



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:46 PM UTC

PDB ID : 4UXG / pdb_00004uxg
Title : Crystal structure of the carboxy-terminal region of the bacteriophage T4 proximal long tail fibre protein gp34, R32 native crystal
Authors : Granell, M.; Alvira, S.; Garcia-Doval, C.; Singh, A.K.; van Raaij, M.J.
Deposited on : 2014-08-22
Resolution : 3.00 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

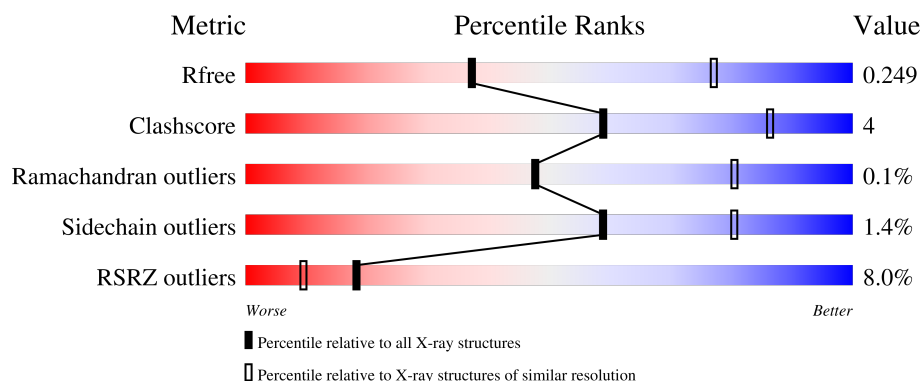
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



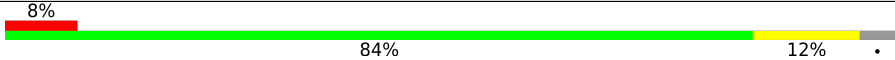
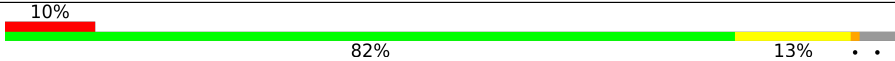
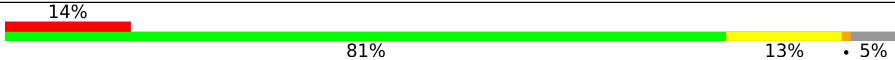
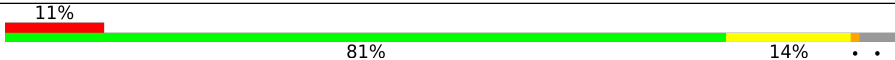
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	410	 3% 88% 8% .
1	B	410	 2% 89% 7% .
1	C	410	 % 89% 8% .
1	D	410	 9% 80% 16% . .
1	E	410	 10% 84% 12% . .

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Mol	Chain	Length	Quality of chain
1	F	410	
1	G	410	
1	H	410	
1	I	410	
1	J	410	
1	K	410	
1	L	410	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 36241 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 LARGE TAIL FIBER PROTEIN P34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3020	1886	532	597	5			
1	B	395	Total	C	N	O	S	0	0	0
			3020	1886	532	597	5			
1	C	398	Total	C	N	O	S	0	0	0
			3043	1898	536	604	5			
1	D	395	Total	C	N	O	S	0	0	0
			3020	1886	532	597	5			
1	E	398	Total	C	N	O	S	0	0	0
			3043	1898	536	604	5			
1	F	396	Total	C	N	O	S	0	0	0
			3027	1891	533	598	5			
1	G	395	Total	C	N	O	S	0	0	0
			3020	1886	532	597	5			
1	H	394	Total	C	N	O	S	0	0	0
			3013	1881	531	596	5			
1	I	394	Total	C	N	O	S	0	0	0
			3014	1883	531	595	5			
1	J	394	Total	C	N	O	S	0	0	0
			3014	1883	531	595	5			
1	K	391	Total	C	N	O	S	0	0	0
			2987	1864	527	591	5			
1	L	395	Total	C	N	O	S	0	0	0
			3020	1886	532	597	5			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	880	MET	-	expression tag	UNP P18771
A	881	GLY	-	expression tag	UNP P18771
A	882	SER	-	expression tag	UNP P18771
A	883	SER	-	expression tag	UNP P18771
A	884	HIS	-	expression tag	UNP P18771

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Chain	Residue	Modelled	Actual	Comment	Reference
A	885	HIS	-	expression tag	UNP P18771
A	886	HIS	-	expression tag	UNP P18771
A	887	HIS	-	expression tag	UNP P18771
A	888	HIS	-	expression tag	UNP P18771
A	889	HIS	-	expression tag	UNP P18771
A	890	SER	-	expression tag	UNP P18771
A	891	GLN	-	expression tag	UNP P18771
A	892	ASP	-	expression tag	UNP P18771
A	893	PRO	-	expression tag	UNP P18771
B	880	MET	-	expression tag	UNP P18771
B	881	GLY	-	expression tag	UNP P18771
B	882	SER	-	expression tag	UNP P18771
B	883	SER	-	expression tag	UNP P18771
B	884	HIS	-	expression tag	UNP P18771
B	885	HIS	-	expression tag	UNP P18771
B	886	HIS	-	expression tag	UNP P18771
B	887	HIS	-	expression tag	UNP P18771
B	888	HIS	-	expression tag	UNP P18771
B	889	HIS	-	expression tag	UNP P18771
B	890	SER	-	expression tag	UNP P18771
B	891	GLN	-	expression tag	UNP P18771
B	892	ASP	-	expression tag	UNP P18771
B	893	PRO	-	expression tag	UNP P18771
C	880	MET	-	expression tag	UNP P18771
C	881	GLY	-	expression tag	UNP P18771
C	882	SER	-	expression tag	UNP P18771
C	883	SER	-	expression tag	UNP P18771
C	884	HIS	-	expression tag	UNP P18771
C	885	HIS	-	expression tag	UNP P18771
C	886	HIS	-	expression tag	UNP P18771
C	887	HIS	-	expression tag	UNP P18771
C	888	HIS	-	expression tag	UNP P18771
C	889	HIS	-	expression tag	UNP P18771
C	890	SER	-	expression tag	UNP P18771
C	891	GLN	-	expression tag	UNP P18771
C	892	ASP	-	expression tag	UNP P18771
C	893	PRO	-	expression tag	UNP P18771
D	880	MET	-	expression tag	UNP P18771
D	881	GLY	-	expression tag	UNP P18771
D	882	SER	-	expression tag	UNP P18771
D	883	SER	-	expression tag	UNP P18771
D	884	HIS	-	expression tag	UNP P18771

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Chain	Residue	Modelled	Actual	Comment	Reference
D	885	HIS	-	expression tag	UNP P18771
D	886	HIS	-	expression tag	UNP P18771
D	887	HIS	-	expression tag	UNP P18771
D	888	HIS	-	expression tag	UNP P18771
D	889	HIS	-	expression tag	UNP P18771
D	890	SER	-	expression tag	UNP P18771
D	891	GLN	-	expression tag	UNP P18771
D	892	ASP	-	expression tag	UNP P18771
D	893	PRO	-	expression tag	UNP P18771
E	880	MET	-	expression tag	UNP P18771
E	881	GLY	-	expression tag	UNP P18771
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E	883	SER	-	expression tag	UNP P18771
E	884	HIS	-	expression tag	UNP P18771
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E	892	ASP	-	expression tag	UNP P18771
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F	888	HIS	-	expression tag	UNP P18771
F	889	HIS	-	expression tag	UNP P18771
F	890	SER	-	expression tag	UNP P18771
F	891	GLN	-	expression tag	UNP P18771
F	892	ASP	-	expression tag	UNP P18771
F	893	PRO	-	expression tag	UNP P18771
G	880	MET	-	expression tag	UNP P18771
G	881	GLY	-	expression tag	UNP P18771
G	882	SER	-	expression tag	UNP P18771
G	883	SER	-	expression tag	UNP P18771
G	884	HIS	-	expression tag	UNP P18771

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Chain	Residue	Modelled	Actual	Comment	Reference
G	885	HIS	-	expression tag	UNP P18771
G	886	HIS	-	expression tag	UNP P18771
G	887	HIS	-	expression tag	UNP P18771
G	888	HIS	-	expression tag	UNP P18771
G	889	HIS	-	expression tag	UNP P18771
G	890	SER	-	expression tag	UNP P18771
G	891	GLN	-	expression tag	UNP P18771
G	892	ASP	-	expression tag	UNP P18771
G	893	PRO	-	expression tag	UNP P18771
H	880	MET	-	expression tag	UNP P18771
H	881	GLY	-	expression tag	UNP P18771
H	882	SER	-	expression tag	UNP P18771
H	883	SER	-	expression tag	UNP P18771
H	884	HIS	-	expression tag	UNP P18771
H	885	HIS	-	expression tag	UNP P18771
H	886	HIS	-	expression tag	UNP P18771
H	887	HIS	-	expression tag	UNP P18771
H	888	HIS	-	expression tag	UNP P18771
H	889	HIS	-	expression tag	UNP P18771
H	890	SER	-	expression tag	UNP P18771
H	891	GLN	-	expression tag	UNP P18771
H	892	ASP	-	expression tag	UNP P18771
H	893	PRO	-	expression tag	UNP P18771
I	880	MET	-	expression tag	UNP P18771
I	881	GLY	-	expression tag	UNP P18771
I	882	SER	-	expression tag	UNP P18771
I	883	SER	-	expression tag	UNP P18771
I	884	HIS	-	expression tag	UNP P18771
I	885	HIS	-	expression tag	UNP P18771
I	886	HIS	-	expression tag	UNP P18771
I	887	HIS	-	expression tag	UNP P18771
I	888	HIS	-	expression tag	UNP P18771
I	889	HIS	-	expression tag	UNP P18771
I	890	SER	-	expression tag	UNP P18771
I	891	GLN	-	expression tag	UNP P18771
I	892	ASP	-	expression tag	UNP P18771
I	893	PRO	-	expression tag	UNP P18771
J	880	MET	-	expression tag	UNP P18771
J	881	GLY	-	expression tag	UNP P18771
J	882	SER	-	expression tag	UNP P18771
J	883	SER	-	expression tag	UNP P18771
J	884	HIS	-	expression tag	UNP P18771

