Full wwPDB EM Validation Report ⓘ

Jun 25, 2025 – 06:14 PM JST

PDB ID	:	8WVX / pdb_00008wvx
EMDB ID	:	EMD-37875
Title	:	Cryo-EM structure of LGR4 in complex with Norrin(dimer)
Authors	:	Lin, C.; Chang, Z.
Deposited on	:	2023-10-24
Resolution	:	3.32 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

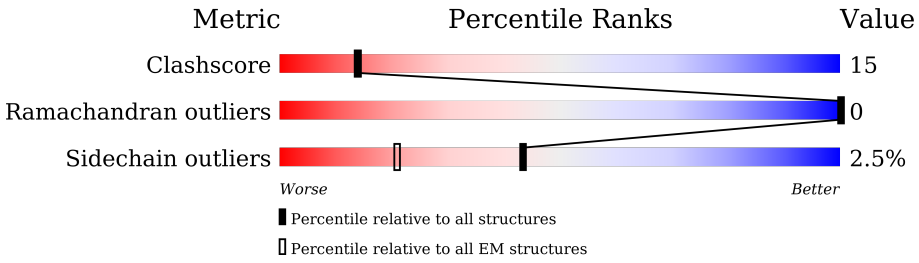
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.32 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	832	16% 53% 29% 5% 13%
1	B	832	17% 53% 31% . 12%
2	C	103	. 55% 37% 5% .
2	D	103	. 51% 38% 7% .

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11460 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Leucine-rich repeat-containing G-protein coupled receptor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	725	Total	C	N	O	S	0	0
			4931	3091	876	948	16		
1	B	731	Total	C	N	O	S	0	0
			4964	3110	884	953	17		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9BXB1
A	2	LYS	-	expression tag	UNP Q9BXB1
A	3	THR	-	expression tag	UNP Q9BXB1
A	4	ILE	-	expression tag	UNP Q9BXB1
A	5	ILE	-	expression tag	UNP Q9BXB1
A	6	ALA	-	expression tag	UNP Q9BXB1
A	7	LEU	-	expression tag	UNP Q9BXB1
A	8	SER	-	expression tag	UNP Q9BXB1
A	9	TYR	-	expression tag	UNP Q9BXB1
A	10	ILE	-	expression tag	UNP Q9BXB1
A	11	PHE	-	expression tag	UNP Q9BXB1
A	12	CYS	-	expression tag	UNP Q9BXB1
A	13	LEU	-	expression tag	UNP Q9BXB1
A	14	VAL	-	expression tag	UNP Q9BXB1
A	15	PHE	-	expression tag	UNP Q9BXB1
A	16	ALA	-	expression tag	UNP Q9BXB1
A	17	ASP	-	expression tag	UNP Q9BXB1
A	18	TYR	-	expression tag	UNP Q9BXB1
A	19	LYS	-	expression tag	UNP Q9BXB1
A	20	ASP	-	expression tag	UNP Q9BXB1
A	21	ASP	-	expression tag	UNP Q9BXB1
A	22	ASP	-	expression tag	UNP Q9BXB1
A	23	ASP	-	expression tag	UNP Q9BXB1
B	1	MET	-	initiating methionine	UNP Q9BXB1
B	2	LYS	-	expression tag	UNP Q9BXB1
B	3	THR	-	expression tag	UNP Q9BXB1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	ILE	-	expression tag	UNP Q9BXB1
B	5	ILE	-	expression tag	UNP Q9BXB1
B	6	ALA	-	expression tag	UNP Q9BXB1
B	7	LEU	-	expression tag	UNP Q9BXB1
B	8	SER	-	expression tag	UNP Q9BXB1
B	9	TYR	-	expression tag	UNP Q9BXB1
B	10	ILE	-	expression tag	UNP Q9BXB1
B	11	PHE	-	expression tag	UNP Q9BXB1
B	12	CYS	-	expression tag	UNP Q9BXB1
B	13	LEU	-	expression tag	UNP Q9BXB1
B	14	VAL	-	expression tag	UNP Q9BXB1
B	15	PHE	-	expression tag	UNP Q9BXB1
B	16	ALA	-	expression tag	UNP Q9BXB1
B	17	ASP	-	expression tag	UNP Q9BXB1
B	18	TYR	-	expression tag	UNP Q9BXB1
B	19	LYS	-	expression tag	UNP Q9BXB1
B	20	ASP	-	expression tag	UNP Q9BXB1
B	21	ASP	-	expression tag	UNP Q9BXB1
B	22	ASP	-	expression tag	UNP Q9BXB1
B	23	ASP	-	expression tag	UNP Q9BXB1

- Molecule 2 is a protein called Norrin.

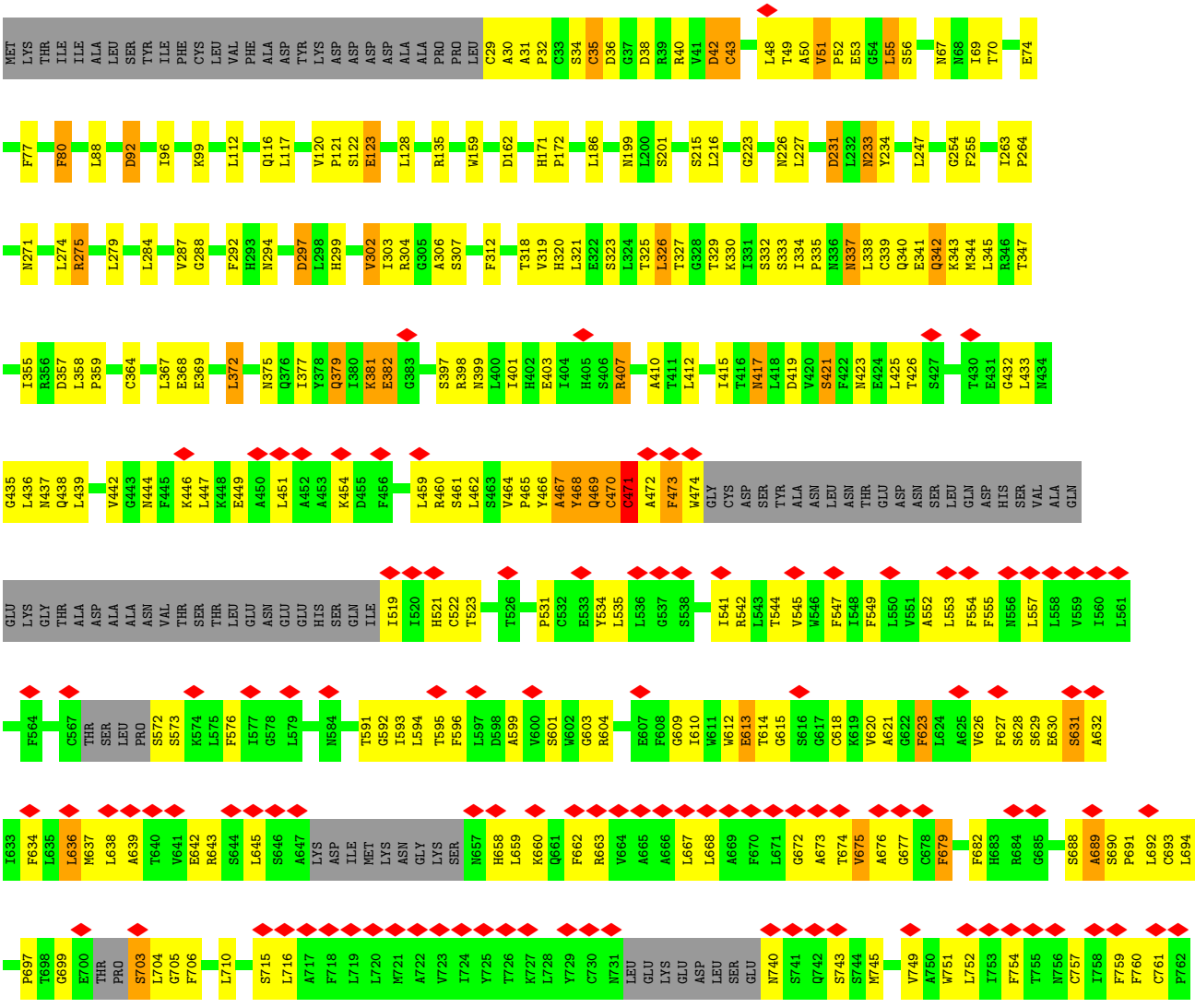
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	100	Total	C	N	O	S	0	0
			783	477	154	139	13		
2	D	99	Total	C	N	O	S	0	0
			782	477	153	138	14		

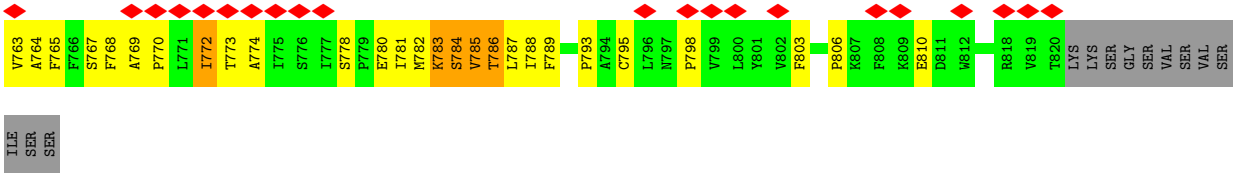
3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Leucine-rich repeat-containing G-protein coupled receptor 4

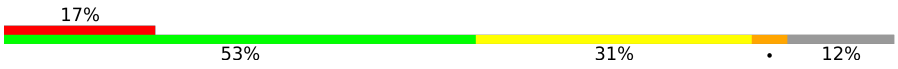
Chain A:

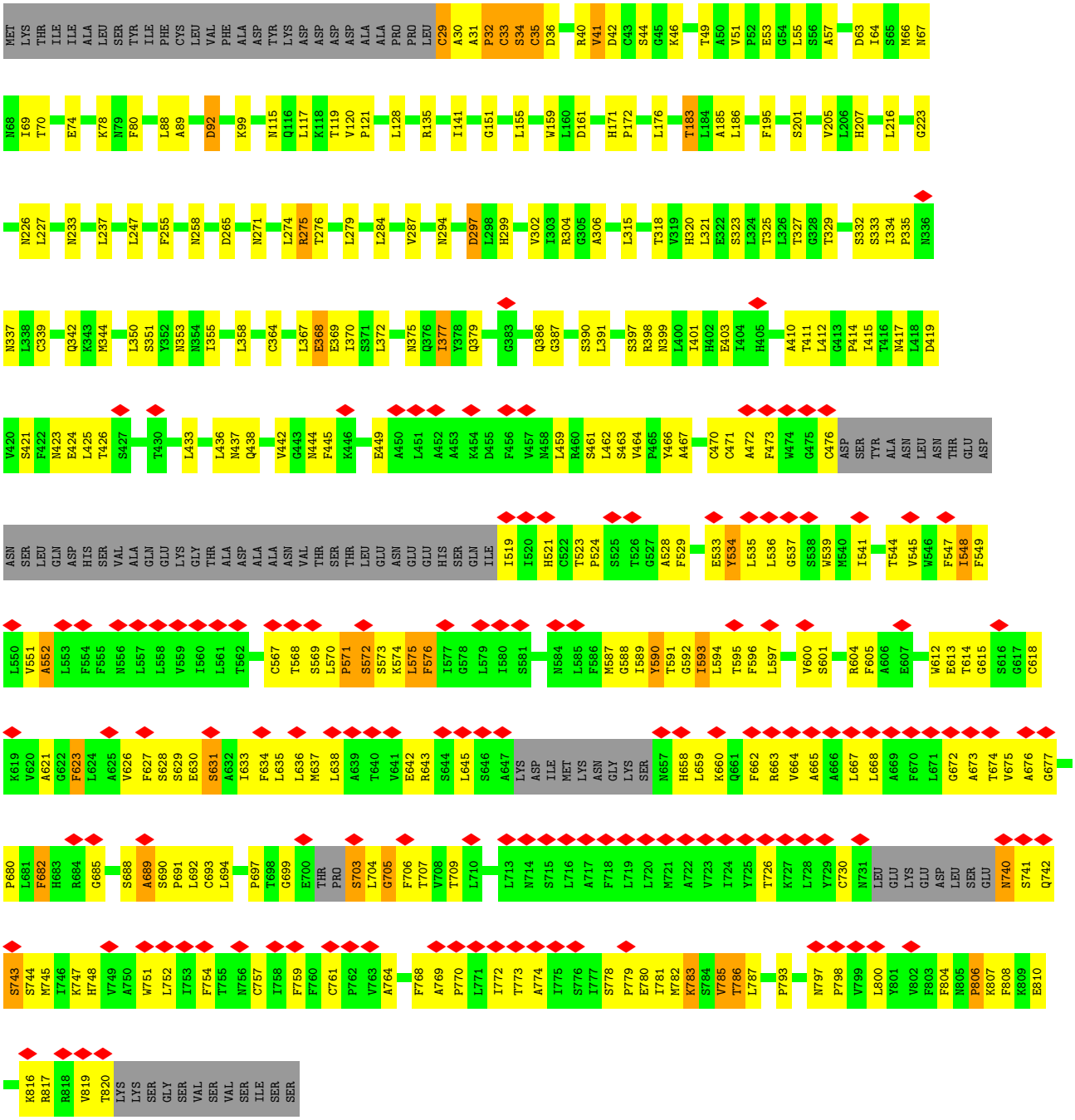




• Molecule 1: Leucine-rich repeat-containing G-protein coupled receptor 4

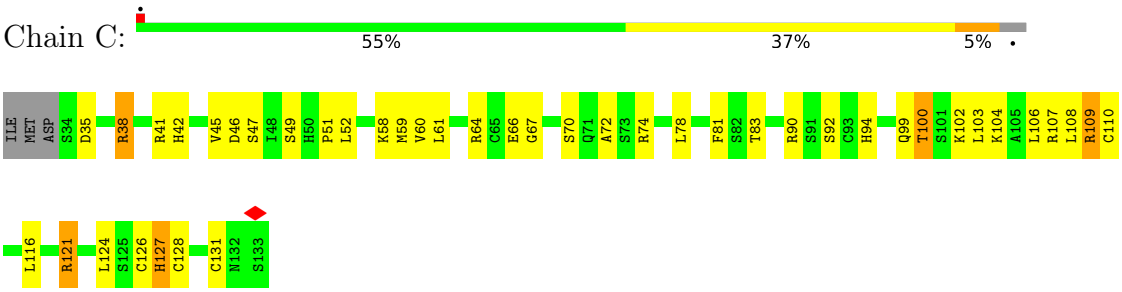
Chain B:





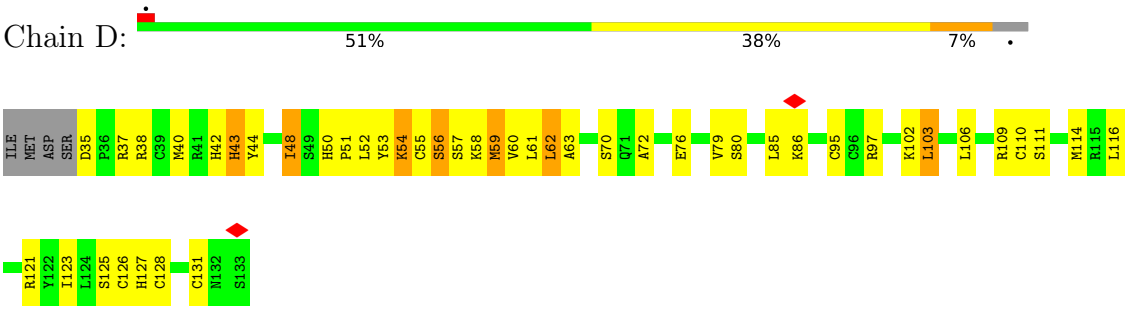
• Molecule 2: Norrin

Chain C:



