



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:46 AM UTC

PDB ID : 2Q4K / pdb_00002q4k
Title : Ensemble refinement of the protein crystal structure of gene product from Homo sapiens Hs.433573
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-31
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

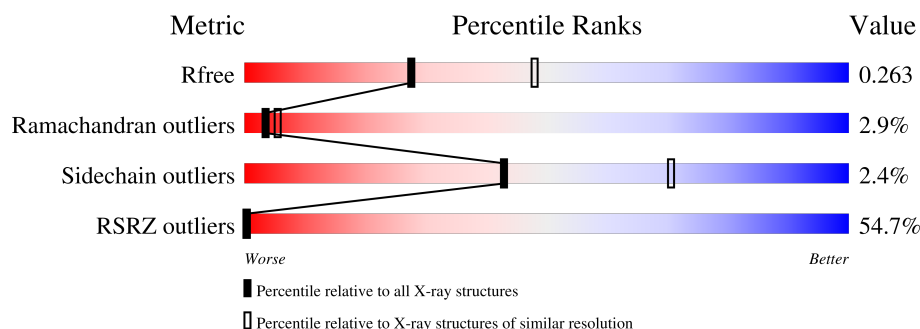
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



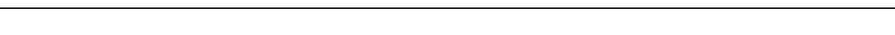
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	1-A	251	58% 84% 7% 9%
1	1-B	251	54% 86% 7% 6%
1	1-C	251	35% 86% • 12%
1	10-A	251	88% • 9%
1	10-B	251	89% • 6%
1	10-C	251	86% • 12%
1	11-A	251	86% 5% 9%

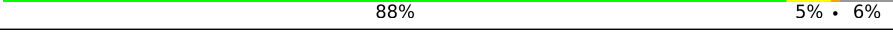
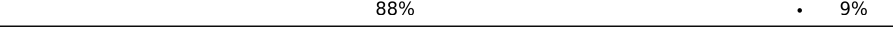
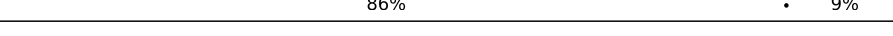
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Mol	Chain	Length	Quality of chain
1	11-B	251	 88%6%6%
1	11-C	251	 88%12%
1	12-A	251	 86%5%9%
1	12-B	251	 87%7%6%
1	12-C	251	 86%12%
1	13-A	251	 85%6%9%
1	13-B	251	 88%6%6%
1	13-C	251	 85%12%
1	14-A	251	 84%6%9%
1	14-B	251	 86%8%6%
1	14-C	251	 86%12%
1	15-A	251	 84%6%9%
1	15-B	251	 85%9%6%
1	15-C	251	 86%12%
1	16-A	251	 86%9%
1	16-B	251	 90%6%
1	16-C	251	 84%12%
1	2-A	251	 87%9%
1	2-B	251	 86%7%6%
1	2-C	251	 87%12%
1	3-A	251	 87%9%
1	3-B	251	 90%6%
1	3-C	251	 87%12%
1	4-A	251	 86%9%
1	4-B	251	 88%5%6%

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Mol	Chain	Length	Quality of chain
1	4-C	251	 84% 12%
1	5-A	251	 84% 7% 9%
1	5-B	251	 87% 6% 6%
1	5-C	251	 86% 12%
1	6-A	251	 84% 6% 9%
1	6-B	251	 88% 5% 6%
1	6-C	251	 86% 12%
1	7-A	251	 86% 9%
1	7-B	251	 88% 5% 6%
1	7-C	251	 86% 12%
1	8-A	251	 88% 9%
1	8-B	251	 90% 6%
1	8-C	251	 86% 12%
1	9-A	251	 86% 9%
1	9-B	251	 88% 5% 6%
1	9-C	251	 84% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 88208 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 Uncharacterized protein C11orf68.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	2-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	3-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	4-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	5-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	6-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	7-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	8-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	9-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	10-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	11-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	12-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	13-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	14-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	15-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	16-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	2-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	3-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	4-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	5-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	6-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	7-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	8-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	9-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	10-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	11-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	12-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	13-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	14-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	15-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	16-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	1-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	2-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	3-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	4-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	5-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	6-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	7-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	8-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	9-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	10-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	11-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	12-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	13-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	14-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	15-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	16-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q9H3H3
A	30	MSE	MET	modified residue	UNP Q9H3H3
A	34	MSE	MET	modified residue	UNP Q9H3H3
A	131	MSE	MET	modified residue	UNP Q9H3H3
B	1	MSE	MET	modified residue	UNP Q9H3H3
B	30	MSE	MET	modified residue	UNP Q9H3H3
B	34	MSE	MET	modified residue	UNP Q9H3H3
B	131	MSE	MET	modified residue	UNP Q9H3H3
C	1	MSE	MET	modified residue	UNP Q9H3H3
C	30	MSE	MET	modified residue	UNP Q9H3H3
C	34	MSE	MET	modified residue	UNP Q9H3H3
C	131	MSE	MET	modified residue	UNP Q9H3H3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	50	Total 50	O 50	0	0
2	2-A	55	Total 55	O 55	0	0
2	3-A	56	Total 56	O 56	0	0
2	4-A	55	Total 55	O 55	0	0
2	5-A	55	Total 55	O 55	0	0
2	6-A	56	Total 56	O 56	0	0
2	7-A	54	Total 54	O 54	0	0
2	8-A	56	Total 56	O 56	0	0
2	9-A	57	Total 57	O 57	0	0
2	10-A	56	Total 56	O 56	0	0
2	11-A	58	Total 58	O 58	0	0
2	12-A	55	Total 55	O 55	0	0
2	13-A	53	Total 53	O 53	0	0
2	14-A	56	Total 56	O 56	0	0
2	15-A	53	Total 53	O 53	0	0
2	16-A	53	Total 53	O 53	0	0
2	1-B	91	Total 91	O 91	0	0
2	2-B	88	Total 88	O 88	0	0
2	3-B	88	Total 88	O 88	0	0
2	4-B	90	Total 90	O 90	0	0
2	5-B	89	Total 89	O 89	0	0
2	6-B	89	Total 89	O 89	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	7-B	89	Total O 89 89	0	0
2	8-B	88	Total O 88 88	0	0
2	9-B	88	Total O 88 88	0	0
2	10-B	88	Total O 88 88	0	0
2	11-B	87	Total O 87 87	0	0
2	12-B	87	Total O 87 87	0	0
2	13-B	91	Total O 91 91	0	0
2	14-B	87	Total O 87 87	0	0
2	15-B	91	Total O 91 91	0	0
2	16-B	91	Total O 91 91	0	0
2	1-C	76	Total O 76 76	0	0
2	2-C	74	Total O 74 74	0	0
2	3-C	73	Total O 73 73	0	0
2	4-C	72	Total O 72 72	0	0
2	5-C	73	Total O 73 73	0	0
2	6-C	72	Total O 72 72	0	0
2	7-C	74	Total O 74 74	0	0
2	8-C	73	Total O 73 73	0	0
2	9-C	72	Total O 72 72	0	0
2	10-C	73	Total O 73 73	0	0
2	11-C	72	Total O 72 72	0	0

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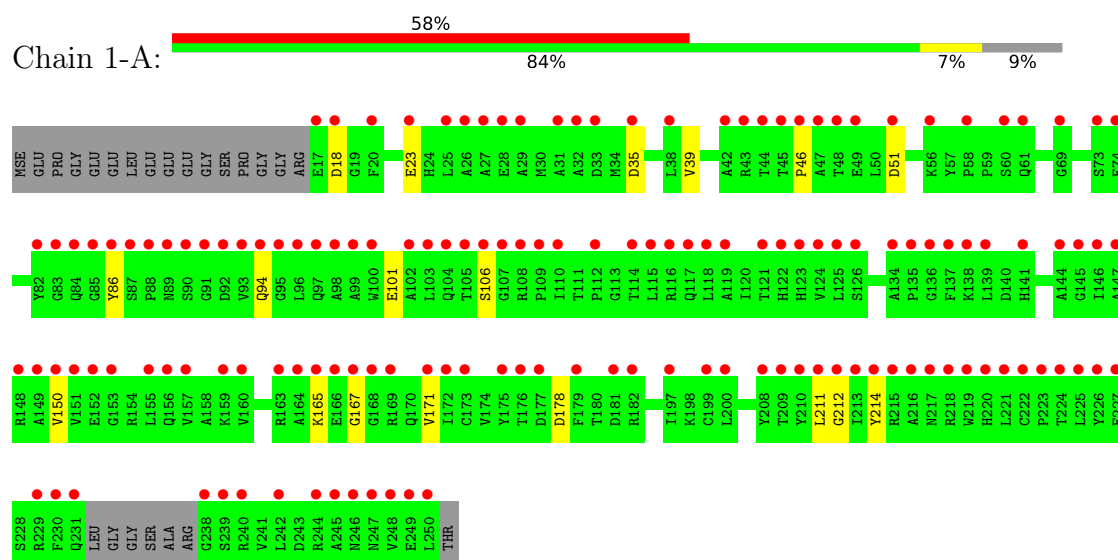
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	12-C	75	Total 75	O 75	0	0
2	13-C	73	Total 73	O 73	0	0
2	14-C	74	Total 74	O 74	0	0
2	15-C	73	Total 73	O 73	0	0
2	16-C	73	Total 73	O 73	0	0