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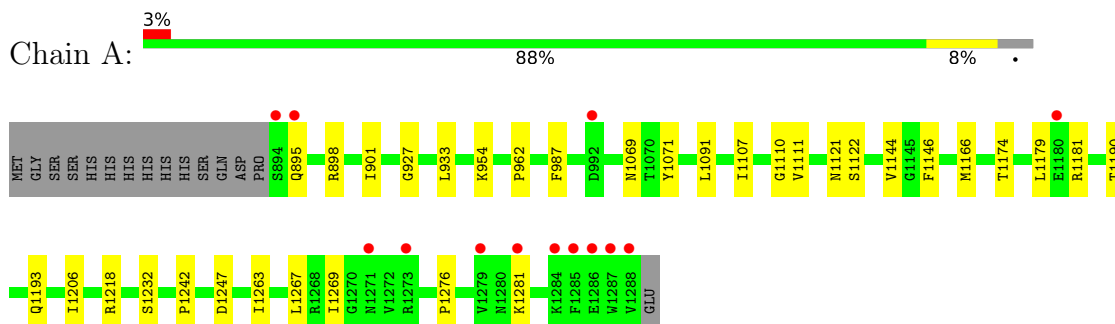
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Chain	Residue	Modelled	Actual	Comment	Reference
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J	887	HIS	-	expression tag	UNP P18771
J	888	HIS	-	expression tag	UNP P18771
J	889	HIS	-	expression tag	UNP P18771
J	890	SER	-	expression tag	UNP P18771
J	891	GLN	-	expression tag	UNP P18771
J	892	ASP	-	expression tag	UNP P18771
J	893	PRO	-	expression tag	UNP P18771
K	880	MET	-	expression tag	UNP P18771
K	881	GLY	-	expression tag	UNP P18771
K	882	SER	-	expression tag	UNP P18771
K	883	SER	-	expression tag	UNP P18771
K	884	HIS	-	expression tag	UNP P18771
K	885	HIS	-	expression tag	UNP P18771
K	886	HIS	-	expression tag	UNP P18771
K	887	HIS	-	expression tag	UNP P18771
K	888	HIS	-	expression tag	UNP P18771
K	889	HIS	-	expression tag	UNP P18771
K	890	SER	-	expression tag	UNP P18771
K	891	GLN	-	expression tag	UNP P18771
K	892	ASP	-	expression tag	UNP P18771
K	893	PRO	-	expression tag	UNP P18771
L	880	MET	-	expression tag	UNP P18771
L	881	GLY	-	expression tag	UNP P18771
L	882	SER	-	expression tag	UNP P18771
L	883	SER	-	expression tag	UNP P18771
L	884	HIS	-	expression tag	UNP P18771
L	885	HIS	-	expression tag	UNP P18771
L	886	HIS	-	expression tag	UNP P18771
L	887	HIS	-	expression tag	UNP P18771
L	888	HIS	-	expression tag	UNP P18771
L	889	HIS	-	expression tag	UNP P18771
L	890	SER	-	expression tag	UNP P18771
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L	893	PRO	-	expression tag	UNP P18771

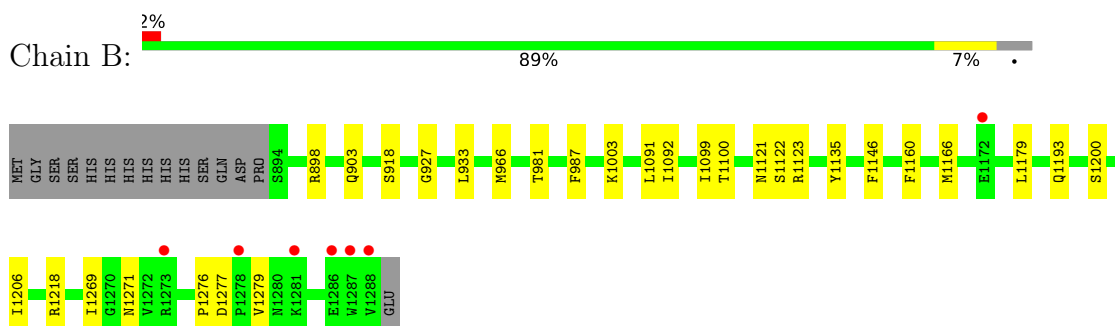
3 Residue-property plots

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.

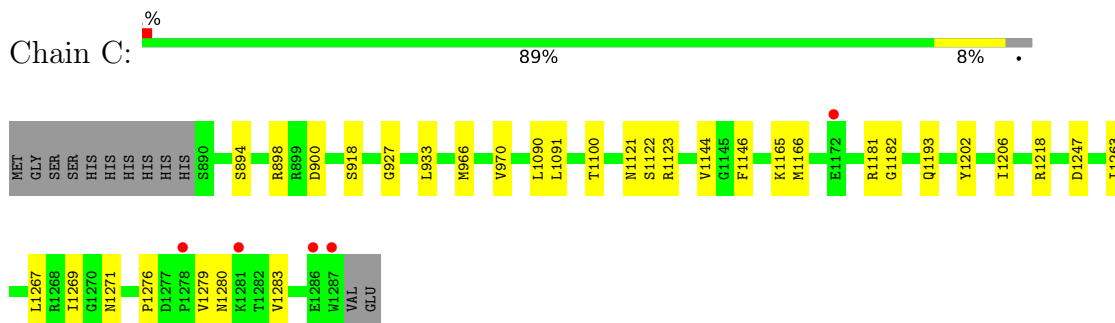
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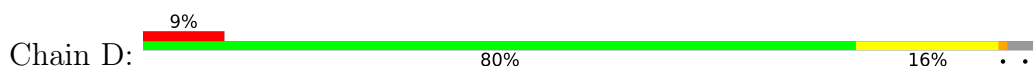
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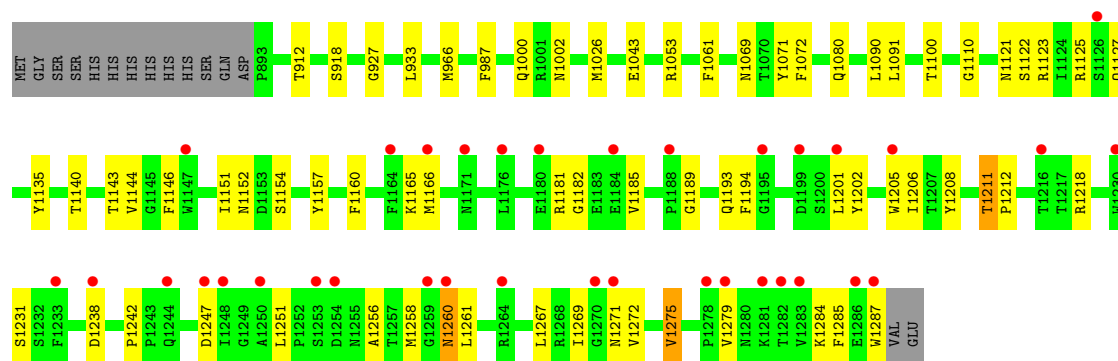


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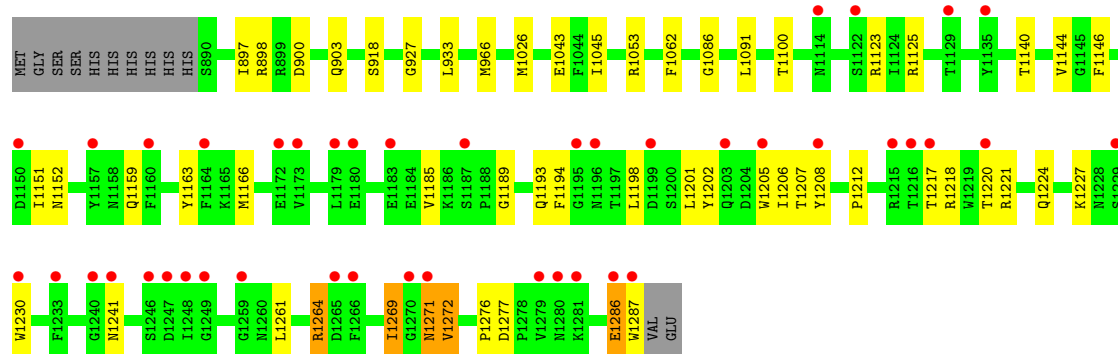
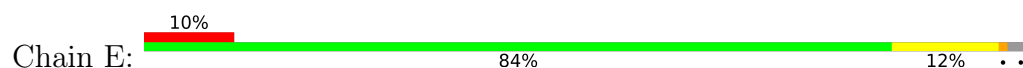


• Molecule 1: LARGE TAIL FIBER PROTEIN P34

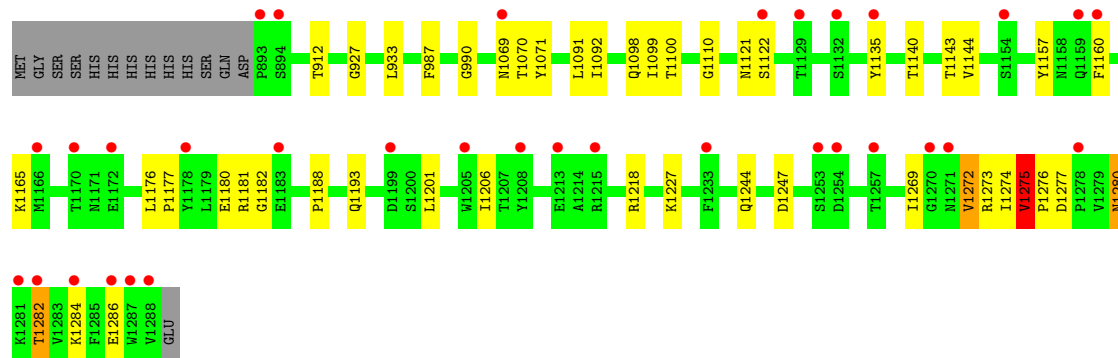
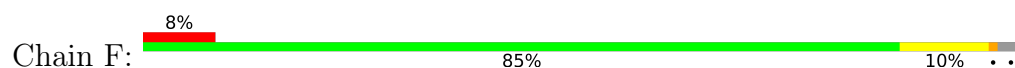




