



Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 11:22 AM JST

PDB ID : 6LU9
EMDB ID : EMD-0979
Title : Rat ionotropic Glutamate Delta-2 receptor in complex with 7-CKA and Calcium
Authors : Kumar, J.; Burada, A.P.
Deposited on : 2020-01-27
Resolution : 8.80 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

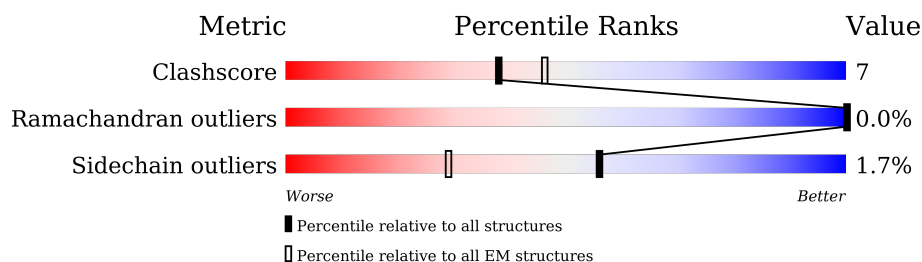
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.80 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 $\leq 5\%$. 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	877	
1	B	877	
1	C	877	
1	D	877	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20992 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 Glutamate receptor ionotropic, delta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	660	Total	C	N	O	S	0	0
			5248	3314	910	999	25		
1	B	660	Total	C	N	O	S	0	0
			5248	3314	910	999	25		
1	C	660	Total	C	N	O	S	0	0
			5248	3314	910	999	25		
1	D	660	Total	C	N	O	S	0	0
			5248	3314	910	999	25		

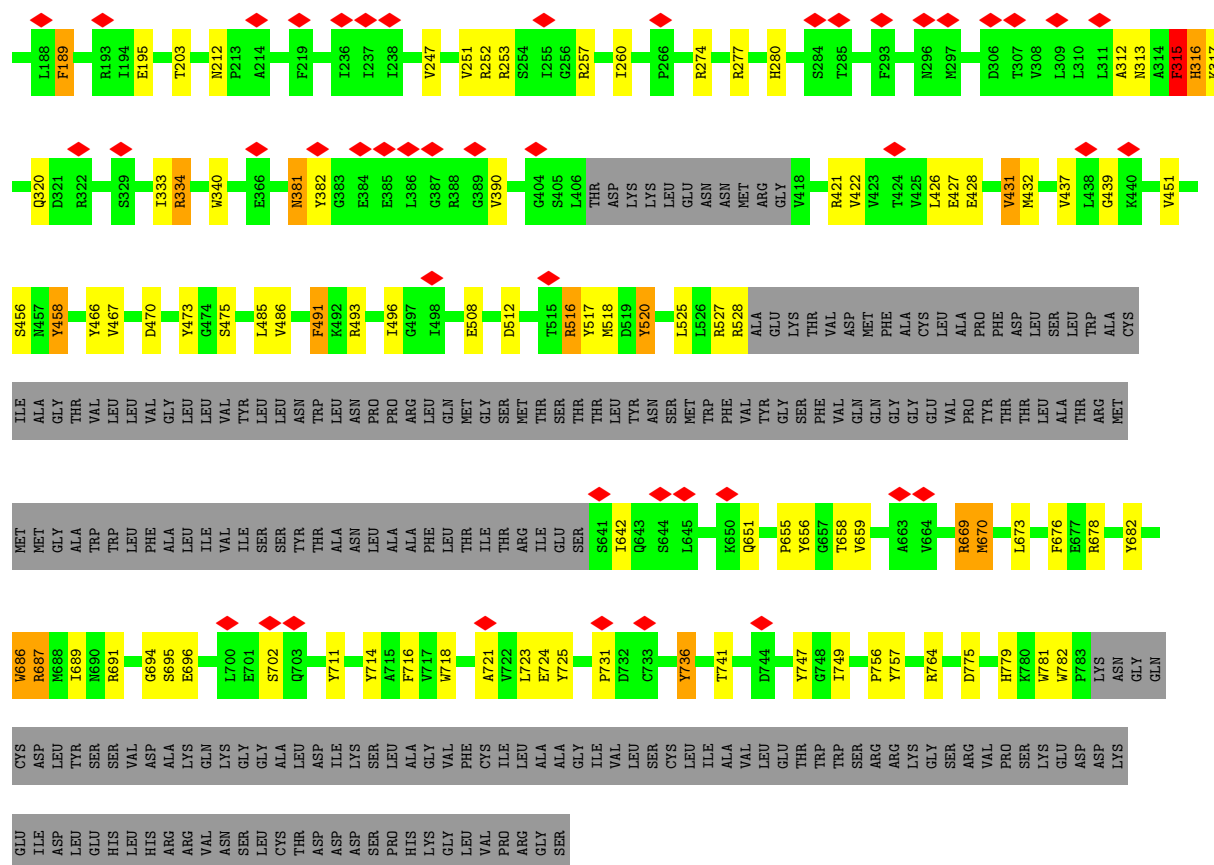
There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	GLN	GLU	conflict	UNP Q63226
A	871	GLY	-	expression tag	UNP Q63226
A	872	LEU	-	expression tag	UNP Q63226
A	873	VAL	-	expression tag	UNP Q63226
A	874	PRO	-	expression tag	UNP Q63226
A	875	ARG	-	expression tag	UNP Q63226
A	876	GLY	-	expression tag	UNP Q63226
A	877	SER	-	expression tag	UNP Q63226
B	320	GLN	GLU	conflict	UNP Q63226
B	871	GLY	-	expression tag	UNP Q63226
B	872	LEU	-	expression tag	UNP Q63226
B	873	VAL	-	expression tag	UNP Q63226
B	874	PRO	-	expression tag	UNP Q63226
B	875	ARG	-	expression tag	UNP Q63226
B	876	GLY	-	expression tag	UNP Q63226
B	877	SER	-	expression tag	UNP Q63226
C	320	GLN	GLU	conflict	UNP Q63226
C	871	GLY	-	expression tag	UNP Q63226
C	872	LEU	-	expression tag	UNP Q63226
C	873	VAL	-	expression tag	UNP Q63226
C	874	PRO	-	expression tag	UNP Q63226
C	875	ARG	-	expression tag	UNP Q63226

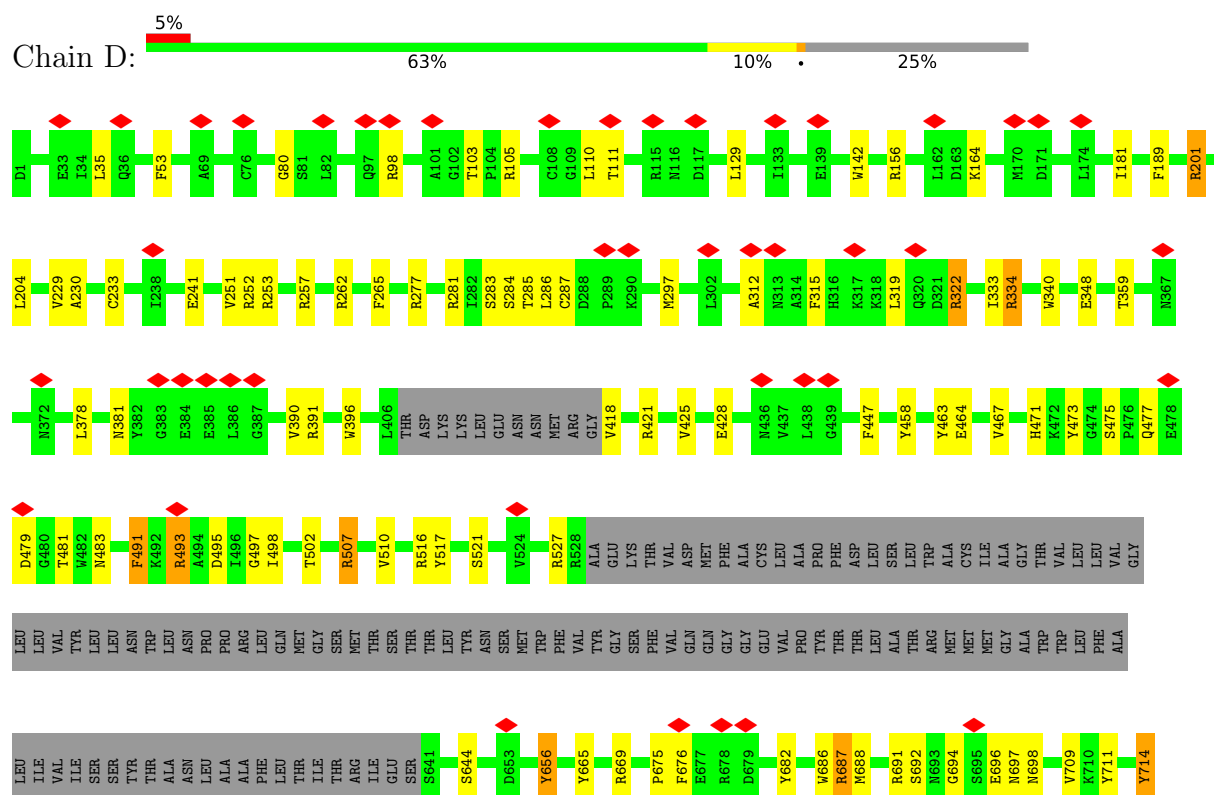
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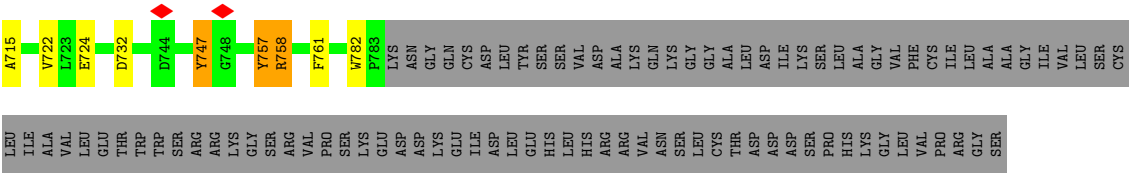
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Chain	Residue	Modelled	Actual	Comment	Reference
C	876	GLY	-	expression tag	UNP Q63226
C	877	SER	-	expression tag	UNP Q63226
D	320	GLN	GLU	conflict	UNP Q63226
D	871	GLY	-	expression tag	UNP Q63226
D	872	LEU	-	expression tag	UNP Q63226
D	873	VAL	-	expression tag	UNP Q63226
D	874	PRO	-	expression tag	UNP Q63226
D	875	ARG	-	expression tag	UNP Q63226
D	876	GLY	-	expression tag	UNP Q63226
D	877	SER	-	expression tag	UNP Q63226



• Molecule 1: Glutamate receptor ionotropic, delta-2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	7977	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 ($e^-/\text{\AA}^2$)	40.38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.958	Depositor
Minimum map value	-0.463	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.316	Depositor
Map size (Å)	392.0, 392.0, 392.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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	1.15	17/5352 (0.3%)	1.38	53/7251 (0.7%)
1	B	1.17	13/5352 (0.2%)	1.41	53/7251 (0.7%)
1	C	1.21	19/5352 (0.4%)	1.49	65/7251 (0.9%)
1	D	1.21	18/5352 (0.3%)	1.40	43/7251 (0.6%)
All	All	1.18	67/21408 (0.3%)	1.42	214/29004 (0.7%)

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	A	0	7
1	B	0	7
1	C	0	12
1	D	0	17
All	All	0	43