• Molecule 2: Norrin

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	584272	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	63	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.200	Depositor
Minimum map value	-1.486	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	306.0, 306.0, 306.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.63	124/5011 (2.5%)	1.62	138/6862 (2.0%)
1	B	1.62	132/5045 (2.6%)	1.53	144/6908 (2.1%)
2	C	1.23	11/799 (1.4%)	1.29	4/1072 (0.4%)
2	D	1.61	20/798 (2.5%)	1.21	13/1070 (1.2%)
All	All	1.60	287/11653 (2.5%)	1.54	299/15912 (1.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (287) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	541	ILE	C-N	19.08	1.58	1.33
1	B	601	SER	C-N	18.94	1.59	1.33
1	A	601	SER	C-N	18.43	1.59	1.33
1	B	472	ALA	C-N	17.48	1.56	1.33
1	A	469	GLN	C-N	16.64	1.54	1.33
1	A	470	CYS	C-N	16.44	1.53	1.33
1	A	473	PHE	C-N	16.38	1.56	1.33
1	A	472	ALA	C-N	15.26	1.53	1.33
1	A	784	SER	C-N	14.73	1.52	1.33
1	A	752	LEU	C-N	14.64	1.52	1.33
1	B	752	LEU	C-N	14.46	1.52	1.33
1	B	774	ALA	C-N	14.15	1.52	1.33
1	B	628	SER	C-N	13.98	1.51	1.33
1	A	628	SER	C-N	13.94	1.51	1.33
1	B	772	ILE	C-N	13.85	1.53	1.33
2	D	57	SER	C-N	13.74	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	615	GLY	C-O	13.52	1.38	1.23
1	A	615	GLY	C-O	13.44	1.38	1.23
1	A	690	SER	C-N	13.40	1.48	1.34
1	A	554	PHE	C-N	13.32	1.51	1.33
1	A	468	TYR	C-N	13.19	1.50	1.33
1	B	674	THR	C-N	13.07	1.50	1.33
1	A	674	THR	C-N	13.04	1.50	1.33
1	B	605	PHE	C-N	13.04	1.50	1.33
1	A	223	GLY	C-N	12.88	1.50	1.33
2	D	125	SER	C-N	12.78	1.51	1.33
1	B	690	SER	C-N	12.72	1.48	1.34
1	B	570	LEU	C-N	12.38	1.49	1.33
1	A	772	ILE	C-N	12.03	1.50	1.33
1	A	294	ASN	C-N	11.98	1.49	1.33
1	A	785	VAL	C-N	11.87	1.49	1.33
1	B	571	PRO	C-N	11.86	1.50	1.33
2	D	40	MET	C-N	11.85	1.49	1.33
1	B	589	ILE	C-N	11.61	1.49	1.33
1	A	623	PHE	C-N	11.52	1.49	1.33
1	A	67	ASN	C-N	11.49	1.50	1.33
1	B	631	SER	C-N	11.38	1.48	1.33
1	A	631	SER	C-N	11.31	1.48	1.33
1	B	575	LEU	C-N	11.30	1.49	1.33
1	A	675	VAL	C-N	11.20	1.48	1.33
2	D	58	LYS	C-N	11.14	1.48	1.33
1	B	785	VAL	C-N	11.13	1.48	1.33
1	B	783	LYS	C-N	10.98	1.48	1.33
1	B	536	LEU	C-N	10.93	1.49	1.33
1	A	603	GLY	C-N	10.87	1.49	1.33
1	A	783	LYS	C-N	10.72	1.48	1.33
2	D	61	LEU	C-N	10.68	1.48	1.33
2	D	106	LEU	C-N	10.54	1.47	1.33
1	B	463	SER	C-N	10.16	1.43	1.33
1	B	660	LYS	C-N	10.16	1.48	1.34
1	B	612	TRP	C-N	10.13	1.49	1.33
1	B	375	ASN	C-N	10.12	1.48	1.33
1	B	685	GLY	C-N	10.06	1.47	1.33
1	A	660	LYS	C-N	9.98	1.47	1.34
1	B	223	GLY	C-N	9.97	1.46	1.33
1	B	332	SER	C-N	9.83	1.47	1.33
1	B	387	GLY	C-N	9.76	1.46	1.33
2	D	56	SER	C-N	9.72	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	595	THR	C-N	9.70	1.46	1.33
1	B	541	ILE	C-N	9.60	1.46	1.33
1	B	572	SER	C-N	9.56	1.46	1.33
1	B	689	ALA	C-N	9.55	1.43	1.33
1	B	663	ARG	C-N	-9.43	1.22	1.33
2	C	74	ARG	C-N	9.43	1.45	1.33
1	A	74	GLU	C-N	-9.35	1.21	1.33
1	B	42	ASP	C-N	-9.26	1.21	1.33
1	B	34	SER	C-N	-9.25	1.20	1.33
1	A	128	LEU	C-N	9.25	1.46	1.33
2	D	123	ILE	C-N	-9.24	1.20	1.33
1	A	643	ARG	C-N	-9.20	1.21	1.33
1	B	743	SER	C-N	9.15	1.45	1.33
1	B	33	CYS	C-N	-9.09	1.21	1.33
1	B	467	ALA	C-N	-9.06	1.21	1.33
1	B	549	PHE	C-N	9.05	1.46	1.34
1	B	128	LEU	C-N	9.05	1.46	1.33
1	A	599	ALA	C-N	9.04	1.45	1.33
1	B	667	LEU	C-N	-9.05	1.21	1.33
1	B	519	ILE	C-N	8.98	1.45	1.33
1	A	264	PRO	C-N	8.89	1.46	1.33
1	B	265	ASP	C-N	8.84	1.46	1.33
1	B	523	THR	C-N	8.83	1.46	1.34
2	D	59	MET	C-N	8.80	1.45	1.33
1	B	117	LEU	C-N	-8.80	1.21	1.33
1	A	663	ARG	C-N	-8.76	1.22	1.33
1	A	645	LEU	C-N	8.71	1.45	1.33
1	A	519	ILE	C-N	8.67	1.44	1.33
1	A	332	SER	C-N	8.66	1.45	1.33
1	B	778	SER	C-N	-8.63	1.23	1.33
1	A	379	GLN	C-N	-8.59	1.23	1.33
1	A	667	LEU	C-N	-8.58	1.22	1.33
1	A	471	CYS	C-N	8.55	1.44	1.33
1	A	523	THR	C-N	8.47	1.45	1.34
1	A	594	LEU	C-N	8.33	1.45	1.33
1	B	688	SER	C-N	8.21	1.45	1.33
1	A	688	SER	C-N	8.17	1.45	1.33
1	A	368	GLU	C-N	-8.15	1.22	1.33
1	B	594	LEU	C-N	8.13	1.44	1.33
1	B	403	GLU	C-N	-8.12	1.23	1.33
1	A	612	TRP	C-N	8.12	1.45	1.33
1	A	636	LEU	C-N	-8.12	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	636	LEU	C-N	-8.07	1.22	1.34
1	A	553	LEU	C-N	8.07	1.45	1.33
1	B	521	HIS	C-N	8.03	1.44	1.33
1	B	30	ALA	C-N	8.01	1.47	1.34
1	B	466	TYR	C-N	8.01	1.44	1.33
1	A	254	GLY	C-N	-7.98	1.22	1.33
1	A	460	ARG	C-N	-7.92	1.22	1.33
2	D	79	VAL	C-N	7.90	1.45	1.33
1	A	545	VAL	C-N	-7.88	1.23	1.33
1	A	292	PHE	C-N	-7.86	1.22	1.33
1	A	323	SER	C-N	-7.85	1.23	1.33
1	A	765	PHE	C-N	7.83	1.45	1.33
1	A	637	MET	C-N	7.80	1.44	1.33
1	A	689	ALA	C-N	7.80	1.42	1.33
1	A	407	ARG	C-N	7.77	1.44	1.33
1	A	521	HIS	C-N	7.76	1.43	1.33
1	A	302	VAL	C-N	7.76	1.43	1.33
2	D	35	ASP	C-N	-7.74	1.26	1.34
1	A	764	ALA	C-N	-7.67	1.23	1.33
1	B	444	ASN	C-N	-7.64	1.23	1.33
1	B	368	GLU	C-N	-7.63	1.23	1.33
1	B	539	TRP	C-N	-7.63	1.23	1.33
1	A	377	ILE	C-N	7.62	1.44	1.33
1	A	613	GLU	C-N	7.61	1.44	1.33
2	D	70	SER	C-N	7.60	1.44	1.33
1	B	544	THR	C-N	7.54	1.43	1.33
1	A	596	PHE	C-N	-7.54	1.24	1.33
1	B	337	ASN	C-N	7.51	1.43	1.33
1	B	53	GLU	C-N	-7.49	1.22	1.33
1	B	645	LEU	C-N	7.49	1.43	1.33
1	B	637	MET	C-N	7.49	1.44	1.33
1	A	326	LEU	C-N	7.48	1.43	1.33
1	B	545	VAL	C-N	-7.43	1.24	1.33
1	A	231	ASP	C-N	-7.41	1.23	1.33
1	A	740	ASN	C-N	7.38	1.43	1.33
1	B	323	SER	C-N	-7.38	1.23	1.33
1	A	544	THR	C-N	7.38	1.43	1.33
1	B	424	GLU	C-N	-7.38	1.23	1.33
1	A	467	ALA	C-N	7.35	1.43	1.34
1	A	56	SER	C-N	-7.30	1.22	1.33
1	B	764	ALA	C-N	-7.23	1.24	1.33
1	B	780	GLU	C-N	7.22	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	SER	C-N	-7.21	1.23	1.33
1	A	642	GLU	C-N	7.19	1.43	1.33
1	B	74	GLU	C-N	-7.19	1.24	1.33
1	A	761	CYS	C-N	7.17	1.42	1.34
2	C	42	HIS	C-N	7.15	1.43	1.33
1	B	574	LYS	C-N	7.14	1.43	1.33
1	B	676	ALA	C-N	-7.14	1.25	1.33
1	B	740	ASN	C-N	7.12	1.43	1.33
1	A	437	ASN	C-N	-7.12	1.24	1.33
1	B	195	PHE	C-N	7.06	1.43	1.33
1	A	451	LEU	C-N	7.05	1.43	1.33
1	A	676	ALA	C-N	-7.05	1.25	1.33
1	B	642	GLU	C-N	7.04	1.43	1.33
1	B	643	ARG	C-N	-7.04	1.24	1.33
1	A	375	ASN	C-N	7.03	1.44	1.33
1	A	626	VAL	C-N	-7.02	1.24	1.33
1	B	662	PHE	C-N	-7.01	1.24	1.33
1	B	35	CYS	C-N	6.96	1.43	1.33
1	B	761	CYS	C-N	6.93	1.42	1.34
1	A	419	ASP	C-N	-6.91	1.24	1.33
1	B	399	ASN	C-N	-6.90	1.23	1.33
1	B	464	VAL	C-N	6.89	1.43	1.34
2	C	60	VAL	C-N	6.88	1.43	1.33
1	A	444	ASN	C-N	-6.86	1.23	1.33
1	B	297	ASP	C-N	-6.83	1.24	1.33
1	A	767	SER	C-N	6.82	1.42	1.33
1	B	44	SER	C-N	-6.82	1.24	1.33
1	B	67	ASN	C-N	6.82	1.43	1.33
1	B	99	LYS	C-N	6.80	1.42	1.33
2	D	37	ARG	C-N	6.79	1.43	1.33
1	A	233	ASN	C-N	-6.78	1.24	1.33
1	B	121	PRO	C-N	-6.74	1.24	1.33
1	B	626	VAL	C-N	-6.73	1.24	1.33
1	B	419	ASP	C-N	-6.73	1.25	1.33
1	B	770	PRO	C-N	6.72	1.43	1.33
2	C	72	ALA	C-N	6.67	1.43	1.33
1	A	199	ASN	C-N	6.64	1.43	1.33
2	D	72	ALA	C-N	6.63	1.42	1.33
1	A	288	GLY	C-N	6.63	1.42	1.33
1	B	613	GLU	C-N	-6.63	1.24	1.33
1	B	370	ILE	C-N	-6.61	1.24	1.33
1	B	537	GLY	C-N	-6.61	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	275	ARG	C-N	6.61	1.42	1.33
2	D	80	SER	C-N	-6.55	1.24	1.33
1	B	757	CYS	C-N	6.53	1.42	1.33
1	B	29	CYS	C-N	6.52	1.42	1.33
1	B	398	ARG	C-N	6.51	1.42	1.33
1	B	237	LEU	C-N	-6.50	1.24	1.33
1	B	51	VAL	C-N	-6.49	1.25	1.33
1	A	426	THR	C-N	6.49	1.41	1.33
1	A	679	PHE	C-N	-6.48	1.27	1.34
1	A	770	PRO	C-N	6.46	1.42	1.33
1	A	297	ASP	C-N	-6.45	1.25	1.33
1	B	397	SER	C-N	6.42	1.42	1.33
1	A	347	THR	C-N	-6.39	1.25	1.33
1	A	397	SER	C-N	6.36	1.42	1.33
1	A	763	VAL	C-N	-6.36	1.25	1.33
1	A	662	PHE	C-N	-6.33	1.25	1.33
1	B	410	ALA	C-N	-6.32	1.25	1.33
1	A	96	ILE	C-N	-6.29	1.23	1.33
1	A	743	SER	C-N	6.29	1.42	1.33
1	B	590	TYR	C-N	6.26	1.42	1.33
1	A	435	GLY	C-N	6.25	1.41	1.33
1	B	426	THR	C-N	6.20	1.41	1.33
1	B	92	ASP	C-N	6.18	1.42	1.33
1	B	659	LEU	C-N	6.17	1.42	1.33
1	B	377	ILE	C-N	6.14	1.42	1.33
1	A	425	LEU	C-N	6.14	1.43	1.33
1	A	757	CYS	C-N	6.14	1.41	1.33
1	B	623	PHE	C-N	6.14	1.42	1.33
1	B	401	ILE	C-N	6.13	1.43	1.33
1	B	768	PHE	C-N	6.13	1.46	1.33
2	D	62	LEU	C-N	6.09	1.43	1.33
1	A	682	PHE	C-N	6.08	1.41	1.33
2	D	43	HIS	C-N	-6.08	1.25	1.33
1	A	99	LYS	C-N	6.07	1.41	1.33
1	A	552	ALA	C-N	6.06	1.41	1.33
1	B	63	ASP	C-N	-6.05	1.25	1.33
1	A	620	VAL	C-N	-6.02	1.26	1.33
1	A	454	LYS	C-N	6.02	1.42	1.33
1	A	403	GLU	C-N	-6.01	1.26	1.33
1	B	119	THR	C-N	-6.00	1.26	1.33
1	A	275	ARG	C-N	5.99	1.41	1.33
2	D	44	TYR	C-N	5.96	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	433	LEU	C-N	-5.96	1.25	1.33
1	B	552	ALA	C-N	5.94	1.41	1.33
2	C	61	LEU	C-N	-5.93	1.25	1.33
1	A	768	PHE	C-N	5.88	1.45	1.33
1	A	433	LEU	C-N	-5.87	1.25	1.33
1	A	80	PHE	C-N	-5.86	1.26	1.34
2	D	38	ARG	C-N	5.77	1.41	1.33
1	B	390	SER	C-N	-5.77	1.25	1.33
1	B	425	LEU	C-N	5.76	1.42	1.33
2	C	51	PRO	C-N	-5.72	1.26	1.33
1	A	449	GLU	C-N	-5.70	1.25	1.33
2	C	127	HIS	C-N	5.69	1.41	1.33
1	A	417	ASN	C-N	-5.68	1.25	1.33
1	A	372	LEU	C-N	-5.67	1.25	1.33
1	B	445	PHE	C-N	5.67	1.41	1.33
1	B	339	CYS	C-N	-5.66	1.26	1.33
1	A	604	ARG	C-N	5.64	1.41	1.33
1	B	437	ASN	C-N	-5.61	1.26	1.33
1	A	592	GLY	C-N	-5.58	1.26	1.33
1	A	401	ILE	C-N	5.55	1.42	1.33
1	B	333	SER	C-N	-5.53	1.27	1.33
1	B	78	LYS	C-N	5.52	1.41	1.33
2	C	52	LEU	C-N	-5.52	1.25	1.33
1	B	592	GLY	C-N	-5.47	1.27	1.33
1	A	382	GLU	C-N	-5.47	1.25	1.33
1	B	449	GLU	C-N	-5.45	1.25	1.33
1	A	446	LYS	C-N	-5.40	1.25	1.33
1	A	77	PHE	C-N	-5.39	1.25	1.33
1	B	233	ASN	C-N	-5.38	1.25	1.33
2	C	38	ARG	C-N	5.36	1.40	1.33
1	A	432	GLY	C-N	5.35	1.40	1.33
1	B	621	ALA	C-N	-5.34	1.27	1.33
2	D	76	GLU	C-N	-5.32	1.26	1.33
1	B	64	ILE	C-N	-5.31	1.26	1.33
1	A	55	LEU	C-N	5.31	1.40	1.33
1	A	92	ASP	C-N	5.31	1.40	1.33
1	A	673	ALA	C-N	-5.29	1.26	1.33
1	B	372	LEU	C-N	-5.26	1.26	1.33
1	B	534	TYR	C-N	-5.26	1.27	1.33
1	B	379	GLN	C-N	-5.23	1.27	1.33
1	A	234	TYR	C-N	5.23	1.40	1.33
2	C	70	SER	C-N	5.23	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	151	GLY	C-N	5.22	1.41	1.33
1	B	294	ASN	C-N	5.20	1.40	1.33
1	A	621	ALA	C-N	-5.19	1.27	1.33
1	B	89	ALA	C-N	-5.17	1.25	1.33
1	A	410	ALA	C-N	-5.15	1.26	1.33
1	A	399	ASN	C-N	-5.14	1.26	1.33
1	A	535	LEU	C-N	5.12	1.40	1.33
1	B	115	ASN	C-N	5.11	1.40	1.33
1	B	66	MET	C-N	5.10	1.40	1.33
2	C	35	ASP	C-N	-5.10	1.29	1.34
1	B	335	PRO	C-N	5.09	1.40	1.33
1	B	682	PHE	C-N	5.07	1.40	1.33
1	B	588	GLY	C-N	-5.07	1.27	1.33
1	A	549	PHE	C-N	5.06	1.41	1.34
1	B	604	ARG	C-N	5.05	1.40	1.33
1	A	421	SER	C-N	5.05	1.40	1.33
1	B	88	LEU	C-N	-5.04	1.26	1.33
1	A	595	THR	C-N	5.01	1.40	1.33
1	A	760	PHE	C-N	-5.00	1.26	1.33