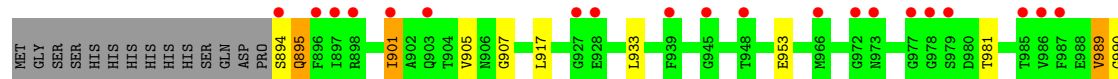
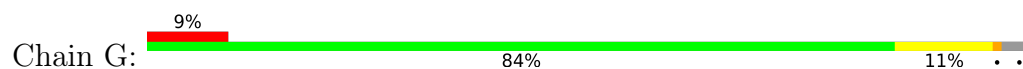
• Molecule 1: LARGE TAIL FIBER PROTEIN P34

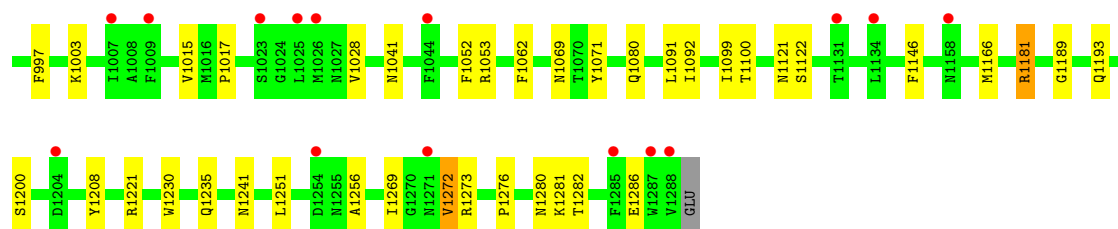


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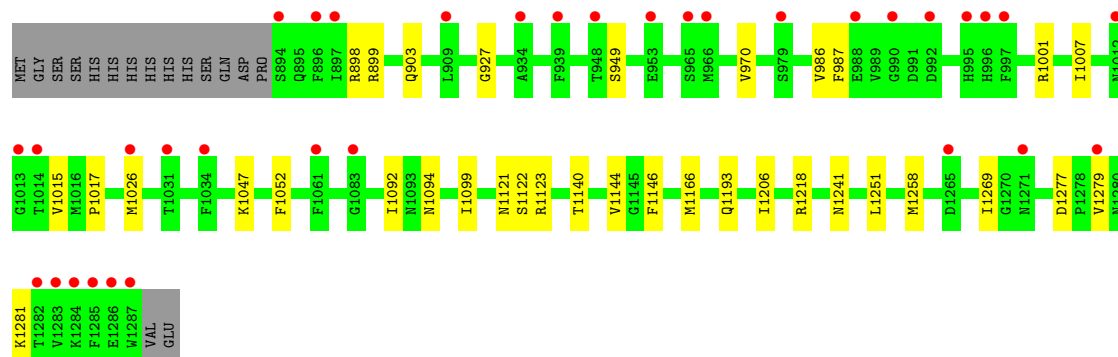
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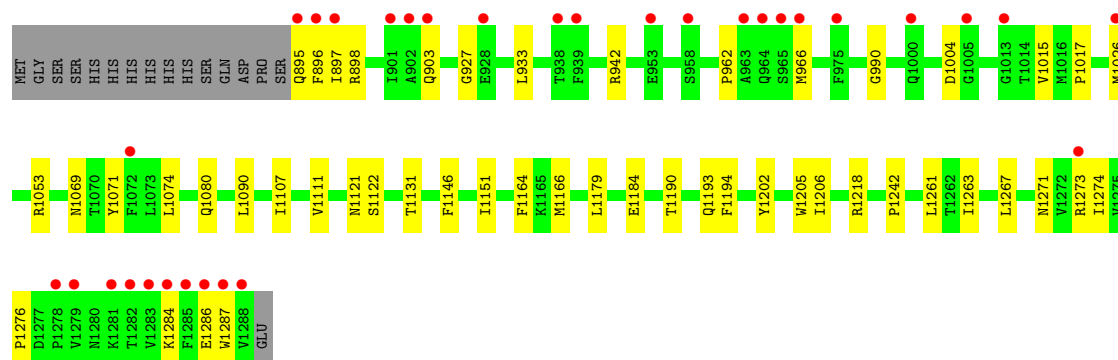
• Molecule 1: LARGE TAIL FIBER PROTEIN P34

Chain H: 8% 88% 9% .



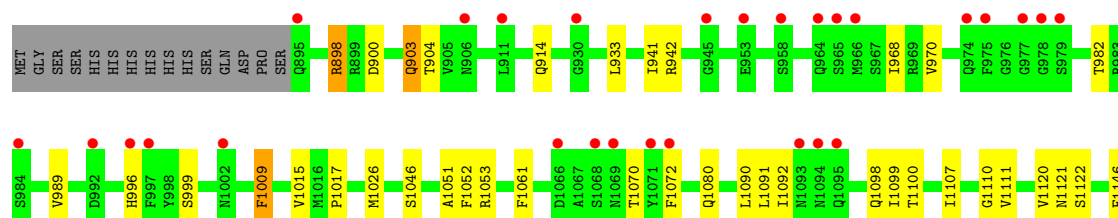
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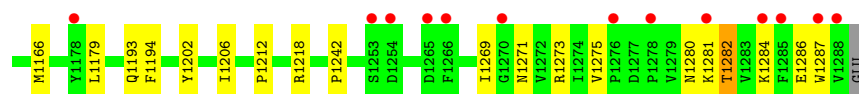
Chain I: 8% 84% 12% .



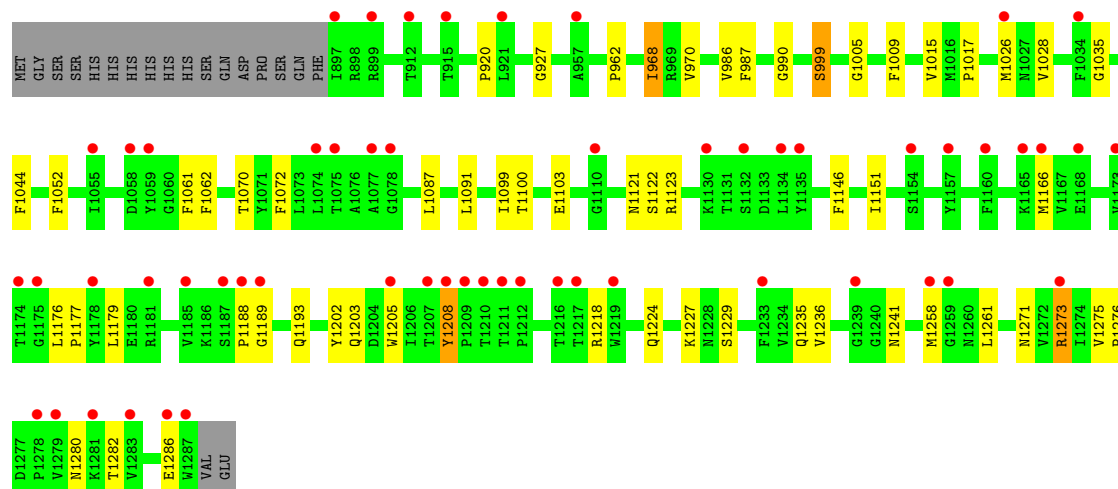
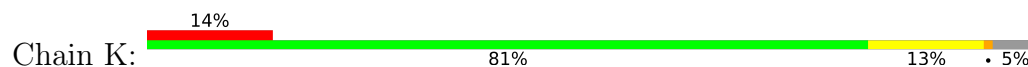
• Molecule 1: LARGE TAIL FIBER PROTEIN P34

Chain J: 10% 82% 13% . .

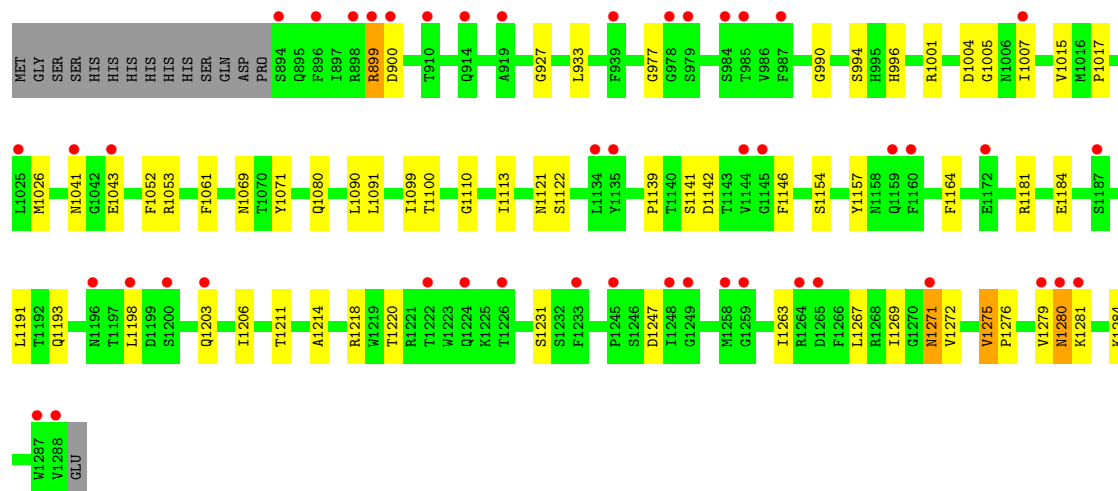
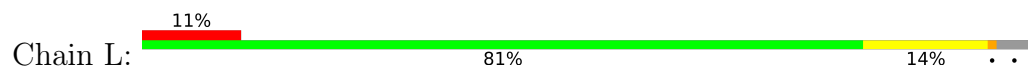




