Full wwPDB EM Validation Report

Oct 22, 2024 – 09:27 AM JST

PDB ID	:	8WVX
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:

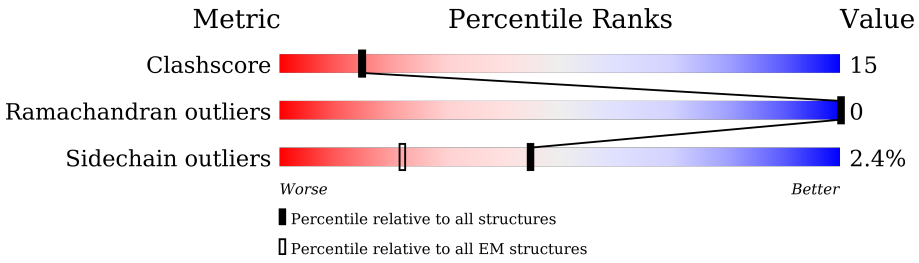
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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% 64% 21% • 13%
1	B	832	17% 65% 22% • 12%
2	C	103	• 64% 31% • •
2	D	103	• 59% 33% • •

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

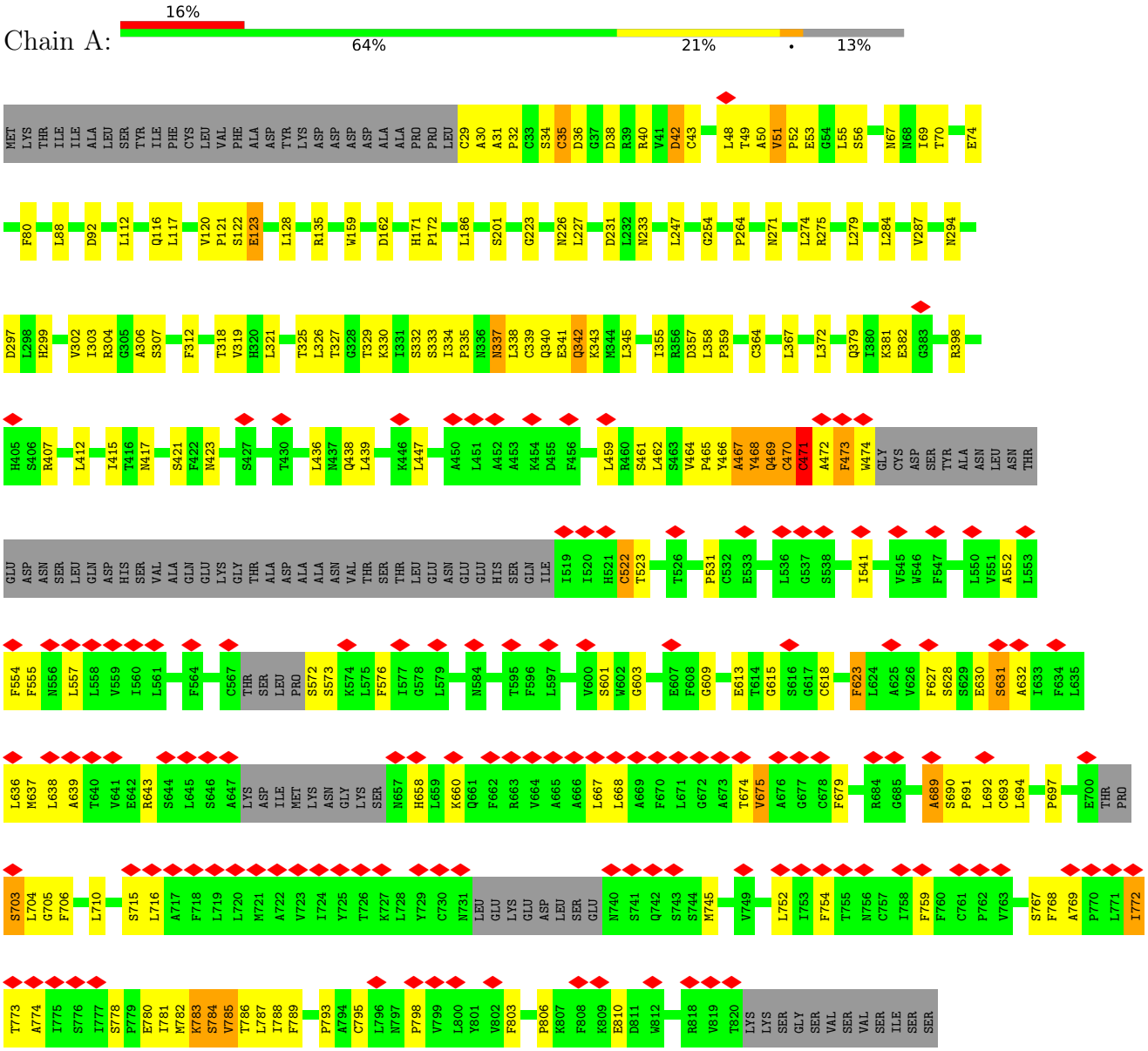
- Molecule 2 is a protein called Norrin.

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)

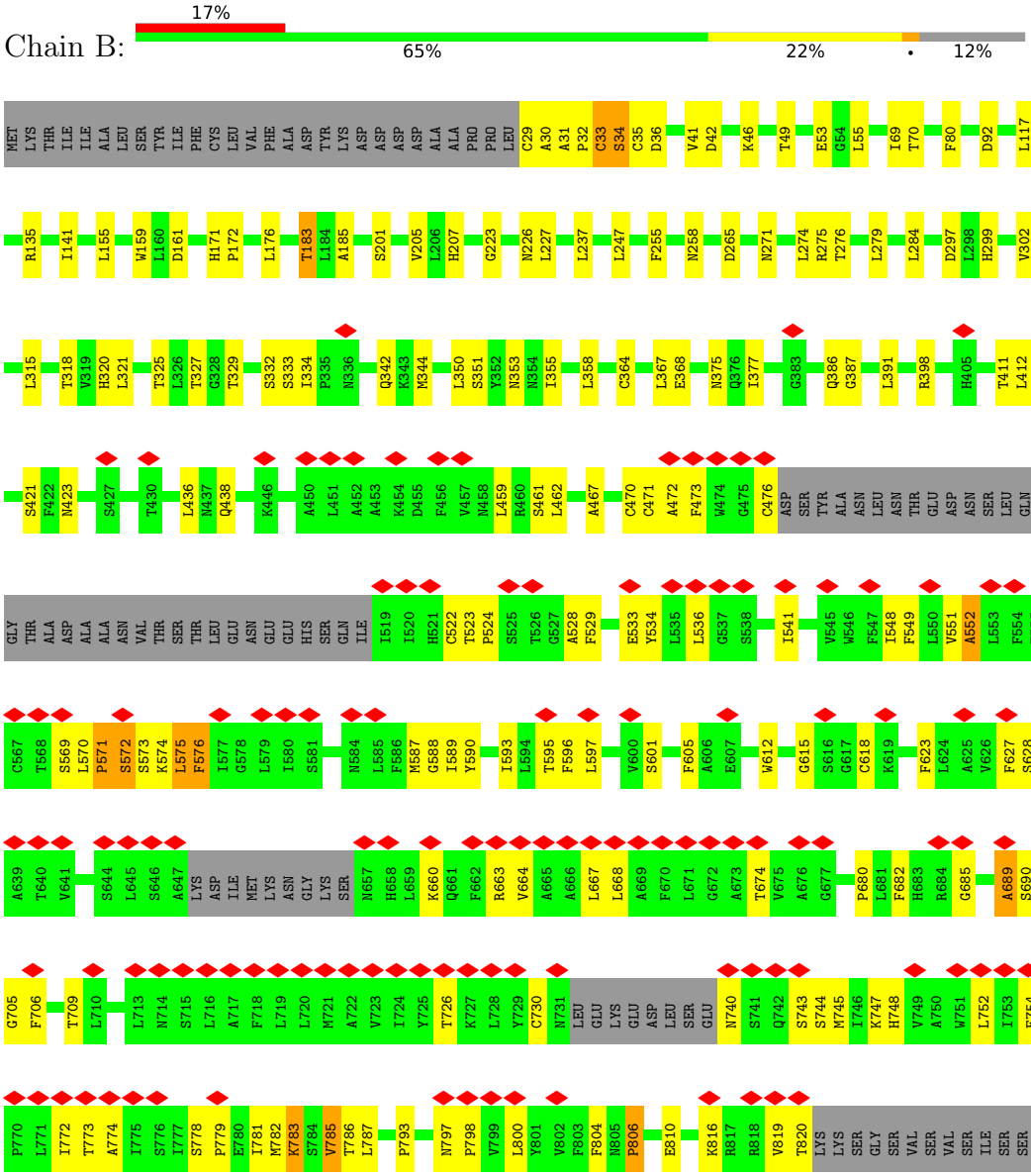
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