All (299) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	573	SER	N-CA-C	-28.02	82.68	114.62
2	C	92	SER	N-CA-C	-18.59	79.38	108.76
1	A	471	CYS	O-C-N	17.44	140.74	122.08
1	A	342	GLN	N-CA-C	-16.70	85.11	109.15
1	A	470	CYS	O-C-N	15.46	138.17	122.09
1	A	472	ALA	O-C-N	15.12	137.64	122.07
1	A	469	GLN	O-C-N	14.48	136.98	122.07
1	A	704	LEU	O-C-N	13.53	139.00	122.35
1	B	704	LEU	O-C-N	13.45	138.89	122.35
1	A	473	PHE	O-C-N	13.43	136.35	122.12
1	A	468	TYR	O-C-N	13.37	137.86	122.22
1	B	808	PHE	N-CA-C	-13.25	97.58	113.88
2	C	92	SER	CB-CA-C	13.23	134.37	110.16
1	A	783	LYS	O-C-N	13.17	136.08	122.12
1	B	745	MET	O-C-N	12.78	135.24	122.07
1	A	704	LEU	CA-C-N	-12.72	104.86	123.95
1	A	704	LEU	C-N-CA	-12.72	104.86	123.95
1	B	573	SER	O-C-N	12.65	135.10	122.07
1	B	704	LEU	CA-C-N	-12.65	104.98	123.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	704	LEU	C-N-CA	-12.65	104.98	123.95
1	B	596	PHE	O-C-N	12.18	134.61	122.07
1	A	469	GLN	CA-C-N	-11.80	104.61	120.54
1	A	469	GLN	C-N-CA	-11.80	104.61	120.54
1	A	471	CYS	CA-C-N	-11.77	105.15	120.44
1	A	471	CYS	C-N-CA	-11.77	105.15	120.44
1	A	667	LEU	O-C-N	-11.29	110.15	122.12
1	A	472	ALA	CA-C-N	-11.10	105.41	120.28
1	A	472	ALA	C-N-CA	-11.10	105.41	120.28
1	A	468	TYR	CA-C-N	-10.81	106.39	120.44
1	A	468	TYR	C-N-CA	-10.81	106.39	120.44
1	B	667	LEU	O-C-N	-10.51	110.97	122.12
1	B	588	GLY	O-C-N	10.34	133.19	122.24
1	B	807	LYS	N-CA-C	10.22	122.38	111.03
1	B	185	ALA	CB-CA-C	-10.21	92.95	109.80
1	B	745	MET	CA-C-N	-10.17	107.74	120.56
1	B	745	MET	C-N-CA	-10.17	107.74	120.56
1	A	638	LEU	O-C-N	-10.11	110.63	122.15
1	B	703	SER	CA-C-N	-10.02	106.60	122.73
1	B	703	SER	C-N-CA	-10.02	106.60	122.73
1	A	703	SER	CA-C-N	-10.01	106.61	122.73
1	A	703	SER	C-N-CA	-10.01	106.61	122.73
1	B	638	LEU	O-C-N	-9.89	110.88	122.15
1	A	783	LYS	CA-C-N	-9.87	106.28	120.29
1	A	783	LYS	C-N-CA	-9.87	106.28	120.29
1	A	745	MET	O-C-N	9.80	132.16	122.07
1	A	541	ILE	O-C-N	9.79	131.91	121.83
1	B	783	LYS	O-C-N	9.71	132.41	122.12
1	B	596	PHE	CA-C-N	-9.64	107.36	120.28
1	B	596	PHE	C-N-CA	-9.64	107.36	120.28
1	B	705	GLY	O-C-N	9.35	127.09	121.85
1	B	574	LYS	O-C-N	9.31	133.72	122.27
1	A	467	ALA	CA-C-N	-9.26	106.95	120.28
1	A	467	ALA	C-N-CA	-9.26	106.95	120.28
2	C	83	THR	N-CA-CB	-9.25	96.80	110.49
1	B	573	SER	CA-C-N	-9.14	106.42	120.31
1	B	573	SER	C-N-CA	-9.14	106.42	120.31
1	B	707	THR	N-CA-C	-9.10	101.32	111.14
1	A	467	ALA	O-C-N	8.87	135.16	122.20
1	A	572	SER	N-CA-C	8.81	135.68	111.00
1	A	638	LEU	CA-C-N	8.79	131.87	120.44
1	A	638	LEU	C-N-CA	8.79	131.87	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	667	LEU	CA-C-N	8.79	132.77	120.29
1	A	667	LEU	C-N-CA	8.79	132.77	120.29
1	A	287	VAL	CA-C-N	8.74	128.31	119.92
1	A	287	VAL	C-N-CA	8.74	128.31	119.92
1	B	576	PHE	O-C-N	8.73	133.74	122.39
1	B	754	PHE	O-C-N	8.67	131.31	122.12
1	B	638	LEU	CA-C-N	8.55	131.56	120.44
1	B	638	LEU	C-N-CA	8.55	131.56	120.44
1	A	552	ALA	O-C-N	8.51	131.14	122.12
1	A	754	PHE	O-C-N	8.49	131.12	122.12
1	B	552	ALA	O-C-N	8.36	130.98	122.12
1	A	287	VAL	O-C-N	-8.27	114.58	123.18
1	B	667	LEU	CA-C-N	8.22	131.97	120.29
1	B	667	LEU	C-N-CA	8.22	131.97	120.29
1	A	637	MET	O-C-N	-8.21	112.17	122.27
2	D	60	VAL	O-C-N	-8.20	113.76	123.02
1	A	342	GLN	CB-CA-C	8.10	122.98	110.67
1	B	637	MET	O-C-N	-8.09	112.32	122.27
1	A	470	CYS	CA-C-N	-8.07	109.57	120.79
1	A	470	CYS	C-N-CA	-8.07	109.57	120.79
1	B	672	GLY	O-C-N	7.98	129.85	122.19
1	B	574	LYS	CA-C-N	-7.96	109.61	120.44
1	B	574	LYS	C-N-CA	-7.96	109.61	120.44
1	A	473	PHE	CA-C-N	-7.93	107.43	121.70
1	A	473	PHE	C-N-CA	-7.93	107.43	121.70
1	A	745	MET	CA-C-N	-7.90	110.60	120.56
1	A	745	MET	C-N-CA	-7.90	110.60	120.56
1	B	576	PHE	CA-C-N	-7.82	109.75	120.46
1	B	576	PHE	C-N-CA	-7.82	109.75	120.46
1	B	664	VAL	O-C-N	-7.78	114.32	121.87
2	D	56	SER	O-C-N	-7.74	113.55	122.68
1	A	784	SER	O-C-N	7.70	130.93	122.15
1	A	675	VAL	O-C-N	7.68	129.89	121.90
1	B	629	SER	O-C-N	7.67	129.97	122.07
1	A	767	SER	O-C-N	-7.66	113.42	122.15
1	A	541	ILE	CA-C-N	-7.63	110.52	120.44
1	A	541	ILE	C-N-CA	-7.63	110.52	120.44
1	B	569	SER	O-C-N	-7.59	113.95	123.06
1	A	535	LEU	O-C-N	7.52	130.15	122.03
1	A	629	SER	O-C-N	7.44	129.74	122.07
1	A	672	GLY	O-C-N	7.40	129.29	122.19
1	B	588	GLY	CA-C-N	-7.35	109.98	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	588	GLY	C-N-CA	-7.35	109.98	120.42
1	A	263	ILE	O-C-N	-7.33	116.75	121.37
1	A	668	LEU	O-C-N	-7.32	113.80	122.15
1	B	783	LYS	CA-C-N	-7.26	109.98	120.29
1	B	783	LYS	C-N-CA	-7.26	109.98	120.29
1	B	673	ALA	O-C-N	7.22	129.77	122.12
1	B	575	LEU	O-C-N	7.15	129.82	122.09
2	C	83	THR	N-CA-C	7.15	122.17	113.17
1	A	553	LEU	O-C-N	7.07	129.35	122.07
1	B	535	LEU	O-C-N	7.07	129.66	122.03
1	A	637	MET	CA-C-N	7.03	130.27	120.29
1	A	637	MET	C-N-CA	7.03	130.27	120.29
1	B	630	GLU	O-C-N	6.97	130.85	122.27
2	D	58	LYS	O-C-N	-6.95	115.50	123.42
1	B	551	VAL	O-C-N	6.94	131.24	122.57
1	A	659	LEU	O-C-N	6.93	130.33	122.22
1	B	637	MET	CA-C-N	6.91	130.10	120.29
1	B	637	MET	C-N-CA	6.91	130.10	120.29
1	A	630	GLU	O-C-N	6.89	130.75	122.27
1	B	665	ALA	O-C-N	-6.87	114.84	122.12
1	A	545	VAL	O-C-N	-6.86	114.77	121.83
1	A	381	LYS	O-C-N	6.85	130.69	122.68
1	A	573	SER	N-CA-CB	6.84	121.99	111.18
1	A	552	ALA	CA-C-N	-6.83	111.56	120.44
1	A	552	ALA	C-N-CA	-6.83	111.56	120.44
1	B	548	ILE	O-C-N	6.77	128.54	121.91
1	A	689	ALA	O-C-N	-6.74	113.33	122.36
1	A	786	THR	O-C-N	6.72	128.99	122.07
1	B	552	ALA	CA-C-N	-6.71	111.72	120.44
1	B	552	ALA	C-N-CA	-6.71	111.72	120.44
1	B	633	ILE	O-C-N	6.70	128.48	121.91
1	B	668	LEU	O-C-N	-6.68	114.54	122.15
1	B	333	SER	O-C-N	6.62	131.76	123.15
2	D	60	VAL	CA-C-N	6.62	131.86	122.72
2	D	60	VAL	C-N-CA	6.62	131.86	122.72
1	A	96	ILE	O-C-N	-6.59	116.21	123.20
1	A	784	SER	CA-C-N	-6.58	112.14	120.56
1	A	784	SER	C-N-CA	-6.58	112.14	120.56
1	B	287	VAL	CA-C-N	6.54	126.31	120.10
1	B	287	VAL	C-N-CA	6.54	126.31	120.10
1	B	754	PHE	CA-C-N	-6.54	111.01	120.29
1	B	754	PHE	C-N-CA	-6.54	111.01	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	689	ALA	O-C-N	-6.52	113.62	122.36
1	B	614	THR	O-C-N	6.52	130.75	122.28
1	A	591	THR	O-C-N	6.50	129.01	122.12
1	A	547	PHE	O-C-N	-6.48	114.76	122.15
1	A	675	VAL	CA-C-N	-6.46	111.63	120.28
1	A	675	VAL	C-N-CA	-6.46	111.63	120.28
1	B	630	GLU	CA-C-N	-6.43	111.66	120.28
1	B	630	GLU	C-N-CA	-6.43	111.66	120.28
1	A	754	PHE	CA-C-N	-6.40	111.20	120.29
1	A	754	PHE	C-N-CA	-6.40	111.20	120.29
1	A	630	GLU	CA-C-N	-6.38	111.73	120.28
1	A	630	GLU	C-N-CA	-6.38	111.73	120.28
1	A	333	SER	O-C-N	6.35	131.40	123.15
1	B	764	ALA	O-C-N	6.31	129.34	122.15
1	B	591	THR	O-C-N	6.27	128.77	122.12
1	B	662	PHE	O-C-N	-6.27	115.47	122.12
1	B	287	VAL	O-C-N	-6.21	116.72	123.18
1	B	703	SER	O-C-N	6.19	132.91	123.00
1	B	786	THR	O-C-N	6.19	128.45	122.07
1	A	658	HIS	O-C-N	6.18	130.90	122.37
1	A	764	ALA	O-C-N	6.18	129.20	122.15
1	A	216	LEU	O-C-N	-6.17	116.08	123.31
1	A	668	LEU	CA-C-N	6.16	129.04	120.29
1	A	668	LEU	C-N-CA	6.16	129.04	120.29
1	A	703	SER	O-C-N	6.16	132.86	123.00
1	A	614	THR	O-C-N	6.14	130.76	122.59
1	A	535	LEU	CA-C-N	-6.13	112.10	120.44
1	A	535	LEU	C-N-CA	-6.13	112.10	120.44
1	A	593	ILE	O-C-N	6.09	127.78	121.87
1	A	534	TYR	O-C-N	6.08	130.47	123.29
1	B	41	VAL	O-C-N	6.07	129.87	122.95
1	A	615	GLY	O-C-N	-6.03	116.38	123.55
1	A	591	THR	CA-C-N	-6.02	113.30	119.98
1	A	591	THR	C-N-CA	-6.02	113.30	119.98
1	B	658	HIS	O-C-N	6.01	130.67	122.37
1	A	379	GLN	O-C-N	6.01	130.44	123.17
1	B	545	VAL	O-C-N	-6.00	115.65	121.83
1	B	333	SER	CA-C-N	-5.99	114.84	123.28
1	B	333	SER	C-N-CA	-5.99	114.84	123.28
1	A	377	ILE	O-C-N	-5.95	115.82	122.66
1	B	32	PRO	N-CA-CB	-5.95	97.82	102.28
1	B	659	LEU	O-C-N	5.95	129.18	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	35	CYS	O-C-N	5.94	130.49	122.59
1	B	537	GLY	O-C-N	-5.93	114.98	122.70
1	B	817	ARG	N-CA-C	-5.91	104.17	111.33
1	A	547	PHE	CA-C-N	5.91	128.00	120.56
1	A	547	PHE	C-N-CA	5.91	128.00	120.56
1	B	398	ARG	O-C-N	-5.87	112.40	122.20
1	B	807	LYS	CB-CA-C	-5.86	101.87	110.95
1	B	664	VAL	CA-C-N	5.85	128.12	120.28
1	B	664	VAL	C-N-CA	5.85	128.12	120.28
1	A	704	LEU	N-CA-C	-5.85	106.05	112.72
1	B	704	LEU	N-CA-C	-5.85	106.05	112.72
1	A	55	LEU	O-C-N	5.83	129.50	122.85
1	B	593	ILE	O-C-N	5.82	127.52	121.87
1	A	610	ILE	O-C-N	5.81	127.81	121.83
1	B	535	LEU	CA-C-N	-5.77	112.59	120.44
1	B	535	LEU	C-N-CA	-5.77	112.59	120.44
1	A	785	VAL	O-C-N	5.76	127.89	121.90
1	B	591	THR	CA-C-N	-5.76	113.58	119.98
1	B	591	THR	C-N-CA	-5.76	113.58	119.98
1	B	369	GLU	O-C-N	5.76	130.15	123.30
1	B	665	ALA	CA-C-N	5.75	127.92	120.44
1	B	665	ALA	C-N-CA	5.75	127.92	120.44
2	D	102	LYS	O-C-N	5.73	129.91	123.27
1	B	551	VAL	CA-C-N	-5.69	112.66	120.28
1	B	551	VAL	C-N-CA	-5.69	112.66	120.28
1	A	381	LYS	CA-C-N	-5.68	113.06	120.44
1	A	381	LYS	C-N-CA	-5.68	113.06	120.44
1	B	677	GLY	O-C-N	5.67	127.69	122.19
1	B	547	PHE	O-C-N	-5.66	115.70	122.15
1	A	615	GLY	N-CA-C	5.66	119.83	110.55
1	B	595	THR	O-C-N	5.65	128.19	122.09
1	B	615	GLY	N-CA-C	5.64	119.80	110.55
1	A	634	PHE	O-C-N	5.63	128.09	122.12
1	B	549	PHE	O-C-N	5.63	128.09	122.12
1	B	668	LEU	CA-C-N	5.63	128.28	120.29
1	B	668	LEU	C-N-CA	5.63	128.28	120.29
1	B	634	PHE	O-C-N	5.59	128.04	122.12
1	B	216	LEU	O-C-N	-5.56	116.81	123.31
1	B	398	ARG	CA-C-N	5.53	131.67	122.54
1	B	398	ARG	C-N-CA	5.53	131.67	122.54
1	B	51	VAL	CA-C-N	-5.53	114.56	120.03
1	B	51	VAL	C-N-CA	-5.53	114.56	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	672	GLY	CA-C-N	-5.52	112.88	120.28
1	B	672	GLY	C-N-CA	-5.52	112.88	120.28
1	B	615	GLY	O-C-N	-5.50	117.00	123.55
1	A	369	GLU	O-C-N	5.50	129.84	123.30
1	A	767	SER	CA-C-N	5.50	130.26	122.24
1	A	767	SER	C-N-CA	5.50	130.26	122.24
1	B	40	ARG	O-C-N	5.48	129.60	123.40
1	A	398	ARG	O-C-N	-5.48	113.05	122.20
1	B	764	ALA	CA-C-N	-5.46	113.34	120.44
1	B	764	ALA	C-N-CA	-5.46	113.34	120.44
1	A	658	HIS	CA-C-N	-5.46	112.42	120.28
1	A	658	HIS	C-N-CA	-5.46	112.42	120.28
1	B	595	THR	CA-C-N	-5.44	113.36	120.44
1	B	595	THR	C-N-CA	-5.44	113.36	120.44
1	A	542	ARG	O-C-N	-5.42	116.49	122.07
1	B	785	VAL	O-C-N	5.42	127.54	121.90
1	A	604	ARG	O-C-N	-5.42	115.28	121.99
1	A	786	THR	CA-C-N	-5.39	113.05	120.28
1	A	786	THR	C-N-CA	-5.39	113.05	120.28
1	A	688	SER	O-C-N	-5.39	115.53	122.21
1	B	600	VAL	O-C-N	-5.39	116.28	121.83
1	A	659	LEU	CA-C-N	-5.38	112.66	120.29
1	A	659	LEU	C-N-CA	-5.38	112.66	120.29
1	A	544	THR	O-C-N	-5.37	116.29	122.09
1	B	621	ALA	O-C-N	5.36	127.81	122.12
2	D	56	SER	CA-C-N	5.35	131.74	122.64
2	D	56	SER	C-N-CA	5.35	131.74	122.64
1	B	387	GLY	O-C-N	-5.33	115.77	122.70
1	B	817	ARG	CA-C-N	-5.33	112.72	120.29
1	B	817	ARG	C-N-CA	-5.33	112.72	120.29
1	A	677	GLY	O-C-N	5.32	127.35	122.19
1	B	673	ALA	CA-C-N	-5.32	112.73	120.29
1	B	673	ALA	C-N-CA	-5.32	112.73	120.29
1	B	751	TRP	O-C-N	5.32	127.75	122.12
1	B	57	ALA	N-CA-C	-5.31	106.38	112.92
1	B	658	HIS	CA-C-N	-5.30	112.65	120.28
1	B	658	HIS	C-N-CA	-5.30	112.65	120.28
1	B	51	VAL	O-C-N	5.29	126.89	121.07
1	A	660	LYS	O-C-N	5.29	128.18	122.15
2	D	58	LYS	CA-C-N	5.27	130.58	122.93
2	D	58	LYS	C-N-CA	5.27	130.58	122.93
1	B	569	SER	CA-C-N	5.24	130.87	121.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	569	SER	C-N-CA	5.24	130.87	121.76
1	B	742	GLN	O-C-N	5.23	127.66	122.12
2	D	103	LEU	O-C-N	-5.21	116.71	122.86
1	A	534	TYR	CA-C-N	-5.21	113.55	120.63
1	A	534	TYR	C-N-CA	-5.21	113.55	120.63
1	B	34	SER	O-C-N	5.21	129.33	122.30
1	B	675	VAL	O-C-N	5.18	127.29	121.90
1	A	263	ILE	CA-C-N	5.18	125.12	119.78
1	A	263	ILE	C-N-CA	5.18	125.12	119.78
1	B	547	PHE	CA-C-N	5.17	127.07	120.56
1	B	547	PHE	C-N-CA	5.17	127.07	120.56
1	B	636	LEU	O-C-N	-5.13	116.21	122.22
1	B	690	SER	O-C-N	-5.12	118.43	121.71
1	A	398	ARG	CA-C-N	5.12	130.98	122.54
1	A	398	ARG	C-N-CA	5.12	130.98	122.54
2	D	57	SER	O-C-N	5.11	128.97	123.10
1	A	764	ALA	CA-C-N	-5.10	113.44	120.28
1	A	764	ALA	C-N-CA	-5.10	113.44	120.28
1	B	548	ILE	CA-C-N	-5.09	113.45	120.28
1	B	548	ILE	C-N-CA	-5.09	113.45	120.28
1	A	751	TRP	O-C-N	5.08	127.50	122.12
2	D	80	SER	O-C-N	-5.04	117.11	123.27
1	A	255	PHE	O-C-N	5.04	128.24	121.99
1	A	96	ILE	CA-C-N	5.04	127.65	120.49
1	A	96	ILE	C-N-CA	5.04	127.65	120.49
1	B	741	SER	O-C-N	5.03	127.25	122.07
1	B	186	LEU	N-CA-CB	5.03	119.87	111.53
1	A	749	VAL	O-C-N	-5.01	116.67	121.83