• Molecule 1: LARGE TAIL FIBER PROTEIN P34



• Molecule 1: LARGE TAIL FIBER PROTEIN P34



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	228.49Å 228.49Å 1069.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.99 – 3.00 29.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.99-3.00) 99.8 (29.99-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 3.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.226 , 0.249 0.225 , 0.249	Depositor DCC
R_{free} test set	3005 reflections (1.40%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	1.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	36241	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.51% 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	0.43	0/3085	0.79	1/4197 (0.0%)
1	B	0.43	0/3085	0.78	2/4197 (0.0%)
1	C	0.44	0/3109	0.79	1/4230 (0.0%)
1	D	0.40	0/3086	0.79	2/4198 (0.0%)
1	E	0.40	0/3109	0.83	4/4230 (0.1%)
1	F	0.40	0/3093	0.80	7/4208 (0.2%)
1	G	0.32	0/3085	0.78	2/4197 (0.0%)
1	H	0.32	0/3078	0.77	3/4187 (0.1%)
1	I	0.33	0/3079	0.77	1/4189 (0.0%)
1	J	0.34	0/3079	0.78	1/4189 (0.0%)
1	K	0.33	0/3051	0.81	4/4151 (0.1%)
1	L	0.34	0/3085	0.78	2/4197 (0.0%)
All	All	0.38	0/37024	0.79	30/50370 (0.1%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1277	ASP	CA-C-N	6.81	126.77	119.28
1	E	1277	ASP	C-N-CA	6.81	126.77	119.28
1	L	990	GLY	N-CA-C	6.49	118.88	110.45
1	H	1277	ASP	CA-C-N	6.38	126.30	119.28
1	H	1277	ASP	C-N-CA	6.38	126.30	119.28
1	K	1208	TYR	CA-C-N	6.11	125.87	119.76
1	K	1208	TYR	C-N-CA	6.11	125.87	119.76
1	F	1110	GLY	N-CA-C	5.73	119.42	112.48
1	F	1275	VAL	CA-C-N	5.70	125.61	119.85
1	F	1275	VAL	C-N-CA	5.70	125.61	119.85
1	E	1062	PHE	N-CA-C	5.64	117.65	109.07
1	B	1277	ASP	CA-C-N	5.60	125.44	119.28
1	B	1277	ASP	C-N-CA	5.60	125.44	119.28
1	G	1272	VAL	N-CA-C	5.57	116.13	107.99
1	K	1062	PHE	N-CA-C	5.45	117.36	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1110	GLY	N-CA-C	5.40	119.42	112.18
1	F	1272	VAL	N-CA-C	5.35	115.81	107.99
1	J	1110	GLY	N-CA-C	5.33	118.93	112.48
1	F	990	GLY	N-CA-C	5.32	117.36	110.45
1	F	1280	ASN	CB-CA-C	-5.29	109.45	117.07
1	C	894	SER	N-CA-C	-5.20	105.60	112.94
1	F	1280	ASN	CA-C-O	5.20	120.96	117.94
1	A	1110	GLY	N-CA-C	5.20	118.77	112.48
1	D	1279	VAL	N-CA-C	5.12	115.34	110.42
1	K	990	GLY	N-CA-C	5.10	117.08	110.45
1	L	1110	GLY	N-CA-C	5.10	118.65	112.48
1	G	1062	PHE	N-CA-C	5.09	116.80	109.07
1	I	990	GLY	N-CA-C	5.07	117.04	110.45
1	E	1189	GLY	N-CA-C	5.05	118.83	110.55
1	H	949	SER	N-CA-C	5.02	116.47	108.79

