87%)	3363 (95%)	172 (5%)	21 (1%)	22	39

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	187	ARG
1	I	187	ARG
1	K	187	ARG
1	J	187	ARG
1	A	187	ARG
1	E	187	ARG
1	K	82	SER
1	A	123	VAL
1	B	123	VAL
1	C	123	VAL
1	D	123	VAL
1	E	123	VAL
1	F	123	VAL
1	G	123	VAL
1	H	123	VAL
1	I	123	VAL
1	J	123	VAL
1	K	123	VAL
1	L	123	VAL
1	M	123	VAL
1	N	123	VAL

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	238/257 (93%)	234 (98%)	4 (2%)	56	79
1	B	238/257 (93%)	236 (99%)	2 (1%)	79	91
1	C	238/257 (93%)	236 (99%)	2 (1%)	79	91
1	D	238/257 (93%)	235 (99%)	3 (1%)	65	85
1	E	238/257 (93%)	236 (99%)	2 (1%)	79	91
1	F	238/257 (93%)	235 (99%)	3 (1%)	65	85
1	G	238/257 (93%)	237 (100%)	1 (0%)	89	96
1	H	238/257 (93%)	235 (99%)	3 (1%)	65	85
1	I	238/257 (93%)	236 (99%)	2 (1%)	79	91
1	J	238/257 (93%)	236 (99%)	2 (1%)	79	91
1	K	238/257 (93%)	237 (100%)	1 (0%)	89	96
1	L	238/257 (93%)	236 (99%)	2 (1%)	79	91
1	M	238/257 (93%)	236 (99%)	2 (1%)	79	91
1	N	238/257 (93%)	235 (99%)	3 (1%)	65	85
All	All	3332/3598 (93%)	3300 (99%)	32 (1%)	73	88

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ILE
1	A	82	SER
1	A	186	SER
1	A	231	ASN
1	B	186	SER
1	B	231	ASN
1	C	142	SER
1	C	231	ASN
1	D	196	ASP
1	D	197	GLN
1	D	231	ASN
1	E	82	SER
1	E	231	ASN
1	F	82	SER
1	F	197	GLN
1	F	231	ASN
1	G	231	ASN

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Mol	Chain	Res	Type
1	H	80	ILE
1	H	82	SER
1	H	231	ASN
1	I	197	GLN
1	I	231	ASN
1	J	92	GLU
1	J	231	ASN
1	K	231	ASN
1	L	82	SER
1	L	231	ASN
1	M	186	SER
1	M	231	ASN
1	N	82	SER
1	N	186	SER
1	N	231	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	HIS
1	A	164	ASN
1	A	217	ASN
1	A	231	ASN
1	A	292	ASN
1	A	295	ASN
1	B	127	HIS
1	B	164	ASN
1	B	217	ASN
1	B	231	ASN
1	B	292	ASN
1	B	295	ASN
1	C	127	HIS
1	C	164	ASN
1	C	217	ASN
1	C	231	ASN
1	C	292	ASN
1	C	295	ASN
1	D	127	HIS
1	D	164	ASN
1	D	217	ASN
1	D	228	ASN
1	D	231	ASN

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Mol	Chain	Res	Type
1	D	292	ASN
1	D	295	ASN
1	E	127	HIS
1	E	164	ASN
1	E	217	ASN
1	E	231	ASN
1	E	295	ASN
1	F	127	HIS
1	F	164	ASN
1	F	197	GLN
1	F	217	ASN
1	F	231	ASN
1	F	292	ASN
1	F	295	ASN
1	G	127	HIS
1	G	164	ASN
1	G	217	ASN
1	G	231	ASN
1	G	295	ASN
1	H	127	HIS
1	H	164	ASN
1	H	217	ASN
1	H	231	ASN
1	H	295	ASN
1	I	127	HIS
1	I	164	ASN
1	I	217	ASN
1	I	231	ASN
1	I	292	ASN
1	I	295	ASN
1	J	127	HIS
1	J	164	ASN
1	J	217	ASN
1	J	231	ASN
1	J	295	ASN
1	K	127	HIS
1	K	164	ASN
1	K	217	ASN
1	K	231	ASN
1	K	292	ASN
1	K	295	ASN
1	L	127	HIS