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	475	SER	CA-CB	7.71	1.64	1.52
1	C	466	TYR	CD1-CE1	7.59	1.50	1.39
1	D	340	TRP	CD2-CE2	7.54	1.50	1.41
1	C	508	GLU	CG-CD	7.51	1.63	1.51
1	B	421	ARG	CZ-NH2	7.33	1.42	1.33
1	C	520	TYR	CG-CD1	7.13	1.48	1.39
1	D	396	TRP	CD2-CE2	7.08	1.49	1.41
1	A	782	TRP	NE1-CE2	-7.03	1.28	1.37
1	D	724	GLU	CG-CD	6.92	1.62	1.51
1	A	761	PHE	CG-CD1	6.82	1.49	1.38
1	C	458	TYR	CG-CD1	6.76	1.48	1.39
1	B	466	TYR	CE2-CZ	6.75	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	516	ARG	NE-CZ	6.74	1.41	1.33
1	D	473	TYR	CG-CD2	6.64	1.47	1.39
1	B	757	TYR	CE2-CZ	6.64	1.47	1.38
1	D	463	TYR	CD2-CE2	6.39	1.49	1.39
1	C	517	TYR	CZ-OH	6.32	1.48	1.37
1	C	724	GLU	CD-OE1	6.16	1.32	1.25
1	D	644	SER	CA-CB	6.07	1.62	1.52
1	D	669	ARG	CD-NE	5.98	1.56	1.46
1	D	757	TYR	CD2-CE2	5.93	1.48	1.39
1	D	447	PHE	CB-CG	5.90	1.61	1.51
1	C	456	SER	CA-CB	5.87	1.61	1.52
1	A	466	TYR	CG-CD1	5.83	1.46	1.39
1	C	439	GLY	CA-C	-5.77	1.42	1.51
1	C	736	TYR	CD1-CE1	5.75	1.48	1.39
1	C	764	ARG	NE-CZ	5.69	1.40	1.33
1	B	480	GLY	N-CA	-5.66	1.37	1.46
1	D	142	TRP	CD2-CE2	-5.65	1.34	1.41
1	A	716	PHE	CB-CG	5.63	1.60	1.51
1	D	493	ARG	CZ-NH2	5.62	1.40	1.33
1	B	757	TYR	CG-CD1	5.59	1.46	1.39
1	C	694	GLY	CA-C	-5.57	1.43	1.51
1	C	714	TYR	CE2-CZ	5.53	1.45	1.38
1	C	421	ARG	CZ-NH2	5.51	1.40	1.33
1	D	714	TYR	CZ-OH	5.51	1.47	1.37
1	A	428	GLU	CG-CD	5.50	1.60	1.51
1	A	516	ARG	CZ-NH2	5.49	1.40	1.33
1	B	736	TYR	CG-CD2	5.46	1.46	1.39
1	D	464	GLU	CB-CG	5.46	1.62	1.52
1	C	528	ARG	NE-CZ	5.45	1.40	1.33
1	A	511	VAL	CB-CG2	5.44	1.64	1.52
1	B	714	TYR	CE1-CZ	5.43	1.45	1.38
1	D	758	ARG	CZ-NH1	5.41	1.40	1.33
1	A	444	TYR	CE1-CZ	5.40	1.45	1.38
1	B	456	SER	CB-OG	5.40	1.49	1.42
1	A	436	ASN	CB-CG	5.36	1.63	1.51
1	C	682	TYR	CG-CD2	5.32	1.46	1.39
1	C	678	ARG	CZ-NH2	5.28	1.40	1.33
1	B	508	GLU	CD-OE1	5.27	1.31	1.25
1	A	683	SER	CA-CB	5.22	1.60	1.52
1	B	745	ARG	NE-CZ	5.22	1.39	1.33
1	B	725	TYR	CE2-CZ	5.21	1.45	1.38
1	D	521	SER	CB-OG	5.21	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	421	ARG	CZ-NH2	5.21	1.39	1.33
1	C	516	ARG	NE-CZ	5.17	1.39	1.33
1	B	480	GLY	CA-C	-5.16	1.43	1.51
1	C	475	SER	CB-OG	5.15	1.49	1.42
1	A	692	SER	CA-CB	5.15	1.60	1.52
1	B	444	TYR	CG-CD1	5.15	1.45	1.39
1	A	493	ARG	NE-CZ	5.14	1.39	1.33
1	A	528	ARG	CD-NE	5.12	1.55	1.46
1	A	676	PHE	CG-CD1	5.11	1.46	1.38
1	A	714	TYR	CZ-OH	5.10	1.46	1.37
1	A	757	TYR	CE2-CZ	5.08	1.45	1.38
1	C	702	SER	CA-CB	5.01	1.60	1.52
1	A	714	TYR	CG-CD2	5.01	1.45	1.39

All (214) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	761	PHE	CB-CG-CD1	19.40	134.38	120.80
1	C	527	ARG	NE-CZ-NH2	-16.78	111.91	120.30
1	C	691	ARG	NE-CZ-NH2	15.10	127.85	120.30
1	C	691	ARG	NE-CZ-NH1	-14.35	113.13	120.30
1	D	687	ARG	NE-CZ-NH1	14.13	127.36	120.30
1	C	527	ARG	NE-CZ-NH1	13.35	126.97	120.30
1	B	491	PHE	CB-CG-CD1	-13.22	111.55	120.80
1	B	458	TYR	CB-CG-CD1	13.16	128.90	121.00
1	A	761	PHE	CB-CG-CD2	-12.74	111.88	120.80
1	A	463	TYR	CB-CG-CD2	12.63	128.58	121.00
1	A	676	PHE	CB-CG-CD2	-12.55	112.02	120.80
1	A	691	ARG	NE-CZ-NH2	-11.83	114.38	120.30
1	B	735	PHE	CB-CG-CD2	-11.68	112.62	120.80
1	B	665	TYR	CB-CG-CD2	-11.47	114.12	121.00
1	C	714	TYR	CB-CG-CD2	-11.27	114.24	121.00
1	C	516	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	B	757	TYR	CB-CG-CD2	10.95	127.57	121.00
1	B	491	PHE	CB-CG-CD2	10.14	127.90	120.80
1	B	761	PHE	CB-CG-CD1	10.05	127.84	120.80
1	C	711	TYR	CB-CG-CD2	10.00	127.00	121.00
1	B	682	TYR	CB-CG-CD2	-9.89	115.07	121.00
1	B	691	ARG	NE-CZ-NH1	9.81	125.21	120.30
1	B	653	ASP	CB-CG-OD2	-9.76	109.52	118.30
1	D	253	ARG	NE-CZ-NH2	-9.65	115.47	120.30
1	C	491	PHE	CB-CG-CD1	-9.61	114.07	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	ARG	NE-CZ-NH1	9.57	125.09	120.30
1	A	516	ARG	NE-CZ-NH1	9.47	125.04	120.30
1	A	262	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	B	687	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	A	473	TYR	CB-CG-CD2	9.25	126.55	121.00
1	C	458	TYR	CB-CG-CD1	-9.16	115.50	121.00
1	A	757	TYR	CB-CG-CD2	-9.01	115.59	121.00
1	A	473	TYR	CB-CG-CD1	-8.97	115.62	121.00
1	B	691	ARG	NE-CZ-NH2	8.96	124.78	120.30
1	B	665	TYR	CB-CG-CD1	8.94	126.37	121.00
1	C	421	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	B	691	ARG	NH1-CZ-NH2	-8.66	109.87	119.40
1	B	493	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	C	315	PHE	CB-CG-CD1	8.37	126.66	120.80
1	C	669	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	B	761	PHE	CB-CG-CD2	-8.28	115.00	120.80
1	B	98	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	D	669	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	A	506	ASP	CB-CG-OD2	-8.20	110.92	118.30
1	D	747	TYR	CB-CG-CD2	-8.18	116.09	121.00
1	D	391	ARG	NE-CZ-NH2	8.16	124.38	120.30
1	B	520	TYR	CB-CG-CD2	-8.04	116.18	121.00
1	A	98	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	B	112	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	B	262	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	A	463	TYR	CB-CG-CD1	-7.86	116.29	121.00
1	C	491	PHE	CB-CG-CD2	7.78	126.25	120.80
1	A	719	ASP	CB-CG-OD1	-7.77	111.30	118.30
1	D	687	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	B	735	PHE	CB-CG-CD1	7.73	126.21	120.80
1	B	516	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	C	315	PHE	CB-CG-CD2	-7.67	115.43	120.80
1	A	714	TYR	CG-CD1-CE1	-7.59	115.23	121.30
1	D	656	TYR	CZ-CE2-CD2	-7.56	113.00	119.80
1	A	495	ASP	CB-CG-OD1	-7.48	111.57	118.30
1	A	506	ASP	CB-CG-OD1	7.46	125.01	118.30
1	C	714	TYR	CG-CD1-CE1	-7.43	115.36	121.30
1	C	686	TRP	CE3-CZ3-CH2	7.35	129.28	121.20
1	D	758	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	B	479	ASP	CB-CG-OD1	7.26	124.83	118.30
1	C	382	TYR	CB-CG-CD2	-7.19	116.68	121.00
1	C	528	ARG	NE-CZ-NH2	-7.19	116.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	761	PHE	CB-CG-CD2	-7.18	115.78	120.80
1	A	669	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	C	473	TYR	CB-CG-CD2	-7.09	116.74	121.00
1	D	507	ARG	NE-CZ-NH2	7.07	123.83	120.30
1	D	732	ASP	CB-CG-OD1	7.05	124.65	118.30
1	D	281	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	D	761	PHE	CB-CG-CD1	6.95	125.67	120.80
1	A	782	TRP	CH2-CZ2-CE2	6.92	124.32	117.40
1	C	670	MET	CG-SD-CE	-6.90	89.16	100.20
1	C	98	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	C	518	MET	CG-SD-CE	-6.74	89.41	100.20
1	C	676	PHE	CB-CG-CD2	-6.72	116.09	120.80
1	A	493	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	D	156	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	B	727	ALA	CB-CA-C	-6.67	100.10	110.10
1	C	714	TYR	CD1-CG-CD2	6.66	125.23	117.90
1	C	686	TRP	CZ3-CH2-CZ2	-6.65	113.62	121.60
1	C	736	TYR	CB-CG-CD1	6.59	124.95	121.00
1	D	447	PHE	CB-CG-CD2	-6.49	116.25	120.80
1	B	527	ARG	NE-CZ-NH1	-6.49	117.06	120.30
1	C	189	PHE	CB-CG-CD2	-6.49	116.26	120.80
1	B	458	TYR	CB-CG-CD2	-6.44	117.13	121.00
1	B	495	ASP	CB-CG-OD1	-6.38	112.56	118.30
1	B	479	ASP	CB-CG-OD2	-6.37	112.56	118.30
1	D	714	TYR	CG-CD1-CE1	-6.36	116.21	121.30
1	C	63	MET	CG-SD-CE	-6.32	90.08	100.20
1	C	189	PHE	CB-CG-CD1	6.32	125.22	120.80
1	C	277	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	B	745	ARG	N-CA-CB	6.31	121.95	110.60
1	C	725	TYR	CD1-CE1-CZ	-6.27	114.15	119.80
1	A	444	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	A	720	ALA	N-CA-CB	6.24	118.84	110.10
1	C	437	VAL	CA-CB-CG2	-6.22	101.57	110.90
1	C	382	TYR	CB-CG-CD1	6.20	124.72	121.00
1	C	686	TRP	CG-CD2-CE3	-6.16	128.36	133.90
1	C	170	MET	CG-SD-CE	-6.12	90.41	100.20
1	A	782	TRP	NE1-CE2-CD2	6.09	113.39	107.30
1	A	782	TRP	CD2-CE2-CZ2	-6.05	115.04	122.30
1	D	142	TRP	CG-CD2-CE3	-6.01	128.49	133.90
1	D	340	TRP	NE1-CE2-CZ2	5.99	136.99	130.40
1	B	656	TYR	CZ-CE2-CD2	5.99	125.19	119.80
1	B	757	TYR	CG-CD2-CE2	5.96	126.07	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	473	TYR	CB-CG-CD1	5.96	124.58	121.00
1	B	725	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	A	463	TYR	CG-CD1-CE1	5.95	126.06	121.30
1	B	652	THR	CA-CB-CG2	-5.95	104.08	112.40
1	D	425	VAL	CA-CB-CG1	5.94	119.81	110.90
1	A	458	TYR	CA-CB-CG	5.92	124.66	113.40
1	A	675	PRO	N-CA-CB	5.90	110.39	103.30
1	B	205	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	747	TYR	CG-CD2-CE2	-5.87	116.60	121.30
1	A	687	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	688	MET	CG-SD-CE	-5.87	90.81	100.20
1	C	721	ALA	N-CA-CB	5.86	118.31	110.10
1	A	461	PHE	CB-CG-CD2	-5.86	116.70	120.80
1	B	757	TYR	CB-CG-CD1	-5.85	117.49	121.00
1	D	421	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	C	659	VAL	CA-CB-CG2	-5.77	102.25	110.90
1	B	670	MET	CG-SD-CE	-5.77	90.97	100.20
1	D	334	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	470	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	B	662	SER	O-C-N	-5.72	113.55	122.70
1	B	493	ARG	NH1-CZ-NH2	-5.71	113.12	119.40
1	C	528	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	528	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	D	516	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	D	517	TYR	CG-CD2-CE2	-5.68	116.76	121.30
1	D	517	TYR	CB-CG-CD1	-5.66	117.60	121.00
1	A	687	ARG	CA-CB-CG	5.64	125.81	113.40
1	D	782	TRP	N-CA-C	-5.63	95.80	111.00
1	A	513	PHE	CB-CG-CD2	-5.63	116.86	120.80
1	A	427	GLU	OE1-CD-OE2	5.62	130.04	123.30
1	A	458	TYR	CB-CG-CD2	-5.61	117.64	121.00
1	C	512	ASP	CB-CG-OD1	5.60	123.34	118.30
1	C	451	VAL	CA-CB-CG2	-5.58	102.52	110.90
1	D	253	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	494	ALA	CB-CA-C	-5.56	101.75	110.10
1	A	723	LEU	CB-CG-CD2	5.56	120.45	111.00
1	C	749	ILE	O-C-N	5.54	131.57	122.70
1	C	316	HIS	CA-CB-CG	5.54	123.01	113.60
1	D	516	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	C	317	LYS	N-CA-CB	-5.52	100.67	110.60
1	D	692	SER	N-CA-CB	5.51	118.77	110.50
1	B	655	PRO	N-CD-CG	5.51	111.47	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	656	TYR	CG-CD2-CE2	-5.51	116.89	121.30
1	C	473	TYR	CD1-CE1-CZ	-5.48	114.87	119.80
1	C	156	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	C	316	HIS	CB-CA-C	-5.47	99.46	110.40
1	C	686	TRP	CA-CB-CG	5.46	124.08	113.70
1	D	686	TRP	CB-CG-CD2	-5.46	119.50	126.60
1	D	491	PHE	CB-CG-CD2	-5.44	116.99	120.80
1	A	444	TYR	CB-CG-CD1	5.44	124.26	121.00
1	B	520	TYR	CB-CG-CD1	5.41	124.25	121.00
1	D	156	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	C	458	TYR	CG-CD1-CE1	-5.40	116.98	121.30
1	D	396	TRP	NE1-CE2-CZ2	5.39	136.33	130.40
1	B	461	PHE	CB-CG-CD1	5.39	124.57	120.80
1	C	696	GLU	C-N-CA	5.38	135.14	121.70
1	C	725	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	C	527	ARG	CD-NE-CZ	-5.37	116.09	123.60
1	C	658	THR	N-CA-C	-5.36	96.52	111.00
1	C	716	PHE	CB-CG-CD2	5.36	124.55	120.80
1	A	205	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	768	LEU	CB-CG-CD1	-5.35	101.90	111.00
1	B	461	PHE	CB-CG-CD2	-5.34	117.06	120.80
1	C	695	SER	N-CA-CB	5.34	118.51	110.50
1	C	135	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	512	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	D	105	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	436	ASN	N-CA-CB	5.30	120.14	110.60
1	A	719	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	669	ARG	CA-CB-CG	5.29	125.03	113.40
1	A	445	GLN	N-CA-C	-5.28	96.74	111.00
1	C	486	VAL	CA-CB-CG2	-5.26	103.00	110.90
1	D	189	PHE	CB-CG-CD1	-5.26	117.11	120.80
1	B	253	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	253	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	437	VAL	N-CA-C	-5.23	96.88	111.00
1	C	470	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	C	253	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	714	TYR	CB-CG-CD2	-5.21	117.88	121.00
1	D	498	ILE	N-CA-C	-5.20	96.97	111.00
1	A	513	PHE	CG-CD2-CE2	-5.20	115.09	120.80
1	B	759	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	B	718	TRP	CA-CB-CG	5.18	123.53	113.70
1	C	431	VAL	CG1-CB-CG2	-5.17	102.62	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	782	TRP	CE2-CD2-CG	5.17	111.44	107.30
1	D	497	GLY	N-CA-C	-5.17	100.18	113.10
1	A	730	ASP	CB-CG-OD2	5.15	122.93	118.30
1	C	655	PRO	N-CA-CB	5.15	109.48	103.30
1	D	142	TRP	CD1-NE1-CE2	-5.14	104.38	109.00
1	A	699	VAL	CA-CB-CG1	-5.13	103.20	110.90
1	D	418	VAL	CA-CB-CG1	5.12	118.58	110.90
1	D	491	PHE	CZ-CE2-CD2	5.12	126.24	120.10
1	B	747	TYR	CG-CD1-CE1	-5.11	117.22	121.30
1	D	262	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	C	725	TYR	CG-CD2-CE2	-5.08	117.23	121.30
1	D	516	ARG	NH1-CZ-NH2	5.07	124.98	119.40
1	B	647	ASP	CB-CG-OD2	5.06	122.86	118.30
1	D	510	VAL	CA-CB-CG1	-5.06	103.31	110.90
1	A	759	ASP	CB-CA-C	-5.06	100.29	110.40
1	A	105	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	B	669	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	452	LEU	O-C-N	-5.03	114.66	122.70
1	C	781	TRP	CB-CG-CD1	-5.02	120.47	127.00
1	C	253	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C	682	TYR	CB-CG-CD1	5.01	124.00	121.00