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	3020	0	2921	21	0
1	B	3020	0	2921	20	0
1	C	3043	0	2936	22	0
1	D	3020	0	2920	47	0
1	E	3043	0	2936	42	0
1	F	3027	0	2929	30	0
1	G	3020	0	2921	30	0
1	H	3013	0	2912	24	0
1	I	3014	0	2916	34	0
1	J	3014	0	2916	43	0
1	K	2987	0	2890	43	0
1	L	3020	0	2921	41	0
All	All	36241	0	35039	313	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (313) 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:A:1190:THR:HG1	1:B:1200:SER:HG	1.16	0.86
1:G:989:VAL:HG12	1:G:990:GLY:H	1.46	0.79
1:E:1207:THR:HG22	1:E:1217:THR:H	1.50	0.76
1:F:1275:VAL:HG13	1:F:1284:LYS:HB2	1.66	0.76
1:J:904:THR:O	1:L:899:ARG:NH2	2.21	0.73
1:B:898:ARG:N	1:B:903:GLN:OE1	2.16	0.73
1:D:1166:MET:HE1	1:D:1242:PRO:HD2	1.71	0.72
1:A:1269:ILE:HG22	1:C:1276:PRO:HG3	1.71	0.71
1:K:1123:ARG:NH1	1:L:1141:SER:O	2.24	0.71
1:C:1181:ARG:NH2	1:C:1247:ASP:OD2	2.20	0.69
1:F:1273:ARG:HB2	1:F:1286:GLU:HB2	1.73	0.69
1:D:1211:THR:HG22	1:D:1212:PRO:HD2	1.73	0.69
1:D:1269:ILE:HG22	1:F:1276:PRO:HG3	1.75	0.69
1:F:1193:GLN:HE21	1:F:1201:LEU:HD11	1.59	0.67
1:A:1069:ASN:HD22	1:A:1091:LEU:HD13	1.59	0.67
1:D:1218:ARG:HD2	1:E:1220:THR:HG21	1.77	0.67
1:E:1152:ASN:OD1	1:E:1208:TYR:OH	2.13	0.66
1:D:1152:ASN:OD1	1:D:1208:TYR:OH	2.12	0.66
1:I:1166:MET:HE2	1:I:1242:PRO:HD2	1.78	0.66
1:I:1273:ARG:HB3	1:I:1286:GLU:HB3	1.79	0.65
1:J:1206:ILE:HG13	1:J:1218:ARG:HG2	1.79	0.65
1:J:914:GLN:HE22	1:K:920:PRO:HB2	1.60	0.64
1:K:1276:PRO:HG3	1:L:1269:ILE:HG22	1.78	0.64
1:E:897:ILE:HG23	1:E:903:GLN:HG2	1.79	0.64
1:H:1015:VAL:HG22	1:H:1017:PRO:HD3	1.80	0.64
1:G:1166:MET:HE3	1:G:1241:ASN:HA	1.80	0.63
1:H:987:PHE:HB2	1:I:966:MET:HE2	1.80	0.63
1:I:898:ARG:N	1:I:903:GLN:OE1	2.23	0.63
1:D:1125:ARG:NH2	1:D:1127:GLN:OE1	2.31	0.63
1:E:1206:ILE:HG13	1:E:1218:ARG:HG2	1.82	0.62
1:G:1269:ILE:HG22	1:I:1276:PRO:HG3	1.80	0.62
1:D:1258:MET:HE2	1:E:1261:LEU:HD11	1.82	0.61
1:K:1151:ILE:HD12	1:K:1205:TRP:HZ3	1.66	0.61
1:B:1276:PRO:HG3	1:C:1269:ILE:HG22	1.84	0.60
1:E:1264:ARG:HG3	1:E:1264:ARG:HH11	1.67	0.60
1:I:1015:VAL:HG22	1:I:1017:PRO:HD3	1.83	0.59
1:A:1276:PRO:HG3	1:B:1269:ILE:HG22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1258:MET:HE1	1:D:1261:LEU:HD22	1.85	0.58
1:E:1286:GLU:OE1	1:E:1287:TRP:N	2.36	0.58
1:G:1276:PRO:HG3	1:H:1269:ILE:HG22	1.84	0.58
1:G:1052:PHE:CE2	1:H:1052:PHE:HB3	2.39	0.58
1:A:1206:ILE:HG13	1:A:1218:ARG:HG2	1.85	0.58
1:D:1123:ARG:HD2	1:E:1144:VAL:O	2.04	0.58
1:G:1092:ILE:HG12	1:G:1099:ILE:HG12	1.85	0.58
1:J:898:ARG:NH1	1:J:900:ASP:OD1	2.38	0.57
1:D:1193:GLN:HE21	1:D:1201:LEU:HD11	1.70	0.56
1:A:1166:MET:HE2	1:A:1242:PRO:HD2	1.87	0.56
1:A:1166:MET:HE3	1:A:1179:LEU:HB3	1.87	0.56
1:D:1275:VAL:HG13	1:D:1284:LYS:HB2	1.87	0.56
1:E:1193:GLN:HE21	1:E:1201:LEU:HD11	1.71	0.56
1:L:1001:ARG:NH1	1:L:1005:GLY:O	2.39	0.56
1:E:1091:LEU:HG	1:E:1100:THR:HB	1.87	0.56
1:H:898:ARG:H	1:H:903:GLN:HG3	1.71	0.56
1:J:1271:ASN:HB3	1:J:1287:TRP:CZ3	2.40	0.55
1:E:1269:ILE:HG23	1:E:1272:VAL:HG13	1.88	0.55
1:A:927:GLY:O	1:B:933:LEU:HD12	2.07	0.55
1:G:1280:ASN:O	1:G:1282:THR:HG23	2.06	0.55
1:J:1273:ARG:HB3	1:J:1286:GLU:HB2	1.87	0.55
1:L:1280:ASN:OD1	1:L:1281:LYS:N	2.37	0.55
1:A:1181:ARG:NH2	1:A:1247:ASP:OD2	2.40	0.55
1:G:1273:ARG:HB2	1:G:1286:GLU:HB2	1.89	0.55
1:I:1166:MET:HE3	1:I:1179:LEU:HB3	1.90	0.54
1:J:1053:ARG:NE	1:L:1043:GLU:OE2	2.40	0.54
1:L:1271:ASN:O	1:L:1271:ASN:ND2	2.39	0.54
1:C:898:ARG:HG2	1:C:900:ASP:OD1	2.08	0.54
1:G:981:THR:O	1:G:1003:LYS:HD2	2.08	0.54
1:J:1194:PHE:HB2	1:J:1202:TYR:CE1	2.43	0.53
1:J:1015:VAL:HG22	1:J:1017:PRO:HD3	1.90	0.53
1:E:1224:GLN:OE1	1:E:1227:LYS:HD2	2.08	0.53
1:J:1053:ARG:NH1	1:J:1080:GLN:O	2.39	0.53
1:D:1193:GLN:NE2	1:D:1201:LEU:HD11	2.24	0.53
1:G:1015:VAL:HG22	1:G:1017:PRO:HD3	1.91	0.53
1:A:898:ARG:HG2	1:A:901:ILE:HG12	1.91	0.53
1:D:1165:LYS:O	1:D:1182:GLY:N	2.40	0.52
1:G:894:SER:OG	1:G:895:GLN:N	2.42	0.52
1:H:1166:MET:HE3	1:H:1241:ASN:HA	1.89	0.52
1:J:996:HIS:HA	1:L:1007:ILE:HD13	1.90	0.52
1:D:1206:ILE:HG13	1:D:1218:ARG:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1166:MET:HE2	1:J:1242:PRO:HD2	1.90	0.52
1:J:1280:ASN:OD1	1:J:1282:THR:OG1	2.27	0.52
1:I:1206:ILE:HG13	1:I:1218:ARG:HG2	1.91	0.51
1:J:1271:ASN:HB3	1:J:1287:TRP:HZ3	1.74	0.51
1:B:1166:MET:HE3	1:B:1179:LEU:HB3	1.92	0.51
1:J:1091:LEU:HG	1:J:1100:THR:HB	1.93	0.51
1:K:999:SER:OG	1:L:996:HIS:ND1	2.36	0.51
1:E:1151:ILE:HD12	1:E:1205:TRP:HZ3	1.76	0.50
1:J:1166:MET:HE3	1:J:1179:LEU:HB3	1.93	0.50
1:C:1206:ILE:HG13	1:C:1218:ARG:HG2	1.94	0.50
1:D:1271:ASN:HB2	1:D:1287:TRP:CD1	2.46	0.50
1:L:1053:ARG:NH1	1:L:1080:GLN:O	2.43	0.49
1:F:1069:ASN:HB2	1:F:1071:TYR:CE1	2.47	0.49
1:F:1181:ARG:NH2	1:F:1247:ASP:OD2	2.44	0.49
1:H:1092:ILE:HG12	1:H:1099:ILE:HG12	1.94	0.49
1:I:1053:ARG:NH1	1:I:1080:GLN:O	2.44	0.49
1:A:1069:ASN:HB2	1:A:1071:TYR:CE1	2.47	0.49
1:E:1043:GLU:HB3	1:E:1045:ILE:HD11	1.94	0.49
1:E:1151:ILE:HD12	1:E:1205:TRP:CZ3	2.47	0.49
1:F:1206:ILE:HG13	1:F:1218:ARG:HG2	1.94	0.49
1:A:1144:VAL:O	1:C:1123:ARG:HD3	2.12	0.49
1:E:898:ARG:NH2	1:E:900:ASP:OD2	2.46	0.49
1:B:981:THR:O	1:B:1003:LYS:HD2	2.13	0.49
1:J:1052:PHE:CE2	1:K:1052:PHE:HB3	2.48	0.49
1:K:1273:ARG:HD2	1:K:1286:GLU:HB3	1.95	0.49
1:E:1086:GLY:HA3	1:K:1005:GLY:HA3	1.95	0.48
1:E:1123:ARG:NH1	1:E:1125:ARG:HG3	2.27	0.48
1:K:1070:THR:HG21	1:L:1061:PHE:CD2	2.48	0.48
1:D:933:LEU:HD12	1:F:927:GLY:O	2.12	0.48
1:G:989:VAL:HG12	1:G:990:GLY:N	2.23	0.48
1:K:927:GLY:O	1:L:933:LEU:HD12	2.14	0.48
1:H:1206:ILE:HG13	1:H:1218:ARG:HG2	1.95	0.48
1:I:1194:PHE:HB2	1:I:1202:TYR:CE1	2.48	0.48
1:K:1258:MET:SD	1:K:1261:LEU:HB2	2.53	0.48
1:L:1263:ILE:HD13	1:L:1267:LEU:HB2	1.96	0.48
1:K:1123:ARG:HD3	1:L:1142:ASP:O	2.13	0.48
1:L:1139:PRO:HG2	1:L:1198:LEU:HD21	1.96	0.48
1:J:1269:ILE:HG22	1:L:1276:PRO:HG3	1.96	0.48
1:K:1091:LEU:HG	1:K:1100:THR:HB	1.95	0.48
1:E:1212:PRO:HA	1:F:1227:LYS:HE2	1.95	0.47
1:E:1217:THR:HG22	1:E:1241:ASN:ND2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1180:GLU:HA	1:F:1244:GLN:HE22	1.79	0.47
1:G:1069:ASN:HB2	1:G:1071:TYR:CE1	2.49	0.47
1:L:900:ASP:OD1	1:L:900:ASP:N	2.46	0.47
1:K:1026:MET:HE3	1:K:1028:VAL:HG23	1.95	0.47
1:A:1146:PHE:HA	1:A:1193:GLN:O	2.13	0.47
1:E:1140:THR:O	1:E:1144:VAL:HG23	2.14	0.47
1:F:1092:ILE:HG12	1:F:1099:ILE:HG12	1.96	0.47
1:B:927:GLY:O	1:C:933:LEU:HD12	2.14	0.47
1:G:1146:PHE:HA	1:G:1193:GLN:O	2.15	0.47
1:I:1164:PHE:HE1	1:I:1184:GLU:HB2	1.79	0.47
1:G:1181:ARG:NH2	1:G:1235:GLN:OE1	2.47	0.47
1:J:1121:ASN:HA	1:J:1122:SER:HA	1.55	0.47
1:K:1146:PHE:HA	1:K:1193:GLN:O	2.14	0.47
1:L:1206:ILE:HG13	1:L:1218:ARG:HG2	1.95	0.47
1:D:1135:TYR:HB2	1:D:1160:PHE:CE1	2.49	0.47
1:E:1194:PHE:HB2	1:E:1202:TYR:CE1	2.49	0.47
1:F:1091:LEU:HG	1:F:1100:THR:HB	1.96	0.47
1:C:1271:ASN:OD1	1:C:1271:ASN:N	2.47	0.47
1:D:1043:GLU:OE2	1:E:1053:ARG:NE	2.43	0.47
1:C:1121:ASN:HA	1:C:1122:SER:HA	1.55	0.46
1:E:1166:MET:HE3	1:E:1241:ASN:HA	1.97	0.46
1:C:1091:LEU:HG	1:C:1100:THR:HB	1.97	0.46
1:C:1263:ILE:HD13	1:C:1267:LEU:HB2	1.97	0.46
1:G:1121:ASN:HA	1:G:1122:SER:HA	1.54	0.46
1:K:1099:ILE:HD11	1:L:1090:LEU:HB2	1.98	0.46
1:G:1251:LEU:HD11	1:G:1256:ALA:HB1	1.97	0.46
1:I:895:GLN:HA	1:I:896:PHE:HA	1.54	0.46
1:J:1098:GLN:HG2	1:K:1103:GLU:O	2.16	0.46
1:C:1279:VAL:HG13	1:C:1280:ASN:OD1	2.16	0.46
1:H:1099:ILE:HD11	1:I:1090:LEU:HB2	1.98	0.46
1:B:1099:ILE:HD11	1:C:1090:LEU:HB2	1.98	0.46
1:B:987:PHE:HB2	1:C:966:MET:SD	2.56	0.46