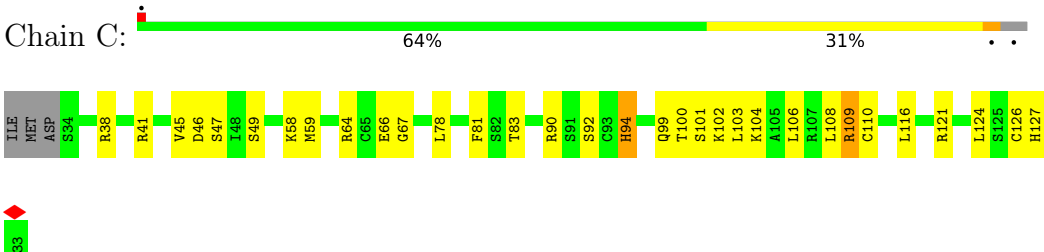
• Molecule 1: Leucine-rich repeat-containing G-protein coupled receptor 4

Chain B:



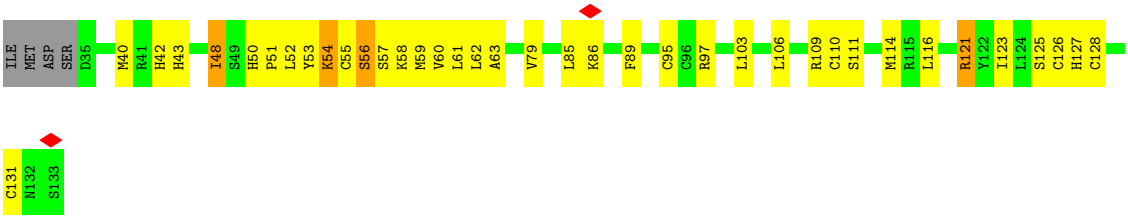
• Molecule 2: Norrin

Chain C:



• Molecule 2: Norrin

Chain D:


ILE
MET
ASP
SER
D35
M40
R41
H42
H43
I48
S49
H50
P51
L52
Y53
K54
C55
S56
S57
K58
M59
V60
L61
L62
A63
V79
L85
K86
F89
C95
C96
R97
L103
L106
R109
C110
S111
M114
R115
L116
R121
Y122
I123
L124
S125
C126
H127
C128
C131
N132
S133

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 (i)

5.1 Standard geometry (i)

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	1.00	35/5011 (0.7%)	1.09	51/6862 (0.7%)
1	B	1.01	44/5045 (0.9%)	1.06	36/6908 (0.5%)
2	C	0.77	0/799	0.96	3/1072 (0.3%)
2	D	0.99	9/798 (1.1%)	0.96	2/1070 (0.2%)
All	All	0.99	88/11653 (0.8%)	1.06	92/15912 (0.6%)

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 (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	601	SER	C-N	11.26	1.59	1.34
1	A	601	SER	C-N	10.95	1.59	1.34
1	A	541	ILE	C-N	10.46	1.58	1.34
1	B	472	ALA	C-N	9.78	1.56	1.34
1	A	473	PHE	C-N	9.67	1.56	1.34
1	B	536	LEU	C-N	9.11	1.49	1.33
1	B	615	GLY	C-O	9.08	1.38	1.23
1	A	615	GLY	C-O	9.02	1.38	1.23
1	A	469	GLN	C-N	8.98	1.54	1.34
1	A	472	ALA	C-N	8.64	1.53	1.34
1	A	470	CYS	C-N	8.50	1.53	1.34
1	B	772	ILE	C-N	8.28	1.53	1.34
1	B	774	ALA	C-N	8.19	1.52	1.34
1	A	784	SER	C-N	7.97	1.52	1.34
1	A	752	LEU	C-N	7.95	1.52	1.34
1	B	570	LEU	C-N	7.88	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	752	LEU	C-N	7.85	1.52	1.34
2	D	125	SER	C-N	7.74	1.51	1.34
1	B	628	SER	C-N	7.65	1.51	1.34
1	A	628	SER	C-N	7.62	1.51	1.34
1	A	554	PHE	C-N	7.54	1.51	1.34
1	A	690	SER	C-N	7.50	1.48	1.34
1	B	265	ASP	C-N	7.42	1.46	1.33
1	B	690	SER	C-N	7.35	1.48	1.34
1	A	67	ASN	C-N	7.34	1.50	1.34
2	D	57	SER	C-N	7.28	1.50	1.34
1	A	468	TYR	C-N	7.21	1.50	1.34
1	A	772	ILE	C-N	7.17	1.50	1.34
1	B	605	PHE	C-N	7.13	1.50	1.34
1	B	674	THR	C-N	7.07	1.50	1.34
1	A	674	THR	C-N	7.05	1.50	1.34
1	A	223	GLY	C-N	7.03	1.50	1.34
1	B	571	PRO	C-N	6.96	1.50	1.34
1	A	623	PHE	C-N	6.86	1.49	1.34
1	A	294	ASN	C-N	6.64	1.49	1.34
1	B	589	ILE	C-N	6.64	1.49	1.34
1	B	575	LEU	C-N	6.58	1.49	1.34
1	B	612	TRP	C-N	6.56	1.49	1.34
1	A	603	GLY	C-N	6.52	1.49	1.34
2	D	40	MET	C-N	6.52	1.49	1.34
1	A	785	VAL	C-N	6.48	1.49	1.34
1	B	783	LYS	C-N	6.44	1.48	1.34
1	B	375	ASN	C-N	6.43	1.48	1.34
1	A	675	VAL	C-N	6.33	1.48	1.34
2	D	61	LEU	C-N	6.32	1.48	1.34
2	D	58	LYS	C-N	6.31	1.48	1.34
1	A	783	LYS	C-N	6.29	1.48	1.34
1	B	631	SER	C-N	6.21	1.48	1.34
1	B	523	THR	C-N	6.18	1.46	1.34
1	A	631	SER	C-N	6.17	1.48	1.34
1	B	785	VAL	C-N	6.07	1.48	1.34
1	B	660	LYS	C-N	6.05	1.48	1.34
1	B	53	GLU	C-N	-5.98	1.22	1.33
1	B	685	GLY	C-N	5.98	1.47	1.34
1	A	660	LYS	C-N	5.95	1.47	1.34
2	D	106	LEU	C-N	5.95	1.47	1.34
1	B	30	ALA	C-N	5.94	1.47	1.34
1	A	523	THR	C-N	5.92	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	332	SER	C-N	5.80	1.47	1.34
1	B	34	SER	C-N	-5.79	1.20	1.34
2	D	56	SER	C-N	5.77	1.47	1.34
2	D	123	ILE	C-N	-5.75	1.20	1.34
1	B	467	ALA	C-N	-5.67	1.21	1.34
1	B	778	SER	C-N	-5.59	1.23	1.34
1	B	33	CYS	C-N	-5.57	1.21	1.34
1	A	74	GLU	C-N	-5.54	1.21	1.34
1	B	42	ASP	C-N	-5.51	1.21	1.34
1	B	223	GLY	C-N	5.49	1.46	1.34
1	B	667	LEU	C-N	-5.40	1.21	1.34
1	B	549	PHE	C-N	5.39	1.46	1.34
1	B	387	GLY	C-N	5.39	1.46	1.34
1	A	128	LEU	C-N	5.38	1.46	1.34
1	A	264	PRO	C-N	5.33	1.46	1.34
1	B	117	LEU	C-N	-5.33	1.21	1.34
1	B	768	PHE	C-N	5.30	1.46	1.34
1	A	643	ARG	C-N	-5.29	1.21	1.34
1	B	595	THR	C-N	5.29	1.46	1.34
1	B	128	LEU	C-N	5.26	1.46	1.34
1	B	541	ILE	C-N	5.23	1.46	1.34
1	B	663	ARG	C-N	-5.23	1.22	1.34
1	B	572	SER	C-N	5.21	1.46	1.34
1	A	667	LEU	C-N	-5.13	1.22	1.34
1	A	254	GLY	C-N	-5.12	1.22	1.34
2	D	79	VAL	C-N	5.11	1.45	1.34
1	A	332	SER	C-N	5.08	1.45	1.34
1	A	768	PHE	C-N	5.08	1.45	1.34
1	B	237	LEU	C-N	-5.02	1.24	1.33
1	A	56	SER	C-N	-5.00	1.22	1.34