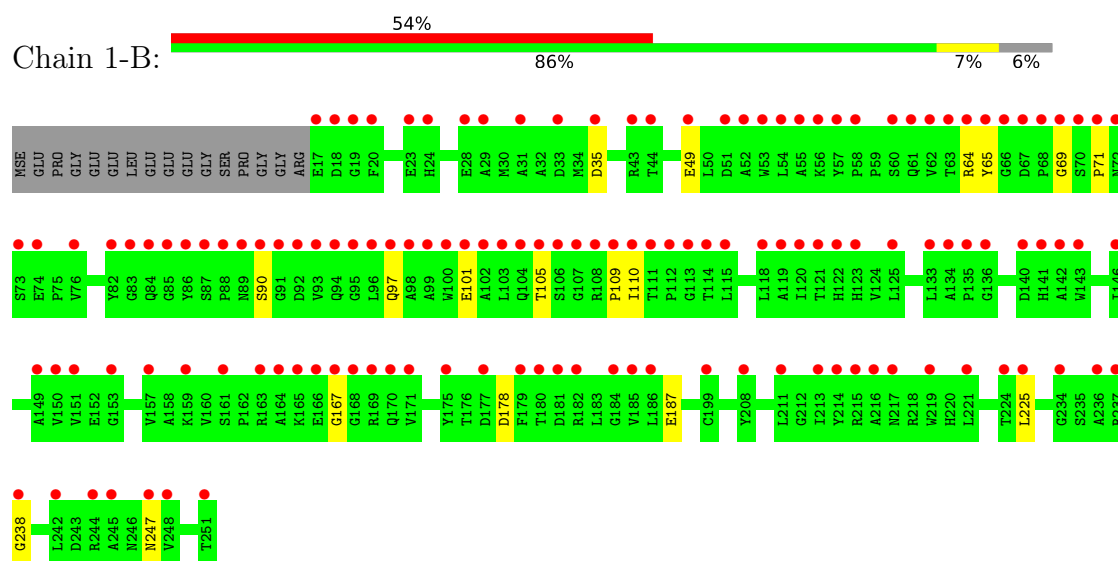
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

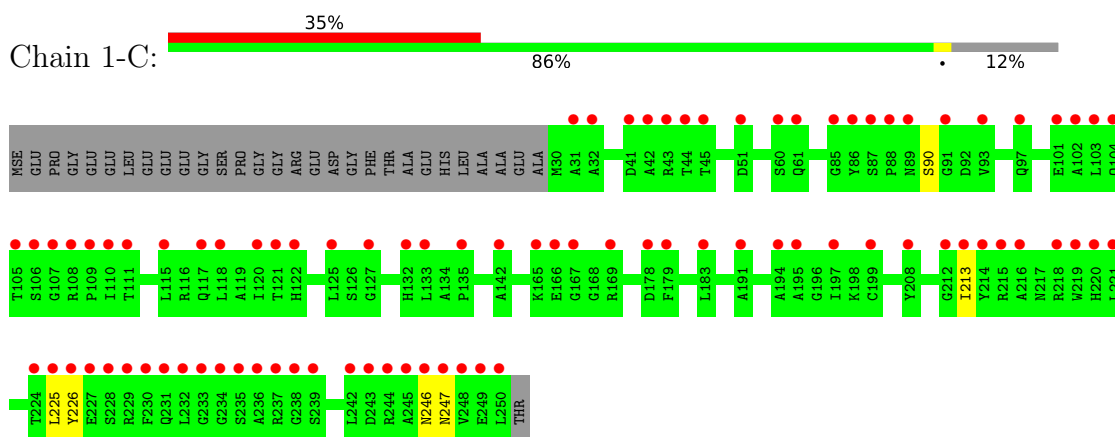
• Molecule 1: Uncharacterized protein C11orf68



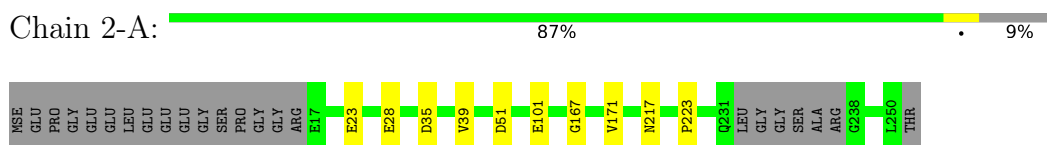
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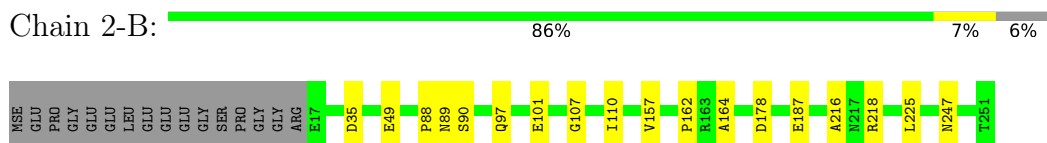
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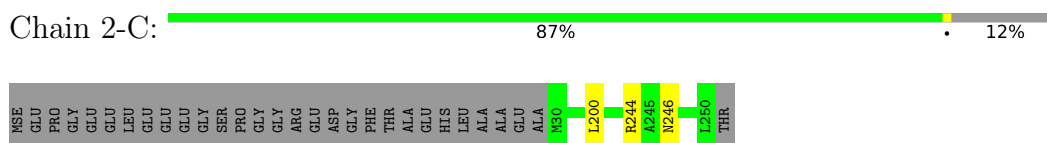
- Molecule 1: Uncharacterized protein C11orf68



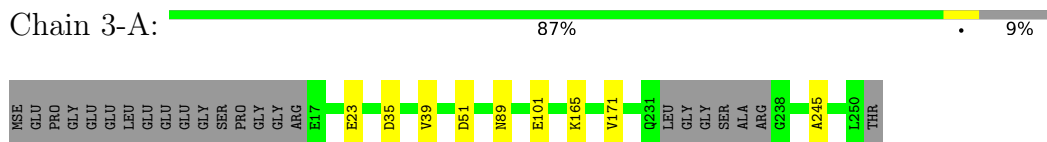
- Molecule 1: Uncharacterized protein C11orf68



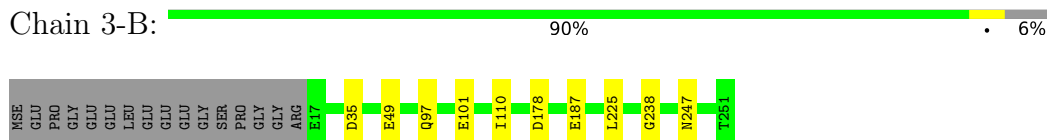
- Molecule 1: Uncharacterized protein C11orf68



- Molecule 1: Uncharacterized protein C11orf68

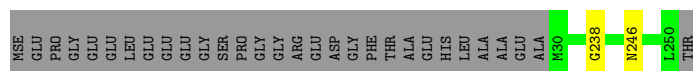


- Molecule 1: Uncharacterized protein C11orf68



- Molecule 1: Uncharacterized protein C11orf68

Chain 3-C:  87% 12%



- Molecule 1: Uncharacterized protein C11orf68

Chain 4-A:  86% 9%



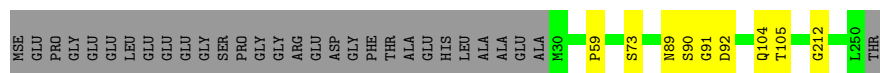
- Molecule 1: Uncharacterized protein C11orf68

Chain 4-B:  88% 5% 6%



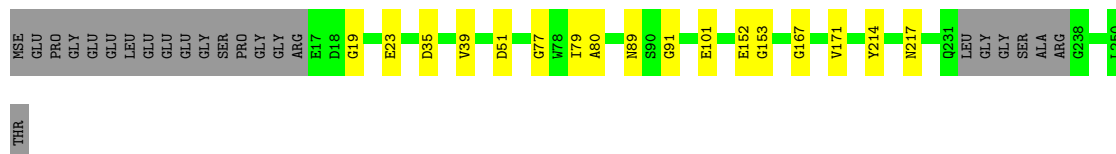
- Molecule 1: Uncharacterized protein C11orf68

Chain 4-C:  84% 12%



- Molecule 1: Uncharacterized protein C11orf68

Chain 5-A:  84% 7% 9%



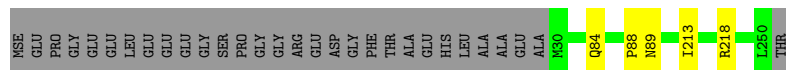
- Molecule 1: Uncharacterized protein C11orf68

Chain 5-B:  87% 6% 6%



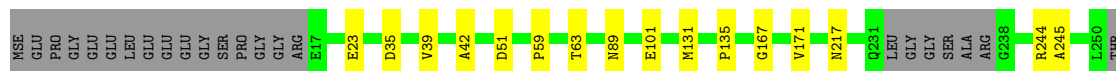
- Molecule 1: Uncharacterized protein C11orf68

Chain 5-C:  86% 12%



- Molecule 1: Uncharacterized protein C11orf68

Chain 6-A:  84% 6% 9%



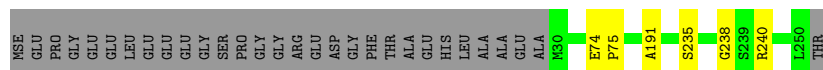
- Molecule 1: Uncharacterized protein C11orf68

Chain 6-B:  88% 5% 6%



- Molecule 1: Uncharacterized protein C11orf68

Chain 6-C:  86% 12%



- Molecule 1: Uncharacterized protein C11orf68

Chain 7-A:  86% 9%



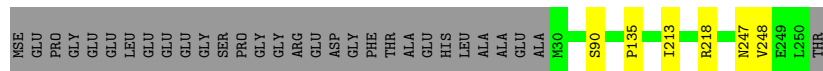
- Molecule 1: Uncharacterized protein C11orf68

Chain 7-B:  88% 5% 6%



- Molecule 1: Uncharacterized protein C11orf68

Chain 7-C:  86% 12%



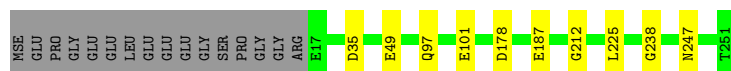
- Molecule 1: Uncharacterized protein C11orf68

Chain 8-A:  88% 9%



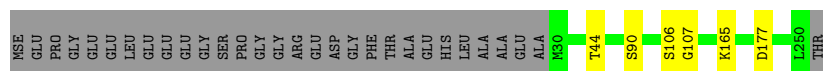
- Molecule 1: Uncharacterized protein C11orf68