1:G:1272:VAL:HA	1:G:1286:GLU:O	2.16	0.46
1:D:1061:PHE:CD2	1:F:1070:THR:HG21	2.51	0.46
1:B:1092:ILE:HG12	1:B:1099:ILE:HG12	1.98	0.45
1:D:927:GLY:O	1:E:933:LEU:HD12	2.16	0.45
1:I:1121:ASN:HA	1:I:1122:SER:HA	1.49	0.45
1:J:914:GLN:NE2	1:K:920:PRO:HB2	2.28	0.45
1:J:1092:ILE:HG12	1:J:1099:ILE:HG12	1.97	0.45
1:K:1035:GLY:HA2	1:L:1041:ASN:HD22	1.82	0.45
1:K:1235:GLN:NE2	1:K:1241:ASN:HB3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1121:ASN:HA	1:D:1122:SER:HA	1.67	0.45
1:E:1123:ARG:HD2	1:F:1144:VAL:O	2.16	0.45
1:F:1121:ASN:HA	1:F:1122:SER:HA	1.59	0.45
1:F:1272:VAL:HA	1:F:1286:GLU:O	2.17	0.45
1:I:1069:ASN:HB2	1:I:1071:TYR:CE1	2.51	0.45
1:K:1280:ASN:ND2	1:K:1282:THR:OG1	2.50	0.45
1:H:927:GLY:O	1:I:933:LEU:HD12	2.15	0.45
1:I:1274:ILE:HA	1:I:1284:LYS:O	2.17	0.45
1:C:1146:PHE:HA	1:C:1193:GLN:O	2.17	0.45
1:H:1026:MET:HE1	1:I:1026:MET:CE	2.46	0.45
1:K:1166:MET:HG3	1:K:1179:LEU:HB3	1.99	0.45
1:E:1159:GLN:OE1	1:E:1159:GLN:N	2.50	0.45
1:L:1275:VAL:HG13	1:L:1284:LYS:HG3	1.98	0.45
1:B:1091:LEU:HG	1:B:1100:THR:HB	1.99	0.45
1:D:1026:MET:SD	1:E:1026:MET:HE1	2.57	0.45
1:H:970:VAL:HG12	1:I:962:PRO:HG3	1.99	0.45
1:I:1273:ARG:NH2	1:I:1286:GLU:HG2	2.32	0.45
1:G:1091:LEU:HG	1:G:1100:THR:HB	1.99	0.44
1:K:1044:PHE:HB2	1:L:1052:PHE:HD1	1.81	0.44
1:K:1235:GLN:HE21	1:K:1241:ASN:HB3	1.82	0.44
1:E:1193:GLN:NE2	1:E:1201:LEU:HD11	2.31	0.44
1:F:1277:ASP:OD2	1:F:1280:ASN:ND2	2.48	0.44
1:J:970:VAL:HG12	1:K:962:PRO:HG3	1.99	0.44
1:F:1135:TYR:HB2	1:F:1160:PHE:CE1	2.53	0.44
1:F:1277:ASP:HB3	1:F:1282:THR:HG23	1.98	0.44
1:K:1189:GLY:HA2	1:K:1208:TYR:CD2	2.53	0.44
1:D:1053:ARG:NH1	1:D:1080:GLN:O	2.47	0.44
1:H:1140:THR:O	1:H:1144:VAL:HG13	2.17	0.44
1:H:1146:PHE:HA	1:H:1193:GLN:O	2.17	0.44
1:I:1271:ASN:O	1:I:1287:TRP:HA	2.17	0.44
1:D:987:PHE:HB2	1:E:966:MET:SD	2.58	0.44
1:J:1206:ILE:HD13	1:K:1202:TYR:CE2	2.53	0.44
1:K:1218:ARG:HH21	1:L:1220:THR:HB	1.81	0.44
1:A:954:LYS:HA	1:A:962:PRO:HG2	2.00	0.44
1:E:1146:PHE:HA	1:E:1193:GLN:O	2.18	0.44
1:E:1221:ARG:HD2	1:E:1230:TRP:HB3	2.00	0.44
1:E:1271:ASN:O	1:E:1271:ASN:ND2	2.37	0.44
1:L:1069:ASN:HB2	1:L:1071:TYR:CE1	2.52	0.44
1:D:1251:LEU:HD11	1:D:1256:ALA:HB1	1.99	0.44
1:E:1217:THR:HG22	1:E:1241:ASN:CG	2.43	0.44
1:C:900:ASP:OD1	1:C:900:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1146:PHE:HA	1:D:1193:GLN:O	2.18	0.44
1:J:903:GLN:HG2	1:L:899:ARG:HH12	1.83	0.44
1:J:1146:PHE:HA	1:J:1193:GLN:O	2.18	0.44
1:B:1135:TYR:HB2	1:B:1160:PHE:CE1	2.53	0.43
1:D:1181:ARG:NH2	1:D:1247:ASP:OD2	2.51	0.43
1:F:1140:THR:H	1:F:1143:THR:HG1	1.61	0.43
1:H:1121:ASN:HA	1:H:1122:SER:HA	1.59	0.43
1:H:1206:ILE:HD13	1:I:1202:TYR:CE2	2.53	0.43
1:K:1061:PHE:CE1	1:K:1072:PHE:HB3	2.52	0.43
1:K:1273:ARG:HD3	1:K:1275:VAL:HG23	1.99	0.43
1:A:933:LEU:HD12	1:C:927:GLY:O	2.18	0.43
1:F:1165:LYS:O	1:F:1182:GLY:N	2.51	0.43
1:G:1189:GLY:HA2	1:G:1208:TYR:CD2	2.53	0.43
1:K:1166:MET:CG	1:K:1179:LEU:HB3	2.49	0.43
1:L:1091:LEU:HG	1:L:1100:THR:HB	2.00	0.43
1:G:1200:SER:OG	1:I:1190:THR:OG1	2.24	0.43
1:J:1202:TYR:CE2	1:L:1206:ILE:HD13	2.53	0.43
1:A:1281:LYS:HA	1:B:1271:ASN:HD21	1.84	0.43
1:D:966:MET:SD	1:F:987:PHE:HB2	2.58	0.43
1:E:1276:PRO:CG	1:F:1269:ILE:HG22	2.49	0.43
1:H:1094:ASN:HA	1:I:1074:LEU:HD13	1.99	0.43
1:J:1026:MET:HE1	1:L:1026:MET:SD	2.59	0.43
1:J:1212:PRO:HA	1:K:1227:LYS:HE2	1.99	0.43
1:L:1121:ASN:HA	1:L:1122:SER:HA	1.57	0.43
1:J:914:GLN:NE2	1:K:920:PRO:O	2.52	0.43
1:L:1164:PHE:HE1	1:L:1184:GLU:HB2	1.84	0.43
1:B:1206:ILE:HG13	1:B:1218:ARG:HG2	2.01	0.43
1:E:1264:ARG:HH11	1:E:1264:ARG:CG	2.30	0.43
1:G:1028:VAL:HG21	1:I:1026:MET:SD	2.58	0.43
1:L:1154:SER:HA	1:L:1157:TYR:CE2	2.54	0.43
1:F:1176:LEU:HA	1:F:1177:PRO:HD3	1.84	0.43
1:J:933:LEU:HD12	1:L:927:GLY:O	2.18	0.43
1:C:1165:LYS:O	1:C:1166:MET:HE2	2.18	0.42
1:D:1123:ARG:HH21	1:D:1125:ARG:HD3	1.83	0.42
1:D:1000:GLN:NE2	1:D:1002:ASN:OD1	2.47	0.42
1:D:1260:ASN:OD1	1:D:1260:ASN:N	2.52	0.42
1:K:1121:ASN:HA	1:K:1122:SER:HA	1.59	0.42
1:L:1191:LEU:HD11	1:L:1203:GLN:NE2	2.33	0.42
1:D:912:THR:HA	1:E:918:SER:OG	2.19	0.42
1:G:933:LEU:HD12	1:I:927:GLY:O	2.19	0.42
1:H:1281:LYS:HB3	1:I:1287:TRP:CZ3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1107:ILE:HG21	1:I:1111:VAL:HG22	2.01	0.42
1:L:1146:PHE:HA	1:L:1193:GLN:O	2.19	0.42
1:G:901:ILE:HD12	1:G:901:ILE:HA	1.84	0.42
1:J:1120:VAL:HG22	1:L:1113:ILE:HD12	2.01	0.42
1:I:1146:PHE:HA	1:I:1193:GLN:O	2.20	0.42
1:I:1263:ILE:HD13	1:I:1267:LEU:HB2	2.01	0.42
1:J:1273:ARG:HG2	1:J:1275:VAL:HG23	2.01	0.42
1:A:1107:ILE:HG21	1:A:1111:VAL:HG22	2.01	0.42
1:D:918:SER:OG	1:F:912:THR:HA	2.20	0.42
1:B:1123:ARG:HD3	1:C:1144:VAL:O	2.19	0.42
1:C:1165:LYS:O	1:C:1182:GLY:N	2.48	0.42
1:D:1140:THR:O	1:D:1144:VAL:HG13	2.20	0.42
1:K:1188:PRO:HB2	1:K:1208:TYR:CZ	2.54	0.42
1:A:962:PRO:HG3	1:C:970:VAL:HG12	2.01	0.42
1:A:987:PHE:HB2	1:B:966:MET:SD	2.60	0.42
1:G:1053:ARG:NH1	1:G:1080:GLN:O	2.48	0.42
1:D:1154:SER:HA	1:D:1157:TYR:CE2	2.55	0.42
1:E:1144:VAL:HG13	1:E:1201:LEU:HD13	2.00	0.42
1:J:903:GLN:CG	1:L:899:ARG:HH12	2.33	0.42
1:H:970:VAL:HA	1:H:986:VAL:O	2.19	0.41
1:L:1001:ARG:NH2	1:L:1007:ILE:HD11	2.35	0.41
1:B:1146:PHE:HA	1:B:1193:GLN:O	2.19	0.41
1:K:1176:LEU:HA	1:K:1177:PRO:HD3	1.81	0.41
1:B:1206:ILE:HD13	1:C:1202:TYR:CE2	2.56	0.41
1:F:1274:ILE:HA	1:F:1284:LYS:O	2.20	0.41
1:I:1151:ILE:HD12	1:I:1205:TRP:CZ3	2.55	0.41
1:J:1009:PHE:CD1	1:J:1009:PHE:C	2.98	0.41
1:J:1061:PHE:CE1	1:J:1072:PHE:HB3	2.56	0.41
1:A:1121:ASN:HA	1:A:1122:SER:HA	1.57	0.41
1:H:899:ARG:HB2	1:I:897:ILE:HG13	2.02	0.41
1:J:1090:LEU:HB2	1:L:1099:ILE:HD11	2.01	0.41
1:K:968:ILE:O	1:K:968:ILE:HG13	2.19	0.41
1:D:1061:PHE:CE1	1:D:1072:PHE:HB3	2.55	0.41
1:G:953:GLU:OE2	1:I:942:ARG:HD3	2.21	0.41
1:G:1041:ASN:HA	1:H:1047:LYS:HB2	2.02	0.41
1:H:1258:MET:HE3	1:I:1261:LEU:HD11	2.02	0.41
1:J:1107:ILE:HG21	1:J:1111:VAL:HG22	2.02	0.41
1:D:1194:PHE:HB2	1:D:1202:TYR:CE1	2.56	0.41
1:J:1070:THR:HG21	1:K:1061:PHE:CD2	2.55	0.41
1:D:1069:ASN:HB2	1:D:1071:TYR:CE1	2.56	0.41
1:D:1151:ILE:HD12	1:D:1205:TRP:CZ3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1163:TYR:HB3	1:E:1207:THR:HG21	2.03	0.41
1:B:1121:ASN:HA	1:B:1122:SER:HA	1.60	0.41
1:J:1009:PHE:C	1:J:1009:PHE:HD1	2.29	0.41
1:D:1090:LEU:HB2	1:F:1099:ILE:HD11	2.03	0.41
1:E:1276:PRO:HG3	1:F:1269:ILE:HG22	2.03	0.41
1:G:905:VAL:HG12	1:G:907:GLY:H	1.86	0.41
1:J:1046:SER:HB3	1:J:1051:ALA:HB1	2.03	0.41
1:K:968:ILE:HD13	1:K:987:PHE:CZ	2.56	0.41
1:K:970:VAL:HA	1:K:986:VAL:O	2.20	0.41
1:K:1218:ARG:HB2	1:K:1236:VAL:HB	2.03	0.41
1:L:1211:THR:OG1	1:L:1214:ALA:HB2	2.21	0.41
1:D:1189:GLY:HA2	1:D:1208:TYR:CD1	2.56	0.41
1:D:1238:ASP:OD1	1:D:1238:ASP:N	2.54	0.41
1:G:1221:ARG:HD2	1:G:1230:TRP:HB3	2.02	0.41
1:J:968:ILE:HG12	1:J:989:VAL:HG22	2.03	0.40
1:D:1140:THR:H	1:D:1143:THR:HG1	1.67	0.40
1:G:1251:LEU:HD23	1:H:1251:LEU:HD22	2.03	0.40
1:K:1015:VAL:HG22	1:K:1017:PRO:HD3	2.04	0.40
1:L:1015:VAL:HG22	1:L:1017:PRO:HD3	2.02	0.40
1:L:1181:ARG:NH2	1:L:1247:ASP:OD2	2.51	0.40
1:A:1263:ILE:HD13	1:A:1267:LEU:HB2	2.02	0.40
1:D:1271:ASN:OD1	1:D:1271:ASN:N	2.50	0.40
1:D:1284:LYS:C	1:D:1285:PHE:HD1	2.29	0.40
1:F:1157:TYR:CZ	1:F:1188:PRO:HD3	2.57	0.40
1:D:1061:PHE:HE1	1:D:1072:PHE:HB3	1.86	0.40
1:D:1091:LEU:HG	1:D:1100:THR:HB	2.03	0.40
1:E:927:GLY:O	1:F:933:LEU:HD12	2.22	0.40
1:H:1001:ARG:NH2	1:H:1007:ILE:HD11	2.37	0.40
1:J:1275:VAL:HB	1:J:1284:LYS:HB2	2.04	0.40
1:K:1224:GLN:NE2	1:K:1227:LYS:HD2	2.36	0.40