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	806	PRO	Mainchain

5.2 Too-close contacts (i)

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	4931	0	4290	131	0
1	B	4964	0	4332	128	0
2	C	783	0	765	42	0
2	D	782	0	772	44	0
All	All	11460	0	10159	333	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 15.

All (333) 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)
2:C:45:VAL:CG1	2:C:59:MET:HG2	1.68	1.23
1:B:29:CYS:SG	1:B:35:CYS:CB	2.28	1.21
2:C:131:CYS:SG	2:D:131:CYS:SG	1.48	1.18
1:B:412:LEU:O	1:B:412:LEU:HD12	1.44	1.17
1:A:412:LEU:HD12	1:A:412:LEU:O	1.44	1.16
2:C:99:GLN:HB2	2:C:127:HIS:CD2	1.80	1.15
2:C:45:VAL:HG11	2:C:59:MET:HG2	1.19	1.13
1:B:207:HIS:CE1	2:D:59:MET:HG3	1.85	1.11
1:A:49:THR:HA	1:A:69:ILE:HG12	1.31	1.07
1:B:29:CYS:SG	1:B:35:CYS:SG	1.21	1.07
1:A:468:TYR:HA	1:A:471:CYS:HB2	1.08	1.06
2:D:55:CYS:HA	2:D:110:CYS:HA	1.09	1.06
1:B:207:HIS:CE1	2:D:59:MET:CG	2.40	1.05
2:C:99:GLN:HB2	2:C:127:HIS:HD2	1.08	1.03
1:A:334:ILE:HB	1:A:359:PRO:HG3	1.39	1.02
1:A:468:TYR:CA	1:A:471:CYS:HB2	1.91	1.00
1:B:572:SER:O	1:B:576:PHE:N	1.95	0.99
1:B:207:HIS:HE1	2:D:59:MET:HG3	1.20	0.99
2:C:131:CYS:CB	2:D:131:CYS:SG	2.50	0.99
2:D:85:LEU:HD23	2:D:86:LYS:O	1.65	0.97
1:B:819:VAL:O	1:B:820:THR:O	1.81	0.96
2:D:55:CYS:HA	2:D:110:CYS:CA	1.93	0.96
1:A:474:TRP:HZ3	1:A:522:CYS:H	1.02	0.93
1:A:343:LYS:HE2	1:A:343:LYS:HA	1.52	0.92
2:D:85:LEU:HD23	2:D:86:LYS:N	1.84	0.91
1:B:29:CYS:CB	1:B:35:CYS:SG	2.59	0.90
1:A:782:MET:O	1:A:786:THR:N	2.04	0.89
2:D:85:LEU:CD2	2:D:86:LYS:O	2.21	0.88
1:A:781:ILE:O	1:A:785:VAL:N	2.08	0.86
1:A:468:TYR:HA	1:A:471:CYS:CB	2.01	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:TYR:HB2	1:A:469:GLN:HG2	1.59	0.85
1:A:467:ALA:HA	1:A:470:CYS:HB2	1.60	0.84
1:A:783:LYS:O	1:A:787:LEU:N	2.10	0.83
2:C:45:VAL:HG11	2:C:59:MET:CG	2.08	0.81
2:D:54:LYS:HB2	2:D:111:SER:OG	1.80	0.81
1:A:162:ASP:OD1	1:A:186:LEU:CD1	2.30	0.80
1:B:706:PHE:HA	1:B:709:THR:CB	2.10	0.80
2:C:131:CYS:SG	2:D:131:CYS:CB	2.70	0.79
2:D:85:LEU:HD23	2:D:86:LYS:H	1.45	0.79
2:C:58:LYS:HE2	2:C:106:LEU:HD11	1.65	0.78
2:C:100:THR:O	2:C:124:LEU:HB2	1.84	0.78
2:C:102:LYS:O	2:C:121:ARG:HA	1.85	0.77
2:D:55:CYS:CA	2:D:110:CYS:HA	2.03	0.76
1:A:49:THR:HG23	1:A:69:ILE:HG23	1.67	0.75
1:B:705:GLY:O	1:B:709:THR:N	2.21	0.74
1:A:162:ASP:OD1	1:A:186:LEU:HD13	1.87	0.74
1:A:806:PRO:HB2	1:A:810:GLU:CB	2.17	0.74
1:B:32:PRO:CB	1:B:46:LYS:HE2	2.18	0.74
1:B:572:SER:HA	1:B:575:LEU:CB	2.18	0.73
1:B:34:SER:O	1:B:35:CYS:SG	2.46	0.73
1:B:334:ILE:HD11	1:B:355:ILE:HD13	1.70	0.73
1:B:247:LEU:O	1:B:271:ASN:ND2	2.22	0.72
1:B:321:LEU:O	1:B:344:MET:HB3	1.90	0.72
1:A:334:ILE:HD11	1:A:355:ILE:HD13	1.71	0.72
2:C:99:GLN:CB	2:C:127:HIS:CD2	2.69	0.71
1:A:447:LEU:O	1:A:469:GLN:NE2	2.23	0.71
1:B:34:SER:C	1:B:36:ASP:H	1.98	0.71
1:B:274:LEU:O	1:B:297:ASP:HB2	1.90	0.71
2:D:53:TYR:C	2:D:55:CYS:H	1.98	0.71
2:C:58:LYS:HE2	2:C:106:LEU:CD1	2.20	0.70
1:B:412:LEU:O	1:B:412:LEU:CD1	2.33	0.70
2:C:110:CYS:SG	2:C:116:LEU:HD23	2.32	0.70
1:A:466:TYR:HB2	1:A:469:GLN:CG	2.21	0.69
1:A:465:PRO:HG2	1:A:469:GLN:HG3	1.74	0.69
2:C:58:LYS:CE	2:C:106:LEU:HD11	2.24	0.68
1:B:769:ALA:O	1:B:773:THR:N	2.27	0.67
1:B:34:SER:C	1:B:36:ASP:N	2.52	0.67
1:B:29:CYS:SG	1:B:35:CYS:HB3	2.31	0.67
2:C:58:LYS:HE2	2:C:106:LEU:CG	2.25	0.66
2:C:81:PHE:HE2	2:D:48:ILE:HG23	1.60	0.66
1:A:464:VAL:HB	1:A:465:PRO:HD2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:PRO:O	1:B:575:LEU:N	2.29	0.66
1:A:474:TRP:CE3	1:A:522:CYS:SG	2.87	0.66
2:C:99:GLN:CB	2:C:127:HIS:HD2	1.96	0.65
1:A:306:ALA:HB3	1:A:329:THR:HG22	1.77	0.65
1:A:162:ASP:OD1	1:A:186:LEU:HD12	1.96	0.65
1:B:462:LEU:CD2	1:B:473:PHE:CD1	2.80	0.65
2:D:53:TYR:HB3	2:D:110:CYS:HB3	1.79	0.65
2:D:85:LEU:CD2	2:D:86:LYS:H	2.10	0.65
1:A:466:TYR:H	1:A:469:GLN:HG3	1.61	0.64
1:A:52:PRO:HB2	1:A:55:LEU:HD11	1.79	0.64
2:C:38:ARG:O	2:C:67:GLY:HA3	1.97	0.64
1:A:412:LEU:O	1:A:412:LEU:CD1	2.33	0.64
2:C:94:HIS:HB3	2:C:128:CYS:SG	2.38	0.64
1:B:689:ALA:HB3	1:B:697:PRO:HG2	1.79	0.64
1:A:302:VAL:HA	1:A:325:THR:HB	1.80	0.64
1:A:689:ALA:HB3	1:A:697:PRO:HG2	1.79	0.63
2:D:56:SER:N	2:D:109:ARG:O	2.25	0.63
1:A:320:HIS:HA	1:A:344:MET:HE3	1.80	0.63
1:A:783:LYS:O	1:A:787:LEU:CB	2.46	0.63
1:A:29:CYS:SG	1:A:30:ALA:N	2.72	0.63
1:A:304:ARG:HG2	1:A:327:THR:CG2	2.29	0.62
1:A:703:SER:C	1:A:705:GLY:H	2.06	0.62
1:B:471:CYS:O	1:B:476:CYS:HA	1.99	0.62
1:A:120:VAL:O	1:A:121:PRO:C	2.42	0.62
1:A:412:LEU:CD1	1:A:415:ILE:HG21	2.29	0.62
1:B:275:ARG:HG2	1:B:297:ASP:HB3	1.80	0.62
1:B:55:LEU:HD12	1:B:80:PHE:CZ	2.35	0.62
2:C:58:LYS:CE	2:C:106:LEU:HD21	2.29	0.62
1:A:275:ARG:HG2	1:A:297:ASP:HB3	1.81	0.61
1:A:459:LEU:HD21	1:A:462:LEU:HB2	1.82	0.61
1:A:474:TRP:HE3	1:A:522:CYS:HG	1.45	0.61
1:B:275:ARG:O	1:B:299:HIS:CE1	2.53	0.61
2:D:53:TYR:C	2:D:55:CYS:N	2.58	0.61
2:C:64:ARG:NH1	2:C:66:GLU:OE1	2.25	0.61
1:B:315:LEU:HD13	1:B:342:GLN:HE22	1.65	0.61
1:B:797:ASN:N	1:B:798:PRO:HD2	2.16	0.61
1:A:784:SER:O	1:A:788:ILE:N	2.31	0.60
1:B:412:LEU:CD1	1:B:415:ILE:HG21	2.30	0.60
1:B:572:SER:C	1:B:575:LEU:H	2.09	0.60
1:A:474:TRP:HZ3	1:A:522:CYS:N	1.86	0.60
1:A:692:LEU:HD12	1:A:694:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:LEU:HD23	1:B:247:LEU:HD13	1.85	0.59
2:D:56:SER:OG	2:D:109:ARG:O	2.11	0.59
1:A:675:VAL:O	1:A:679:PHE:N	2.30	0.58
1:A:345:LEU:O	1:A:367:LEU:HA	2.03	0.58
1:A:55:LEU:HD12	1:A:80:PHE:CZ	2.38	0.58
1:B:819:VAL:O	1:B:820:THR:C	2.46	0.58
1:A:247:LEU:O	1:A:271:ASN:ND2	2.36	0.58
2:C:103:LEU:HD12	2:C:121:ARG:HG2	1.84	0.58
1:A:227:LEU:HD23	1:A:247:LEU:HD13	1.86	0.58
1:B:627:PHE:O	1:B:631:SER:CB	2.51	0.58
1:B:275:ARG:O	1:B:299:HIS:ND1	2.37	0.58
1:B:694:LEU:HD12	1:B:697:PRO:HB3	1.86	0.58
1:A:474:TRP:HE3	1:A:522:CYS:SG	2.24	0.58
1:B:315:LEU:HB3	1:B:342:GLN:NE2	2.18	0.58
2:C:58:LYS:HE3	2:C:106:LEU:HD21	1.85	0.58
2:D:50:HIS:CG	2:D:51:PRO:HD2	2.39	0.57
1:A:116:GLN:C	1:A:117:LEU:HD12	2.30	0.57
1:A:632:ALA:O	1:A:636:LEU:N	2.31	0.57
1:A:694:LEU:HD12	1:A:697:PRO:HB3	1.86	0.57
1:A:627:PHE:O	1:A:631:SER:CB	2.52	0.57
1:B:35:CYS:HA	1:B:41:VAL:HG22	1.86	0.57
1:A:38:ASP:O	1:A:40:ARG:HG3	2.04	0.57
1:B:415:ILE:O	1:B:436:LEU:HD23	2.05	0.57
1:B:70:THR:HG22	1:B:92:ASP:HB3	1.87	0.56
1:B:703:SER:C	1:B:705:GLY:H	2.06	0.56
2:C:58:LYS:HG3	2:C:108:LEU:CD1	2.35	0.56
1:B:120:VAL:HG23	1:B:141:ILE:HG21	1.88	0.56
1:B:623:PHE:O	1:B:627:PHE:CB	2.54	0.56
1:B:692:LEU:HB2	1:B:694:LEU:HG	1.86	0.56
1:A:692:LEU:HB2	1:A:694:LEU:HG	1.88	0.55
2:D:103:LEU:HB2	2:D:121:ARG:CZ	2.36	0.55
2:C:58:LYS:HE2	2:C:106:LEU:HG	1.87	0.55
1:A:759:PHE:CB	1:A:793:PRO:HG3	2.37	0.55
1:B:351:SER:O	1:B:353:ASN:ND2	2.39	0.55
1:B:692:LEU:HD12	1:B:694:LEU:HD11	1.88	0.55
1:B:816:LYS:O	1:B:819:VAL:N	2.40	0.55
1:B:800:LEU:O	1:B:804:PHE:CB	2.56	0.54
2:C:49:SER:HA	2:C:108:LEU:HD21	1.88	0.54
1:B:49:THR:C	1:B:69:ILE:HG12	2.33	0.54
1:A:769:ALA:O	1:A:773:THR:N	2.41	0.54
1:B:386:GLN:HA	1:B:411:THR:OG1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:LEU:O	1:B:353:ASN:ND2	2.39	0.53
1:B:302:VAL:HA	1:B:325:THR:HB	1.89	0.53
1:A:304:ARG:HG2	1:A:327:THR:HG22	1.89	0.53
1:A:623:PHE:O	1:A:627:PHE:CB	2.56	0.53
1:B:680:PRO:C	1:B:682:PHE:H	2.16	0.53
1:A:439:LEU:HB3	1:A:459:LEU:HD11	1.91	0.53
2:C:102:LYS:O	2:C:121:ARG:CA	2.55	0.53
1:B:32:PRO:CA	1:B:46:LYS:HE2	2.38	0.53
1:B:706:PHE:C	1:B:709:THR:H	2.17	0.53