Chain 8-B:  90% 6%



- Molecule 1: Uncharacterized protein C11orf68

Chain 8-C:  86% 12%



- Molecule 1: Uncharacterized protein C11orf68

Chain 9-A:  86% 9%



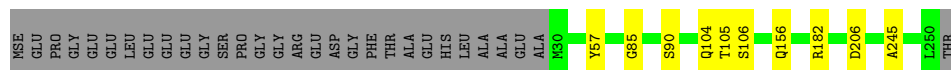
- Molecule 1: Uncharacterized protein C11orf68

Chain 9-B:  88% 5% 6%



- Molecule 1: Uncharacterized protein C11orf68

Chain 9-C:  84% 12%



- Molecule 1: Uncharacterized protein C11orf68

Chain 10-A:  88% 9%



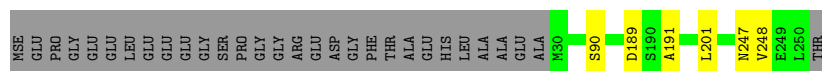
- Molecule 1: Uncharacterized protein C11orf68

Chain 10-B:  89% 6%



- Molecule 1: Uncharacterized protein C11orf68

Chain 10-C:  86% 12%



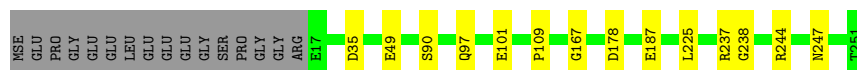
- Molecule 1: Uncharacterized protein C11orf68

Chain 11-A:  86% 5% 9%



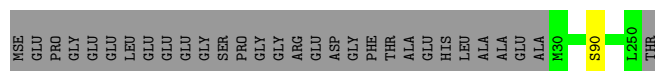
- Molecule 1: Uncharacterized protein C11orf68

Chain 11-B:  88% 6% 6%



- Molecule 1: Uncharacterized protein C11orf68

Chain 11-C:  88% 12%



- Molecule 1: Uncharacterized protein C11orf68

Chain 12-A:  86% 5% 9%



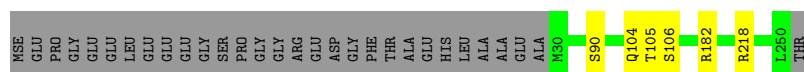
- Molecule 1: Uncharacterized protein C11orf68

Chain 12-B:  87% 7% 6%



- Molecule 1: Uncharacterized protein C11orf68

Chain 12-C:  86% 12%



- Molecule 1: Uncharacterized protein C11orf68

Chain 13-A:  85% 6% 9%



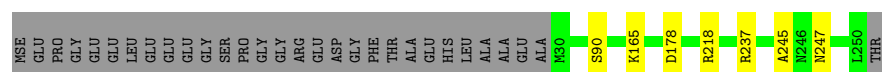
- Molecule 1: Uncharacterized protein C11orf68

Chain 13-B:  88% 6% 6%



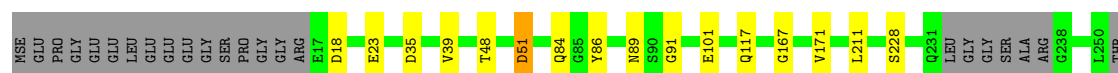
- Molecule 1: Uncharacterized protein C11orf68

Chain 13-C:  85% 12%



- Molecule 1: Uncharacterized protein C11orf68

Chain 14-A:  84% 6% 9%



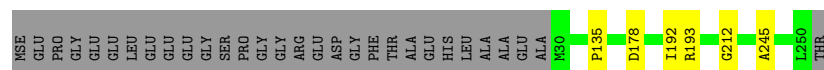
- Molecule 1: Uncharacterized protein C11orf68

Chain 14-B:  86% 8% 6%



- Molecule 1: Uncharacterized protein C11orf68

Chain 14-C:  86% 12%



- Molecule 1: Uncharacterized protein C11orf68

Chain 15-A:  84% 6% 9%



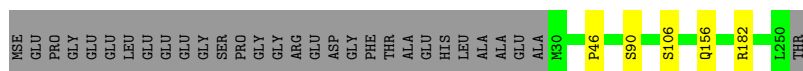
- Molecule 1: Uncharacterized protein C11orf68

Chain 15-B:  85% 9% 6%



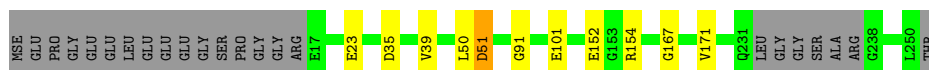
- Molecule 1: Uncharacterized protein C11orf68

Chain 15-C:  86% • 12%



- Molecule 1: Uncharacterized protein C11orf68

Chain 16-A:  86% • 9%



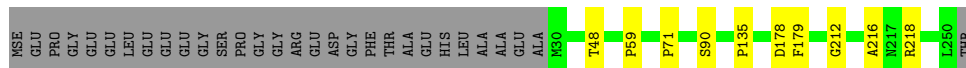
- Molecule 1: Uncharacterized protein C11orf68

Chain 16-B:  90% • 6%



- Molecule 1: Uncharacterized protein C11orf68

Chain 16-C:  84% • 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.55Å 116.81Å 123.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.97 – 2.50 43.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (43.97-2.50) 98.0 (43.97-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.166 , 0.236 0.193 , 0.263	Depositor DCC
R_{free} test set	1607 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.02 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	88208	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 4.51% 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	1-A	0.18	0/1813	0.34	1/2468 (0.0%)
1	1-B	0.19	0/1860	0.34	0/2531
1	1-C	0.21	0/1756	0.38	0/2392
1	2-A	0.18	0/1813	0.34	1/2468 (0.0%)
1	2-B	0.19	0/1860	0.34	0/2531
1	2-C	0.21	0/1756	0.38	0/2392
1	3-A	0.18	0/1813	0.34	1/2468 (0.0%)
1	3-B	0.19	0/1860	0.34	0/2531
1	3-C	0.21	0/1756	0.38	0/2392
1	4-A	0.18	0/1813	0.34	1/2468 (0.0%)
1	4-B	0.19	0/1860	0.34	0/2531
1	4-C	0.21	0/1756	0.38	0/2392
1	5-A	0.18	0/1813	0.34	1/2468 (0.0%)
1	5-B	0.19	0/1860	0.34	0/2531
1	5-C	0.21	0/1756	0.38	0/2392
1	6-A	0.18	0/1813	0.34	1/2468 (0.0%)
1	6-B	0.19	0/1860	0.34	0/2531
1	6-C	0.21	0/1756	0.38	0/2392
1	7-A	0.18	0/1813	0.34	1/2468 (0.0%)
1	7-B	0.19	0/1860	0.34	0/2531
1	7-C	0.21	0/1756	0.38	0/2392
1	8-A	0.18	0/1813	0.34	1/2468 (0.0%)
1	8-B	0.19	0/1860	0.34	0/2531
1	8-C	0.21	0/1756	0.38	0/2392
1	9-A	0.18	0/1813	0.34	1/2468 (0.0%)
1	9-B	0.19	0/1860	0.34	0/2531
1	9-C	0.21	0/1756	0.38	0/2392
1	10-A	0.18	0/1813	0.34	1/2468 (0.0%)
1	10-B	0.19	0/1860	0.34	0/2531
1	10-C	0.21	0/1756	0.38	0/2392
1	11-A	0.18	0/1813	0.34	1/2468 (0.0%)
1	11-B	0.19	0/1860	0.34	0/2531
1	11-C	0.21	0/1756	0.38	0/2392
1	12-A	0.18	0/1813	0.34	1/2468 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	12-B	0.19	0/1860	0.34	0/2531
1	12-C	0.21	0/1756	0.38	0/2392
1	13-A	0.18	0/1813	0.34	1/2468 (0.0%)
1	13-B	0.19	0/1860	0.34	0/2531
1	13-C	0.21	0/1756	0.38	0/2392
1	14-A	0.18	0/1813	0.34	1/2468 (0.0%)
1	14-B	0.19	0/1860	0.34	0/2531
1	14-C	0.21	0/1756	0.38	0/2392
1	15-A	0.18	0/1813	0.34	1/2468 (0.0%)
1	15-B	0.19	0/1860	0.34	0/2531
1	15-C	0.21	0/1756	0.38	0/2392
1	16-A	0.18	0/1813	0.34	1/2468 (0.0%)
1	16-B	0.19	0/1860	0.34	0/2531
1	16-C	0.21	0/1756	0.38	0/2392
All	All	0.19	0/86864	0.35	16/118256 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	39	VAL	N-CA-C	5.00	115.68	108.48
1	2-A	39	VAL	N-CA-C	5.00	115.68	108.48
1	3-A	39	VAL	N-CA-C	5.00	115.68	108.48
1	4-A	39	VAL	N-CA-C	5.00	115.68	108.48
1	5-A	39	VAL	N-CA-C	5.00	115.68	108.48
1	6-A	39	VAL	N-CA-C	5.00	115.68	108.48
1	7-A	39	VAL	N-CA-C	5.00	115.68	108.48
1	8-A	39	VAL	N-CA-C	5.00	115.68	108.48
1	9-A	39	VAL	N-CA-C	5.00	115.68	108.48
1	10-A	39	VAL	N-CA-C	5.00	115.68	108.48
1	11-A	39	VAL	N-CA-C	5.00	115.68	108.48
1	12-A	39	VAL	N-CA-C	5.00	115.68	108.48
1	13-A	39	VAL	N-CA-C	5.00	115.68	108.48
1	14-A	39	VAL	N-CA-C	5.00	115.68	108.48
1	15-A	39	VAL	N-CA-C	5.00	115.68	108.48
1	16-A	39	VAL	N-CA-C	5.00	115.68	108.48