There are no symmetry-related clashes.

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	393/410 (96%)	379 (96%)	14 (4%)	0	100	100
1	B	393/410 (96%)	379 (96%)	14 (4%)	0	100	100
1	C	396/410 (97%)	379 (96%)	17 (4%)	0	100	100
1	D	393/410 (96%)	379 (96%)	14 (4%)	0	100	100
1	E	396/410 (97%)	382 (96%)	14 (4%)	0	100	100
1	F	394/410 (96%)	379 (96%)	15 (4%)	0	100	100
1	G	393/410 (96%)	377 (96%)	13 (3%)	3 (1%)	16	50
1	H	392/410 (96%)	378 (96%)	14 (4%)	0	100	100
1	I	392/410 (96%)	376 (96%)	16 (4%)	0	100	100
1	J	392/410 (96%)	377 (96%)	14 (4%)	1 (0%)	36	70
1	K	389/410 (95%)	375 (96%)	14 (4%)	0	100	100
1	L	393/410 (96%)	376 (96%)	14 (4%)	3 (1%)	16	50
All	All	4716/4920 (96%)	4536 (96%)	173 (4%)	7 (0%)	48	80

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1279	VAL
1	J	1281	LYS
1	L	1280	ASN
1	G	1281	LYS
1	L	977	GLY
1	G	895	GLN
1	G	989	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	329/343 (96%)	326 (99%)	3 (1%)	70	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	329/343 (96%)	327 (99%)	2 (1%)	78	88
1	C	332/343 (97%)	330 (99%)	2 (1%)	78	88
1	D	329/343 (96%)	322 (98%)	7 (2%)	47	75
1	E	332/343 (97%)	325 (98%)	7 (2%)	47	75
1	F	330/343 (96%)	327 (99%)	3 (1%)	70	85
1	G	329/343 (96%)	325 (99%)	4 (1%)	63	82
1	H	328/343 (96%)	326 (99%)	2 (1%)	78	88
1	I	328/343 (96%)	326 (99%)	2 (1%)	78	88
1	J	328/343 (96%)	320 (98%)	8 (2%)	43	73
1	K	325/343 (95%)	317 (98%)	8 (2%)	42	72
1	L	329/343 (96%)	322 (98%)	7 (2%)	47	75
All	All	3948/4116 (96%)	3893 (99%)	55 (1%)	59	80

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	895	GLN
1	A	1174	THR
1	A	1232	SER
1	B	918	SER
1	B	1279	VAL
1	C	918	SER
1	C	1283	VAL
1	D	1185	VAL
1	D	1211	THR
1	D	1231	SER
1	D	1260	ASN
1	D	1267	LEU
1	D	1272	VAL
1	D	1275	VAL
1	E	1185	VAL
1	E	1198	LEU
1	E	1264	ARG
1	E	1269	ILE
1	E	1271	ASN
1	E	1272	VAL
1	E	1286	GLU
1	F	1098	GLN

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Mol	Chain	Res	Type
1	F	1275	VAL
1	F	1282	THR
1	G	901	ILE
1	G	917	LEU
1	G	997	PHE
1	G	1181	ARG
1	H	1123	ARG
1	H	1279	VAL
1	I	1004	ASP
1	I	1131	THR
1	J	898	ARG
1	J	903	GLN
1	J	941	ILE
1	J	942	ARG
1	J	982	THR
1	J	999	SER
1	J	1009	PHE
1	J	1282	THR
1	K	968	ILE
1	K	999	SER
1	K	1009	PHE
1	K	1087	LEU
1	K	1203	GLN
1	K	1229	SER
1	K	1271	ASN
1	K	1273	ARG
1	L	899	ARG
1	L	994	SER
1	L	1004	ASP
1	L	1231	SER
1	L	1271	ASN
1	L	1272	VAL
1	L	1275	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	964	GLN
1	A	1241	ASN
1	B	1127	GLN
1	C	1127	GLN
1	D	1094	ASN

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Mol	Chain	Res	Type
1	D	1235	GLN
1	E	914	GLN
1	E	916	ASN
1	E	1193	GLN
1	E	1224	GLN
1	F	1127	GLN
1	G	936	ASN
1	G	1027	ASN
1	G	1127	GLN
1	G	1159	GLN
1	G	1255	ASN
1	G	1280	ASN
1	H	914	GLN
1	H	936	ASN
1	H	1027	ASN
1	I	936	ASN
1	I	964	GLN
1	I	1127	GLN
1	I	1193	GLN
1	I	1280	ASN
1	J	914	GLN
1	J	1121	ASN
1	J	1127	GLN
1	J	1241	ASN
1	J	1255	ASN
1	K	916	ASN
1	K	964	GLN
1	K	1121	ASN
1	K	1127	GLN
1	K	1255	ASN
1	L	903	GLN
1	L	914	GLN
1	L	1041	ASN
1	L	1093	ASN
1	L	1098	GLN
1	L	1127	GLN
1	L	1193	GLN
1	L	1203	GLN
1	L	1235	GLN
1	L	1241	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	395/410 (96%)	-0.25	13 (3%)	49	28	4, 19, 62, 121	0
1	B	395/410 (96%)	-0.24	7 (1%)	67	44	5, 21, 56, 130	0
1	C	398/410 (97%)	-0.25	5 (1%)	75	53	4, 19, 62, 124	0
1	D	395/410 (96%)	0.45	35 (8%)	15	8	5, 42, 92, 135	0
1	E	398/410 (97%)	0.49	43 (10%)	11	6	5, 42, 94, 129	0
1	F	396/410 (96%)	0.43	33 (8%)	17	9	4, 43, 93, 125	0
1	G	395/410 (96%)	0.92	35 (8%)	15	8	36, 69, 103, 125	0
1	H	394/410 (96%)	0.78	34 (8%)	16	8	31, 64, 100, 137	0
1	I	394/410 (96%)	0.82	32 (8%)	18	9	26, 65, 100, 134	0
1	J	394/410 (96%)	0.87	41 (10%)	11	6	28, 62, 99, 134	0
1	K	391/410 (95%)	1.01	56 (14%)	6	3	27, 64, 105, 143	0
1	L	395/410 (96%)	0.90	47 (11%)	9	5	28, 64, 104, 152	0
All	All	4740/4920 (96%)	0.49	381 (8%)	18	9	4, 52, 97, 152	0