1:B:438:GLN:HG3	1:B:461:SER:HB3	1.91	0.52
1:B:255:PHE:O	1:B:258:ASN:ND2	2.41	0.52
1:B:159:TRP:HA	1:B:183:THR:HG23	1.91	0.52
1:B:804:PHE:C	1:B:806:PRO:HD3	2.35	0.52
1:A:306:ALA:O	1:A:329:THR:HA	2.09	0.52
1:B:804:PHE:O	1:B:806:PRO:HD3	2.10	0.52
2:D:85:LEU:HD21	2:D:86:LYS:O	2.05	0.51
1:A:70:THR:HG22	1:A:92:ASP:HB3	1.93	0.51
1:A:320:HIS:CA	1:A:344:MET:HE3	2.40	0.51
1:A:706:PHE:O	1:A:710:LEU:N	2.33	0.51
1:B:306:ALA:HB3	1:B:329:THR:HG22	1.93	0.51
1:B:368:GLU:O	1:B:391:LEU:HD12	2.11	0.51
2:C:58:LYS:HG3	2:C:108:LEU:HD12	1.92	0.51
2:D:52:LEU:O	2:D:53:TYR:HB2	2.10	0.51
1:A:312:PHE:CZ	1:A:338:LEU:HD22	2.46	0.50
2:C:116:LEU:H	2:C:116:LEU:HD22	1.76	0.50
1:B:548:ILE:O	1:B:552:ALA:N	2.36	0.50
1:B:631:SER:O	1:B:635:LEU:N	2.34	0.50
1:A:42:ASP:OD1	1:A:42:ASP:N	2.45	0.50
2:D:97:ARG:N	2:D:127:HIS:O	2.36	0.50
1:B:31:ALA:HB3	1:B:32:PRO:HD3	1.93	0.50
1:A:201:SER:O	1:A:226:ASN:ND2	2.45	0.49
1:B:743:SER:O	1:B:747:LYS:N	2.39	0.49
1:A:338:LEU:C	1:A:340:GLN:H	2.20	0.49
1:B:255:PHE:CZ	1:B:279:LEU:HB3	2.47	0.49
1:B:759:PHE:CB	1:B:793:PRO:HG3	2.42	0.49
1:A:468:TYR:CD1	1:A:609:GLY:HA3	2.48	0.49
2:D:85:LEU:HD23	2:D:86:LYS:C	2.35	0.49
1:A:49:THR:HG22	1:A:50:ALA:H	1.77	0.49
1:A:275:ARG:O	1:A:299:HIS:CE1	2.66	0.49
2:D:53:TYR:CE1	2:D:114:MET:SD	3.06	0.49
1:B:279:LEU:HD13	1:B:284:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:LEU:O	1:B:414:PRO:O	2.30	0.49
1:A:55:LEU:HD12	1:A:80:PHE:HZ	1.78	0.48
2:D:50:HIS:CD2	2:D:51:PRO:HD2	2.48	0.48
1:A:88:LEU:HB2	1:A:112:LEU:HD23	1.96	0.48
1:B:279:LEU:HD12	1:B:279:LEU:O	2.14	0.48
1:B:459:LEU:HD21	1:B:462:LEU:HB2	1.94	0.48
2:D:103:LEU:HB2	2:D:121:ARG:NH2	2.29	0.48
1:A:279:LEU:HD12	1:A:279:LEU:O	2.14	0.48
1:A:795:CYS:O	1:A:798:PRO:HG2	2.14	0.48
1:B:726:THR:O	1:B:730:CYS:N	2.46	0.48
1:A:319:VAL:HG12	1:A:341:GLU:HB2	1.95	0.47
1:A:703:SER:C	1:A:705:GLY:N	2.67	0.47
1:A:122:SER:O	1:A:123:GLU:C	2.56	0.47
2:C:102:LYS:HD2	2:C:104:LYS:HG3	1.95	0.47
1:A:464:VAL:HG11	1:A:473:PHE:HB2	1.95	0.47
1:A:468:TYR:HE2	1:A:613:GLU:CB	2.27	0.47
1:B:120:VAL:HG22	1:B:141:ILE:HD13	1.95	0.47
1:A:382:GLU:HA	1:A:407:ARG:HB2	1.96	0.47
1:A:135:ARG:HG2	1:A:159:TRP:CE3	2.49	0.47
1:B:462:LEU:HD22	1:B:473:PHE:CD1	2.49	0.47
2:D:103:LEU:HB2	2:D:121:ARG:NH1	2.30	0.47
1:A:43:CYS:SG	1:A:52:PRO:HG2	2.55	0.47
1:A:52:PRO:HB2	1:A:55:LEU:CD1	2.45	0.47
1:A:803:PHE:O	1:A:806:PRO:HD3	2.15	0.47
1:B:782:MET:O	1:B:786:THR:N	2.28	0.47
1:A:470:CYS:HA	1:A:473:PHE:HB3	1.97	0.47
1:B:32:PRO:O	1:B:33:CYS:SG	2.72	0.47
1:A:438:GLN:HG3	1:A:461:SER:HB3	1.97	0.46
1:B:320:HIS:HA	1:B:344:MET:SD	2.55	0.46
1:B:783:LYS:O	1:B:787:LEU:N	2.31	0.46
1:B:358:LEU:HD11	1:B:377:ILE:HD13	1.98	0.46
2:D:85:LEU:CG	2:D:86:LYS:H	2.28	0.46
1:A:358:LEU:HD21	1:A:372:LEU:HD13	1.98	0.46
1:A:466:TYR:N	1:A:469:GLN:HG3	2.29	0.46
1:B:533:GLU:HG3	1:B:534:TYR:H	1.80	0.46
1:A:773:THR:O	1:A:774:ALA:C	2.59	0.46
1:A:49:THR:HG22	1:A:50:ALA:N	2.30	0.46
1:A:171:HIS:HB3	1:A:172:PRO:HD3	1.98	0.46
2:D:85:LEU:CD2	2:D:86:LYS:N	2.66	0.46
1:A:715:SER:O	1:A:716:LEU:C	2.56	0.46
2:D:53:TYR:O	2:D:55:CYS:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LEU:O	1:A:297:ASP:HB2	2.15	0.46
1:B:744:SER:O	1:B:748:HIS:N	2.37	0.46
2:D:42:HIS:O	2:D:63:ALA:HA	2.16	0.46
1:A:379:GLN:NE2	1:A:381:LYS:HE3	2.31	0.46
1:A:279:LEU:HD13	1:A:284:LEU:HD11	1.98	0.45
1:A:555:PHE:C	1:A:557:LEU:H	2.24	0.45
1:B:171:HIS:HB3	1:B:172:PRO:HD3	1.99	0.45
2:C:41:ARG:HA	2:C:64:ARG:O	2.17	0.45
1:B:417:ASN:HD22	1:B:438:GLN:HB3	1.79	0.45
2:C:109:ARG:HB3	2:C:109:ARG:NH1	2.32	0.45
1:A:772:ILE:C	1:A:774:ALA:H	2.24	0.45
1:A:778:SER:CB	1:A:782:MET:H	2.30	0.45
1:B:55:LEU:HB2	1:B:80:PHE:CE1	2.51	0.45
1:B:462:LEU:HD22	1:B:473:PHE:CG	2.52	0.45
1:A:50:ALA:O	1:A:51:VAL:HG22	2.16	0.45
1:B:593:ILE:O	1:B:597:LEU:CB	2.65	0.45
1:A:307:SER:O	1:A:330:LYS:NZ	2.34	0.45
1:A:31:ALA:HB1	1:A:32:PRO:HD2	1.99	0.44
1:B:135:ARG:HG2	1:B:159:TRP:CE3	2.53	0.44
1:B:364:CYS:HB3	1:B:367:LEU:HB2	1.99	0.44
1:B:462:LEU:HD21	1:B:473:PHE:CE1	2.53	0.44
1:A:697:PRO:C	1:A:699:GLY:H	2.25	0.44
1:A:785:VAL:O	1:A:789:PHE:N	2.39	0.44
1:A:31:ALA:HB1	1:A:32:PRO:CD	2.48	0.44
1:A:307:SER:O	1:A:330:LYS:HG3	2.18	0.44
1:B:781:ILE:O	1:B:785:VAL:N	2.35	0.44
1:A:576:PHE:CB	1:A:639:ALA:HB2	2.48	0.44
1:B:567:CYS:O	1:B:568:THR:C	2.61	0.44
1:B:680:PRO:C	1:B:682:PHE:N	2.75	0.44
1:B:740:ASN:O	1:B:744:SER:N	2.40	0.44
1:B:587:MET:O	1:B:590:TYR:N	2.51	0.44
2:C:78:LEU:HD21	2:C:90:ARG:HE	1.83	0.44
1:A:231:ASP:OD1	1:A:233:ASN:ND2	2.51	0.43
1:B:34:SER:O	1:B:36:ASP:N	2.51	0.43
1:A:415:ILE:O	1:A:436:LEU:HD23	2.18	0.43
1:B:572:SER:O	1:B:575:LEU:N	2.52	0.43
1:A:465:PRO:HG2	1:A:469:GLN:CG	2.46	0.43
1:A:531:PRO:HD2	1:A:691:PRO:HG3	1.99	0.43
1:B:703:SER:C	1:B:705:GLY:N	2.67	0.43
1:A:474:TRP:CZ3	1:A:522:CYS:N	2.73	0.43
2:C:81:PHE:CE2	2:D:48:ILE:HG23	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:VAL:CG1	2:D:59:MET:SD	3.07	0.43
1:B:159:TRP:HA	1:B:183:THR:CG2	2.48	0.43
1:B:470:CYS:SG	1:B:524:PRO:HD2	2.58	0.43
1:B:697:PRO:C	1:B:699:GLY:H	2.26	0.43
2:D:50:HIS:ND1	2:D:53:TYR:HD2	2.17	0.43
1:A:421:SER:O	1:A:423:ASN:ND2	2.52	0.42
1:B:135:ARG:HA	1:B:159:TRP:HB2	2.01	0.42
1:B:205:VAL:HG11	2:D:59:MET:SD	2.59	0.42
1:B:315:LEU:CD1	1:B:342:GLN:HE22	2.31	0.42
1:A:417:ASN:HD22	1:A:438:GLN:HB3	1.84	0.42
1:B:462:LEU:HD21	1:B:473:PHE:CD1	2.53	0.42
1:B:806:PRO:O	1:B:810:GLU:CB	2.68	0.42
2:C:109:ARG:HD2	2:C:109:ARG:O	2.19	0.42
2:D:95:CYS:O	2:D:128:CYS:HA	2.20	0.42
1:A:464:VAL:HG21	1:A:470:CYS:HA	2.02	0.42
2:C:107:ARG:O	2:C:108:LEU:C	2.63	0.42
1:B:207:HIS:HB2	2:D:59:MET:HE1	1.63	0.42
1:A:468:TYR:CE2	1:A:613:GLU:CB	3.02	0.42
1:B:207:HIS:NE2	2:D:59:MET:SD	2.72	0.42
1:B:417:ASN:ND2	1:B:438:GLN:HB3	2.35	0.42
1:B:318:THR:HG22	1:B:321:LEU:HG	2.02	0.41
1:B:55:LEU:HD12	1:B:80:PHE:HZ	1.81	0.41
1:B:694:LEU:HB2	1:B:697:PRO:HB3	2.02	0.41
2:C:116:LEU:HD22	2:C:116:LEU:N	2.35	0.41
2:D:116:LEU:HD12	2:D:116:LEU:HA	1.87	0.41
1:A:303:ILE:HB	1:A:326:LEU:HD23	2.02	0.41
1:A:338:LEU:O	1:A:342:GLN:HG2	2.20	0.41
1:B:155:LEU:HD23	1:B:176:LEU:HD13	2.03	0.41
1:B:528:ALA:HB3	1:B:779:PRO:HB2	2.02	0.41
2:D:43:HIS:HA	2:D:62:LEU:O	2.21	0.41
1:A:135:ARG:HA	1:A:159:TRP:HB2	2.01	0.41
1:A:337:ASN:O	1:A:340:GLN:HB2	2.21	0.41
1:A:338:LEU:C	1:A:340:GLN:N	2.78	0.41
1:A:341:GLU:O	1:A:343:LYS:N	2.53	0.41
1:B:304:ARG:HG2	1:B:327:THR:CG2	2.50	0.41
1:A:382:GLU:HG3	1:A:407:ARG:CB	2.51	0.41
2:C:116:LEU:H	2:C:116:LEU:CD2	2.34	0.41
1:A:357:ASP:O	1:A:359:PRO:HD3	2.20	0.41
1:B:201:SER:O	1:B:226:ASN:ND2	2.54	0.41
2:C:78:LEU:HD11	2:C:90:ARG:HB2	2.01	0.41
1:B:329:THR:OG1	1:B:353:ASN:OD1	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ALA:CB	1:A:55:LEU:HD23	2.51	0.40
1:B:55:LEU:HD12	1:B:80:PHE:CE1	2.56	0.40
1:B:161:ASP:OD1	1:B:161:ASP:N	2.49	0.40
1:B:421:SER:O	1:B:423:ASN:ND2	2.55	0.40
1:B:276:THR:OG1	1:B:299:HIS:HE1	2.04	0.40
2:C:45:VAL:HG12	2:C:59:MET:HG2	1.84	0.40
2:C:46:ASP:OD1	2:C:47:SER:N	2.50	0.40
1:A:35:CYS:O	1:A:35:CYS:SG	2.75	0.40
1:A:382:GLU:HG3	1:A:407:ARG:CG	2.52	0.40
1:A:780:GLU:O	1:A:784:SER:N	2.49	0.40
1:A:312:PHE:CG	1:A:335:PRO:CD	3.04	0.40
1:A:364:CYS:HB3	1:A:367:LEU:HB2	2.02	0.40
1:B:529:PHE:O	1:B:691:PRO:CD	2.70	0.40
1:A:318:THR:HG22	1:A:321:LEU:HG	2.04	0.40
1:B:529:PHE:O	1:B:691:PRO:HD3	2.20	0.40
1:B:694:LEU:O	1:B:697:PRO:HD3	2.22	0.40