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	1-A	1769	0	1722	0	0
1	1-B	1815	0	1770	0	0
1	1-C	1712	0	1684	0	0
1	2-A	1769	0	1722	0	0
1	2-B	1815	0	1770	0	0
1	2-C	1712	0	1684	0	0
1	3-A	1769	0	1722	0	0
1	3-B	1815	0	1770	0	0
1	3-C	1712	0	1684	0	0
1	4-A	1769	0	1722	0	0
1	4-B	1815	0	1770	0	0
1	4-C	1712	0	1684	0	0
1	5-A	1769	0	1722	0	0
1	5-B	1815	0	1770	0	0
1	5-C	1712	0	1684	0	0
1	6-A	1769	0	1722	0	0
1	6-B	1815	0	1770	0	0
1	6-C	1712	0	1684	0	0
1	7-A	1769	0	1722	0	0
1	7-B	1815	0	1770	0	0
1	7-C	1712	0	1684	0	0
1	8-A	1769	0	1722	0	0
1	8-B	1815	0	1770	0	0
1	8-C	1712	0	1684	0	0
1	9-A	1769	0	1722	0	0
1	9-B	1815	0	1770	0	0
1	9-C	1712	0	1684	0	0
1	10-A	1769	0	1722	0	0
1	10-B	1815	0	1770	0	0
1	10-C	1712	0	1684	0	0
1	11-A	1769	0	1722	0	0
1	11-B	1815	0	1770	0	0
1	11-C	1712	0	1684	0	0
1	12-A	1769	0	1722	0	0
1	12-B	1815	0	1770	0	0
1	12-C	1712	0	1684	0	0
1	13-A	1769	0	1722	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13-B	1815	0	1770	0	0
1	13-C	1712	0	1684	0	0
1	14-A	1769	0	1722	0	0
1	14-B	1815	0	1770	0	0
1	14-C	1712	0	1684	0	0
1	15-A	1769	0	1722	0	0
1	15-B	1815	0	1770	0	0
1	15-C	1712	0	1684	0	0
1	16-A	1769	0	1722	0	0
1	16-B	1815	0	1770	0	0
1	16-C	1712	0	1684	0	0
2	1-A	50	0	0	0	0
2	1-B	91	0	0	0	0
2	1-C	76	0	0	0	0
2	2-A	55	0	0	0	0
2	2-B	88	0	0	0	0
2	2-C	74	0	0	0	0
2	3-A	56	0	0	0	0
2	3-B	88	0	0	0	0
2	3-C	73	0	0	0	0
2	4-A	55	0	0	0	0
2	4-B	90	0	0	0	0
2	4-C	72	0	0	0	0
2	5-A	55	0	0	0	0
2	5-B	89	0	0	0	0
2	5-C	73	0	0	0	0
2	6-A	56	0	0	0	0
2	6-B	89	0	0	0	0
2	6-C	72	0	0	0	0
2	7-A	54	0	0	0	0
2	7-B	89	0	0	0	0
2	7-C	74	0	0	0	0
2	8-A	56	0	0	0	0
2	8-B	88	0	0	0	0
2	8-C	73	0	0	0	0
2	9-A	57	0	0	0	0
2	9-B	88	0	0	0	0
2	9-C	72	0	0	0	0
2	10-A	56	0	0	0	0
2	10-B	88	0	0	0	0
2	10-C	73	0	0	0	0
2	11-A	58	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	11-B	87	0	0	0	0
2	11-C	72	0	0	0	0
2	12-A	55	0	0	0	0
2	12-B	87	0	0	0	0
2	12-C	75	0	0	0	0
2	13-A	53	0	0	0	0
2	13-B	91	0	0	0	0
2	13-C	73	0	0	0	0
2	14-A	56	0	0	0	0
2	14-B	87	0	0	0	0
2	14-C	74	0	0	0	0
2	15-A	53	0	0	0	0
2	15-B	91	0	0	0	0
2	15-C	73	0	0	0	0
2	16-A	53	0	0	0	0
2	16-B	91	0	0	0	0
2	16-C	73	0	0	0	0
All	All	88208	0	82816	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1-A	224/251 (89%)	185 (83%)	27 (12%)	12 (5%)	1 1
1	1-B	233/251 (93%)	204 (88%)	19 (8%)	10 (4%)	2 2
1	1-C	219/251 (87%)	193 (88%)	20 (9%)	6 (3%)	4 6
1	2-A	224/251 (89%)	192 (86%)	28 (12%)	4 (2%)	6 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2-B	233/251 (93%)	195 (84%)	28 (12%)	10 (4%)	2	2
1	2-C	219/251 (87%)	198 (90%)	18 (8%)	3 (1%)	9	17
1	3-A	224/251 (89%)	196 (88%)	25 (11%)	3 (1%)	9	18
1	3-B	233/251 (93%)	219 (94%)	12 (5%)	2 (1%)	14	27
1	3-C	219/251 (87%)	202 (92%)	15 (7%)	2 (1%)	14	27
1	4-A	224/251 (89%)	197 (88%)	21 (9%)	6 (3%)	4	6
1	4-B	233/251 (93%)	205 (88%)	23 (10%)	5 (2%)	5	9
1	4-C	219/251 (87%)	186 (85%)	24 (11%)	9 (4%)	2	3
1	5-A	224/251 (89%)	178 (80%)	35 (16%)	11 (5%)	1	2
1	5-B	233/251 (93%)	203 (87%)	22 (9%)	8 (3%)	3	4
1	5-C	219/251 (87%)	201 (92%)	13 (6%)	5 (2%)	5	8
1	6-A	224/251 (89%)	189 (84%)	25 (11%)	10 (4%)	2	2
1	6-B	233/251 (93%)	210 (90%)	18 (8%)	5 (2%)	5	9
1	6-C	219/251 (87%)	200 (91%)	13 (6%)	6 (3%)	4	6
1	7-A	224/251 (89%)	185 (83%)	34 (15%)	5 (2%)	5	9
1	7-B	233/251 (93%)	195 (84%)	29 (12%)	9 (4%)	2	3
1	7-C	219/251 (87%)	192 (88%)	21 (10%)	6 (3%)	4	6
1	8-A	224/251 (89%)	202 (90%)	20 (9%)	2 (1%)	14	27
1	8-B	233/251 (93%)	214 (92%)	17 (7%)	2 (1%)	14	27
1	8-C	219/251 (87%)	199 (91%)	14 (6%)	6 (3%)	4	6
1	9-A	224/251 (89%)	200 (89%)	19 (8%)	5 (2%)	5	9
1	9-B	233/251 (93%)	207 (89%)	21 (9%)	5 (2%)	5	9
1	9-C	219/251 (87%)	193 (88%)	16 (7%)	10 (5%)	2	2
1	10-A	224/251 (89%)	202 (90%)	20 (9%)	2 (1%)	14	27
1	10-B	233/251 (93%)	211 (91%)	19 (8%)	3 (1%)	9	18
1	10-C	219/251 (87%)	198 (90%)	15 (7%)	6 (3%)	4	6
1	11-A	224/251 (89%)	199 (89%)	18 (8%)	7 (3%)	3	5
1	11-B	233/251 (93%)	209 (90%)	18 (8%)	6 (3%)	4	7
1	11-C	219/251 (87%)	203 (93%)	15 (7%)	1 (0%)	24	43
1	12-A	224/251 (89%)	188 (84%)	29 (13%)	7 (3%)	3	5
1	12-B	233/251 (93%)	199 (85%)	25 (11%)	9 (4%)	2	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	12-C	219/251 (87%)	197 (90%)	16 (7%)	6 (3%)	4	6
1	13-A	224/251 (89%)	193 (86%)	23 (10%)	8 (4%)	2	3
1	13-B	233/251 (93%)	208 (89%)	18 (8%)	7 (3%)	3	5
1	13-C	219/251 (87%)	187 (85%)	25 (11%)	7 (3%)	3	4
1	14-A	224/251 (89%)	181 (81%)	32 (14%)	11 (5%)	1	2
1	14-B	233/251 (93%)	194 (83%)	27 (12%)	12 (5%)	1	1
1	14-C	219/251 (87%)	184 (84%)	29 (13%)	6 (3%)	4	6
1	15-A	224/251 (89%)	188 (84%)	26 (12%)	10 (4%)	2	2
1	15-B	233/251 (93%)	195 (84%)	24 (10%)	14 (6%)	1	1
1	15-C	219/251 (87%)	189 (86%)	25 (11%)	5 (2%)	5	8
1	16-A	224/251 (89%)	193 (86%)	25 (11%)	6 (3%)	4	6
1	16-B	233/251 (93%)	207 (89%)	24 (10%)	2 (1%)	14	27
1	16-C	219/251 (87%)	196 (90%)	13 (6%)	10 (5%)	2	2
All	All	10816/12048 (90%)	9461 (88%)	1043 (10%)	312 (3%)	3	5

All (312) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	18	ASP
1	1-A	165	LYS
1	1-A	178	ASP
1	1-A	214	TYR
1	1-B	90	SER
1	1-C	90	SER
1	1-C	226	TYR
1	2-A	217	ASN
1	2-B	89	ASN
1	2-B	164	ALA
1	2-C	200	LEU
1	2-C	244	ARG
1	3-A	245	ALA
1	4-C	89	ASN
1	4-C	90	SER
1	5-A	80	ALA
1	5-B	233	GLY
1	6-A	63	THR
1	6-A	131	MSE

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Mol	Chain	Res	Type
1	6-A	217	ASN
1	6-A	244	ARG
1	6-B	154	ARG
1	7-A	131	MSE
1	7-B	87	SER
1	7-B	178	ASP
1	7-C	90	SER
1	7-C	135	PRO
1	8-C	90	SER
1	8-C	177	ASP
1	9-C	104	GLN
1	9-C	105	THR
1	9-C	206	ASP
1	10-C	90	SER
1	11-A	89	ASN
1	11-A	91	GLY
1	11-B	109	PRO
1	11-B	237	ARG
1	12-A	89	ASN
1	12-B	128	LYS
1	12-C	106	SER
1	13-C	90	SER
1	13-C	178	ASP
1	13-C	237	ARG
1	14-A	51	ASP
1	14-A	84	GLN
1	14-B	90	SER
1	14-B	215	ARG
1	14-C	135	PRO
1	15-A	92	ASP
1	15-A	167	GLY
1	15-B	88	PRO
1	15-B	194	ALA
1	15-B	234	GLY
1	15-B	235	SER
1	15-C	90	SER
1	16-A	152	GLU
1	16-B	237	ARG
1	16-C	90	SER
1	16-C	135	PRO
1	16-C	178	ASP
1	1-A	106	SER