All (381) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	896	PHE	7.7
1	H	1286	GLU	5.4
1	G	1288	VAL	5.3
1	F	893	PRO	4.8
1	D	1286	GLU	4.8
1	J	1288	VAL	4.8
1	G	1287	TRP	4.6
1	D	1287	TRP	4.5
1	F	1129	THR	4.5
1	L	1043	GLU	4.5
1	I	1288	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	1287	TRP	4.3
1	K	1287	TRP	4.3
1	J	1068	SER	4.2
1	D	1247	ASP	4.1
1	G	1134	LEU	4.0
1	I	1286	GLU	4.0
1	L	894	SER	4.0
1	C	1287	TRP	4.0
1	J	966	MET	3.8
1	J	1281	LYS	3.8
1	F	1215	ARG	3.8
1	F	1287	TRP	3.8
1	E	1281	LYS	3.8
1	J	996	HIS	3.8
1	J	895	GLN	3.8
1	L	1265	ASP	3.7
1	B	1287	TRP	3.7
1	I	958	SER	3.7
1	I	895	GLN	3.7
1	H	1285	PHE	3.6
1	H	897	ILE	3.6
1	K	1217	THR	3.6
1	J	1276	PRO	3.6
1	F	1122	SER	3.6
1	L	1287	TRP	3.5
1	G	966	MET	3.5
1	J	1285	PHE	3.5
1	H	1287	TRP	3.5
1	I	897	ILE	3.5
1	E	1216	THR	3.5
1	F	1132	SER	3.5
1	G	979	SER	3.5
1	D	1184	GLU	3.5
1	E	1172	GLU	3.5
1	J	975	PHE	3.5
1	G	901	ILE	3.5
1	B	1286	GLU	3.4
1	C	1286	GLU	3.4
1	H	934	ALA	3.4
1	K	1259	GLY	3.4
1	K	1210	THR	3.3
1	L	1233	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	986	VAL	3.3
1	K	1205	TRP	3.3
1	K	1286	GLU	3.3
1	L	1259	GLY	3.3
1	A	1287	TRP	3.3
1	J	978	GLY	3.2
1	K	1058	ASP	3.2
1	J	953	GLU	3.2
1	F	1233	PHE	3.2
1	L	1288	VAL	3.2
1	D	1281	LYS	3.2
1	I	1281	LYS	3.2
1	J	977	GLY	3.2
1	G	1025	LEU	3.1
1	A	1180	GLU	3.1
1	L	1172	GLU	3.1
1	G	896	PHE	3.1
1	L	1135	TYR	3.1
1	H	894	SER	3.1
1	D	1205	TRP	3.1
1	L	900	ASP	3.1
1	G	978	GLY	3.1
1	F	894	SER	3.1
1	J	1270	GLY	3.1
1	B	1281	LYS	3.1
1	I	966	MET	3.1
1	F	1135	TYR	3.1
1	L	1198	LEU	3.0
1	L	1279	VAL	3.0
1	L	1025	LEU	3.0
1	E	1280	ASN	3.0
1	E	1259	GLY	3.0
1	F	1288	VAL	3.0
1	L	1134	LEU	3.0
1	K	1135	TYR	3.0
1	F	1270	GLY	3.0
1	A	894	SER	3.0
1	D	1176	LEU	3.0
1	G	977	GLY	3.0
1	L	898	ARG	3.0
1	D	1199	ASP	3.0
1	I	1282	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	1278	PRO	2.9
1	I	1285	PHE	2.9
1	G	948	THR	2.9
1	E	1249	GLY	2.9
1	K	1160	PHE	2.9
1	D	1271	ASN	2.9
1	E	1187	SER	2.9
1	G	1009	PHE	2.9
1	J	964	GLN	2.9
1	I	963	ALA	2.9
1	K	1059	TYR	2.9
1	E	1229	SER	2.8
1	E	1247	ASP	2.8
1	H	1014	THR	2.8
1	L	1222	THR	2.8
1	L	1226	THR	2.8
1	A	1288	VAL	2.8
1	F	1281	LYS	2.8
1	K	1077	ALA	2.8
1	H	1279	VAL	2.8
1	G	1204	ASP	2.8
1	H	953	GLU	2.8
1	G	985	THR	2.8
1	K	1211	THR	2.8
1	I	1026	MET	2.8
1	J	1071	TYR	2.8
1	L	1187	SER	2.8
1	G	1007	ILE	2.7
1	I	965	SER	2.7
1	E	1205	TRP	2.7
1	L	1007	ILE	2.7
1	F	1257	THR	2.7
1	H	1031	THR	2.7
1	J	1066	ASP	2.7
1	K	1278	PRO	2.7
1	K	1026	MET	2.7
1	I	1279	VAL	2.7
1	L	1280	ASN	2.7
1	E	1215	ARG	2.7
1	J	1284	LYS	2.7
1	F	1205	TRP	2.7
1	G	1254	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	927	GLY	2.6
1	K	1189	GLY	2.6
1	I	938	THR	2.6
1	H	979	SER	2.6
1	H	966	MET	2.6
1	F	1159	GLN	2.6
1	H	1284	LYS	2.6
1	J	997	PHE	2.6
1	L	1224	GLN	2.6
1	G	1023	SER	2.6
1	K	1154	SER	2.6
1	K	1187	SER	2.6
1	K	1055	ILE	2.6
1	J	1254	ASP	2.6
1	G	1271	ASN	2.6
1	L	1041	ASN	2.6
1	L	1196	ASN	2.6
1	K	1175	GLY	2.6
1	E	1217	THR	2.6
1	K	1074	LEU	2.6
1	E	1279	VAL	2.6
1	K	1219	TRP	2.6
1	D	1264	ARG	2.6
1	K	897	ILE	2.6
1	E	1266	PHE	2.6
1	G	1026	MET	2.6
1	K	1034	PHE	2.6
1	E	1270	GLY	2.6
1	E	1230	TRP	2.6
1	I	1287	TRP	2.6
1	K	1216	THR	2.6
1	K	1258	MET	2.6
1	L	979	SER	2.6
1	H	1083	GLY	2.6
1	I	1013	GLY	2.6
1	K	1078	GLY	2.6
1	E	1179	LEU	2.6
1	J	1178	TYR	2.5
1	K	1132	SER	2.5
1	K	899	ARG	2.5
1	K	1165	LYS	2.5
1	K	957	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	1282	THR	2.5
1	H	1034	PHE	2.5
1	F	1253	SER	2.5
1	J	965	SER	2.5
1	I	1273	ARG	2.5
1	D	1238	ASP	2.5
1	E	1150	ASP	2.5
1	E	1241	ASN	2.5
1	H	939	PHE	2.5
1	L	1160	PHE	2.5
1	K	1208	TYR	2.5
1	E	1240	GLY	2.5
1	H	965	SER	2.5
1	G	897	ILE	2.5
1	A	992	ASP	2.5
1	E	1129	THR	2.5
1	F	1208	TYR	2.5
1	D	1126	SER	2.4
1	H	896	PHE	2.4
1	I	975	PHE	2.4
1	E	1220	THR	2.4
1	K	1174	THR	2.4
1	K	1209	PRO	2.4
1	B	1288	VAL	2.4
1	E	1246	SER	2.4
1	K	1168	GLU	2.4
1	L	1200	SER	2.4
1	G	987	PHE	2.4
1	H	1012	ASN	2.4
1	H	1013	GLY	2.4
1	I	903	GLN	2.4
1	E	1286	GLU	2.4
1	J	1266	PHE	2.4
1	L	899	ARG	2.4
1	E	1122	SER	2.4
1	H	909	LEU	2.4
1	D	1188	PRO	2.4
1	H	1271	ASN	2.4
1	D	1283	VAL	2.4
1	I	1283	VAL	2.4
1	D	1270	GLY	2.4
1	F	1178	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	1095	GLN	2.4
1	L	1203	GLN	2.4
1	D	1253	SER	2.4
1	J	1253	SER	2.4
1	H	1283	VAL	2.4
1	D	1254	ASP	2.4
1	D	1259	GLY	2.4
1	F	1183	GLU	2.4
1	E	1173	VAL	2.4
1	I	1005	GLY	2.3
1	E	1208	TYR	2.3
1	F	1286	GLU	2.3
1	D	1230	TRP	2.3
1	F	1284	LYS	2.3
1	G	1131	THR	2.3
1	K	1181	ARG	2.3
1	H	996	HIS	2.3
1	K	1157	TYR	2.3
1	H	992	ASP	2.3
1	J	1265	ASP	2.3
1	B	1273	ARG	2.3
1	J	945	GLY	2.3
1	F	1282	THR	2.3
1	J	958	SER	2.3
1	J	984	SER	2.3
1	K	1207	THR	2.3
1	L	1271	ASN	2.3
1	A	895	GLN	2.3
1	A	1279	VAL	2.3
1	A	1281	LYS	2.3
1	D	1278	PRO	2.3
1	E	1195	GLY	2.3
1	H	948	THR	2.3
1	K	1134	LEU	2.3
1	E	1157	TYR	2.3
1	D	1233	PHE	2.3
1	J	1094	ASN	2.3
1	H	1265	ASP	2.3
1	F	1213	GLU	2.3
1	I	953	GLU	2.3
1	J	1278	PRO	2.3
1	K	1188	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	1147	TRP	2.3
1	G	894	SER	2.3
1	H	997	PHE	2.3
1	L	987	PHE	2.3
1	K	1281	LYS	2.3
1	L	1159	GLN	2.3
1	H	1026	MET	2.2
1	J	911	LEU	2.2
1	E	1196	ASN	2.2
1	F	1069	ASN	2.2
1	I	964	GLN	2.2
1	J	1069	ASN	2.2
1	D	1180	GLU	2.2
1	B	1278	PRO	2.2
1	K	1212	PRO	2.2
1	K	921	LEU	2.2
1	K	915	THR	2.2
1	E	1135	TYR	2.2
1	J	979	SER	2.2
1	L	984	SER	2.2
1	K	1185	VAL	2.2
1	D	1171	ASN	2.2
1	B	1172	GLU	2.2
1	D	1250	ALA	2.2
1	L	1281	LYS	2.2
1	A	1273	ARG	2.2
1	D	1216	THR	2.2
1	K	912	THR	2.2
1	F	1154	SER	2.2
1	C	1172	GLU	2.2
1	G	945	GLY	2.2
1	I	1278	PRO	2.2
1	L	1145	GLY	2.2
1	E	1160	PHE	2.2
1	I	939	PHE	2.2
1	L	896	PHE	2.2
1	F	1170	THR	2.2
1	L	910	THR	2.2
1	L	985	THR	2.2
1	K	1173	VAL	2.2
1	D	1248	ILE	2.2
1	E	1271	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	1093	ASN	2.2
1	J	930	GLY	2.2
1	K	1110	GLY	2.2
1	L	1249	GLY	2.2
1	I	901	ILE	2.1
1	C	1281	LYS	2.1
1	K	1166	MET	2.1
1	G	972	GLY	2.1
1	L	1264	ARG	2.1
1	A	1271	ASN	2.1
1	K	1233	PHE	2.1
1	E	1199	ASP	2.1
1	J	974	GLN	2.1
1	D	1195	GLY	2.1
1	E	1114	ASN	2.1
1	E	1265	ASP	2.1
1	J	992	ASP	2.1
1	K	1130	LYS	2.1
1	G	898	ARG	2.1
1	E	1203	GLN	2.1
1	I	902	ALA	2.1
1	C	1278	PRO	2.1
1	F	1172	GLU	2.1
1	I	928	GLU	2.1
1	A	1285	PHE	2.1
1	E	1233	PHE	2.1
1	G	1285	PHE	2.1
1	D	1260	ASN	2.1
1	F	1254	ASP	2.1
1	L	1248	ILE	2.1
1	H	1282	THR	2.1
1	G	903	GLN	2.1
1	E	1164	PHE	2.1
1	F	1160	PHE	2.1
1	J	906	ASN	2.1
1	D	1201	LEU	2.1
1	H	995	HIS	2.1
1	K	1075	THR	2.1
1	K	1178	TYR	2.1
1	D	1244	GLN	2.1
1	I	1000	GLN	2.1
1	D	1164	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	1180	GLU	2.1
1	I	1072	PHE	2.1
1	L	1245	PRO	2.1
1	D	1279	VAL	2.0
1	I	1284	LYS	2.0
1	G	973	ASN	2.0
1	G	1158	ASN	2.0
1	J	1002	ASN	2.0
1	K	1273	ARG	2.0
1	F	1199	ASP	2.0
1	L	919	ALA	2.0
1	G	939	PHE	2.0
1	G	1044	PHE	2.0
1	K	1239	GLY	2.0
1	L	978	GLY	2.0
1	A	1284	LYS	2.0
1	A	1286	GLU	2.0
1	G	928	GLU	2.0
1	H	988	GLU	2.0
1	L	1144	VAL	2.0
1	D	1166	MET	2.0
1	F	1166	MET	2.0
1	F	1271	ASN	2.0
1	J	1287	TRP	2.0
1	L	1258	MET	2.0
1	H	990	GLY	2.0
1	H	1061	PHE	2.0
1	J	1072	PHE	2.0
1	L	939	PHE	2.0
1	L	914	GLN	2.0
1	E	1183	GLU	2.0
1	K	1279	VAL	2.0
1	K	1283	VAL	2.0
1	E	1248	ILE	2.0

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

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

6.3 Carbohydrates [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.