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	516	ARG	Sidechain
1	A	527	ARG	Sidechain
1	A	528	ARG	Sidechain
1	A	691	ARG	Sidechain
1	A	711	TYR	Sidechain
1	A	725	TYR	Sidechain
1	A	747	TYR	Sidechain
1	B	507	ARG	Sidechain
1	B	516	ARG	Sidechain
1	B	520	TYR	Sidechain
1	B	527	ARG	Sidechain
1	B	682	TYR	Sidechain
1	B	725	TYR	Sidechain
1	B	779	HIS	Sidechain
1	C	119	TYR	Sidechain
1	C	252	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	257	ARG	Sidechain
1	C	274	ARG	Sidechain
1	C	315	PHE	Sidechain
1	C	458	TYR	Sidechain
1	C	516	ARG	Sidechain
1	C	520	TYR	Sidechain
1	C	656	TYR	Sidechain
1	C	687	ARG	Sidechain
1	C	736	TYR	Sidechain
1	C	747	TYR	Sidechain
1	D	201	ARG	Sidechain
1	D	257	ARG	Sidechain
1	D	277	ARG	Sidechain
1	D	458	TYR	Sidechain
1	D	491	PHE	Sidechain
1	D	493	ARG	Sidechain
1	D	507	ARG	Sidechain
1	D	665	TYR	Sidechain
1	D	682	TYR	Sidechain
1	D	687	ARG	Sidechain
1	D	691	ARG	Sidechain
1	D	711	TYR	Sidechain
1	D	714	TYR	Sidechain
1	D	747	TYR	Sidechain
1	D	757	TYR	Sidechain
1	D	758	ARG	Sidechain
1	D	98	ARG	Sidechain

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	5248	0	5160	107	0
1	B	5248	0	5160	77	0
1	C	5248	0	5158	111	0
1	D	5248	0	5160	91	0
All	All	20992	0	20638	301	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 7.