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Mol	Chain	Res	Type
1	1-A	167	GLY
1	1-A	212	GLY
1	1-B	64	ARG
1	1-B	65	TYR
1	1-B	69	GLY
1	1-B	71	PRO
1	1-B	238	GLY
1	1-C	246	ASN
1	1-C	247	ASN
1	2-B	157	VAL
1	2-C	246	ASN
1	3-A	165	LYS
1	3-B	238	GLY
1	4-A	89	ASN
1	4-A	178	ASP
1	4-B	164	ALA
1	4-B	233	GLY
1	4-C	91	GLY
1	4-C	105	THR
1	5-A	79	ILE
1	5-A	89	ASN
1	5-A	91	GLY
1	5-A	217	ASN
1	5-B	217	ASN
1	5-B	219	TRP
1	5-B	234	GLY
1	5-B	245	ALA
1	5-C	89	ASN
1	6-A	42	ALA
1	6-A	89	ASN
1	6-A	167	GLY
1	6-A	245	ALA
1	6-B	219	TRP
1	6-C	191	ALA
1	6-C	238	GLY
1	7-A	66	GLY
1	7-A	172	ILE
1	7-A	244	ARG
1	7-B	126	SER
1	7-B	165	LYS
1	8-B	212	GLY
1	8-B	238	GLY

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Mol	Chain	Res	Type
1	8-C	106	SER
1	9-A	215	ARG
1	9-A	220	HIS
1	9-B	238	GLY
1	10-A	167	GLY
1	10-C	189	ASP
1	11-B	167	GLY
1	12-A	92	ASP
1	12-B	47	ALA
1	12-B	110	ILE
1	12-B	166	GLU
1	12-C	90	SER
1	12-C	104	GLN
1	12-C	105	THR
1	13-A	226	TYR
1	13-A	248	VAL
1	13-A	249	GLU
1	13-B	21	THR
1	13-B	169	ARG
1	13-C	165	LYS
1	14-A	18	ASP
1	14-A	86	TYR
1	14-A	211	LEU
1	14-B	66	GLY
1	14-B	68	PRO
1	14-B	154	ARG
1	14-B	157	VAL
1	14-B	238	GLY
1	14-C	178	ASP
1	14-C	192	ILE
1	15-A	91	GLY
1	15-A	140	ASP
1	15-A	156	GLN
1	15-A	248	VAL
1	15-B	105	THR
1	15-B	233	GLY
1	15-B	244	ARG
1	16-A	50	LEU
1	16-A	51	ASP
1	16-A	154	ARG
1	16-A	167	GLY
1	1-A	46	PRO

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Mol	Chain	Res	Type
1	1-A	86	TYR
1	1-A	211	LEU
1	2-A	28	GLU
1	2-A	167	GLY
1	2-B	216	ALA
1	2-B	218	ARG
1	3-A	89	ASN
1	3-C	246	ASN
1	4-A	51	ASP
1	4-A	167	GLY
1	4-B	126	SER
1	4-C	73	SER
1	4-C	92	ASP
1	5-A	77	GLY
1	5-A	214	TYR
1	5-B	232	LEU
1	7-B	34	MSE
1	7-C	213	ILE
1	7-C	247	ASN
1	7-C	248	VAL
1	8-A	28	GLU
1	9-A	245	ALA
1	9-B	105	THR
1	9-B	164	ALA
1	9-B	166	GLU
1	9-C	90	SER
1	9-C	245	ALA
1	10-B	216	ALA
1	10-C	191	ALA
1	11-A	167	GLY
1	11-B	90	SER
1	11-B	244	ARG
1	11-C	90	SER
1	12-C	218	ARG
1	13-A	183	LEU
1	13-A	247	ASN
1	13-B	32	ALA
1	13-B	90	SER
1	13-B	165	LYS
1	13-C	247	ASN
1	14-A	48	THR
1	14-A	89	ASN

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Mol	Chain	Res	Type
1	14-A	117	GLN
1	14-B	71	PRO
1	14-B	72	ASN
1	14-B	91	GLY
1	14-C	212	GLY
1	15-A	107	GLY
1	15-B	92	ASP
1	15-B	250	LEU
1	15-C	106	SER
1	16-C	59	PRO
1	16-C	179	PHE
1	16-C	218	ARG
1	1-A	94	GLN
1	1-C	225	LEU
1	2-B	90	SER
1	4-A	38	LEU
1	4-B	235	SER
1	4-C	59	PRO
1	4-C	212	GLY
1	5-A	19	GLY
1	5-B	87	SER
1	5-C	218	ARG
1	6-A	59	PRO
1	6-B	238	GLY
1	6-C	240	ARG
1	7-A	157	VAL
1	7-C	218	ARG
1	8-A	244	ARG
1	8-C	44	THR
1	9-B	215	ARG
1	9-C	106	SER
1	9-C	156	GLN
1	9-C	182	ARG
1	10-B	105	THR
1	11-A	92	ASP
1	12-B	61	GLN
1	12-C	182	ARG
1	13-B	50	LEU
1	13-C	218	ARG
1	13-C	245	ALA
1	14-A	91	GLY
1	14-C	245	ALA

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Mol	Chain	Res	Type
1	15-A	106	SER
1	15-A	215	ARG
1	15-B	23	GLU
1	15-B	181	ASP
1	15-C	156	GLN
1	1-A	150	VAL
1	1-B	105	THR
1	1-B	109	PRO
1	1-B	110	ILE
1	1-C	213	ILE
1	2-B	162	PRO
1	4-A	91	GLY
1	5-B	238	GLY
1	5-C	84	GLN
1	6-B	88	PRO
1	6-B	217	ASN
1	6-C	74	GLU
1	6-C	75	PRO
1	8-C	107	GLY
1	8-C	165	LYS
1	10-A	42	ALA
1	10-C	201	LEU
1	10-C	247	ASN
1	12-A	59	PRO
1	12-A	74	GLU
1	12-B	164	ALA
1	13-A	32	ALA
1	13-A	215	ARG
1	13-B	88	PRO
1	14-A	167	GLY
1	14-A	228	SER
1	14-B	107	GLY
1	15-A	216	ALA
1	15-B	215	ARG
1	16-C	48	THR
1	16-C	216	ALA
1	1-B	167	GLY
1	2-B	107	GLY
1	2-B	110	ILE
1	3-C	238	GLY
1	4-B	110	ILE
1	4-C	104	GLN

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Mol	Chain	Res	Type
1	5-A	152	GLU
1	6-C	235	SER
1	11-A	88	PRO
1	11-A	90	SER
1	12-A	106	SER
1	12-A	131	MSE
1	12-B	106	SER
1	14-C	193	ARG
1	15-B	193	ARG
1	15-C	182	ARG
1	2-A	223	PRO
1	2-B	88	PRO
1	3-B	110	ILE
1	5-A	153	GLY
1	7-B	35	ASP
1	7-B	124	VAL
1	9-C	57	TYR
1	9-C	85	GLY
1	11-A	67	ASP
1	11-B	238	GLY
1	12-B	46	PRO
1	15-C	46	PRO
1	16-C	71	PRO
1	5-A	167	GLY
1	5-C	88	PRO
1	7-B	59	PRO
1	9-A	167	GLY
1	9-A	212	GLY
1	12-A	213	ILE
1	12-B	109	PRO
1	5-C	213	ILE
1	7-B	213	ILE
1	10-C	248	VAL
1	14-B	88	PRO
1	16-B	112	PRO
1	16-C	212	GLY
1	6-A	135	PRO
1	10-B	75	PRO
1	13-A	185	VAL
1	15-B	107	GLY
1	16-A	91	GLY

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	1-A	180/192 (94%)	175 (97%)	5 (3%)	38	66
1	1-B	184/192 (96%)	176 (96%)	8 (4%)	26	51
1	1-C	175/192 (91%)	175 (100%)	0	100	100
1	2-A	180/192 (94%)	175 (97%)	5 (3%)	38	66
1	2-B	184/192 (96%)	176 (96%)	8 (4%)	26	51
1	2-C	175/192 (91%)	175 (100%)	0	100	100
1	3-A	180/192 (94%)	175 (97%)	5 (3%)	38	66
1	3-B	184/192 (96%)	176 (96%)	8 (4%)	26	51
1	3-C	175/192 (91%)	175 (100%)	0	100	100
1	4-A	180/192 (94%)	175 (97%)	5 (3%)	38	66
1	4-B	184/192 (96%)	176 (96%)	8 (4%)	26	51
1	4-C	175/192 (91%)	175 (100%)	0	100	100
1	5-A	180/192 (94%)	175 (97%)	5 (3%)	38	66
1	5-B	184/192 (96%)	176 (96%)	8 (4%)	26	51
1	5-C	175/192 (91%)	175 (100%)	0	100	100
1	6-A	180/192 (94%)	175 (97%)	5 (3%)	38	66
1	6-B	184/192 (96%)	176 (96%)	8 (4%)	26	51
1	6-C	175/192 (91%)	175 (100%)	0	100	100
1	7-A	180/192 (94%)	175 (97%)	5 (3%)	38	66
1	7-B	184/192 (96%)	176 (96%)	8 (4%)	26	51
1	7-C	175/192 (91%)	175 (100%)	0	100	100
1	8-A	180/192 (94%)	175 (97%)	5 (3%)	38	66
1	8-B	184/192 (96%)	176 (96%)	8 (4%)	26	51
1	8-C	175/192 (91%)	175 (100%)	0	100	100
1	9-A	180/192 (94%)	175 (97%)	5 (3%)	38	66
1	9-B	184/192 (96%)	176 (96%)	8 (4%)	26	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	9-C	175/192 (91%)	175 (100%)	0	100	100
1	10-A	180/192 (94%)	175 (97%)	5 (3%)	38	66
1	10-B	184/192 (96%)	176 (96%)	8 (4%)	26	51
1	10-C	175/192 (91%)	175 (100%)	0	100	100
1	11-A	180/192 (94%)	175 (97%)	5 (3%)	38	66
1	11-B	184/192 (96%)	176 (96%)	8 (4%)	26	51
1	11-C	175/192 (91%)	175 (100%)	0	100	100
1	12-A	180/192 (94%)	175 (97%)	5 (3%)	38	66
1	12-B	184/192 (96%)	176 (96%)	8 (4%)	26	51
1	12-C	175/192 (91%)	175 (100%)	0	100	100
1	13-A	180/192 (94%)	175 (97%)	5 (3%)	38	66
1	13-B	184/192 (96%)	176 (96%)	8 (4%)	26	51
1	13-C	175/192 (91%)	175 (100%)	0	100	100
1	14-A	180/192 (94%)	175 (97%)	5 (3%)	38	66
1	14-B	184/192 (96%)	176 (96%)	8 (4%)	26	51
1	14-C	175/192 (91%)	175 (100%)	0	100	100
1	15-A	180/192 (94%)	175 (97%)	5 (3%)	38	66
1	15-B	184/192 (96%)	176 (96%)	8 (4%)	26	51
1	15-C	175/192 (91%)	175 (100%)	0	100	100
1	16-A	180/192 (94%)	175 (97%)	5 (3%)	38	66
1	16-B	184/192 (96%)	176 (96%)	8 (4%)	26	51
1	16-C	175/192 (91%)	175 (100%)	0	100	100
All	All	8624/9216 (94%)	8416 (98%)	208 (2%)	43	70