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	92	SER	CB-CA-C	12.78	134.37	110.10
2	C	92	SER	N-CA-C	-11.71	79.38	111.00
1	B	185	ALA	CB-CA-C	-11.43	92.95	110.10
1	A	471	CYS	O-C-N	11.28	140.74	122.70
1	A	573	SER	N-CA-C	-10.49	82.68	111.00
1	A	470	CYS	O-C-N	9.67	138.17	122.70
1	A	342	GLN	N-CA-C	-9.59	85.11	111.00
1	A	468	TYR	O-C-N	9.47	137.86	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	472	ALA	O-C-N	9.34	137.64	122.70
1	A	704	LEU	O-C-N	9.29	139.00	123.20
1	B	704	LEU	O-C-N	9.23	138.89	123.20
1	A	572	SER	N-CA-C	9.14	135.68	111.00
1	A	469	GLN	O-C-N	8.93	136.98	122.70
1	A	473	PHE	O-C-N	8.53	136.35	122.70
1	A	783	LYS	O-C-N	8.36	136.08	122.70
1	A	704	LEU	C-N-CA	-8.30	104.86	122.30
1	B	704	LEU	C-N-CA	-8.25	104.98	122.30
1	A	704	LEU	CA-C-N	-8.14	99.91	116.20
1	B	704	LEU	CA-C-N	-8.10	100.00	116.20
1	A	667	LEU	O-C-N	-7.84	110.15	122.70
1	B	745	MET	O-C-N	7.84	135.24	122.70
1	A	467	ALA	O-C-N	7.79	135.16	122.70
1	B	573	SER	O-C-N	7.75	135.10	122.70
1	A	573	SER	N-CA-CB	7.66	121.99	110.50
1	A	638	LEU	O-C-N	-7.54	110.63	122.70
1	A	471	CYS	CA-C-N	-7.51	100.69	117.20
1	B	596	PHE	O-C-N	7.45	134.61	122.70
1	B	638	LEU	O-C-N	-7.39	110.88	122.70
1	B	667	LEU	O-C-N	-7.33	110.97	122.70
2	C	83	THR	N-CA-CB	-7.10	96.80	110.30
1	B	576	PHE	O-C-N	6.90	133.74	122.70
1	B	574	LYS	O-C-N	6.89	133.72	122.70
1	A	469	GLN	C-N-CA	-6.83	104.61	121.70
1	A	471	CYS	C-N-CA	-6.62	105.15	121.70
1	A	637	MET	O-C-N	-6.58	112.17	122.70
1	B	588	GLY	O-C-N	6.56	133.19	122.70
1	A	472	ALA	C-N-CA	-6.51	105.41	121.70
1	A	468	TYR	CA-C-N	-6.49	102.92	117.20
1	B	637	MET	O-C-N	-6.49	112.32	122.70
1	B	398	ARG	O-C-N	-6.44	112.40	122.70
1	B	703	SER	O-C-N	6.38	132.91	122.70
1	A	703	SER	O-C-N	6.35	132.86	122.70
1	A	783	LYS	CA-C-N	-6.29	103.35	117.20
1	A	342	GLN	CB-CA-C	6.29	122.98	110.40
1	B	573	SER	CA-C-N	-6.17	103.62	117.20
1	A	783	LYS	C-N-CA	-6.17	106.28	121.70
1	A	468	TYR	C-N-CA	-6.13	106.39	121.70
1	B	573	SER	C-N-CA	-6.11	106.42	121.70
1	B	783	LYS	O-C-N	6.07	132.41	122.70
1	B	703	SER	C-N-CA	-6.04	106.60	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	703	SER	C-N-CA	-6.03	106.61	121.70
1	A	398	ARG	O-C-N	-6.03	113.05	122.70
1	B	745	MET	CA-C-N	-5.98	104.04	117.20
1	A	745	MET	O-C-N	5.92	132.16	122.70
1	A	467	ALA	C-N-CA	-5.90	106.95	121.70
1	A	472	ALA	CA-C-N	-5.86	104.31	117.20
1	A	689	ALA	O-C-N	-5.85	113.33	122.70
1	A	469	GLN	CA-C-N	-5.81	104.42	117.20
1	A	767	SER	O-C-N	-5.80	113.42	122.70
1	A	541	ILE	O-C-N	5.76	131.91	122.70
1	A	470	CYS	CA-C-N	-5.75	104.55	117.20
1	B	596	PHE	C-N-CA	-5.73	107.36	121.70
2	D	56	SER	O-C-N	-5.72	113.55	122.70
1	A	473	PHE	C-N-CA	-5.71	107.43	121.70
1	B	596	PHE	CA-C-N	-5.71	104.64	117.20
1	B	689	ALA	O-C-N	-5.67	113.62	122.70
1	B	333	SER	O-C-N	5.66	131.76	122.70
2	D	60	VAL	O-C-N	-5.59	113.76	122.70
1	B	745	MET	C-N-CA	-5.58	107.74	121.70
1	A	473	PHE	CA-C-N	-5.57	104.95	117.20
1	A	668	LEU	O-C-N	-5.56	113.80	122.70
1	B	569	SER	O-C-N	-5.47	113.95	122.70
1	A	667	LEU	CA-C-N	5.45	129.19	117.20
1	A	333	SER	O-C-N	5.44	131.40	122.70
1	B	754	PHE	O-C-N	5.38	131.31	122.70
1	B	551	VAL	O-C-N	5.34	131.24	122.70
1	A	552	ALA	O-C-N	5.28	131.14	122.70
1	A	754	PHE	O-C-N	5.26	131.12	122.70
1	A	638	LEU	CA-C-N	5.25	128.75	117.20
1	B	664	VAL	O-C-N	-5.24	114.32	122.70
1	B	703	SER	CA-C-N	-5.18	105.80	117.20
1	A	703	SER	CA-C-N	-5.18	105.81	117.20
1	B	552	ALA	O-C-N	5.18	130.98	122.70
1	B	588	GLY	CA-C-N	-5.17	105.81	117.20
1	A	784	SER	O-C-N	5.14	130.93	122.70
1	A	658	HIS	O-C-N	5.13	130.90	122.70
1	B	638	LEU	CA-C-N	5.12	128.47	117.20
1	B	667	LEU	CA-C-N	5.11	128.44	117.20
1	B	668	LEU	O-C-N	-5.10	114.54	122.70
1	B	630	GLU	O-C-N	5.09	130.85	122.70
1	A	287	VAL	O-C-N	-5.07	114.58	123.20
1	A	630	GLU	O-C-N	5.03	130.75	122.70