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 PDB entries followed by that with respect to all EM entries.

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	713/832 (86%)	649 (91%)	64 (9%)	0	100	100
1	B	721/832 (87%)	667 (92%)	54 (8%)	0	100	100
2	C	98/103 (95%)	91 (93%)	7 (7%)	0	100	100
2	D	97/103 (94%)	91 (94%)	6 (6%)	0	100	100
All	All	1629/1870 (87%)	1498 (92%)	131 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	431/730 (59%)	416 (96%)	15 (4%)	31 58
1	B	434/730 (60%)	430 (99%)	4 (1%)	75 85
2	C	91/96 (95%)	87 (96%)	4 (4%)	24 52
2	D	92/96 (96%)	89 (97%)	3 (3%)	33 60
All	All	1048/1652 (63%)	1022 (98%)	26 (2%)	43 67

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	35	CYS
1	A	36	ASP
1	A	42	ASP
1	A	43	CYS
1	A	48	LEU
1	A	51	VAL
1	A	53	GLU
1	A	123	GLU
1	A	337	ASN
1	A	339	CYS
1	A	442	VAL
1	A	471	CYS
1	A	618	CYS
1	A	693	CYS
1	B	183	THR
1	B	442	VAL
1	B	618	CYS
1	B	693	CYS
2	C	100	THR
2	C	109	ARG
2	C	121	ARG
2	C	126	CYS
2	D	48	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	54	LYS
2	D	126	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	163	ASN
1	A	226	ASN
1	A	236	ASN
1	A	278	HIS
1	A	299	HIS
1	A	311	GLN
1	A	362	ASN
1	A	379	GLN
1	A	386	GLN
1	A	444	ASN
1	B	71	GLN
1	B	116	GLN
1	B	163	ASN
1	B	226	ASN
1	B	233	ASN
1	B	278	HIS
1	B	293	HIS
1	B	299	HIS
1	B	311	GLN
1	B	337	ASN
1	B	342	GLN
1	B	379	GLN
1	B	386	GLN
1	B	444	ASN
2	C	87	GLN
2	C	127	HIS
2	D	43	HIS
2	D	94	HIS

5.3.3 RNA

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.

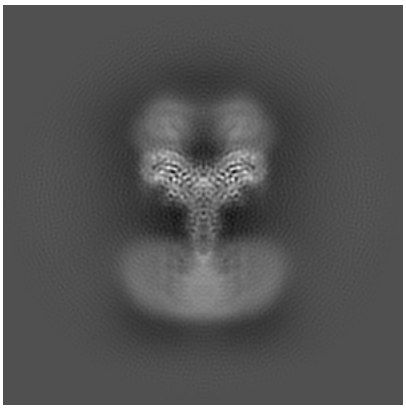
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37875. These allow visual inspection of the internal detail of the map and identification of artifacts.

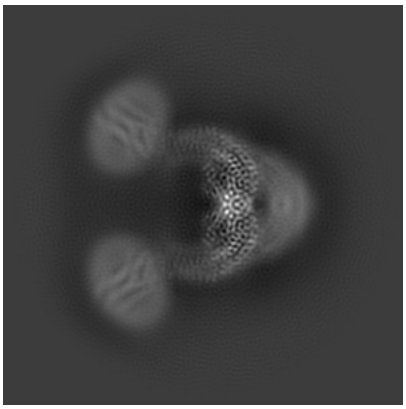
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

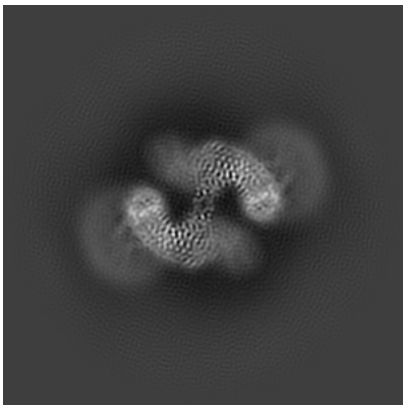
6.1.1 Primary map



X

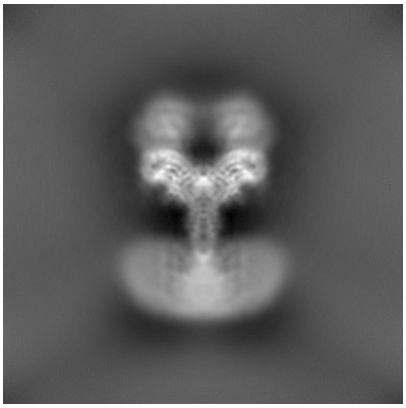


Y

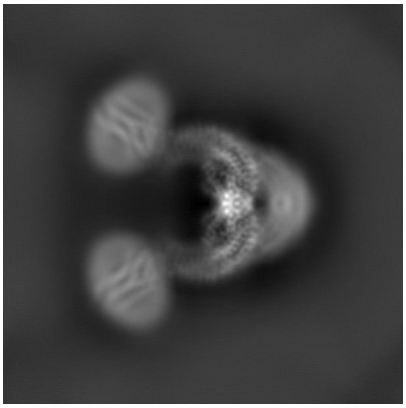


Z

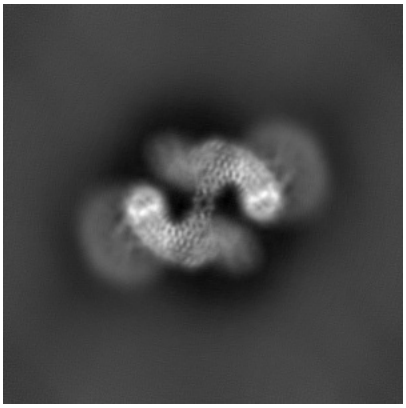
6.1.2 Raw map



X



Y

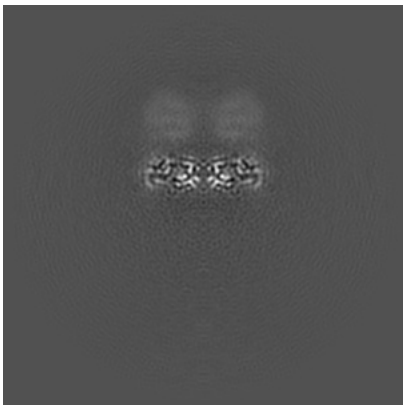


Z

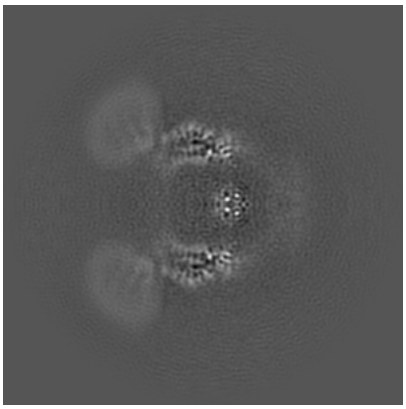
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

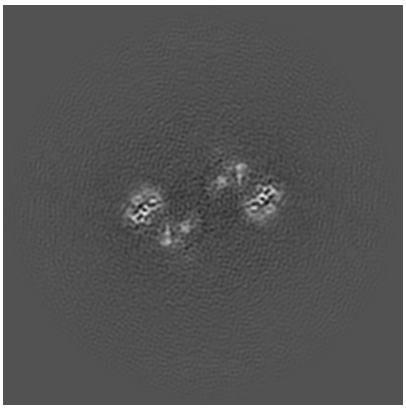
6.2.1 Primary map



X Index: 180

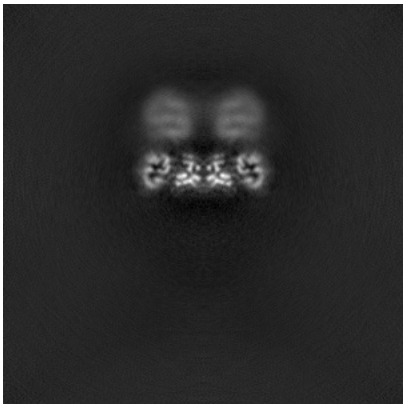


Y Index: 180

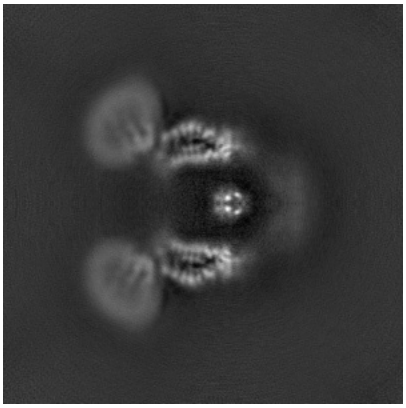


Z Index: 180

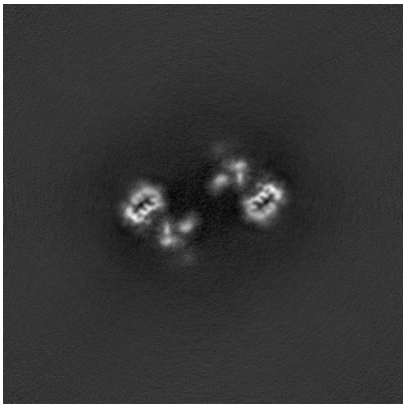
6.2.2 Raw map



X Index: 180



Y Index: 180

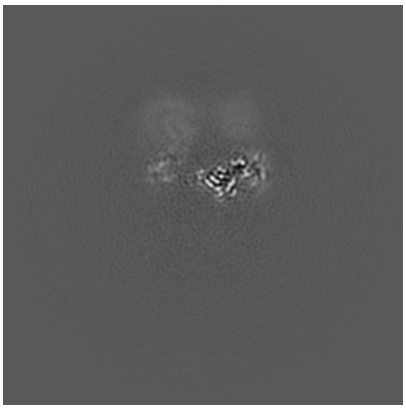


Z Index: 180

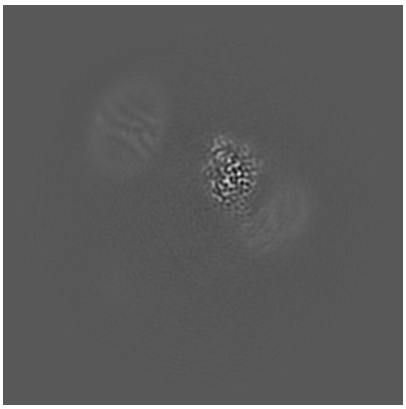
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