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Mol	Chain	Res	Type
1	L	164	ASN
1	L	217	ASN
1	L	231	ASN
1	L	295	ASN
1	M	127	HIS
1	M	164	ASN
1	M	217	ASN
1	M	231	ASN
1	M	295	ASN
1	N	127	HIS
1	N	164	ASN
1	N	217	ASN
1	N	231	ASN
1	N	292	ASN
1	N	295	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	253/291 (86%)	0.03	14 (5%)	32	29	22, 36, 76, 105	0
1	B	253/291 (86%)	-0.01	9 (3%)	46	43	21, 35, 72, 96	0
1	C	253/291 (86%)	0.06	17 (6%)	25	23	17, 34, 72, 98	0
1	D	253/291 (86%)	-0.03	12 (4%)	37	34	21, 34, 72, 104	0
1	E	253/291 (86%)	-0.03	11 (4%)	40	37	21, 35, 74, 106	0
1	F	253/291 (86%)	-0.08	11 (4%)	40	37	21, 36, 76, 98	0
1	G	253/291 (86%)	-0.08	8 (3%)	50	47	20, 34, 67, 96	0
1	H	253/291 (86%)	-0.09	12 (4%)	37	34	21, 36, 76, 104	0
1	I	253/291 (86%)	0.08	22 (8%)	17	16	21, 35, 72, 108	0
1	J	253/291 (86%)	0.04	13 (5%)	34	32	21, 34, 73, 97	0
1	K	253/291 (86%)	-0.04	10 (3%)	43	39	21, 36, 73, 108	0
1	L	253/291 (86%)	-0.00	8 (3%)	50	47	21, 36, 75, 101	0
1	M	253/291 (86%)	0.04	17 (6%)	25	23	21, 35, 72, 105	0
1	N	253/291 (86%)	0.19	19 (7%)	22	20	22, 36, 77, 110	0
All	All	3542/4074 (86%)	0.01	183 (5%)	34	31	17, 35, 75, 110	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	122	PRO	6.7
1	E	122	PRO	6.3
1	C	122	PRO	5.3
1	L	122	PRO	5.1
1	B	122	PRO	4.8
1	I	122	PRO	4.7
1	E	121	SER	4.6
1	J	33	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	121	SER	4.5
1	A	120	LEU	4.4
1	D	120	LEU	4.4
1	N	122	PRO	4.3
1	K	122	PRO	4.3
1	H	120	LEU	4.3
1	N	62	THR	4.2
1	H	122	PRO	4.1
1	L	120	LEU	4.1
1	G	122	PRO	4.1
1	J	122	PRO	4.1
1	H	121	SER	4.0
1	D	121	SER	4.0
1	I	297	ILE	4.0
1	L	121	SER	3.9
1	B	120	LEU	3.9
1	F	121	SER	3.9
1	I	150	ASN	3.8
1	M	37	ASP	3.8
1	I	121	SER	3.8
1	J	291	ASN	3.7
1	A	122	PRO	3.7
1	N	261	SER	3.7
1	F	120	LEU	3.7
1	I	187	ARG	3.7
1	J	187	ARG	3.7
1	C	261	SER	3.6
1	E	33	ASN	3.6
1	L	261	SER	3.6
1	N	120	LEU	3.6
1	J	120	LEU	3.5
1	L	187	ARG	3.5
1	F	122	PRO	3.5
1	G	33	ASN	3.5
1	G	120	LEU	3.4
1	I	290	ASN	3.4
1	K	291	ASN	3.4
1	M	121	SER	3.4
1	G	261	SER	3.3
1	C	191	PRO	3.3
1	C	67	PHE	3.3
1	A	121	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	123	VAL	3.2
1	C	120	LEU	3.2
1	I	33	ASN	3.2
1	N	123	VAL	3.2
1	M	187	ARG	3.2
1	F	33	ASN	3.2
1	H	33	ASN	3.2
1	M	122	PRO	3.2
1	C	121	SER	3.2