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	4287	126	0
1	B	4964	0	4329	124	0
2	C	783	0	765	42	0
2	D	782	0	772	44	0
All	All	11460	0	10153	324	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 (324) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:274:LEU:O	1:B:297:ASP:HB2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:571:PRO:O	1:B:575:LEU:N	2.29	0.66
2:D:53:TYR:C	2:D:55:CYS:H	1.98	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:34:SER:C	1:B:36:ASP:H	1.98	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:56:SER:OG	2:D:109:ARG:O	2.11	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:B:34:SER:C	1:B:36:ASP:N	2.52	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:B:471:CYS:O	1:B:476:CYS:HA	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:LEU:HD21	1:A:462:LEU:HB2	1.82	0.61
1:B:275:ARG:O	1:B:299:HIS:CE1	2.53	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: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
1:B:227:LEU:HD23	1:B:247:LEU:HD13	1.85	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: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:A:703:SER:C	1:A:705:GLY:H	2.06	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:120:VAL:O	1:A:121:PRO:C	2.42	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
2:D:53:TYR:C	2:D:55:CYS:N	2.58	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
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:B:572:SER:C	1:B:575:LEU:H	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:769:ALA:O	1:A:773:THR:N	2.41	0.54
1:B:703:SER:C	1:B:705:GLY:H	2.06	0.54
1:B:386:GLN:HA	1:B:411:THR:OG1	2.07	0.54
1:B:350:LEU:O	1:B:353:ASN:ND2	2.39	0.53
1:B:819:VAL:O	1:B:820:THR:C	2.46	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: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:A:116:GLN:C	1:A:117:LEU:HD12	2.30	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: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: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
2:C:101:SER:HG	2:D:89:PHE:HZ	1.59	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:B:255:PHE:CZ	1:B:279:LEU:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:49:THR:C	1:B:69:ILE:HG12	2.33	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
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
1:B:680:PRO:C	1:B:682:PHE:H	2.16	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:B:706:PHE:C	1:B:709:THR:H	2.17	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
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
1:B:804:PHE:C	1:B:806:PRO:HD3	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:D:53:TYR:O	2:D:55:CYS:N	2.44	0.46
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: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: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:338:LEU:C	1:A:340:GLN:H	2.20	0.45
1:A:35:CYS:O	1:A:35:CYS:SG	2.75	0.44
2:D:85:LEU:HD23	2:D:86:LYS:C	2.35	0.44
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: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:A:703:SER:C	1:A:705:GLY:N	2.67	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:A:715:SER:O	1:A:716:LEU:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:205:VAL:CG1	2:D:59:MET:SD	3.07	0.43
1:A:122:SER:O	1:A:123:GLU:C	2.56	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
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
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
1:A:773:THR:O	1:A:774:ALA:C	2.59	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:680:PRO:C	1:B:682:PHE:N	2.75	0.41
1:A:555:PHE:C	1:A:557:LEU:H	2.24	0.41
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:382:GLU:HG3	1:A:407:ARG:CG	2.52	0.40
1:A:772:ILE:C	1:A:774:ALA:H	2.24	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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%)	417 (97%)	14 (3%)	34 61
1	B	434/730 (60%)	430 (99%)	4 (1%)	75 85
2	C	91/96 (95%)	88 (97%)	3 (3%)	33 60
2	D	92/96 (96%)	88 (96%)	4 (4%)	25 53
All	All	1048/1652 (63%)	1023 (98%)	25 (2%)	45 68

All (25) 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	48	LEU
1	A	51	VAL
1	A	53	GLU
1	A	123	GLU
1	A	337	ASN
1	A	339	CYS
1	A	471	CYS
1	A	522	CYS
1	A	618	CYS
1	A	693	CYS
1	B	183	THR
1	B	522	CYS
1	B	618	CYS

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Mol	Chain	Res	Type
1	B	693	CYS
2	C	94	HIS
2	C	109	ARG
2	C	126	CYS
2	D	48	ILE
2	D	54	LYS
2	D	121	ARG
2	D	126	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) 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	311	GLN
1	A	386	GLN
1	A	423	ASN
1	A	469	GLN
1	B	71	GLN
1	B	226	ASN
1	B	299	HIS
1	B	311	GLN
1	B	337	ASN
1	B	342	GLN
1	B	386	GLN
1	B	423	ASN
2	C	87	GLN
2	C	127	HIS

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.

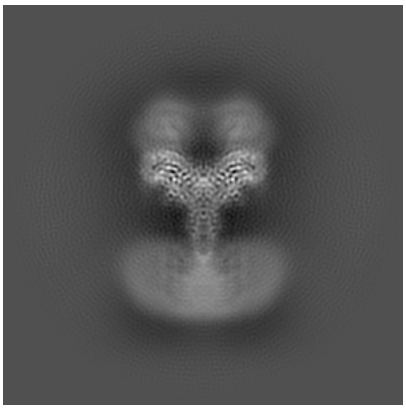
6 Map visualisation

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.

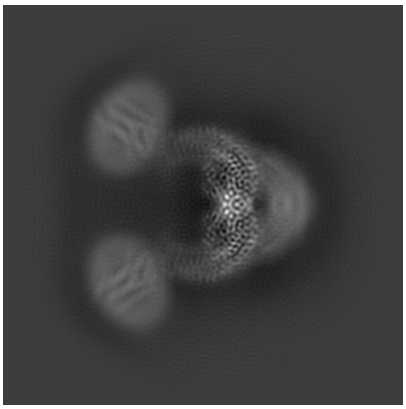
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

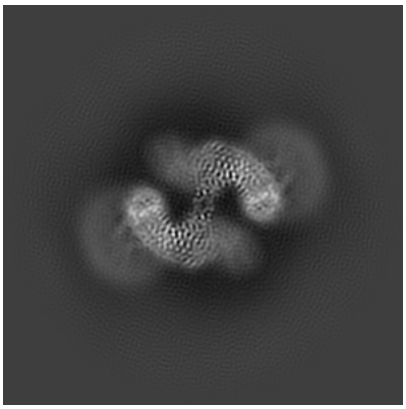
6.1.1 Primary map



X

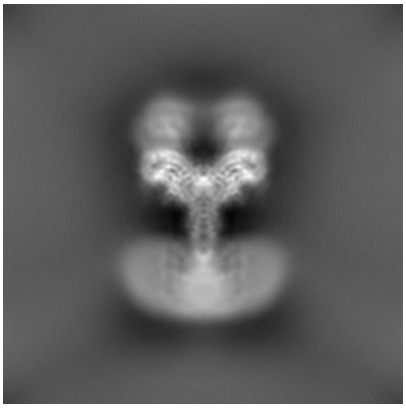


Y

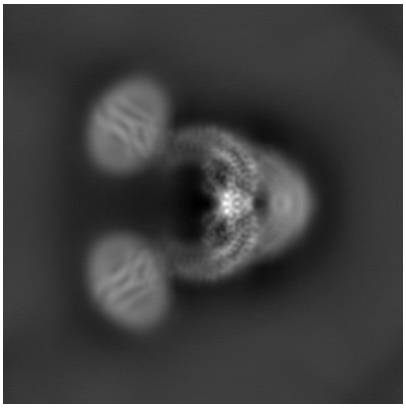


Z

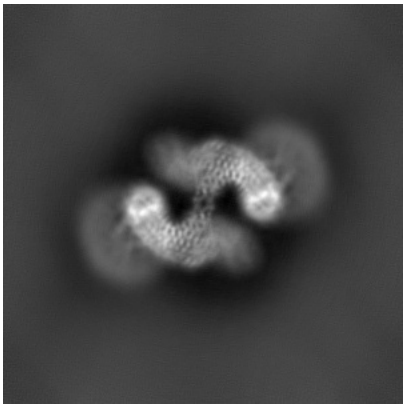
6.1.2 Raw map



X



Y

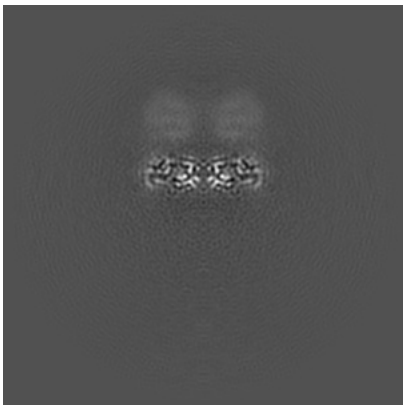


Z

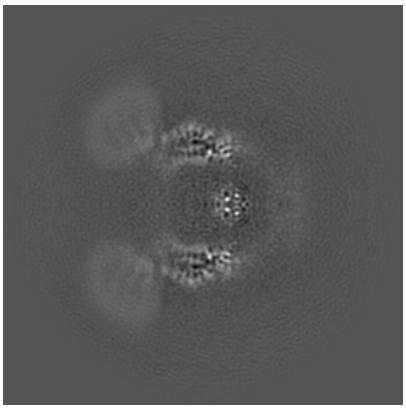
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