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	23	GLU
1	1-A	35	ASP
1	1-A	51	ASP
1	1-A	101	GLU
1	1-A	171	VAL
1	1-B	35	ASP
1	1-B	49	GLU

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Mol	Chain	Res	Type
1	1-B	97	GLN
1	1-B	101	GLU
1	1-B	178	ASP
1	1-B	187	GLU
1	1-B	225	LEU
1	1-B	247	ASN
1	2-A	23	GLU
1	2-A	35	ASP
1	2-A	51	ASP
1	2-A	101	GLU
1	2-A	171	VAL
1	2-B	35	ASP
1	2-B	49	GLU
1	2-B	97	GLN
1	2-B	101	GLU
1	2-B	178	ASP
1	2-B	187	GLU
1	2-B	225	LEU
1	2-B	247	ASN
1	3-A	23	GLU
1	3-A	35	ASP
1	3-A	51	ASP
1	3-A	101	GLU
1	3-A	171	VAL
1	3-B	35	ASP
1	3-B	49	GLU
1	3-B	97	GLN
1	3-B	101	GLU
1	3-B	178	ASP
1	3-B	187	GLU
1	3-B	225	LEU
1	3-B	247	ASN
1	4-A	23	GLU
1	4-A	35	ASP
1	4-A	51	ASP
1	4-A	101	GLU
1	4-A	171	VAL
1	4-B	35	ASP
1	4-B	49	GLU
1	4-B	97	GLN
1	4-B	101	GLU
1	4-B	178	ASP

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Mol	Chain	Res	Type
1	4-B	187	GLU
1	4-B	225	LEU
1	4-B	247	ASN
1	5-A	23	GLU
1	5-A	35	ASP
1	5-A	51	ASP
1	5-A	101	GLU
1	5-A	171	VAL
1	5-B	35	ASP
1	5-B	49	GLU
1	5-B	97	GLN
1	5-B	101	GLU
1	5-B	178	ASP
1	5-B	187	GLU
1	5-B	225	LEU
1	5-B	247	ASN
1	6-A	23	GLU
1	6-A	35	ASP
1	6-A	51	ASP
1	6-A	101	GLU
1	6-A	171	VAL
1	6-B	35	ASP
1	6-B	49	GLU
1	6-B	97	GLN
1	6-B	101	GLU
1	6-B	178	ASP
1	6-B	187	GLU
1	6-B	225	LEU
1	6-B	247	ASN
1	7-A	23	GLU
1	7-A	35	ASP
1	7-A	51	ASP
1	7-A	101	GLU
1	7-A	171	VAL
1	7-B	35	ASP
1	7-B	49	GLU
1	7-B	97	GLN
1	7-B	101	GLU
1	7-B	178	ASP
1	7-B	187	GLU
1	7-B	225	LEU
1	7-B	247	ASN

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Mol	Chain	Res	Type
1	8-A	23	GLU
1	8-A	35	ASP
1	8-A	51	ASP
1	8-A	101	GLU
1	8-A	171	VAL
1	8-B	35	ASP
1	8-B	49	GLU
1	8-B	97	GLN
1	8-B	101	GLU
1	8-B	178	ASP
1	8-B	187	GLU
1	8-B	225	LEU
1	8-B	247	ASN
1	9-A	23	GLU
1	9-A	35	ASP
1	9-A	51	ASP
1	9-A	101	GLU
1	9-A	171	VAL
1	9-B	35	ASP
1	9-B	49	GLU
1	9-B	97	GLN
1	9-B	101	GLU
1	9-B	178	ASP
1	9-B	187	GLU
1	9-B	225	LEU
1	9-B	247	ASN
1	10-A	23	GLU
1	10-A	35	ASP
1	10-A	51	ASP
1	10-A	101	GLU
1	10-A	171	VAL
1	10-B	35	ASP
1	10-B	49	GLU
1	10-B	97	GLN
1	10-B	101	GLU
1	10-B	178	ASP
1	10-B	187	GLU
1	10-B	225	LEU
1	10-B	247	ASN
1	11-A	23	GLU
1	11-A	35	ASP
1	11-A	51	ASP

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Mol	Chain	Res	Type
1	11-A	101	GLU
1	11-A	171	VAL
1	11-B	35	ASP
1	11-B	49	GLU
1	11-B	97	GLN
1	11-B	101	GLU
1	11-B	178	ASP
1	11-B	187	GLU
1	11-B	225	LEU
1	11-B	247	ASN
1	12-A	23	GLU
1	12-A	35	ASP
1	12-A	51	ASP
1	12-A	101	GLU
1	12-A	171	VAL
1	12-B	35	ASP
1	12-B	49	GLU
1	12-B	97	GLN
1	12-B	101	GLU
1	12-B	178	ASP
1	12-B	187	GLU
1	12-B	225	LEU
1	12-B	247	ASN
1	13-A	23	GLU
1	13-A	35	ASP
1	13-A	51	ASP
1	13-A	101	GLU
1	13-A	171	VAL
1	13-B	35	ASP
1	13-B	49	GLU
1	13-B	97	GLN
1	13-B	101	GLU
1	13-B	178	ASP
1	13-B	187	GLU
1	13-B	225	LEU
1	13-B	247	ASN
1	14-A	23	GLU
1	14-A	35	ASP
1	14-A	51	ASP
1	14-A	101	GLU
1	14-A	171	VAL
1	14-B	35	ASP

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Mol	Chain	Res	Type
1	14-B	49	GLU
1	14-B	97	GLN
1	14-B	101	GLU
1	14-B	178	ASP
1	14-B	187	GLU
1	14-B	225	LEU
1	14-B	247	ASN
1	15-A	23	GLU
1	15-A	35	ASP
1	15-A	51	ASP
1	15-A	101	GLU
1	15-A	171	VAL
1	15-B	35	ASP
1	15-B	49	GLU
1	15-B	97	GLN
1	15-B	101	GLU
1	15-B	178	ASP
1	15-B	187	GLU
1	15-B	225	LEU
1	15-B	247	ASN
1	16-A	23	GLU
1	16-A	35	ASP
1	16-A	51	ASP
1	16-A	101	GLU
1	16-A	171	VAL
1	16-B	35	ASP
1	16-B	49	GLU
1	16-B	97	GLN
1	16-B	101	GLU
1	16-B	178	ASP
1	16-B	187	GLU
1	16-B	225	LEU
1	16-B	247	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (178) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	84	GLN
1	1-A	104	GLN
1	1-A	156	GLN
1	1-A	170	GLN
1	1-A	220	HIS

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Mol	Chain	Res	Type
1	1-B	84	GLN
1	1-B	89	ASN
1	1-B	94	GLN
1	1-B	104	GLN
1	1-B	117	GLN
1	1-B	156	GLN
1	1-B	170	GLN
1	1-B	247	ASN
1	1-C	61	GLN
1	1-C	84	GLN
1	1-C	104	GLN
1	1-C	122	HIS
1	1-C	231	GLN
1	2-A	61	GLN
1	2-A	117	GLN
1	2-A	156	GLN
1	2-A	247	ASN
1	2-B	117	GLN
1	2-B	156	GLN
1	2-B	231	GLN
1	2-B	247	ASN
1	2-C	89	ASN
1	2-C	117	GLN
1	2-C	231	GLN
1	3-A	61	GLN
1	3-B	156	GLN
1	3-B	247	ASN
1	3-C	117	GLN
1	3-C	156	GLN
1	3-C	231	GLN
1	3-C	247	ASN
1	4-A	61	GLN
1	4-A	84	GLN
1	4-A	117	GLN
1	4-A	217	ASN
1	4-A	247	ASN
1	4-B	104	GLN
1	4-B	117	GLN
1	4-B	156	GLN
1	4-B	231	GLN
1	4-C	61	GLN
1	4-C	84	GLN

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Mol	Chain	Res	Type
1	4-C	122	HIS
1	4-C	123	HIS
1	4-C	156	GLN
1	4-C	231	GLN
1	4-C	246	ASN
1	4-C	247	ASN
1	5-A	61	GLN
1	5-A	170	GLN
1	5-A	220	HIS
1	5-B	156	GLN
1	5-B	170	GLN
1	5-B	231	GLN
1	5-B	247	ASN
1	5-C	61	GLN
1	5-C	156	GLN
1	5-C	247	ASN
1	6-A	61	GLN
1	6-A	89	ASN
1	6-A	156	GLN
1	6-A	231	GLN
1	6-A	247	ASN
1	6-B	156	GLN
1	6-C	97	GLN
1	6-C	123	HIS
1	6-C	132	HIS
1	6-C	231	GLN
1	6-C	246	ASN
1	7-A	104	GLN
1	7-A	246	ASN
1	7-A	247	ASN
1	7-B	61	GLN
1	7-B	97	GLN
1	7-B	117	GLN
1	7-B	122	HIS
1	7-B	231	GLN
1	7-C	61	GLN
1	7-C	84	GLN
1	7-C	117	GLN
1	8-A	24	HIS
1	8-A	61	GLN
1	8-B	94	GLN
1	8-B	156	GLN