All (301) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:LEU:HD22	1:D:297:MET:SD	1.16	1.71
1:C:334:ARG:CG	1:D:334:ARG:NH2	1.81	1.42
1:A:80:GLY:HA2	1:A:110:LEU:CD2	1.50	1.41
1:D:286:LEU:CD2	1:D:297:MET:SD	2.13	1.36
1:C:333:ILE:CD1	1:D:53:PHE:HE1	1.37	1.35
1:B:316:HIS:NE2	1:B:320:GLN:NE2	1.76	1.33
1:C:35:LEU:HD11	1:C:316:HIS:CA	1.60	1.27
1:C:334:ARG:HG3	1:D:334:ARG:NH2	0.92	1.24
1:A:643:GLN:NE2	1:B:696:GLU:OE1	1.71	1.23
1:A:80:GLY:CA	1:A:110:LEU:HD21	1.68	1.22
1:C:35:LEU:CD1	1:C:316:HIS:HA	1.68	1.22
1:A:80:GLY:CA	1:A:110:LEU:CD2	2.17	1.22
1:A:112:ARG:NH2	1:A:118:ASP:CB	2.02	1.21
1:A:643:GLN:HB3	1:B:696:GLU:CG	1.73	1.18
1:C:35:LEU:HD11	1:C:316:HIS:N	1.60	1.17
1:A:771:SER:O	1:B:440:LYS:HD2	1.44	1.16
1:A:112:ARG:NH2	1:A:118:ASP:CA	2.09	1.16
1:C:333:ILE:CD1	1:D:53:PHE:CE1	2.27	1.16
1:A:112:ARG:HH22	1:A:118:ASP:HB2	1.03	1.14
1:A:646:GLN:OE1	1:B:692:SER:HB3	1.49	1.12
1:A:643:GLN:CB	1:B:696:GLU:HG3	1.79	1.12
1:C:35:LEU:CD2	1:C:316:HIS:HD1	1.63	1.12
1:C:53:PHE:HE1	1:D:333:ILE:HD11	1.15	1.11
1:C:333:ILE:HD11	1:D:53:PHE:HE1	1.09	1.11
1:C:334:ARG:HG3	1:D:334:ARG:CZ	1.79	1.10
1:C:316:HIS:CD2	1:C:320:GLN:OE1	2.03	1.09
1:D:286:LEU:HD13	1:D:297:MET:HE1	1.33	1.08
1:C:35:LEU:HD23	1:C:316:HIS:HD1	1.11	1.07
1:C:779:HIS:CE1	1:D:675:PRO:HG2	1.90	1.06
1:C:35:LEU:HD23	1:C:316:HIS:ND1	1.71	1.04
1:C:333:ILE:HD13	1:D:53:PHE:CE1	1.92	1.04
1:A:112:ARG:NH2	1:A:118:ASP:HB2	1.66	1.03
1:C:53:PHE:CZ	1:D:333:ILE:HG12	1.93	1.03
1:D:694:GLY:O	1:D:698:ASN:OD1	1.73	1.03
1:A:80:GLY:HA2	1:A:110:LEU:HD21	1.08	1.02
1:C:333:ILE:HD13	1:D:53:PHE:HE1	1.25	1.00
1:C:333:ILE:HD11	1:D:53:PHE:CE1	1.96	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLY:CA	1:A:110:LEU:HD22	1.91	0.99
1:C:35:LEU:HG	1:C:316:HIS:HB2	1.44	0.98
1:A:112:ARG:NH2	1:A:118:ASP:HA	1.76	0.98
1:C:35:LEU:HD11	1:C:316:HIS:HA	0.98	0.98
1:C:334:ARG:CG	1:D:334:ARG:CZ	2.39	0.97
1:C:35:LEU:CD2	1:C:316:HIS:ND1	2.25	0.96
1:A:643:GLN:CD	1:B:696:GLU:CD	2.24	0.96
1:A:643:GLN:NE2	1:B:696:GLU:CD	2.18	0.96
1:A:112:ARG:HH22	1:A:118:ASP:CB	1.69	0.95
1:A:112:ARG:NH1	1:A:118:ASP:OD2	1.98	0.95
1:A:643:GLN:CD	1:B:696:GLU:OE1	2.04	0.94
1:A:691:ARG:HB3	1:A:696:GLU:OE1	1.68	0.93
1:C:491:PHE:HD2	1:C:493:ARG:HH11	1.16	0.92
1:A:112:ARG:CZ	1:A:118:ASP:CG	2.39	0.91
1:B:652:THR:HB	1:B:688:MET:CE	2.01	0.91
1:A:771:SER:O	1:B:440:LYS:CD	2.19	0.89
1:A:155:ILE:HD12	1:B:155:ILE:CD1	2.02	0.89
1:C:35:LEU:HG	1:C:316:HIS:CB	2.01	0.89
1:C:53:PHE:CE1	1:D:333:ILE:HD11	2.07	0.89
1:C:334:ARG:HG3	1:D:334:ARG:HH21	1.28	0.89
1:C:35:LEU:CD1	1:C:316:HIS:N	2.36	0.89
1:D:230:ALA:HA	1:D:233:CYS:SG	2.13	0.89
1:A:112:ARG:HH21	1:A:118:ASP:HA	1.36	0.89
1:B:652:THR:HB	1:B:688:MET:HE3	1.54	0.89
1:D:286:LEU:HD13	1:D:297:MET:CE	2.02	0.89
1:C:53:PHE:HE1	1:D:333:ILE:CD1	1.86	0.88
1:C:334:ARG:CG	1:D:334:ARG:HH22	1.61	0.88
1:C:53:PHE:HZ	1:D:333:ILE:HG12	1.33	0.87
1:C:779:HIS:CE1	1:D:675:PRO:CG	2.58	0.87
1:D:204:LEU:HB3	1:D:229:VAL:HG21	1.56	0.86
1:C:35:LEU:CG	1:C:316:HIS:HA	2.06	0.86
1:C:35:LEU:CD1	1:C:316:HIS:CA	2.38	0.85
1:D:467:VAL:HG11	1:D:471:HIS:CD2	2.11	0.85
1:C:334:ARG:HG3	1:D:334:ARG:HH22	1.08	0.85
1:A:155:ILE:CD1	1:B:155:ILE:CD1	2.56	0.84
1:B:676:PHE:CE1	1:C:189:PHE:CD2	2.66	0.84
1:A:776:ILE:HD11	1:B:439:GLY:HA3	1.61	0.82
1:D:467:VAL:HG11	1:D:471:HIS:HD2	1.43	0.82
1:A:643:GLN:HB3	1:B:696:GLU:HG3	0.87	0.82
1:A:80:GLY:HA2	1:A:110:LEU:HD22	1.47	0.80
1:A:80:GLY:HA3	1:A:110:LEU:CD2	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:LEU:HD11	1:C:315:PHE:C	2.01	0.79
1:D:527:ARG:HD3	1:D:709:VAL:O	1.83	0.79
1:A:112:ARG:HH21	1:A:118:ASP:CA	1.92	0.79
1:C:779:HIS:CE1	1:D:676:PHE:CE1	2.71	0.79
1:C:35:LEU:CG	1:C:316:HIS:HD1	1.96	0.78
1:A:155:ILE:HD12	1:B:155:ILE:HD12	1.62	0.78
1:A:771:SER:C	1:B:440:LYS:HD2	2.04	0.78
1:B:35:LEU:H	1:B:316:HIS:HD1	1.30	0.78
1:D:204:LEU:HB3	1:D:229:VAL:CG2	2.13	0.78
1:C:53:PHE:CZ	1:D:333:ILE:CG1	2.67	0.78
1:C:779:HIS:NE2	1:D:675:PRO:HB2	2.01	0.76
1:C:34:ILE:HD13	1:C:313:ASN:HA	1.66	0.76
1:A:112:ARG:CZ	1:A:118:ASP:CB	2.64	0.76
1:A:150:ASP:OD1	1:A:153:TYR:HB2	1.86	0.76
1:C:32:GLU:HB3	1:C:36:GLN:NE2	2.02	0.75
1:B:150:ASP:OD1	1:B:153:TYR:HB2	1.87	0.74
1:D:286:LEU:HD22	1:D:297:MET:CE	2.17	0.74
1:B:193:ARG:O	1:B:197:LEU:HB2	1.88	0.74
1:C:775:ASP:HB2	1:D:676:PHE:HE2	1.53	0.73
1:A:155:ILE:CD1	1:B:155:ILE:HD12	2.17	0.72
1:C:35:LEU:CG	1:C:316:HIS:CA	2.67	0.72
1:B:447:PHE:CE1	1:B:777:LEU:HB2	2.24	0.72
1:A:193:ARG:O	1:A:197:LEU:HB2	1.88	0.72
1:C:779:HIS:HE1	1:D:676:PHE:CE1	2.08	0.71
1:C:34:ILE:HG23	1:C:316:HIS:HB2	1.72	0.71
1:A:155:ILE:HD12	1:B:155:ILE:HD11	1.73	0.71
1:A:80:GLY:HA3	1:A:110:LEU:HD21	1.66	0.71
1:D:286:LEU:CD1	1:D:297:MET:CE	2.69	0.71
1:A:112:ARG:NH1	1:A:118:ASP:CG	2.43	0.70
1:C:35:LEU:CD2	1:C:316:HIS:HA	2.20	0.70
1:C:428:GLU:HG2	1:C:432:MET:HG2	1.74	0.69
1:C:35:LEU:HD21	1:C:316:HIS:HA	1.72	0.69
1:A:646:GLN:OE1	1:B:692:SER:CB	2.36	0.69
1:D:283:SER:HB3	1:D:285:THR:HG22	1.75	0.69
1:A:776:ILE:CD1	1:B:439:GLY:HA3	2.22	0.68
1:B:724:GLU:O	1:B:728:ILE:HG13	1.94	0.68
1:A:643:GLN:CB	1:B:696:GLU:CG	2.53	0.67
1:C:779:HIS:HE1	1:D:675:PRO:HG2	1.53	0.67
1:C:53:PHE:HZ	1:D:333:ILE:CG1	2.04	0.67
1:A:489:LEU:HB2	1:A:511:VAL:HG11	1.77	0.66
1:B:316:HIS:CD2	1:B:320:GLN:NE2	2.62	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:ASN:ND2	1:B:677:GLU:HB3	2.10	0.66
1:C:53:PHE:CE1	1:D:333:ILE:CD1	2.71	0.66
1:C:426:LEU:HG	1:C:467:VAL:HG11	1.78	0.66
1:A:501:LEU:CD1	1:A:507:ARG:NH1	2.60	0.65
1:C:316:HIS:HD2	1:C:320:GLN:OE1	1.75	0.65
1:C:53:PHE:CE1	1:D:333:ILE:CG1	2.80	0.65
1:C:35:LEU:CG	1:C:316:HIS:CB	2.74	0.65
1:A:477:GLN:H	1:A:477:GLN:NE2	1.94	0.65
1:B:447:PHE:HE1	1:B:777:LEU:HB2	1.61	0.64
1:D:204:LEU:O	1:D:229:VAL:HG21	1.97	0.64
1:C:491:PHE:CD2	1:C:493:ARG:NH1	2.67	0.64
1:C:251:VAL:HG11	1:C:381:ASN:HB3	1.80	0.63
1:B:193:ARG:HG2	1:B:196:GLU:HG3	1.81	0.62
1:A:774:MET:HG3	1:A:778:LYS:NZ	2.14	0.62
1:C:53:PHE:CE1	1:D:333:ILE:HG12	2.32	0.62
1:C:334:ARG:HG2	1:D:334:ARG:NH2	2.07	0.62
1:D:230:ALA:O	1:D:233:CYS:SG	2.58	0.62
1:A:487:GLY:O	1:A:491:PHE:HD2	1.81	0.62
1:A:779:HIS:HA	1:A:782:TRP:O	2.00	0.61
1:C:32:GLU:HB3	1:C:36:GLN:CD	2.21	0.61
1:A:501:LEU:HD11	1:A:507:ARG:NH1	2.16	0.61
1:C:35:LEU:HD21	1:C:316:HIS:CA	2.31	0.61
1:A:643:GLN:CB	1:B:696:GLU:CD	2.69	0.61
1:B:111:THR:HG23	1:B:111:THR:O	2.00	0.61
1:A:420:LEU:HD12	1:A:461:PHE:CE1	2.36	0.60
1:B:728:ILE:HG22	1:B:728:ILE:O	2.01	0.60
1:B:316:HIS:CE1	1:B:320:GLN:NE2	2.65	0.60
1:D:696:GLU:HG2	1:D:697:ASN:OD1	2.00	0.60
1:A:193:ARG:HG2	1:A:196:GLU:HG3	1.84	0.60
1:B:429:PRO:HA	1:B:432:MET:HG2	1.83	0.59
1:C:381:ASN:N	1:C:381:ASN:HD22	1.99	0.59
1:A:430:PHE:CG	1:A:500:ALA:HB2	2.38	0.59
1:C:775:ASP:HB2	1:D:676:PHE:CE2	2.37	0.59
1:A:111:THR:HG23	1:A:111:THR:O	2.01	0.59
1:D:322:ARG:HD2	1:D:322:ARG:N	2.14	0.59
1:A:432:MET:HE3	1:A:781:TRP:CZ3	2.37	0.58
1:C:333:ILE:HG12	1:D:53:PHE:CZ	2.39	0.58
1:A:677:GLU:HG3	1:A:677:GLU:O	2.03	0.58
1:C:34:ILE:CG2	1:C:316:HIS:HB2	2.33	0.58
1:C:334:ARG:CD	1:D:334:ARG:CZ	2.82	0.57
1:D:319:LEU:HG	1:D:319:LEU:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:ARG:O	1:D:229:VAL:HG11	2.04	0.57
1:A:334:ARG:CZ	1:B:334:ARG:CZ	2.83	0.57
1:C:426:LEU:HD23	1:C:431:VAL:HG12	1.86	0.57
1:C:422:VAL:HG22	1:C:496:ILE:HD11	1.86	0.57
1:A:696:GLU:C	1:A:698:ASN:H	2.07	0.56
1:D:201:ARG:O	1:D:229:VAL:CG1	2.54	0.56
1:D:477:GLN:O	1:D:481:THR:O	2.24	0.56
1:B:316:HIS:CD2	1:B:320:GLN:CD	2.79	0.56
1:D:286:LEU:CD2	1:D:297:MET:CE	2.80	0.56
1:A:491:PHE:HB2	1:A:493:ARG:NE	2.21	0.56
1:D:527:ARG:CD	1:D:709:VAL:O	2.53	0.56
1:B:673:LEU:HD21	1:B:686:TRP:NE1	2.20	0.56
1:A:776:ILE:HD11	1:B:439:GLY:CA	2.34	0.55
1:B:492:LYS:HG2	1:B:752:GLN:OE1	2.06	0.55
1:C:334:ARG:HD3	1:D:334:ARG:CZ	2.36	0.55
1:A:150:ASP:OD1	1:A:153:TYR:CB	2.54	0.55
1:C:334:ARG:HG2	1:D:334:ARG:HH22	1.65	0.55
1:D:35:LEU:HD21	1:D:315:PHE:HB2	1.88	0.55
1:D:204:LEU:CB	1:D:229:VAL:HG21	2.34	0.55
1:A:421:ARG:NE	1:A:466:TYR:CE2	2.75	0.55
1:B:507:ARG:O	1:B:511:VAL:HG22	2.06	0.55
1:A:112:ARG:NH2	1:A:118:ASP:N	2.55	0.55
1:A:155:ILE:CD1	1:B:155:ILE:HD11	2.31	0.55
1:A:430:PHE:CZ	1:A:747:TYR:CE2	2.94	0.54
1:A:674:ASN:HB3	1:A:677:GLU:HB3	1.89	0.54
1:D:229:VAL:HG23	1:D:229:VAL:O	2.08	0.54
1:A:489:LEU:HB2	1:A:511:VAL:CG1	2.38	0.54
1:A:501:LEU:HD12	1:A:507:ARG:NH1	2.23	0.53
1:B:673:LEU:HD21	1:B:686:TRP:HE1	1.72	0.53
1:A:80:GLY:N	1:A:110:LEU:HD22	2.24	0.53
1:A:689:ILE:HA	1:A:698:ASN:HD21	1.74	0.53
1:C:35:LEU:CG	1:C:316:HIS:ND1	2.67	0.53
1:C:35:LEU:HG	1:C:316:HIS:ND1	2.23	0.53
1:A:432:MET:CE	1:A:781:TRP:CZ3	2.92	0.53
1:C:333:ILE:HG12	1:D:53:PHE:HZ	1.73	0.53
1:A:477:GLN:H	1:A:477:GLN:HE21	1.55	0.53
1:B:110:LEU:HG	1:B:112:ARG:HB2	1.91	0.53
1:A:643:GLN:CD	1:B:696:GLU:CG	2.77	0.52
1:A:430:PHE:CD2	1:A:500:ALA:HB2	2.44	0.52
1:B:316:HIS:NE2	1:B:320:GLN:CD	2.56	0.52
1:A:722:VAL:O	1:A:726:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ILE:HD11	1:B:155:ILE:CD1	2.38	0.52
1:B:110:LEU:CD2	1:B:112:ARG:HB2	2.40	0.52
1:B:150:ASP:OD1	1:B:153:TYR:CB	2.55	0.52
1:D:181:ILE:HD12	1:D:181:ILE:H	1.75	0.51
1:D:265:PHE:CD1	1:D:359:THR:HA	2.46	0.51
1:A:643:GLN:OE1	1:B:696:GLU:OE1	2.28	0.51
1:C:779:HIS:HE1	1:D:676:PHE:CD1	2.29	0.51
1:D:80:GLY:HA3	1:D:110:LEU:HD13	1.91	0.51
1:A:489:LEU:HD13	1:A:750:ALA:HB1	1.93	0.51
1:B:447:PHE:HZ	1:B:774:MET:SD	2.34	0.50
1:A:477:GLN:OE1	1:A:483:ASN:ND2	2.44	0.50
1:C:316:HIS:O	1:C:320:GLN:HG3	2.12	0.50
1:B:434:SER:HB2	1:B:445:GLN:CD	2.32	0.50
1:A:112:ARG:CZ	1:A:118:ASP:HB2	2.33	0.50
1:A:155:ILE:HD11	1:B:155:ILE:HG13	1.93	0.50
1:B:674:ASN:HD22	1:B:677:GLU:HB3	1.75	0.49
1:A:477:GLN:NE2	1:A:477:GLN:N	2.60	0.49
1:C:334:ARG:HG2	1:D:334:ARG:NH1	2.27	0.49
1:D:428:GLU:HG3	1:D:722:VAL:HG13	1.94	0.49
1:A:643:GLN:HB2	1:B:696:GLU:OE2	2.13	0.49
1:A:770:GLN:HG2	1:B:469:PRO:HB3	1.93	0.49
1:C:334:ARG:CG	1:D:334:ARG:NH1	2.76	0.49
1:C:334:ARG:HG2	1:D:334:ARG:CZ	2.39	0.49
1:C:68:LEU:HD22	1:C:340:TRP:CH2	2.48	0.49
1:D:230:ALA:CA	1:D:233:CYS:SG	2.96	0.49
1:A:420:LEU:HD13	1:A:496:ILE:HD13	1.93	0.49
1:A:776:ILE:CG1	1:B:439:GLY:HA3	2.43	0.48
1:C:756:PRO:HG2	1:C:757:TYR:CD2	2.47	0.48
1:D:322:ARG:HD2	1:D:322:ARG:H	1.78	0.48
1:C:33:GLU:OE2	1:C:280:HIS:HB2	2.13	0.48
1:D:204:LEU:C	1:D:229:VAL:HG21	2.33	0.48
1:D:688:MET:HG3	1:D:697:ASN:HD22	1.78	0.48
1:A:433:VAL:O	1:A:433:VAL:HG13	2.14	0.48
1:A:774:MET:HG3	1:A:778:LYS:HZ2	1.79	0.48
1:D:204:LEU:HB3	1:D:229:VAL:HG22	1.96	0.47
1:C:381:ASN:HD22	1:C:381:ASN:H	1.60	0.47
1:C:35:LEU:CD1	1:C:315:PHE:C	2.75	0.47
1:A:660:LEU:HD13	1:A:694:GLY:HA3	1.96	0.47
1:C:333:ILE:O	1:C:333:ILE:HG22	2.13	0.47
1:C:381:ASN:H	1:C:381:ASN:ND2	2.13	0.47
1:C:642:ILE:HD11	1:C:651:GLN:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:PHE:CE2	1:A:747:TYR:CD2	3.02	0.47
1:D:428:GLU:OE2	1:D:722:VAL:CG1	2.63	0.47
1:A:432:MET:HE1	1:A:781:TRP:CE3	2.50	0.46
1:C:779:HIS:CE1	1:D:676:PHE:CZ	3.03	0.46
1:C:525:LEU:N	1:C:723:LEU:HD13	2.30	0.46
1:A:57:GLN:HG3	1:B:333:ILE:HG23	1.98	0.46
1:A:334:ARG:NE	1:B:334:ARG:NE	2.63	0.46
1:B:420:LEU:HD13	1:B:496:ILE:HD13	1.96	0.46
1:C:32:GLU:HB3	1:C:36:GLN:CG	2.46	0.46
1:C:34:ILE:HG23	1:C:316:HIS:CB	2.45	0.46
1:A:645:LEU:HD12	1:A:740:ASN:OD1	2.16	0.46
1:C:35:LEU:HG	1:C:316:HIS:CG	2.51	0.46
1:C:32:GLU:HB3	1:C:36:GLN:HG2	1.98	0.46
1:C:35:LEU:CD2	1:C:316:HIS:CA	2.91	0.46
1:B:427:GLU:HA	1:B:427:GLU:OE1	2.16	0.45
1:C:427:GLU:HA	1:C:427:GLU:OE2	2.17	0.45
1:C:689:ILE:HD12	1:C:689:ILE:HA	1.78	0.45
1:D:164:LYS:HE2	1:D:164:LYS:HA	1.99	0.45
1:C:112:ARG:HH21	1:C:118:ASP:CG	2.20	0.45
1:D:467:VAL:CG1	1:D:471:HIS:CD2	2.92	0.44
1:C:775:ASP:CB	1:D:676:PHE:CE2	2.99	0.44
1:A:501:LEU:HD12	1:A:507:ARG:HH12	1.81	0.44
1:B:524:VAL:CG2	1:B:715:ALA:HB1	2.46	0.44
1:A:778:LYS:O	1:A:782:TRP:HB2	2.18	0.44
1:B:507:ARG:O	1:B:511:VAL:CG2	2.65	0.44
1:D:378:LEU:HB3	1:D:390:VAL:HG11	2.00	0.44
1:C:333:ILE:CG1	1:D:53:PHE:CE1	2.97	0.43
1:C:33:GLU:OE2	1:C:280:HIS:CG	2.71	0.43
1:C:35:LEU:CD2	1:C:316:HIS:CG	3.00	0.43
1:D:284:SER:HA	1:D:287:CYS:SG	2.59	0.43
1:B:509:ASN:ND2	1:C:179:ASN:OD1	2.52	0.43
1:A:155:ILE:HD11	1:B:155:ILE:CG1	2.49	0.43
1:A:776:ILE:HD11	1:B:438:LEU:O	2.19	0.43
1:C:673:LEU:HD21	1:C:686:TRP:CZ2	2.53	0.43
1:A:659:VAL:HG12	1:A:660:LEU:O	2.19	0.43
1:A:504:THR:OG1	1:A:507:ARG:HG3	2.18	0.42
1:C:779:HIS:CE1	1:D:675:PRO:CB	3.01	0.42
1:C:34:ILE:HG21	1:C:312:ALA:O	2.20	0.42
1:D:251:VAL:HG13	1:D:381:ASN:HB3	2.02	0.42
1:D:378:LEU:HB3	1:D:390:VAL:CG1	2.50	0.42
1:B:482:TRP:HB2	1:B:487:GLY:HA2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:676:PHE:CE1	1:C:189:PHE:CE2	3.07	0.41
1:A:28:LEU:HD12	1:A:308:VAL:HG12	2.02	0.41
1:B:316:HIS:O	1:B:320:GLN:HG3	2.20	0.41
1:A:693:ASN:N	1:A:693:ASN:HD22	2.18	0.41
1:C:381:ASN:N	1:C:381:ASN:ND2	2.64	0.41
1:B:427:GLU:OE2	1:B:722:VAL:HG11	2.20	0.41
1:A:643:GLN:HB2	1:B:696:GLU:CD	2.40	0.41
1:B:28:LEU:HD12	1:B:308:VAL:HG12	2.02	0.41
1:C:251:VAL:CG1	1:C:381:ASN:HB3	2.46	0.41
1:C:247:VAL:HG11	1:C:390:VAL:HG21	2.02	0.41
1:A:420:LEU:HD13	1:A:496:ILE:CD1	2.50	0.41
1:C:68:LEU:HD22	1:C:340:TRP:CZ2	2.55	0.41
1:A:80:GLY:HA3	1:A:110:LEU:CD1	2.50	0.41
1:D:35:LEU:HD11	1:D:312:ALA:HA	2.04	0.40
1:A:776:ILE:HG12	1:B:439:GLY:HA3	2.03	0.40
1:B:434:SER:HB2	1:B:445:GLN:CG	2.51	0.40
1:D:283:SER:C	1:D:285:THR:H	2.25	0.40
1:D:656:TYR:HB3	1:D:715:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	654/877 (75%)	636 (97%)	17 (3%)	1 (0%)	44	78
1	B	654/877 (75%)	639 (98%)	15 (2%)	0	100	100
1	C	654/877 (75%)	629 (96%)	25 (4%)	0	100	100
1	D	654/877 (75%)	621 (95%)	33 (5%)	0	100	100
All	All	2616/3508 (75%)	2525 (96%)	90 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	696	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	580/764 (76%)	572 (99%)	8 (1%)	62	75
1	B	580/764 (76%)	575 (99%)	5 (1%)	75	83
1	C	580/764 (76%)	565 (97%)	15 (3%)	41	59
1	D	580/764 (76%)	569 (98%)	11 (2%)	52	69
All	All	2320/3056 (76%)	2281 (98%)	39 (2%)	56	72