1	D	261	SER	3.2
1	N	121	SER	3.2
1	N	187	ARG	3.2
1	C	123	VAL	3.1
1	G	151	LEU	3.1
1	I	120	LEU	3.1
1	I	153	LEU	3.1
1	M	120	LEU	3.1
1	B	33	ASN	3.1
1	L	33	ASN	3.1
1	N	68	ALA	3.1
1	M	151	LEU	3.1
1	J	121	SER	3.1
1	N	33	ASN	3.1
1	N	85	GLY	3.0
1	D	123	VAL	3.0
1	E	123	VAL	3.0
1	C	33	ASN	3.0
1	K	120	LEU	2.9
1	G	187	ARG	2.9
1	F	123	VAL	2.9
1	K	33	ASN	2.9
1	E	120	LEU	2.9
1	D	187	ARG	2.9
1	H	123	VAL	2.8
1	I	148	TYR	2.8
1	C	187	ARG	2.8
1	E	261	SER	2.8
1	F	261	SER	2.8
1	M	36	LYS	2.8
1	A	297	ILE	2.8
1	D	33	ASN	2.7
1	K	151	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	187	ARG	2.7
1	M	189	HIS	2.7
1	M	150	ASN	2.7
1	I	242	SER	2.7
1	H	270	TYR	2.6
1	L	83	ASN	2.6
1	K	261	SER	2.6
1	N	34	SER	2.6
1	J	270	TYR	2.6
1	I	292	ASN	2.6
1	E	187	ARG	2.6
1	A	34	SER	2.5
1	A	123	VAL	2.5
1	K	121	SER	2.5
1	A	33	ASN	2.5
1	C	194	ASN	2.5
1	B	261	SER	2.5
1	D	292	ASN	2.5
1	H	83	ASN	2.5
1	D	151	LEU	2.4
1	M	123	VAL	2.4
1	C	68	ALA	2.4
1	N	58	GLN	2.4
1	A	74	HIS	2.4
1	K	123	VAL	2.4
1	I	291	ASN	2.4
1	L	270	TYR	2.4
1	N	270	TYR	2.4
1	G	121	SER	2.4
1	H	82	SER	2.4
1	N	84	THR	2.4
1	F	270	TYR	2.4
1	H	187	ARG	2.4
1	B	83	ASN	2.3
1	J	71	ASN	2.3
1	M	291	ASN	2.3
1	I	63	ARG	2.3
1	I	145	ARG	2.3
1	I	261	SER	2.3
1	D	63	ARG	2.3
1	A	291	ASN	2.3
1	A	261	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	67	PHE	2.3
1	E	67	PHE	2.3
1	J	290	ASN	2.3
1	C	69	SER	2.2
1	D	36	LYS	2.2
1	I	295	ASN	2.2
1	M	261	SER	2.2
1	F	187	ARG	2.2
1	N	70	PRO	2.2
1	A	82	SER	2.2
1	C	186	SER	2.2
1	M	34	SER	2.2
1	F	63	ARG	2.2
1	H	291	ASN	2.2
1	B	71	ASN	2.2
1	M	33	ASN	2.2
1	N	82	SER	2.1
1	B	123	VAL	2.1
1	F	151	LEU	2.1
1	J	63	ARG	2.1
1	N	35	PRO	2.1
1	A	83	ASN	2.1
1	K	83	ASN	2.1
1	C	189	HIS	2.1
1	J	74	HIS	2.1
1	G	270	TYR	2.1
1	M	270	TYR	2.1
1	M	67	PHE	2.1
1	N	63	ARG	2.1
1	C	118	GLN	2.1
1	E	82	SER	2.1
1	H	261	SER	2.1
1	B	119	ASN	2.1
1	E	189	HIS	2.1
1	E	291	ASN	2.1
1	F	119	ASN	2.1
1	H	119	ASN	2.1
1	I	188	ASN	2.1
1	A	187	ARG	2.0
1	C	193	PRO	2.0
1	J	58	GLN	2.0
1	M	66	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	291	ASN	2.0
1	N	291	ASN	2.0
1	I	289	LEU	2.0
1	I	241	PRO	2.0
1	I	270	TYR	2.0
1	D	58	GLN	2.0
1	J	286	ASN	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 monosaccharides 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.