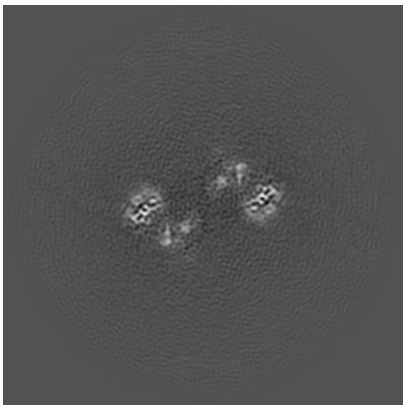
6.2.1 Primary map



X Index: 180

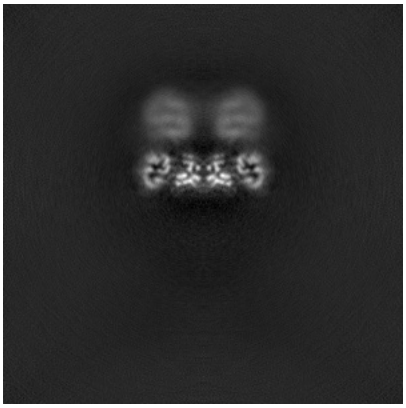


Y Index: 180

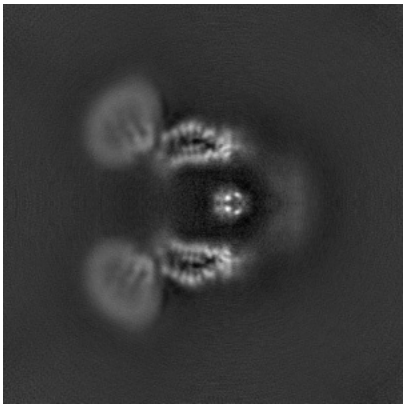


Z Index: 180

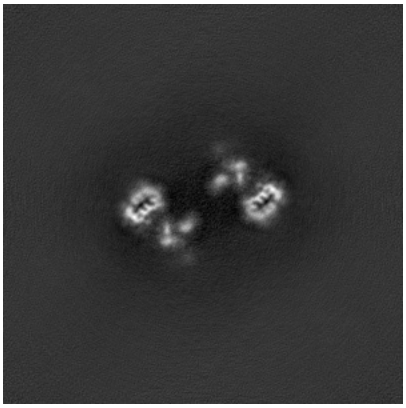
6.2.2 Raw map



X Index: 180



Y Index: 180

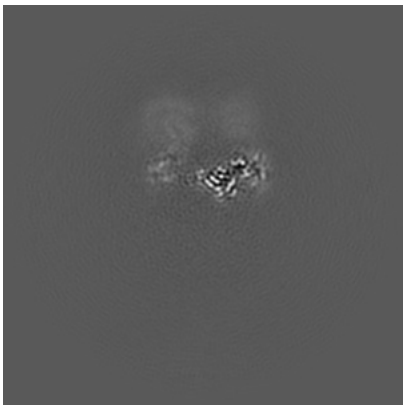


Z Index: 180

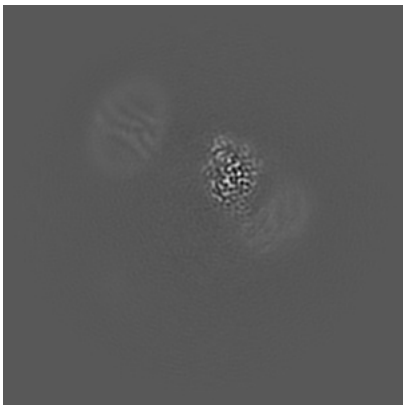
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

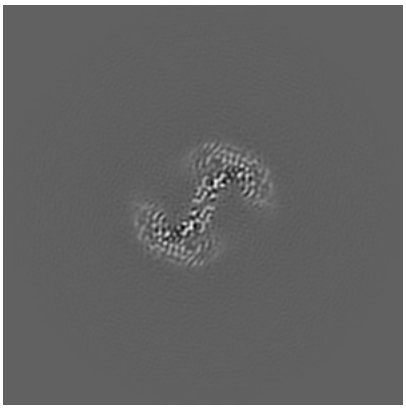
6.3.1 Primary map



X Index: 189

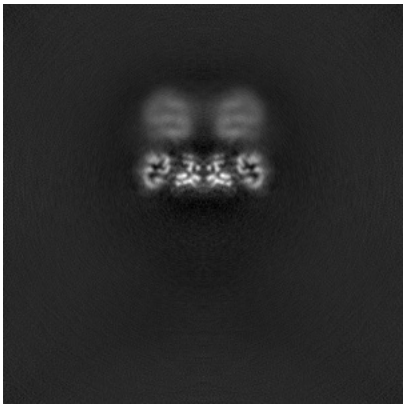


Y Index: 206

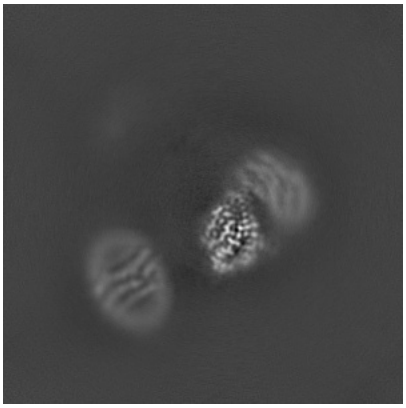


Z Index: 204

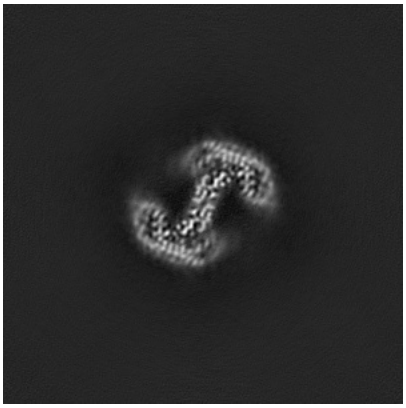
6.3.2 Raw map



X Index: 180



Y Index: 153

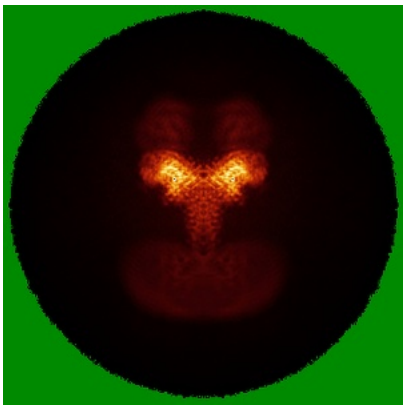


Z Index: 204

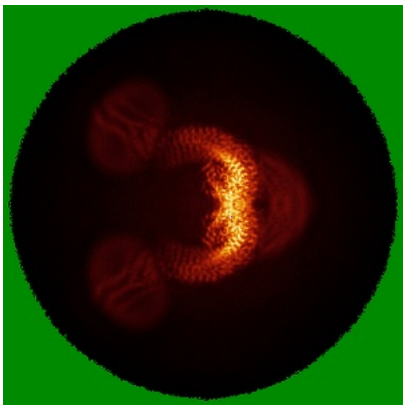
The images above show the largest variance slices of the map in three orthogonal directions.

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

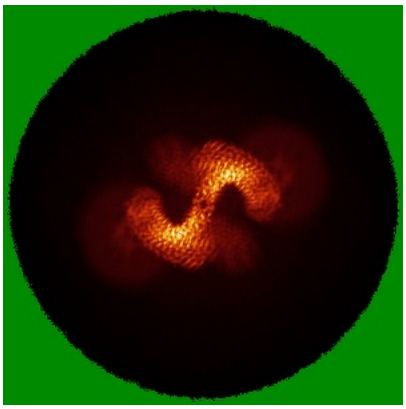
6.4.1 Primary map



X

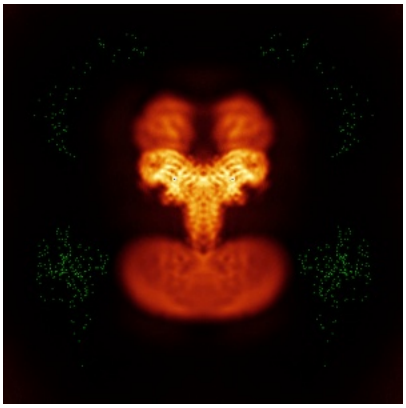


Y

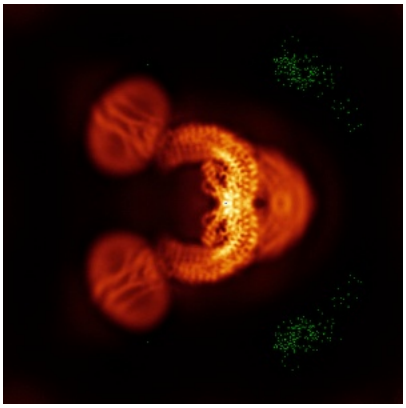


Z

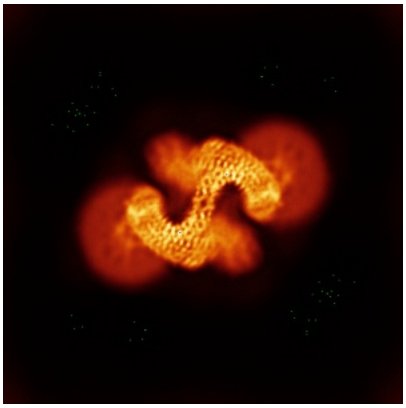
6.4.2 Raw map



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.