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Mol	Chain	Res	Type
1	8-B	170	GLN
1	8-B	247	ASN
1	8-C	247	ASN
1	9-A	61	GLN
1	9-A	122	HIS
1	9-A	231	GLN
1	9-B	84	GLN
1	9-B	104	GLN
1	9-B	156	GLN
1	9-B	170	GLN
1	9-B	247	ASN
1	9-C	61	GLN
1	9-C	89	ASN
1	9-C	117	GLN
1	10-A	61	GLN
1	10-A	217	ASN
1	10-A	231	GLN
1	10-B	84	GLN
1	10-B	94	GLN
1	10-B	132	HIS
1	10-B	156	GLN
1	10-C	123	HIS
1	10-C	170	GLN
1	11-A	61	GLN
1	11-A	122	HIS
1	11-B	61	GLN
1	11-B	156	GLN
1	11-B	231	GLN
1	11-C	89	ASN
1	11-C	97	GLN
1	11-C	104	GLN
1	11-C	231	GLN
1	11-C	246	ASN
1	12-A	24	HIS
1	12-A	61	GLN
1	12-A	84	GLN
1	12-A	97	GLN
1	12-A	122	HIS
1	12-A	246	ASN
1	12-B	84	GLN
1	12-B	117	GLN
1	12-B	156	GLN

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Mol	Chain	Res	Type
1	12-B	231	GLN
1	12-B	247	ASN
1	12-C	61	GLN
1	12-C	123	HIS
1	12-C	141	HIS
1	12-C	156	GLN
1	12-C	246	ASN
1	13-A	156	GLN
1	13-B	247	ASN
1	13-C	117	GLN
1	13-C	122	HIS
1	13-C	123	HIS
1	13-C	231	GLN
1	13-C	246	ASN
1	14-A	104	GLN
1	14-A	117	GLN
1	14-A	217	ASN
1	14-A	231	GLN
1	14-A	247	ASN
1	14-B	122	HIS
1	14-B	231	GLN
1	14-B	247	ASN
1	14-C	61	GLN
1	14-C	94	GLN
1	14-C	117	GLN
1	14-C	246	ASN
1	15-A	170	GLN
1	15-A	220	HIS
1	15-B	141	HIS
1	15-C	89	ASN
1	15-C	156	GLN
1	15-C	231	GLN
1	15-C	246	ASN
1	15-C	247	ASN
1	16-A	104	GLN
1	16-A	117	GLN
1	16-B	89	ASN
1	16-B	104	GLN
1	16-B	117	GLN
1	16-B	170	GLN
1	16-B	247	ASN
1	16-C	61	GLN

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Mol	Chain	Res	Type
1	16-C	141	HIS
1	16-C	156	GLN
1	16-C	170	GLN
1	16-C	231	GLN
1	16-C	246	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	1-A	225/251 (89%)	2.76	146 (64%) 0 0	1, 2, 4, 5	225 (100%)
1	1-B	232/251 (92%)	2.64	135 (58%) 0 0	1, 2, 4, 5	232 (100%)
1	1-C	218/251 (86%)	1.94	88 (40%) 0 0	1, 2, 4, 5	218 (100%)
1	2-A	0/251	-	-	-	-
1	2-B	0/251	-	-	-	-
1	2-C	0/251	-	-	-	-
1	3-A	0/251	-	-	-	-
1	3-B	0/251	-	-	-	-
1	3-C	0/251	-	-	-	-
1	4-A	0/251	-	-	-	-
1	4-B	0/251	-	-	-	-
1	4-C	0/251	-	-	-	-
1	5-A	0/251	-	-	-	-
1	5-B	0/251	-	-	-	-
1	5-C	0/251	-	-	-	-
1	6-A	0/251	-	-	-	-
1	6-B	0/251	-	-	-	-
1	6-C	0/251	-	-	-	-
1	7-A	0/251	-	-	-	-
1	7-B	0/251	-	-	-	-
1	7-C	0/251	-	-	-	-
1	8-A	0/251	-	-	-	-
1	8-B	0/251	-	-	-	-
1	8-C	0/251	-	-	-	-
1	9-A	0/251	-	-	-	-
1	9-B	0/251	-	-	-	-
1	9-C	0/251	-	-	-	-
1	10-A	0/251	-	-	-	-
1	10-B	0/251	-	-	-	-
1	10-C	0/251	-	-	-	-
1	11-A	0/251	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	11-B	0/251	-	-	-	-
1	11-C	0/251	-	-	-	-
1	12-A	0/251	-	-	-	-
1	12-B	0/251	-	-	-	-
1	12-C	0/251	-	-	-	-
1	13-A	0/251	-	-	-	-
1	13-B	0/251	-	-	-	-
1	13-C	0/251	-	-	-	-
1	14-A	0/251	-	-	-	-
1	14-B	0/251	-	-	-	-
1	14-C	0/251	-	-	-	-
1	15-A	0/251	-	-	-	-
1	15-B	0/251	-	-	-	-
1	15-C	0/251	-	-	-	-
1	16-A	0/251	-	-	-	-
1	16-B	0/251	-	-	-	-
1	16-C	0/251	-	-	-	-
All	All	675/12048 (5%)	2.45	369 (54%) 0 0	1, 2, 4, 5	675 (100%)

All (369) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	66	GLY	9.1
1	1-B	69	GLY	8.9
1	1-B	118	LEU	7.8
1	1-B	168	GLY	7.6
1	1-B	121	THR	7.0
1	1-B	103	LEU	7.0
1	1-C	236	ALA	6.7
1	1-A	245	ALA	6.6
1	1-B	122	HIS	6.6
1	1-B	65	TYR	6.6
1	1-C	238	GLY	6.5
1	1-A	138	LYS	6.5
1	1-B	109	PRO	6.5
1	1-A	219	TRP	6.2
1	1-B	153	GLY	6.2
1	1-C	233	GLY	6.2
1	1-B	60	SER	6.1
1	1-B	19	GLY	6.1
1	1-B	119	ALA	6.1
1	1-B	123	HIS	6.0