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	THR
1	A	466	TYR
1	A	477	GLN
1	A	479	ASP
1	A	485	LEU
1	A	648	LEU
1	A	652	THR
1	A	676	PHE
1	B	111	THR
1	B	112	ARG
1	B	438	LEU
1	B	667	HIS
1	B	718	TRP
1	C	103	THR
1	C	112	ARG
1	C	195	GLU
1	C	203	THR
1	C	212	ASN
1	C	260	ILE
1	C	334	ARG
1	C	381	ASN

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Mol	Chain	Res	Type
1	C	485	LEU
1	C	669	ARG
1	C	670	MET
1	C	687	ARG
1	C	718	TRP
1	C	731	PRO
1	C	741	THR
1	D	103	THR
1	D	111	THR
1	D	129	LEU
1	D	241	GLU
1	D	252	ARG
1	D	322	ARG
1	D	348	GLU
1	D	479	ASP
1	D	483	ASN
1	D	495	ASP
1	D	502	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	477	GLN
1	A	483	ASN
1	A	693	ASN
1	A	697	ASN
1	A	698	ASN
1	A	753	HIS
1	B	50	ASN
1	B	320	GLN
1	B	779	HIS
1	C	31	ASN
1	C	90	HIS
1	C	167	GLN
1	C	248	GLN
1	C	367	ASN
1	C	381	ASN
1	C	779	HIS
1	D	36	GLN
1	D	471	HIS
1	D	483	ASN
1	D	698	ASN

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Mol	Chain	Res	Type
1	D	729	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

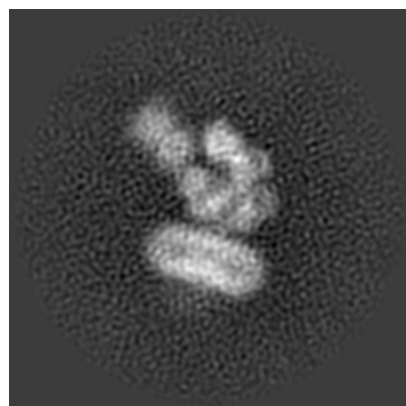
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0979. These allow visual inspection of the internal detail of the map and identification of artifacts.

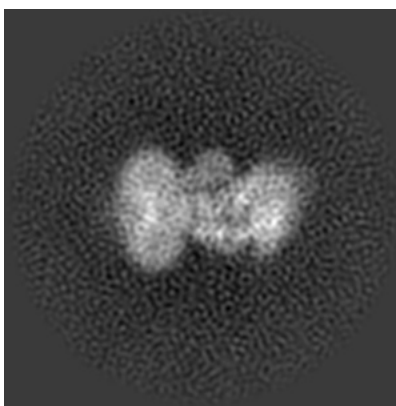
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

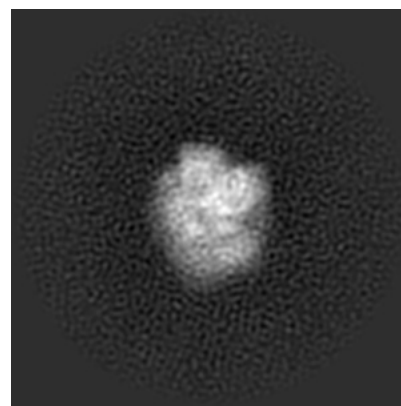
6.1.1 Primary map



X

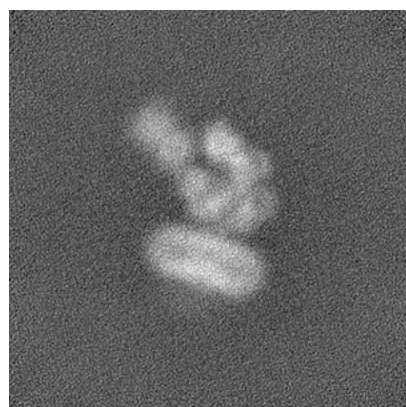


Y

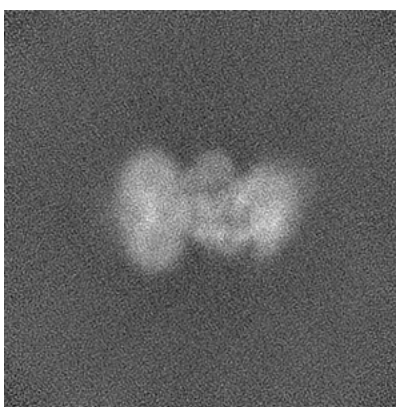


Z

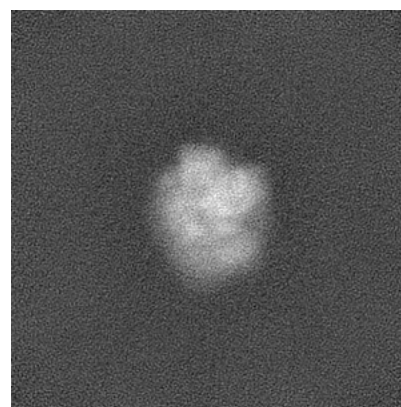
6.1.2 Raw map



X



Y

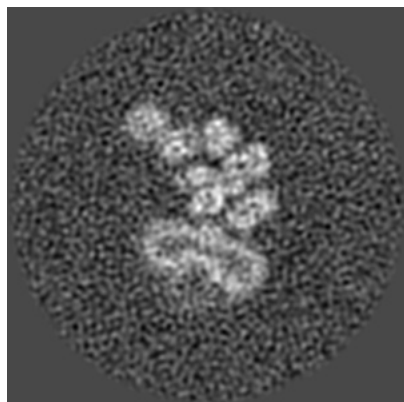


Z

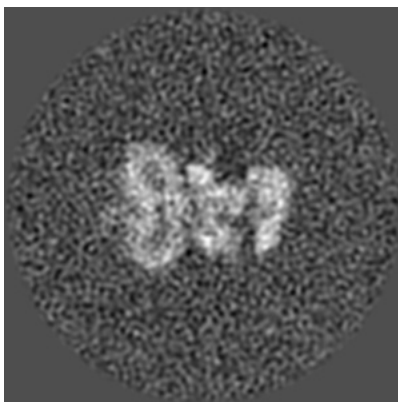
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

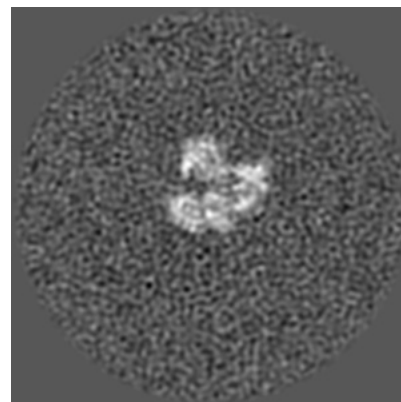
6.2.1 Primary map



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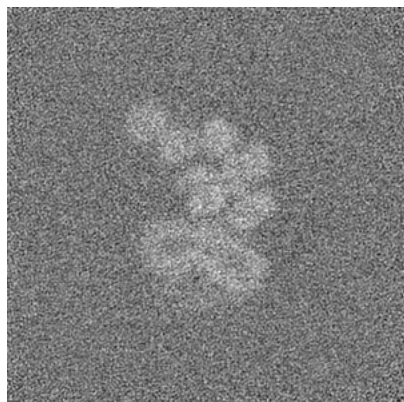