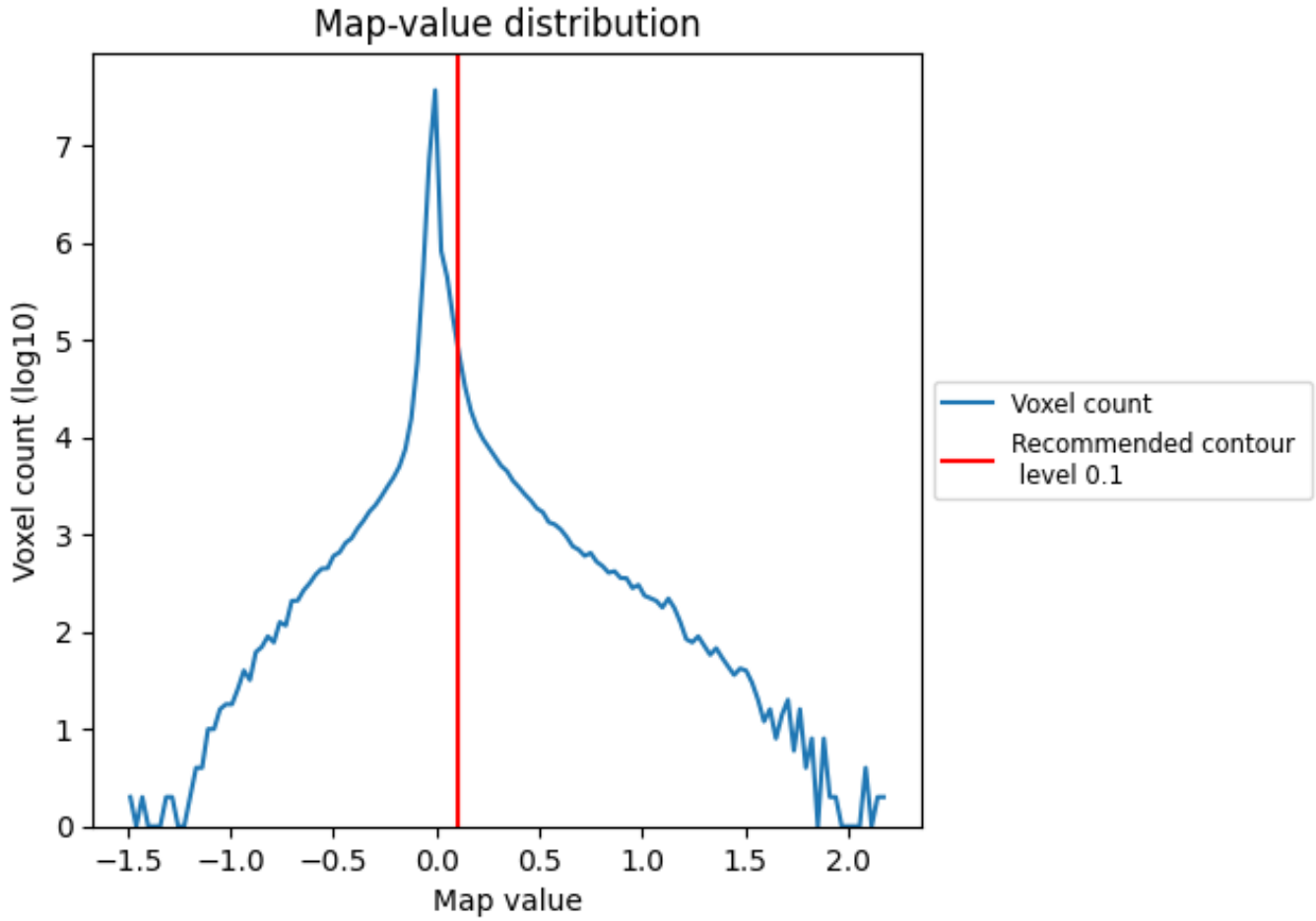
6.6 Mask visualisation (i)

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

7 Map analysis

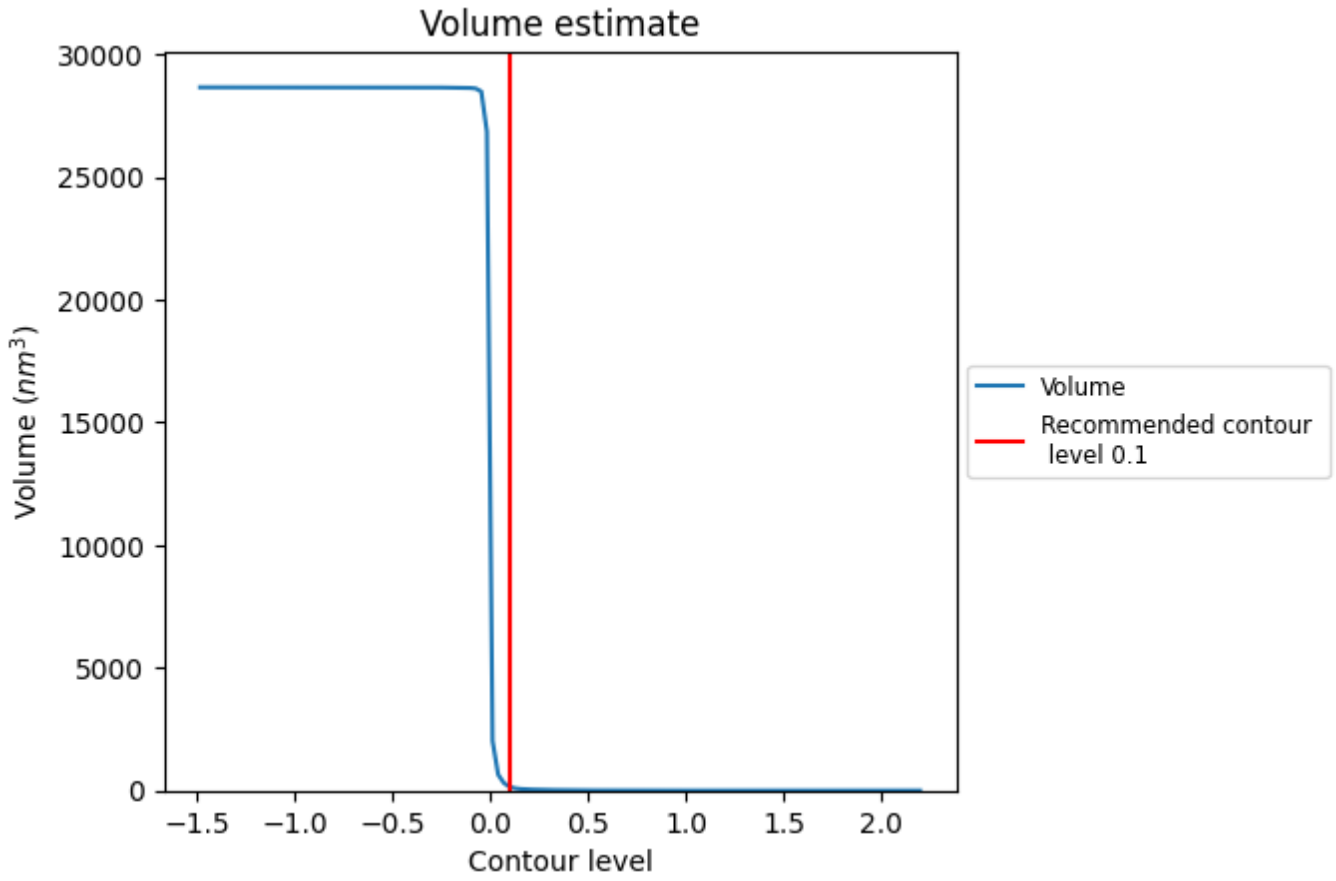
This section contains the results of statistical analysis of the map.