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Mol	Chain	Res	Type	RSRZ
1	1-A	85	GLY	5.9
1	1-A	214	TYR	5.9
1	1-B	18	ASP	5.6
1	1-A	83	GLY	5.6
1	1-B	85	GLY	5.6
1	1-A	124	VAL	5.6
1	1-B	61	GLN	5.6
1	1-C	118	LEU	5.5
1	1-B	120	ILE	5.5
1	1-A	147	ALA	5.4
1	1-A	74	GLU	5.3
1	1-A	217	ASN	5.3
1	1-A	29	ALA	5.3
1	1-A	48	THR	5.3
1	1-C	244	ARG	5.3
1	1-A	218	ARG	5.2
1	1-A	148	ARG	5.2
1	1-A	150	VAL	5.2
1	1-C	109	PRO	5.2
1	1-A	90	SER	5.1
1	1-B	166	GLU	5.0
1	1-B	238	GLY	5.0
1	1-C	213	ILE	5.0
1	1-A	151	VAL	5.0
1	1-A	17	GLU	5.0
1	1-A	213	ILE	4.9
1	1-A	216	ALA	4.9
1	1-A	220	HIS	4.9
1	1-B	90	SER	4.9
1	1-B	171	VAL	4.9
1	1-B	149	ALA	4.9
1	1-C	232	LEU	4.9
1	1-B	161	SER	4.8
1	1-A	86	TYR	4.8
1	1-B	88	PRO	4.8
1	1-A	250	LEU	4.7
1	1-B	110	ILE	4.7
1	1-C	41	ASP	4.7
1	1-A	248	VAL	4.7
1	1-B	63	THR	4.7
1	1-C	85	GLY	4.7
1	1-C	31	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	1-C	245	ALA	4.6
1	1-A	215	ARG	4.6
1	1-C	43	ARG	4.6
1	1-A	26	ALA	4.6
1	1-A	149	ALA	4.6
1	1-A	231	GLN	4.6
1	1-A	108	ARG	4.6
1	1-B	70	SER	4.6
1	1-C	242	LEU	4.6
1	1-A	222	CYS	4.5
1	1-C	166	GLU	4.5
1	1-C	246	ASN	4.5
1	1-A	208	TYR	4.5
1	1-B	114	THR	4.5
1	1-C	212	GLY	4.5
1	1-A	238	GLY	4.4
1	1-A	171	VAL	4.4
1	1-A	109	PRO	4.4
1	1-A	104	GLN	4.4
1	1-C	87	SER	4.4
1	1-B	165	LYS	4.4
1	1-B	99	ALA	4.3
1	1-C	133	LEU	4.3
1	1-B	94	GLN	4.3
1	1-B	97	GLN	4.3
1	1-A	49	GLU	4.3
1	1-B	73	SER	4.3
1	1-A	182	ARG	4.3
1	1-B	84	GLN	4.3
1	1-B	135	PRO	4.3
1	1-A	96	LEU	4.2
1	1-A	242	LEU	4.2
1	1-A	175	TYR	4.2
1	1-B	105	THR	4.2
1	1-B	57	TYR	4.2
1	1-B	107	GLY	4.2
1	1-A	88	PRO	4.1
1	1-C	208	TYR	4.1
1	1-A	95	GLY	4.1
1	1-A	247	ASN	4.1
1	1-A	152	GLU	4.1
1	1-A	210	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	1-A	32	ALA	4.0
1	1-B	133	LEU	4.0
1	1-B	225	LEU	4.0
1	1-C	105	THR	4.0
1	1-A	46	PRO	4.0
1	1-C	243	ASP	4.0
1	1-B	67	ASP	3.9
1	1-A	240	ARG	3.9
1	1-B	208	TYR	3.9
1	1-A	167	GLY	3.9
1	1-B	106	SER	3.9
1	1-C	225	LEU	3.9
1	1-B	112	PRO	3.9
1	1-B	68	PRO	3.9
1	1-C	110	ILE	3.9
1	1-A	25	LEU	3.8
1	1-A	117	GLN	3.8
1	1-B	216	ALA	3.8
1	1-A	97	GLN	3.8
1	1-C	135	PRO	3.8
1	1-A	43	ARG	3.7
1	1-A	110	ILE	3.7
1	1-A	169	ARG	3.7
1	1-C	234	GLY	3.7
1	1-A	115	LEU	3.7
1	1-A	146	ILE	3.7
1	1-A	105	THR	3.7
1	1-B	93	VAL	3.7
1	1-C	132	HIS	3.7
1	1-B	179	PHE	3.7
1	1-A	18	ASP	3.7
1	1-B	64	ARG	3.7
1	1-B	23	GLU	3.6
1	1-C	247	ASN	3.6
1	1-B	181	ASP	3.6
1	1-C	228	SER	3.6
1	1-C	250	LEU	3.6
1	1-B	89	ASN	3.6
1	1-A	163	ARG	3.6
1	1-A	168	GLY	3.6
1	1-A	211	LEU	3.6
1	1-A	225	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	1-A	179	PHE	3.6
1	1-B	71	PRO	3.6
1	1-B	177	ASP	3.6
1	1-C	191	ALA	3.6
1	1-B	24	HIS	3.5
1	1-A	106	SER	3.5
1	1-B	91	GLY	3.5
1	1-C	42	ALA	3.5
1	1-B	92	ASP	3.5
1	1-B	96	LEU	3.5
1	1-C	91	GLY	3.5
1	1-A	92	ASP	3.5
1	1-A	230	PHE	3.5
1	1-B	182	ARG	3.5
1	1-A	224	THR	3.5
1	1-A	229	ARG	3.4
1	1-C	221	LEU	3.4
1	1-A	244	ARG	3.4
1	1-B	169	ARG	3.4
1	1-A	56	LYS	3.4
1	1-A	125	LEU	3.4
1	1-B	214	TYR	3.3
1	1-B	100	TRP	3.3
1	1-B	219	TRP	3.3
1	1-A	157	VAL	3.3
1	1-B	157	VAL	3.3
1	1-C	237	ARG	3.3
1	1-C	226	TYR	3.3
1	1-B	143	TRP	3.3
1	1-C	230	PHE	3.3
1	1-C	220	HIS	3.3
1	1-C	60	SER	3.2
1	1-A	156	GLN	3.2
1	1-B	86	TYR	3.2
1	1-A	212	GLY	3.2
1	1-B	167	GLY	3.2
1	1-A	164	ALA	3.2
1	1-B	98	ALA	3.2
1	1-B	215	ARG	3.2
1	1-A	89	ASN	3.2
1	1-A	221	LEU	3.2
1	1-B	175	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	1-A	249	GLU	3.2
1	1-A	177	ASP	3.2
1	1-A	166	GLU	3.2
1	1-C	120	ILE	3.2
1	1-A	73	SER	3.2
1	1-B	150	VAL	3.2
1	1-C	107	GLY	3.2
1	1-A	47	ALA	3.1
1	1-A	199	CYS	3.1
1	1-C	108	ARG	3.1
1	1-A	165	LYS	3.1
1	1-A	223	PRO	3.1
1	1-B	87	SER	3.1
1	1-B	244	ARG	3.1
1	1-C	121	THR	3.1
1	1-A	94	GLN	3.1
1	1-A	100	TRP	3.1
1	1-A	246	ASN	3.1
1	1-C	45	THR	3.1
1	1-C	97	GLN	3.1
1	1-B	17	GLU	3.1
1	1-A	122	HIS	3.1
1	1-B	184	GLY	3.1
1	1-A	23	GLU	3.0
1	1-B	247	ASN	3.0
1	1-A	27	ALA	3.0
1	1-C	183	LEU	3.0
1	1-B	95	GLY	3.0
1	1-B	180	THR	3.0
1	1-C	249	GLU	3.0
1	1-B	20	PHE	3.0
1	1-B	134	ALA	3.0
1	1-B	108	ARG	3.0
1	1-B	159	LYS	3.0
1	1-C	89	ASN	3.0
1	1-B	185	VAL	2.9
1	1-B	102	ALA	2.9
1	1-B	141	HIS	2.9
1	1-A	107	GLY	2.9
1	1-B	43	ARG	2.9
1	1-B	237	ARG	2.9
1	1-C	195	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	1-A	118	LEU	2.9
1	1-B	251	THR	2.9
1	1-A	51	ASP	2.9
1	1-B	104	GLN	2.9
1	1-C	127	GLY	2.9
1	1-B	53	TRP	2.9
1	1-C	179	PHE	2.9
1	1-B	217	ASN	2.8
1	1-A	135	PRO	2.8
1	1-B	224	THR	2.8
1	1-C	165	LYS	2.8
1	1-B	146	ILE	2.8
1	1-A	112	PRO	2.8
1	1-C	88	PRO	2.8
1	1-A	139	LEU	2.8
1	1-B	186	LEU	2.8
1	1-B	199	CYS	2.8
1	1-B	51	ASP	2.8
1	1-C	227	GLU	2.8
1	1-A	20	PHE	2.8
1	1-A	197	ILE	2.8
1	1-A	98	ALA	2.8
1	1-A	144	ALA	2.8
1	1-B	211	LEU	2.8
1	1-C	102	ALA	2.8
1	1-A	69	GLY	2.8
1	1-A	123	HIS	2.8
1	1-B	248	VAL	2.8
1	1-A	33	ASP	2.8
1	1-A	82	TYR	2.7
1	1-C	248	VAL	2.7
1	1-C	216	ALA	2.7
1	1-A	84	GLN	2.7
1	1-B	170	GLN	2.7
1	1-A	160	VAL	2.7
1	1-A	114	THR	2.7
1	1-B	113	GLY	2.7
1	1-A	28	GLU	2.7
1	1-A	172	ILE	2.7
1	1-A	121	THR	2.7
1	1-A	227	GLU	2.7
1	1-A	145	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	1-B	234	GLY	2.6
1	1-C	117	GLN	2.6
1	1-C	194	ALA	2.6
1	1-A	181	ASP	2.6
1	1-A	116	ARG	2.6
1	1-B	142	ALA	2.6
1	1-C	86	TYR	2.6
1	1-C	214	TYR	2.6
1	1-C	101	GLU	2.6
1	1-A	102	ALA	2.6
1	1-A	134	ALA	2.6
1	1-A	209	THR	2.6
1	1-A	137	PHE	2.6
1	1-C	103	LEU	2.6
1	1-B	76	VAL	2.6
1	1-A	126	SER	2.6
1	1-B	163	ARG	2.5
1	1-B	221	LEU	2.5
1	1-C	178	ASP	2.5
1	1-A	42	ALA	2.5
1	1-B	82	TYR	2.5
1	1-C	219	TRP	2.5
1	1-A	38	LEU	2.5
1	1-B	115	LEU	2.5
1	1-B	125	LEU	2.5
1	1-C	104	GLN	2.5
1	1-A	60	SER	2.5
1	1-B	140	ASP	2.5
1	1-A	200	LEU	2.5
1	1-A	119	ALA	2.5
1	1-A	103	LEU	2.4
1	1-A	31	ALA	2.4
1	1-B	52	ALA	2.4
1	1-A	226	TYR	2.4
1	1-B	245	ALA	2.4
1	1-A	87	SER	2.4
1	1-A	136	GLY	2.4
1	1-C	169	ARG	2.4
1	1-B	164	ALA	2.4
1	1-C	32	ALA	2.4
1	1-C	167	GLY	2.4
1	1-C	61	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	1-A	173	CYS	2.4
1	1-B	101	GLU	2.4
1	1-B	44	THR	2.3
1	1-C	122	HIS	2.3
1	1-B	56	LYS	2.3
1	1-B	29	ALA	2.3
1	1-C	142	ALA	2.3
1	1-C	106	SER	2.3
1	1-A	61	GLN	2.3
1	1-B	242	LEU	2.3
1	1-C	197	ILE	2.3
1	1-C	93	VAL	2.3
1	1-C	111	THR	2.3
1	1-A	91	GLY	2.3
1	1-B	83	GLY	2.3
1	1-A	141	HIS	2.3
1	1-B	74	GLU	2.3
1	1-B	55	ALA	2.3
1	1-C	218	ARG	2.3
1	1-C	231	GLN	2.3
1	1-B	62	VAL	2.3
1	1-B	111	THR	2.2
1	1-B	58	PRO	2.2
1	1-C	199	CYS	2.2
1	1-A	176	THR	2.2
1	1-B	54	LEU	2.2
1	1-A	35	ASP	2.2
1	1-A	93	VAL	2.2
1	1-C	125	LEU	2.2
1	1-B	28	GLU	2.2
1	1-A	45	THR	2.1
1	1-C	215	ARG	2.1
1	1-A	99	ALA	2.1
1	1-C	229	ARG	2.1
1	1-B	33	ASP	2.1
1	1-C	51	ASP	2.1
1	1-C	239	SER	2.1
1	1-A	159	LYS	2.1
1	1-A	155	LEU	2.1
1	1-C	115	LEU	2.1
1	1-B	31	ALA	2.1
1	1-A	153	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	1-B	35	ASP	2.1
1	1-C	235	SER	2.1
1	1-B	151	VAL	2.0
1	1-B	72	ASN	2.0
1	1-A	44	THR	2.0
1	1-C	44	THR	2.0
1	1-C	224	THR	2.0
1	1-A	239	SER	2.0
1	1-B	236	ALA	2.0
1	1-B	49	GLU	2.0
1	1-B	136	GLY	2.0
1	1-B	213	ILE	2.0
1	1-A	58	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.