Y Index: 140

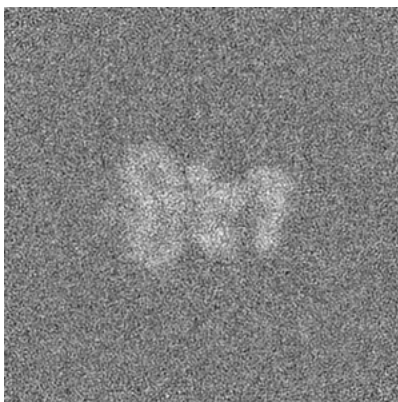


Z Index: 140

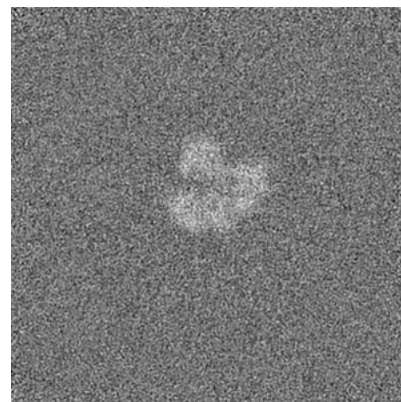
6.2.2 Raw map



X Index: 140



Y Index: 140

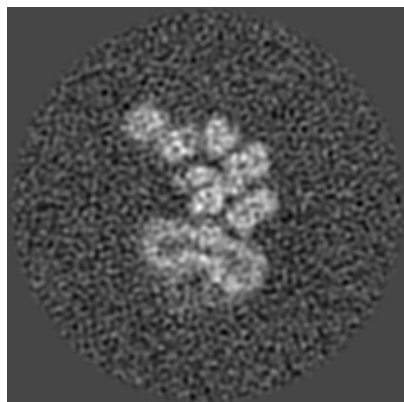


Z Index: 140

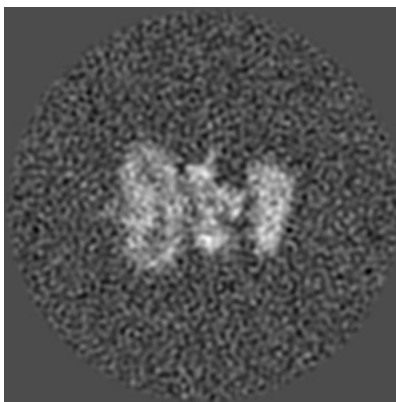
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

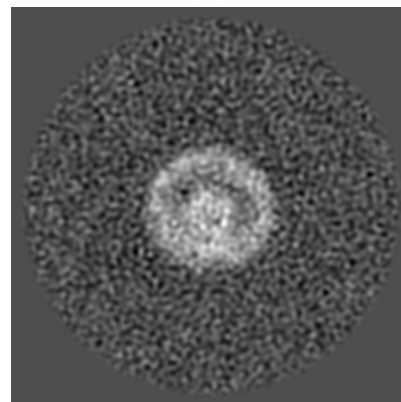
6.3.1 Primary map



X Index: 139

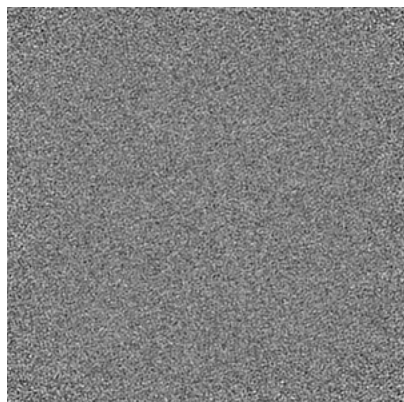


Y Index: 142

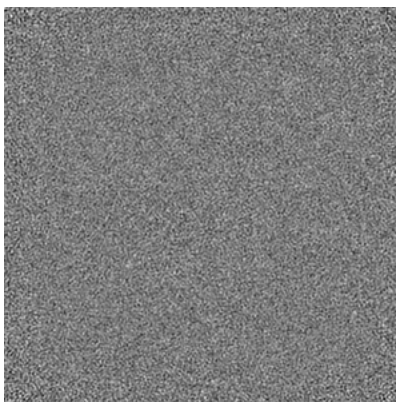


Z Index: 101

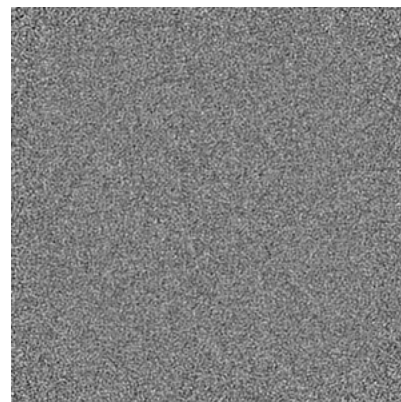
6.3.2 Raw map



X Index: 0



Y Index: 0

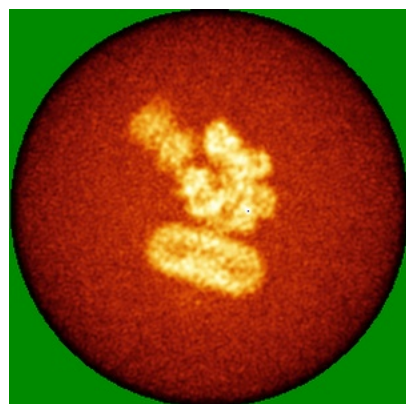


Z Index: 0

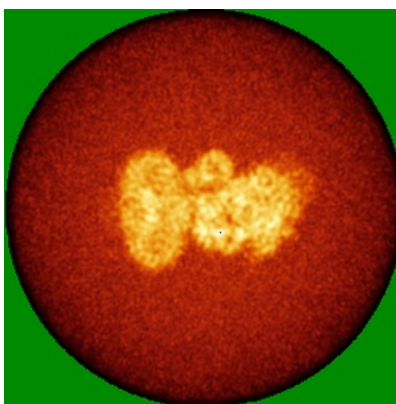
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

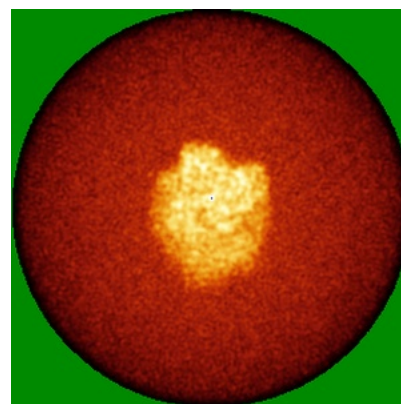
6.4.1 Primary map



X

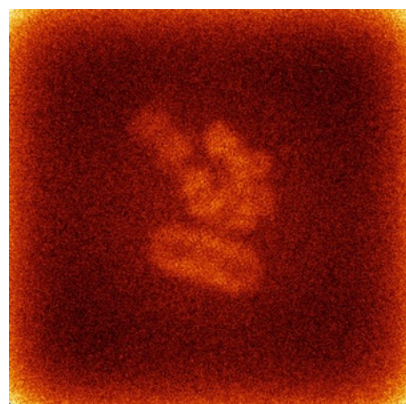


Y

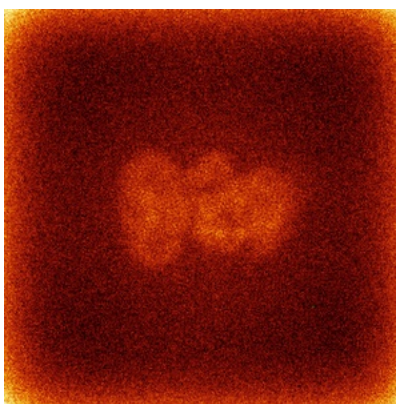


Z

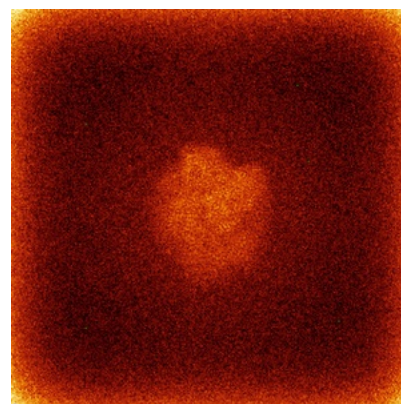
6.4.2 Raw map



X



Y

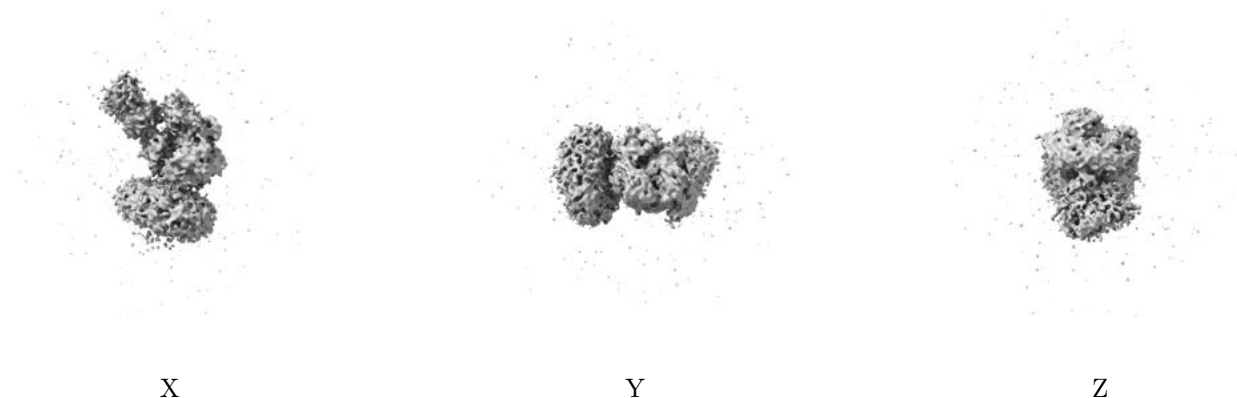


Z

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.

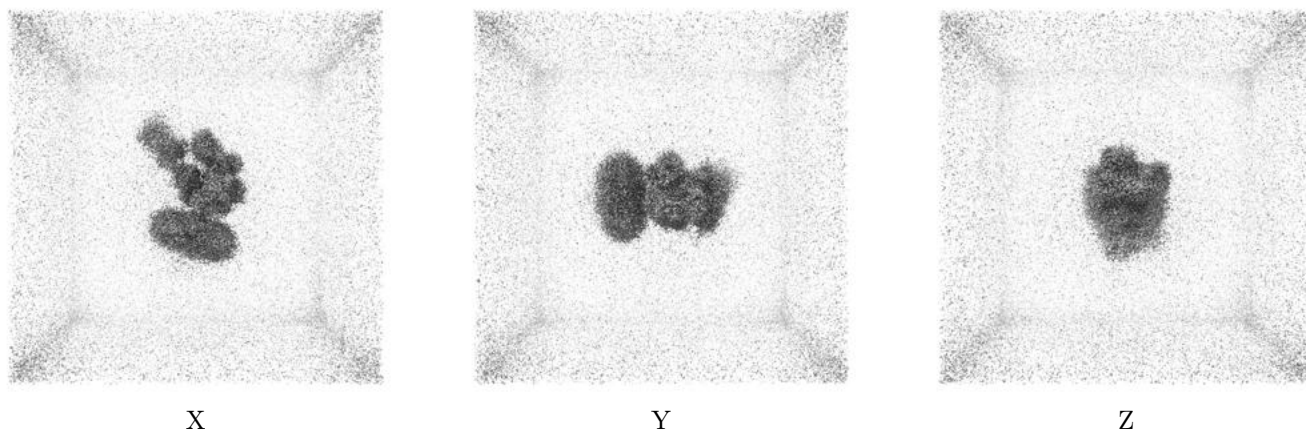
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.316. 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



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.