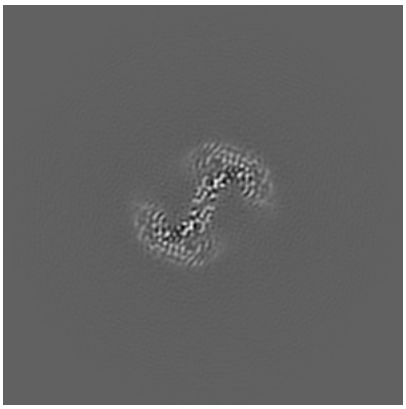
6.3.1 Primary map



X Index: 189

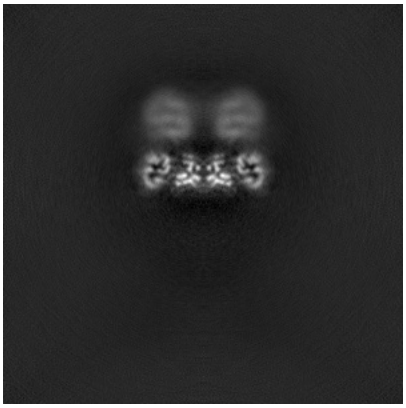


Y Index: 206

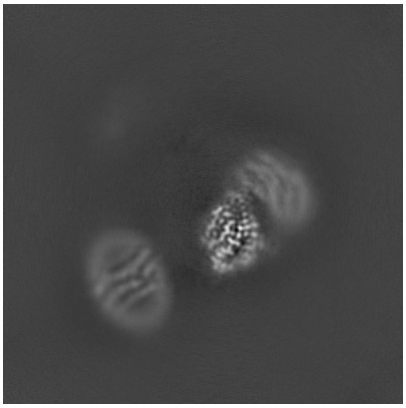


Z Index: 204

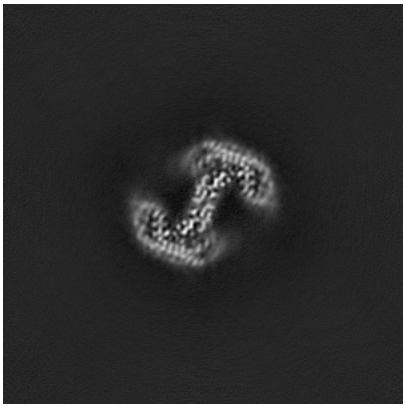
6.3.2 Raw map



X Index: 180



Y Index: 153

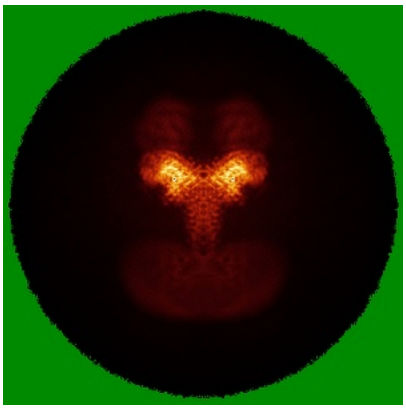


Z Index: 204

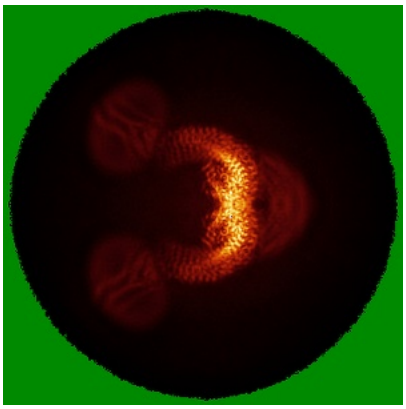
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

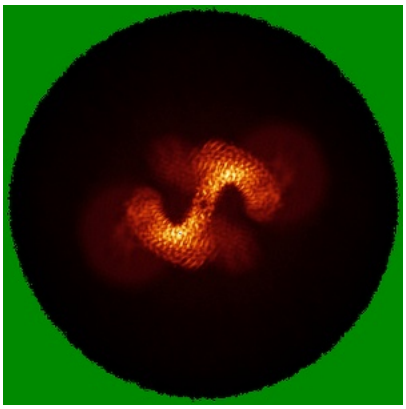
6.4.1 Primary map



X

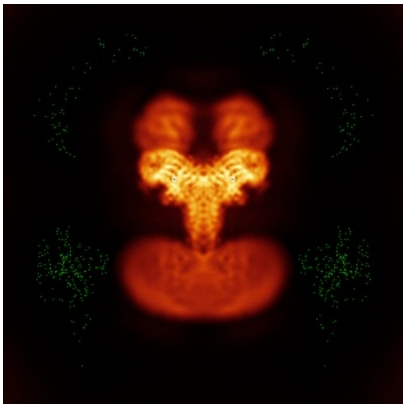


Y

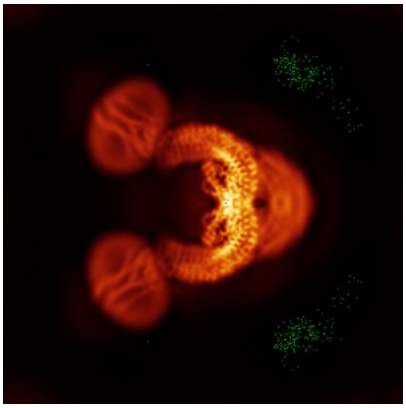


Z

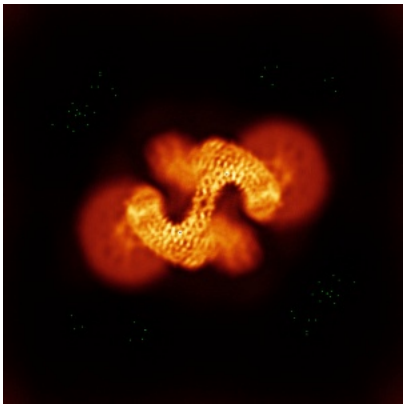
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

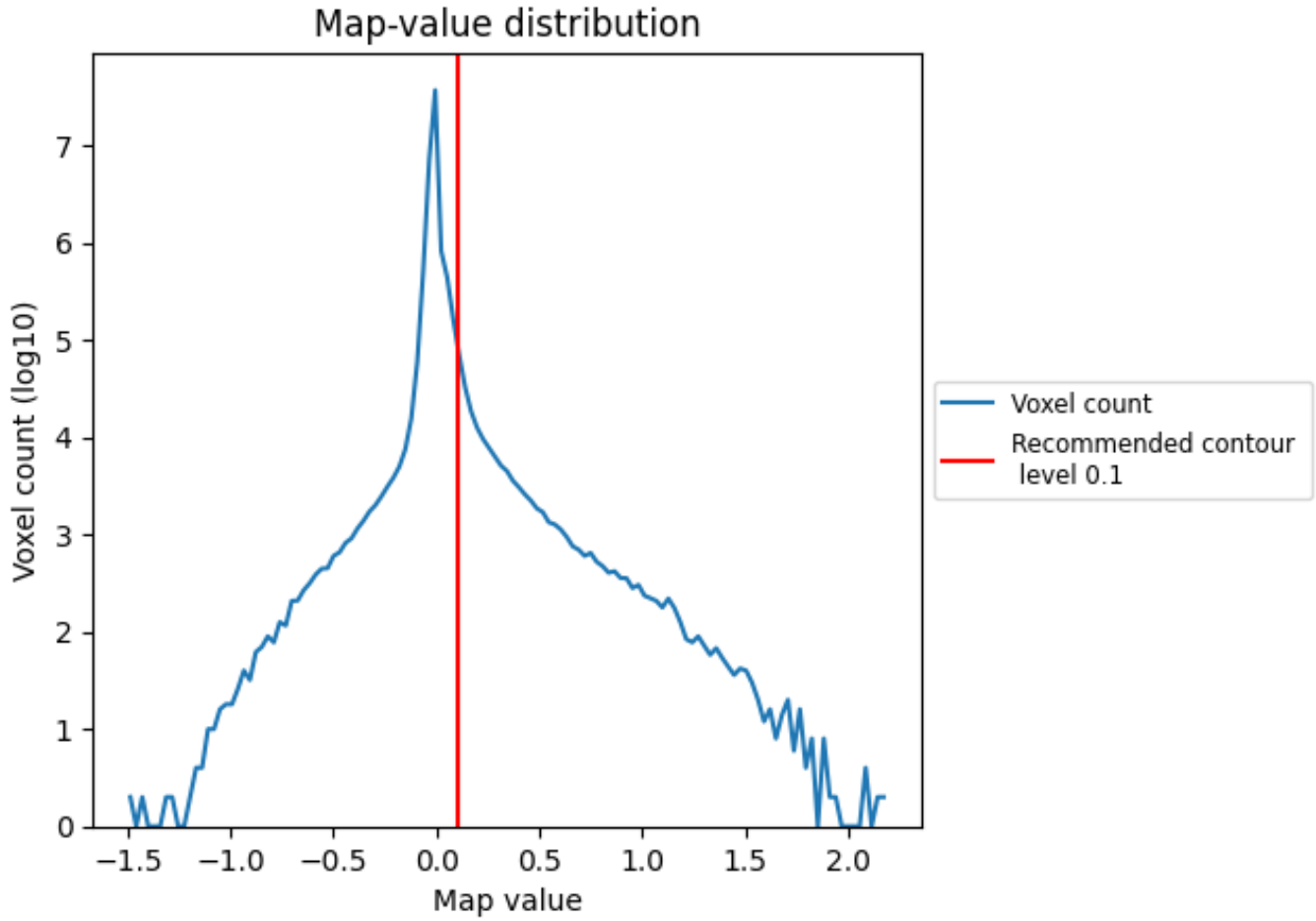
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

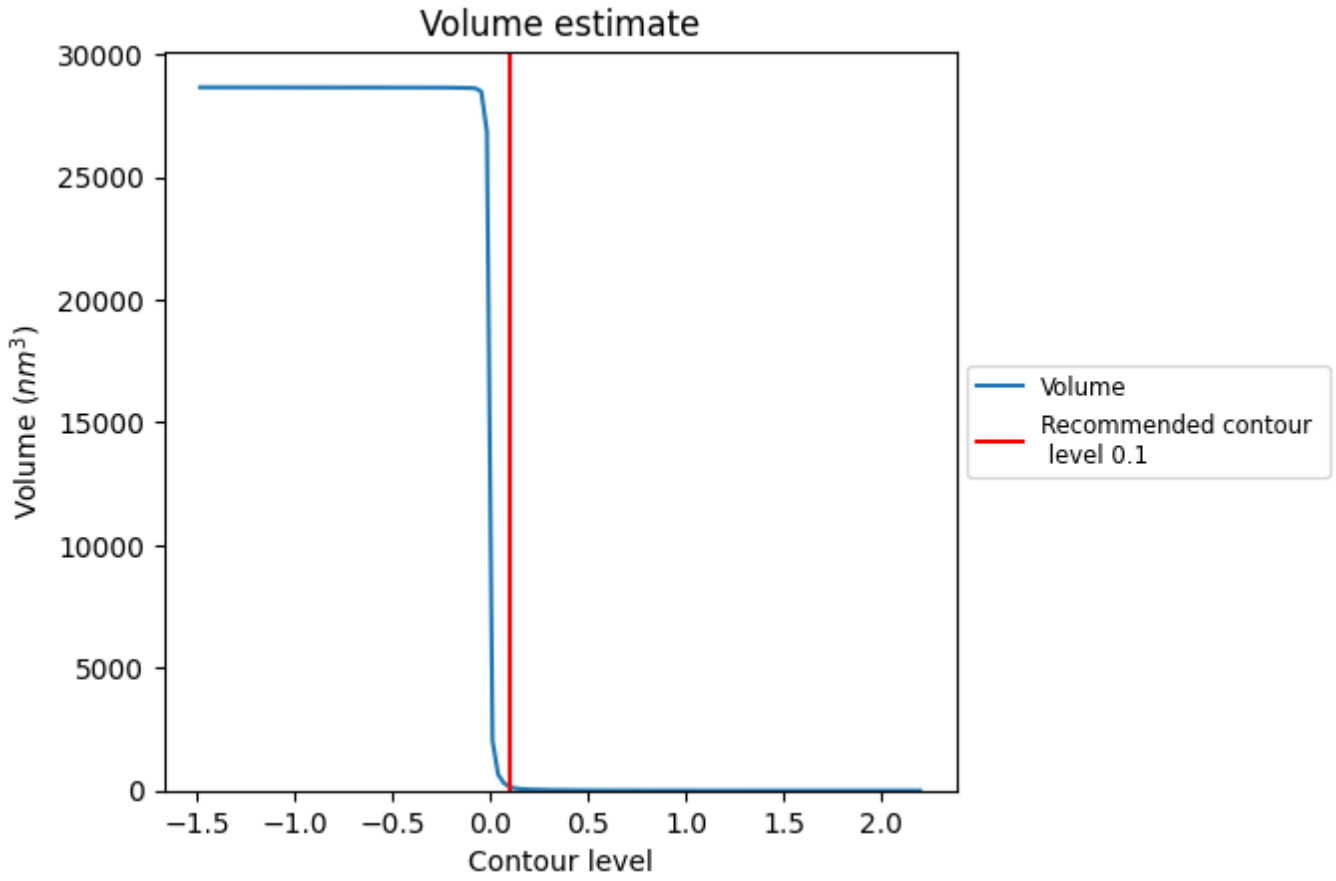
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