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.

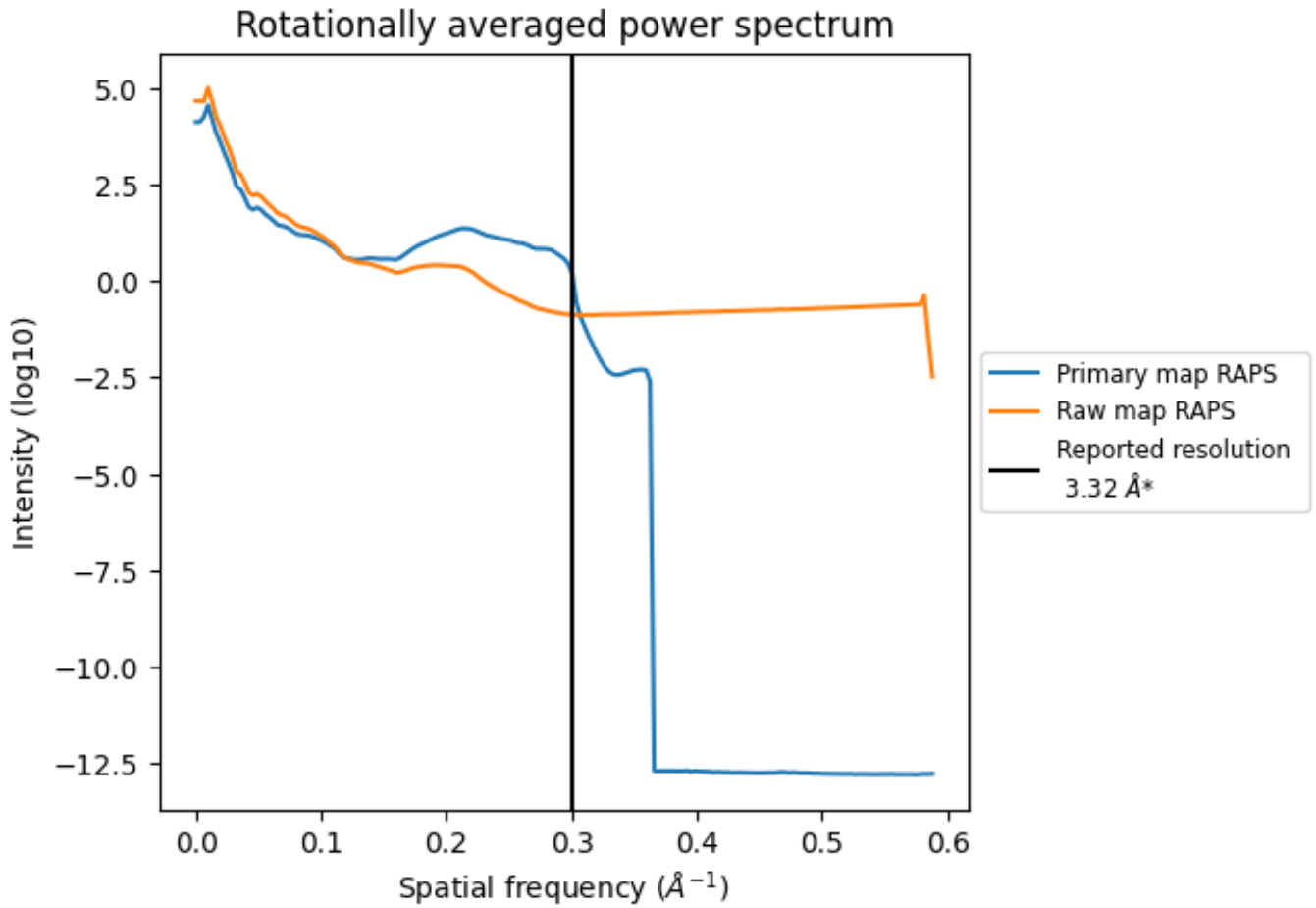
7.2 Volume estimate



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)

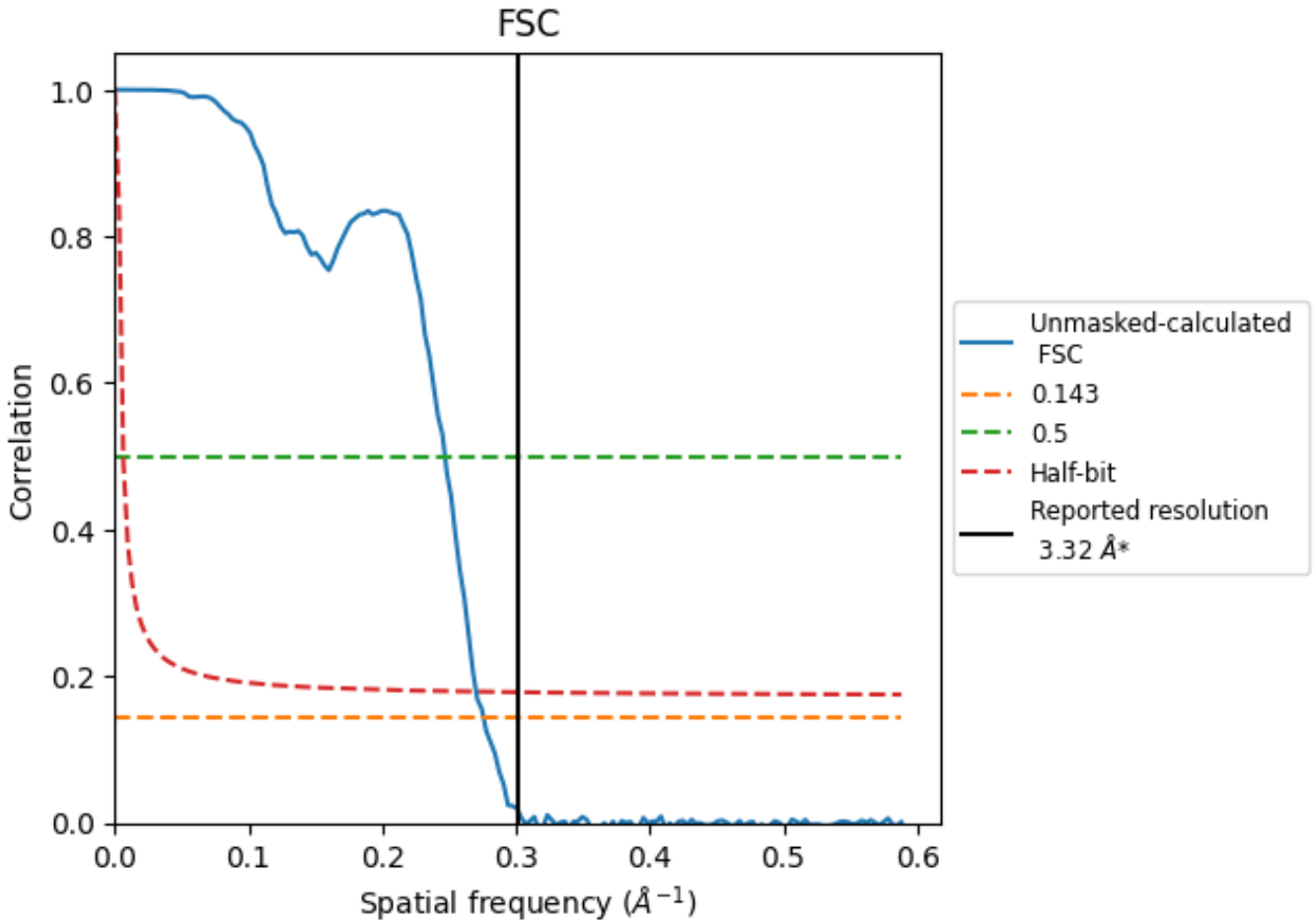


*Reported resolution corresponds to spatial frequency of 0.301 $Å^{-1}$

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)

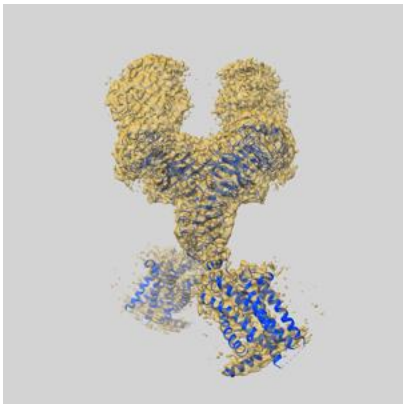
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.32	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.63	4.05	3.70

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

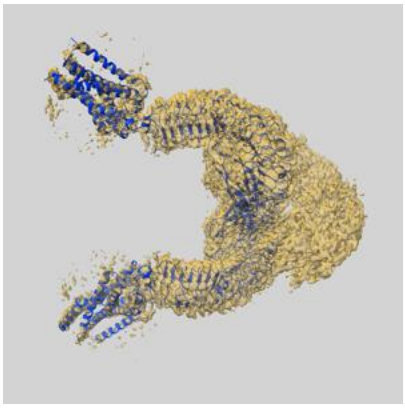
9 Map-model fit

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.