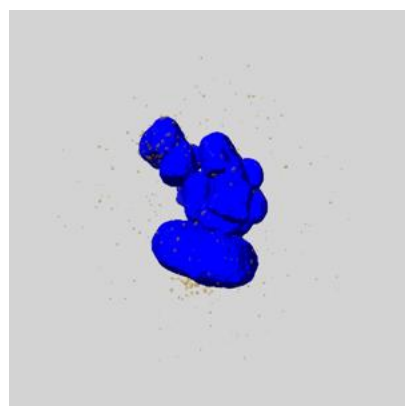
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

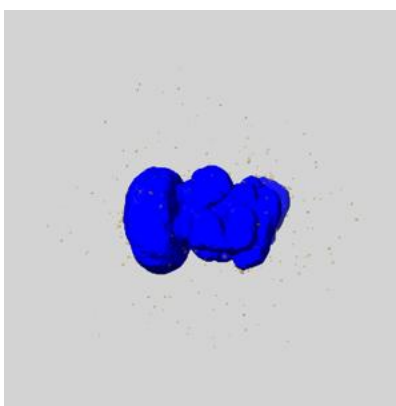
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

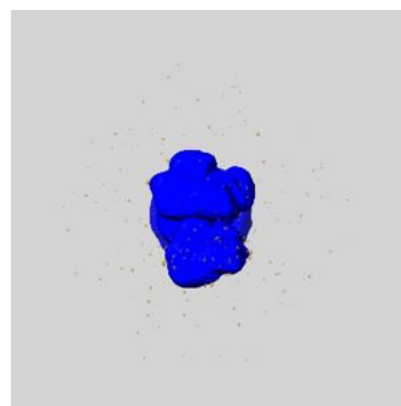
6.6.1 emd_0979_msk_1.map [i](#)



X



Y

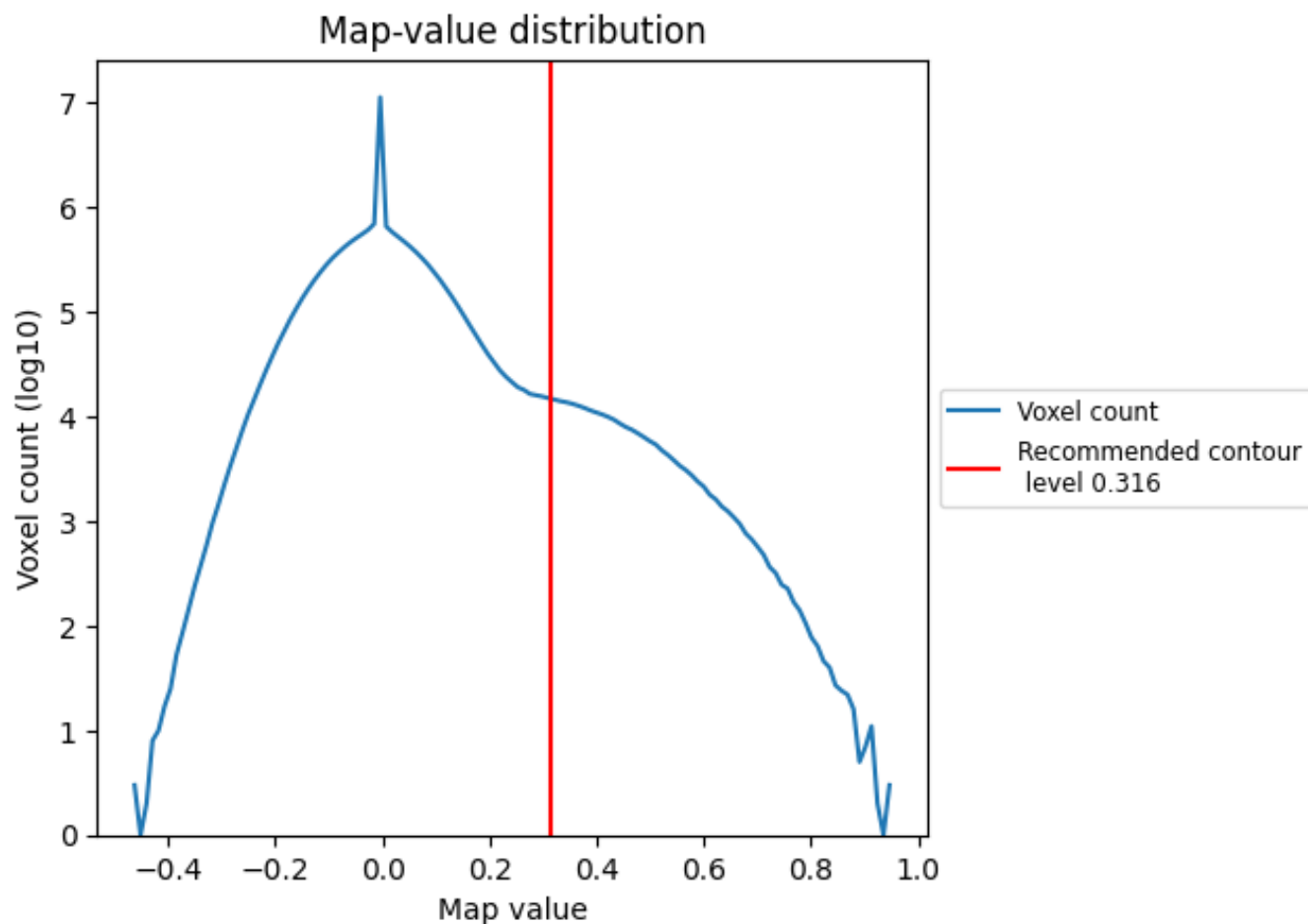


Z

7 Map analysis [i](#)

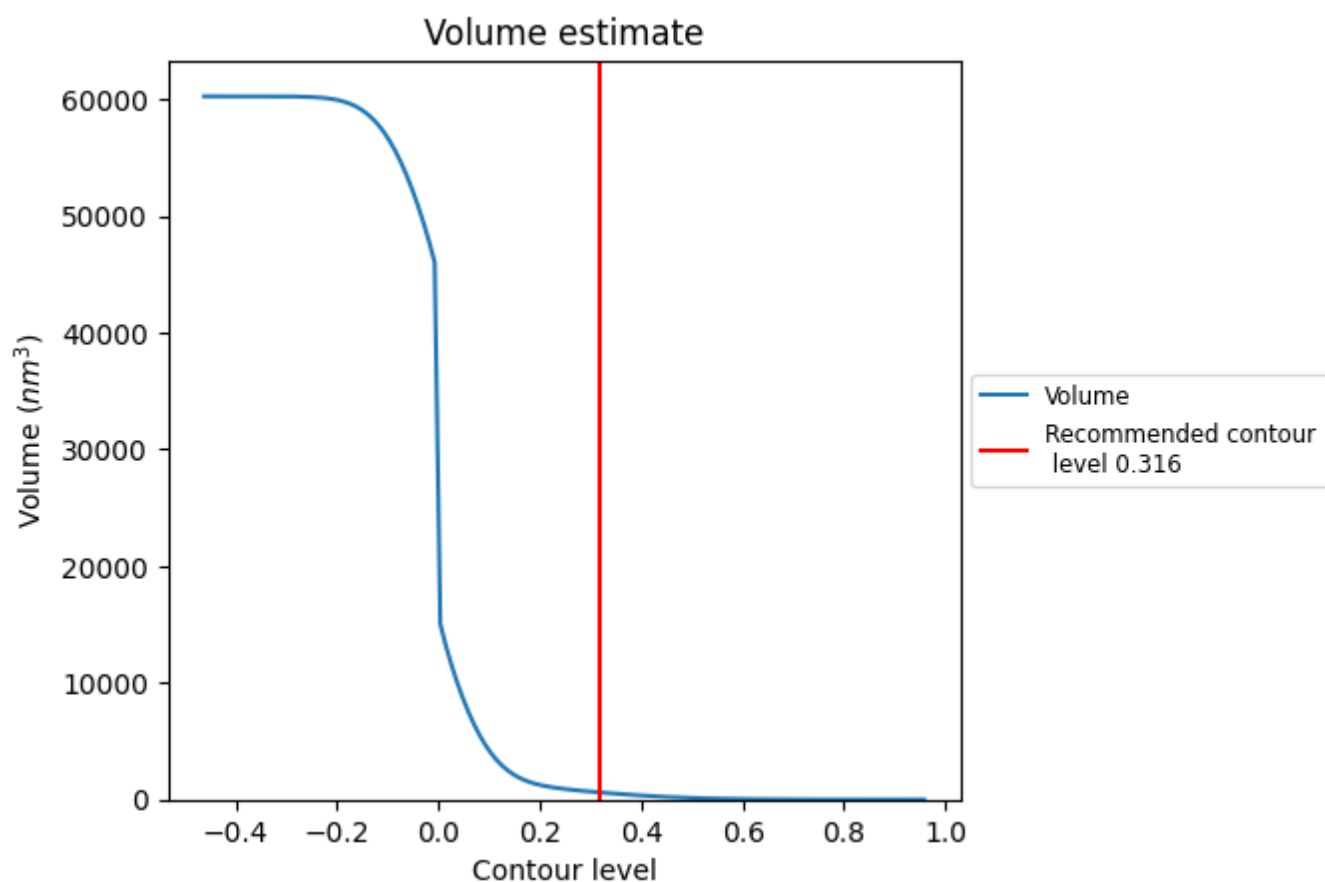
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

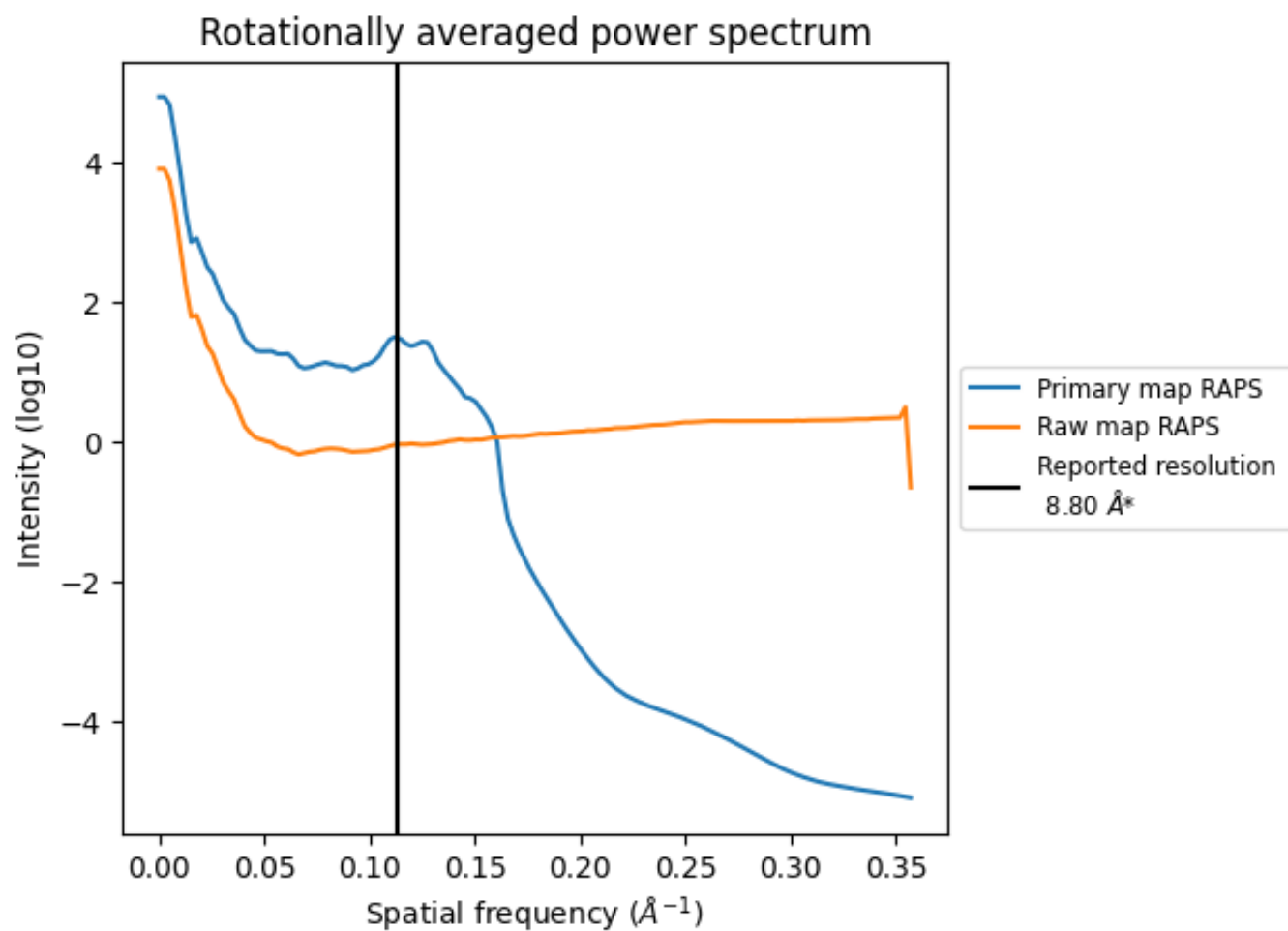
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 621 nm³; this corresponds to an approximate mass of 561 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 ⓘ