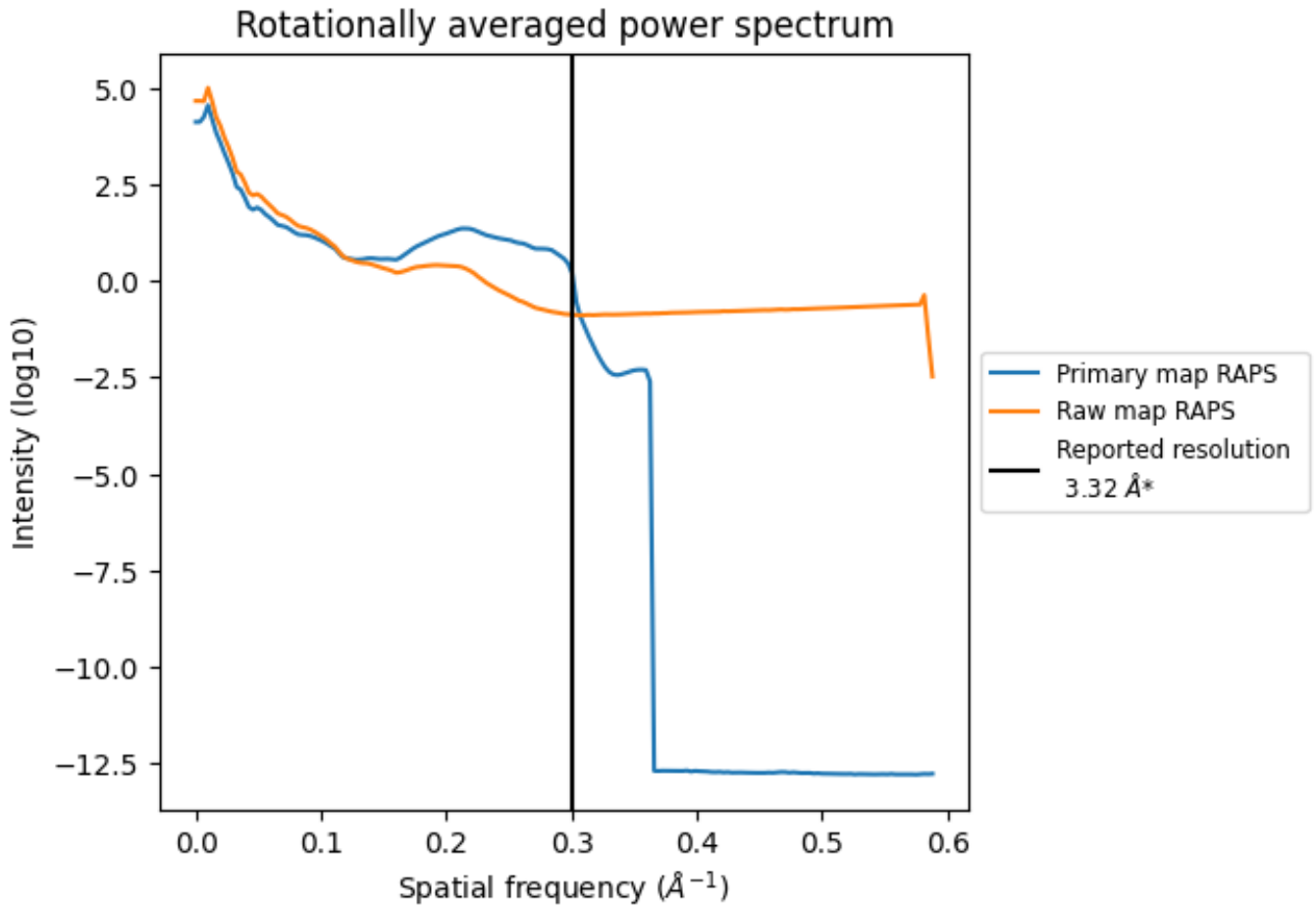
7.2 Volume estimate (i)



The volume at the recommended contour level is 147 nm^3; this corresponds to an approximate mass of 133 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

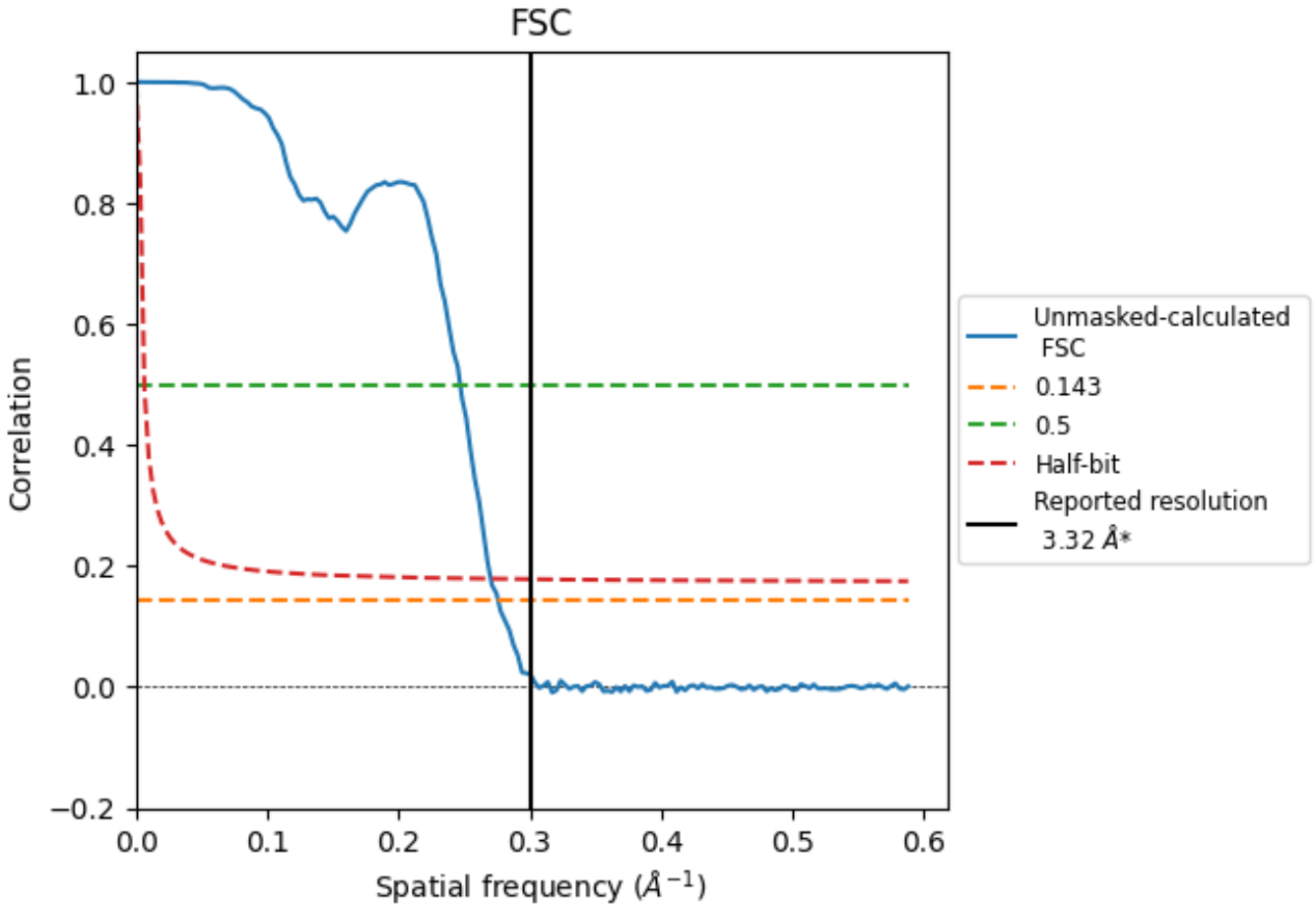


*Reported resolution corresponds to spatial frequency of 0.301 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.301 Å^{-1}

8.2 Resolution estimates (i)

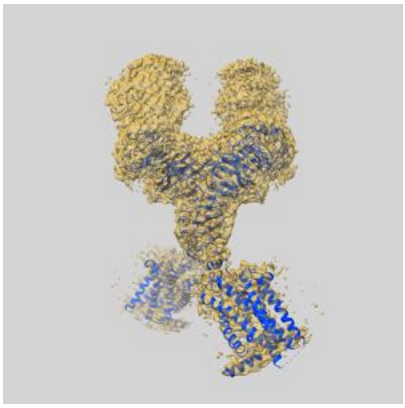
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.32	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.63	4.05	3.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

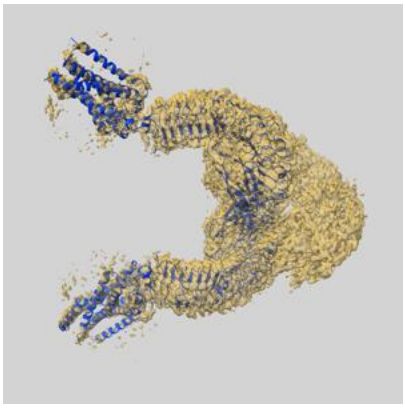
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37875 and PDB model 8WVX. Per-residue inclusion information can be found in section 3 on page 5.

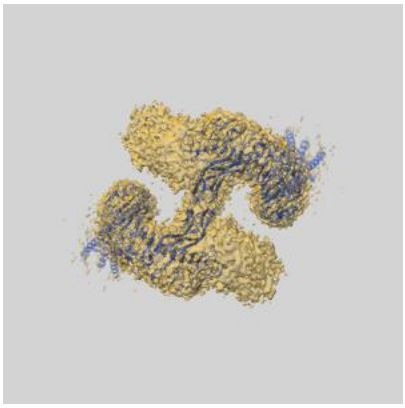
9.1 Map-model overlay



X



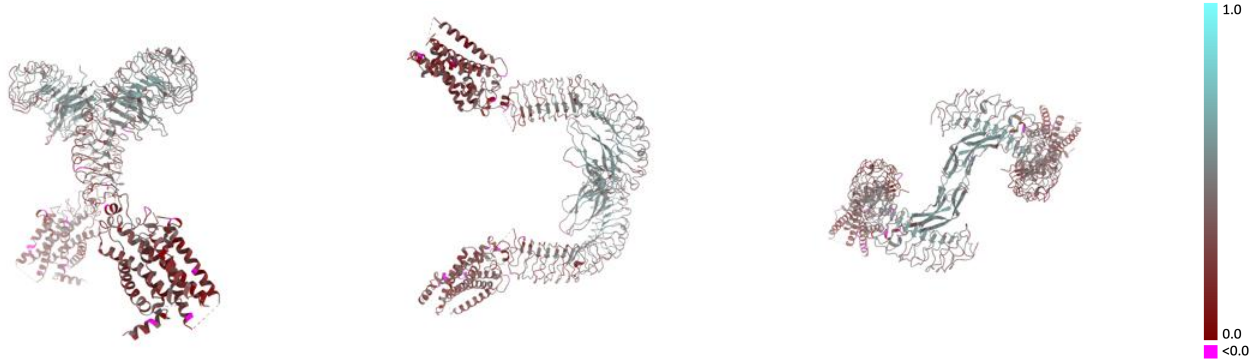
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

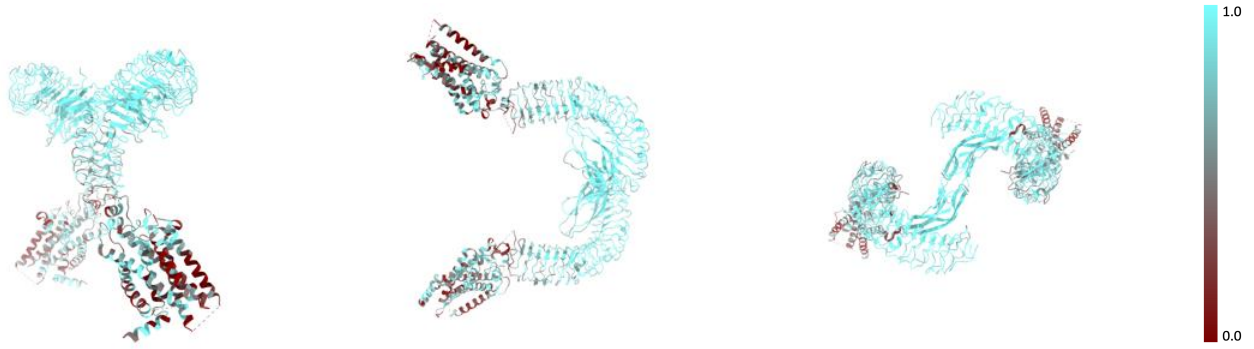
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

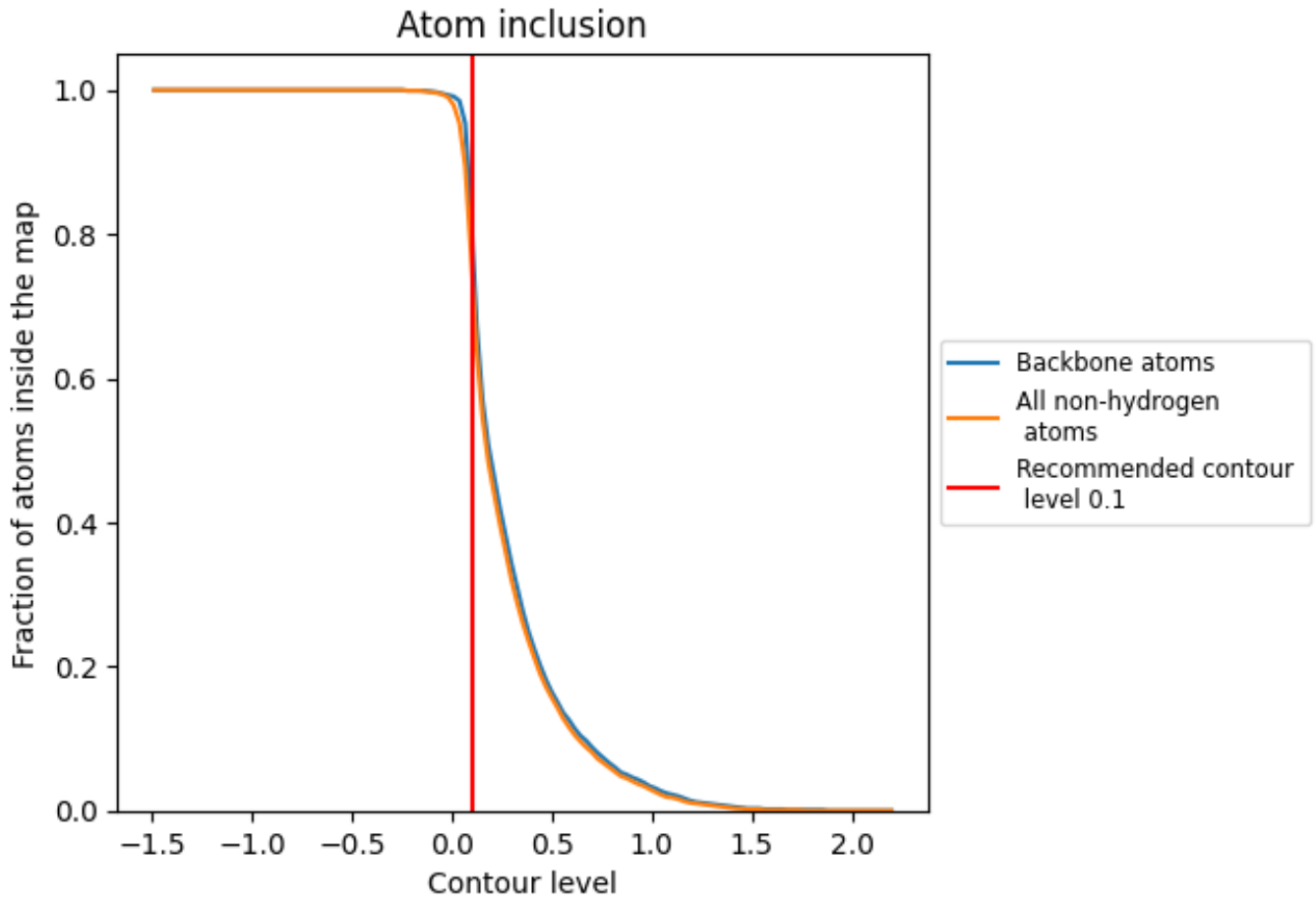
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7600	0.3770
A	0.7410	0.3640
B	0.7330	0.3550
C	0.9260	0.5150
D	0.8850	0.4680