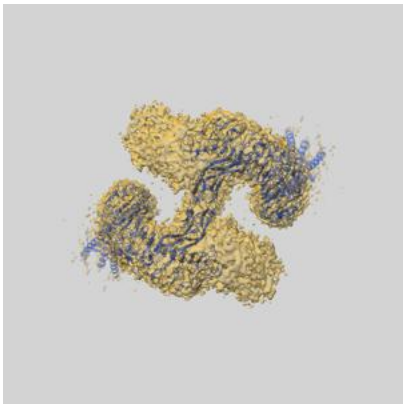
9.1 Map-model overlay



X



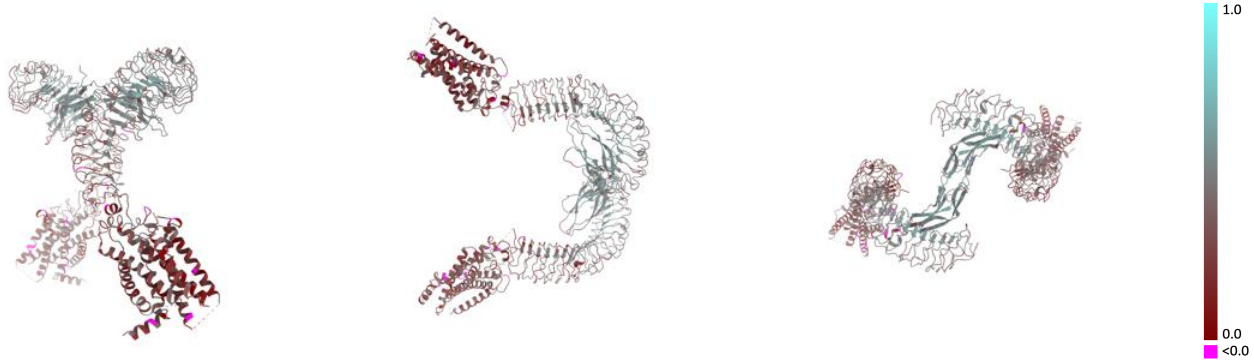
Y



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.

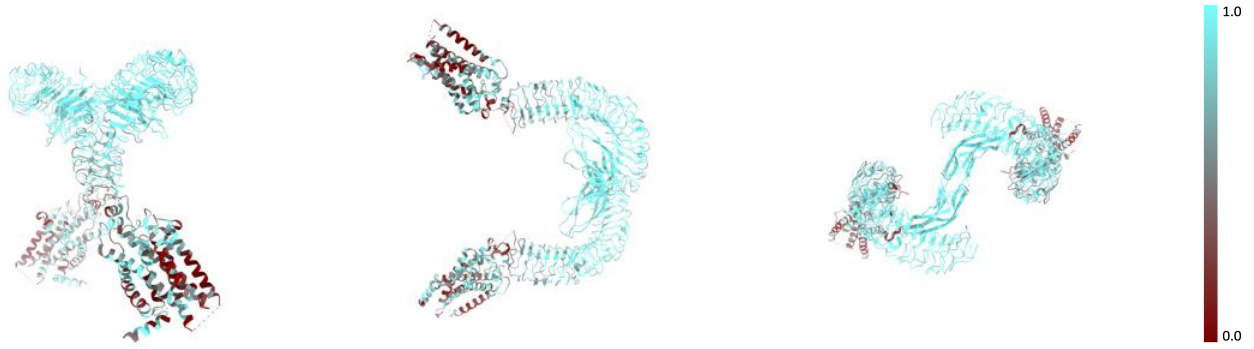
9.2 Q-score mapped to coordinate model (i)



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.

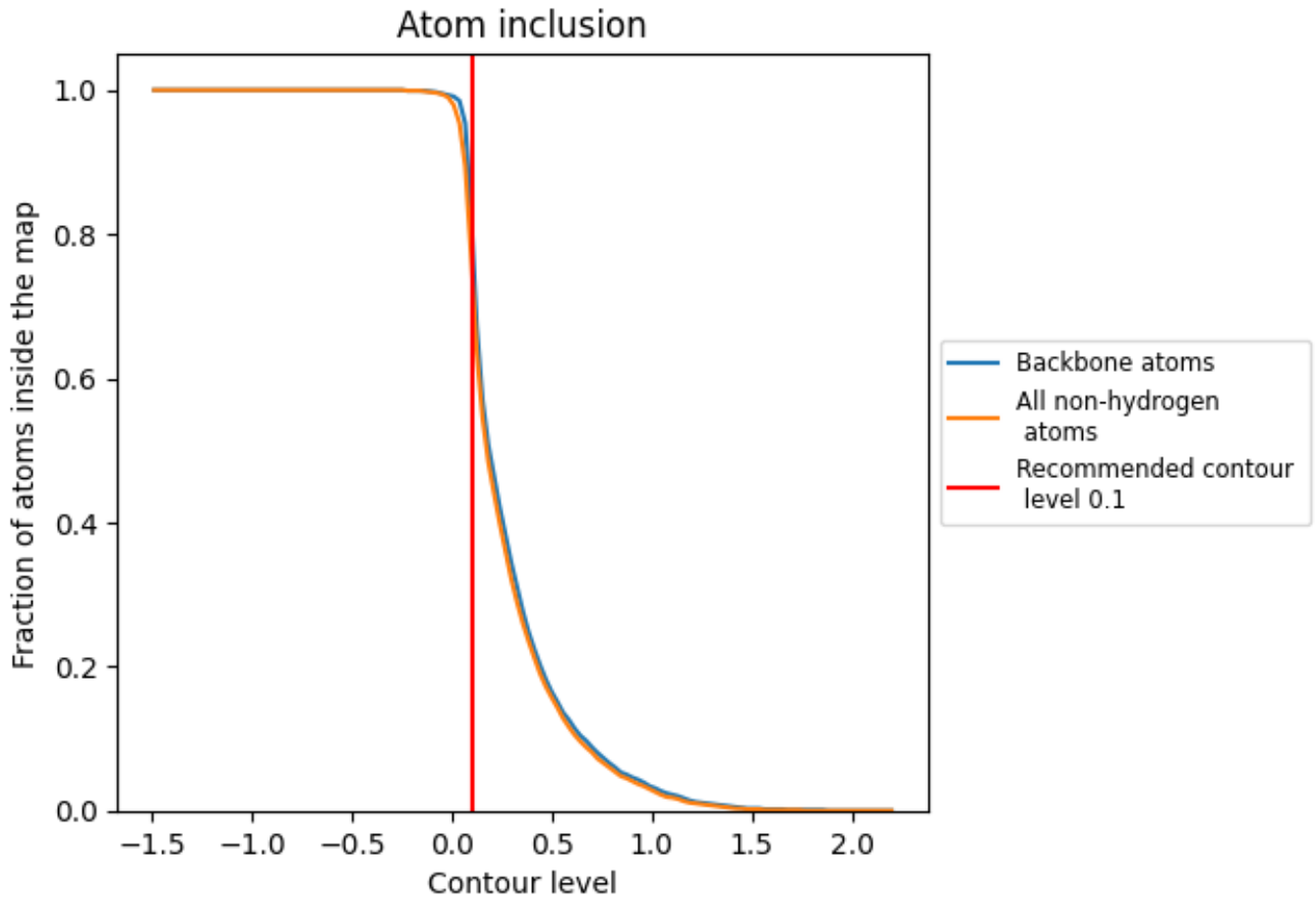
9.3 Atom inclusion mapped to coordinate model (i)



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