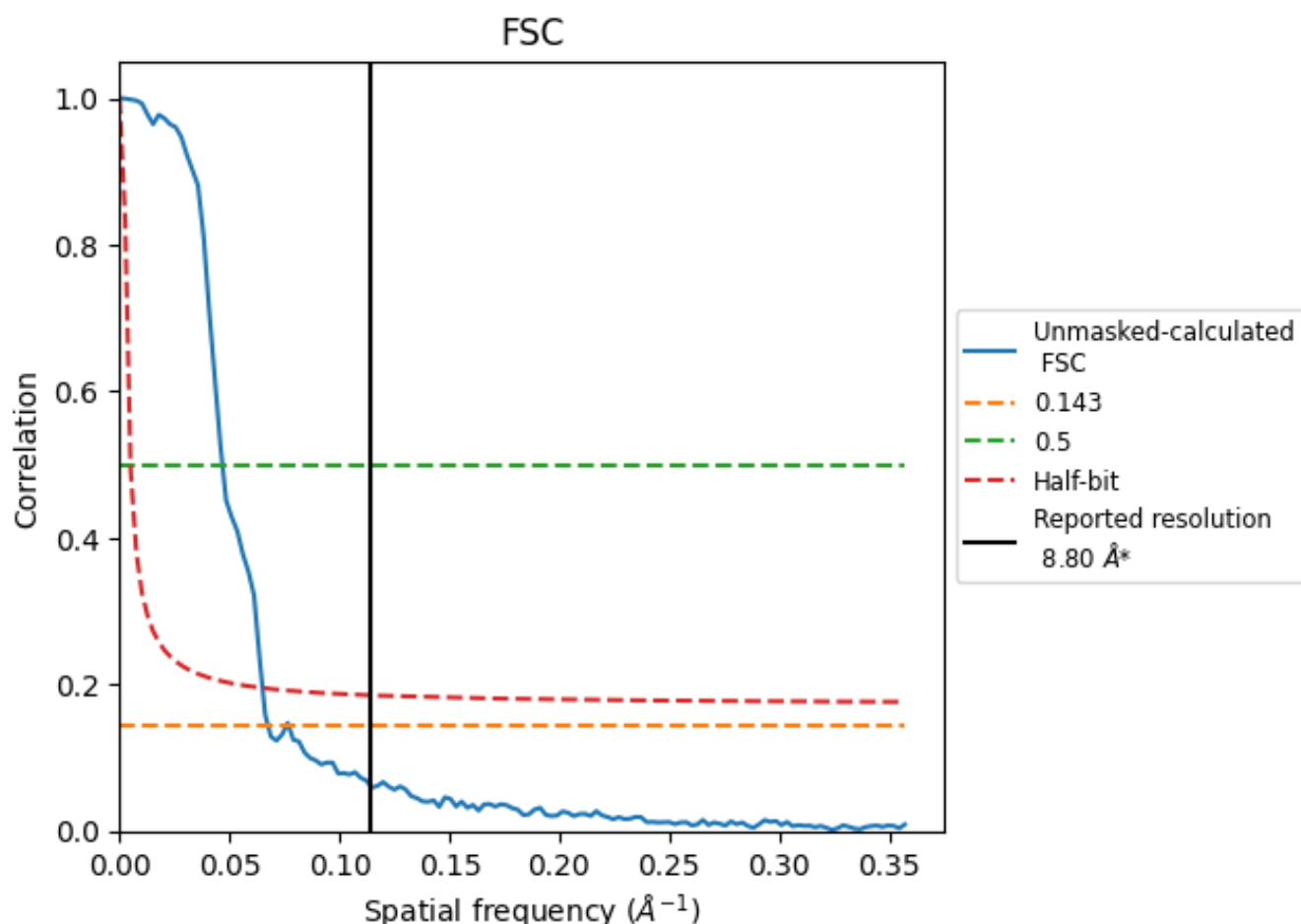


*Reported resolution corresponds to spatial frequency of 0.114 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.114 \AA^{-1}

8.2 Resolution estimates [i](#)

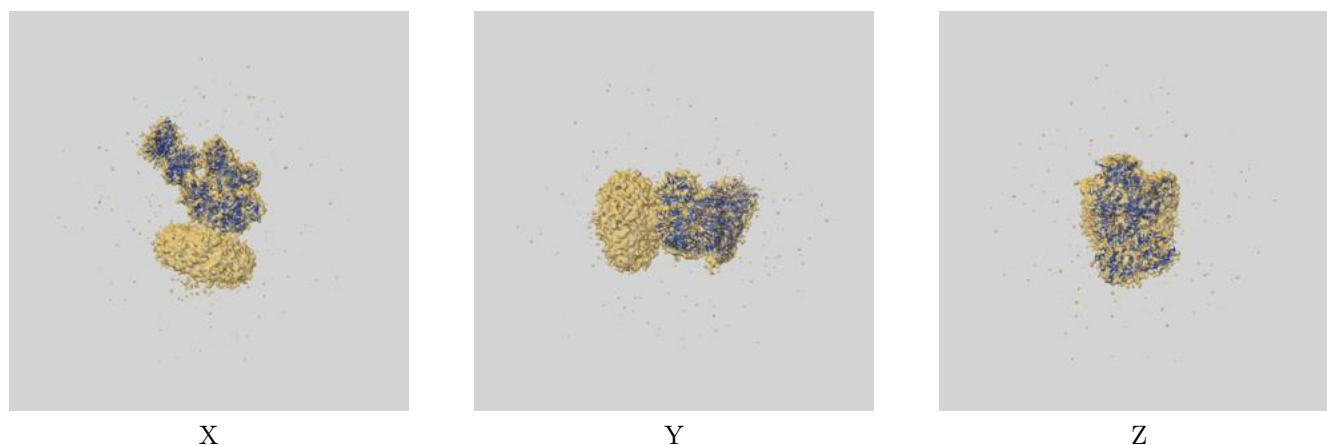
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	14.79	21.37	15.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 14.79 differs from the reported value 8.8 by more than 10 %

9 Map-model fit [i](#)

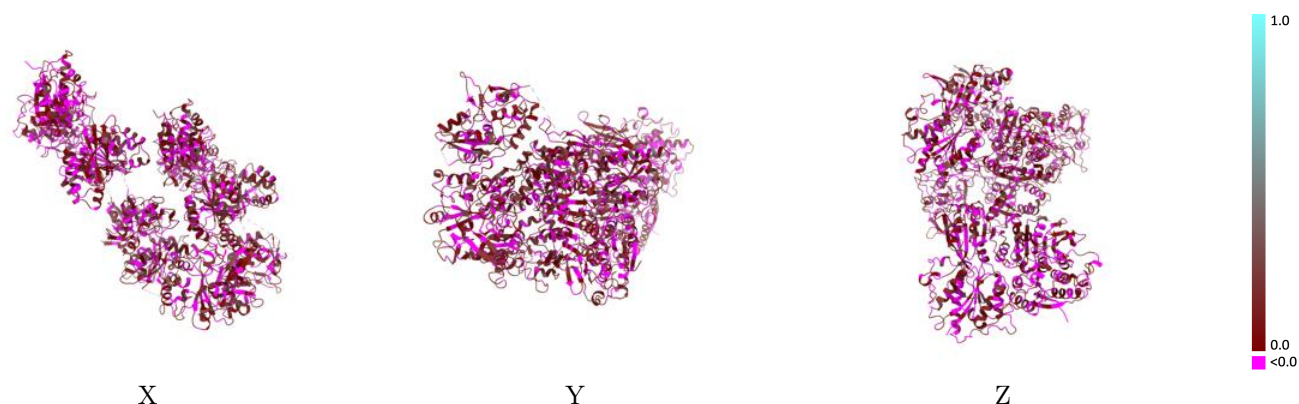
This section contains information regarding the fit between EMDB map EMD-0979 and PDB model 6LU9. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



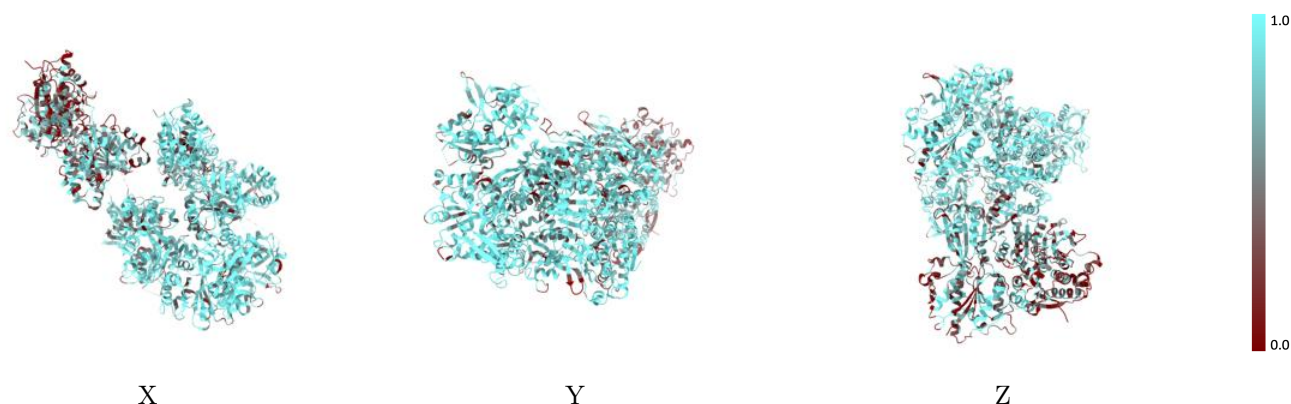
The images above show the 3D surface view of the map at the recommended contour level 0.316 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



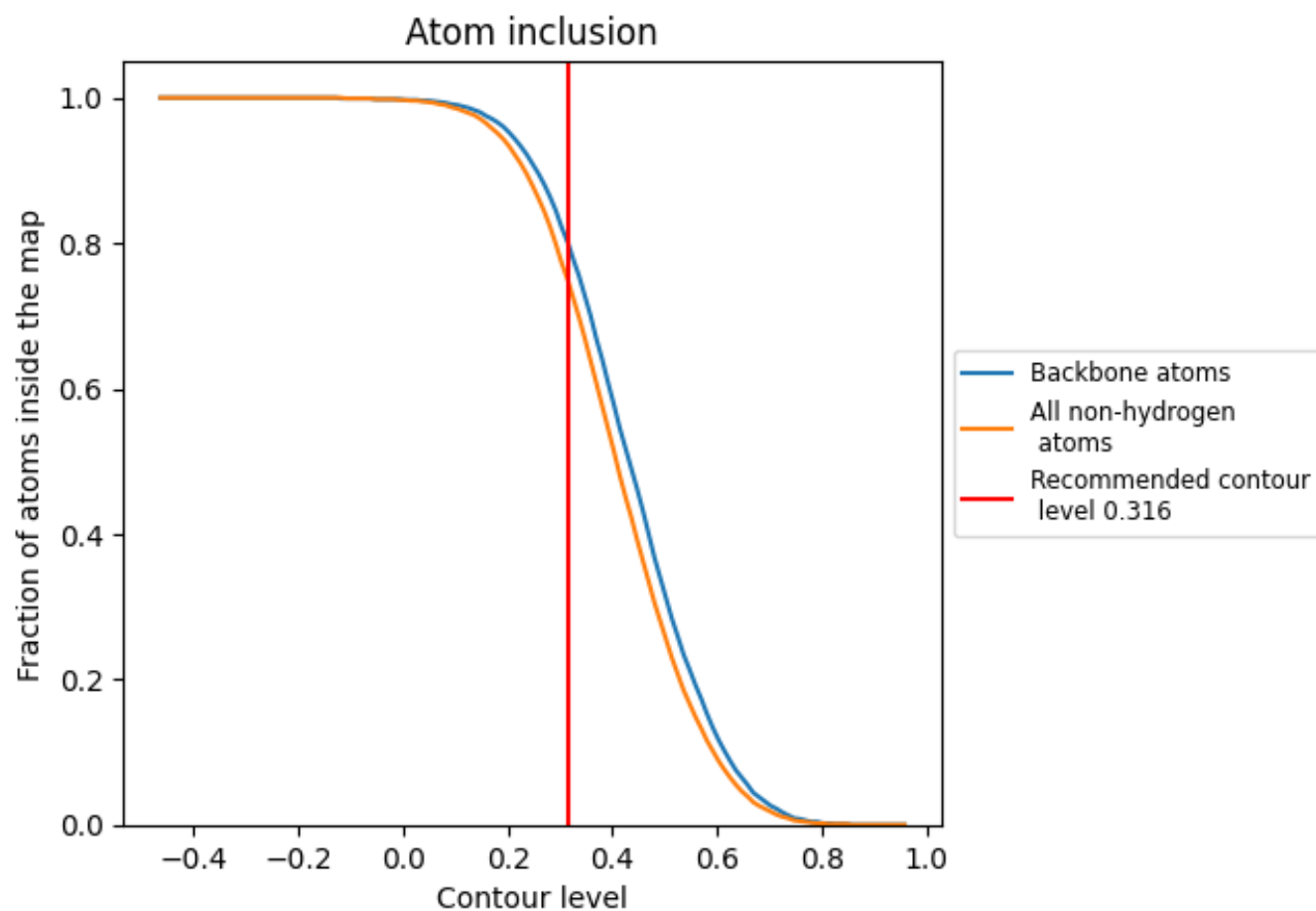
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.316).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 75% 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 (0.316) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7470	<div></div> 0.0650
A	<div></div> 0.6760	<div></div> 0.0450
B	<div></div> 0.6330	<div></div> 0.0550
C	<div></div> 0.8370	<div></div> 0.0860
D	<div></div> 0.8420	<div></div> 0.0730

