



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 05:34 PM UTC

PDB ID : 7TEE / pdb_00007tee
EMDB ID : EMD-25845
Title : Cryo-EM structure of GluN1b-2B NMDAR complexed to Fab2 Non-active2-like
Authors : Tajima, N.; Furukawa, H.
Deposited on : 2022-01-04
Resolution : 6.59 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:

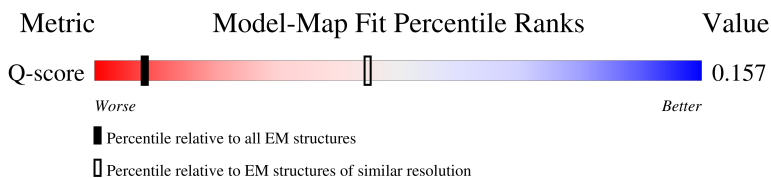
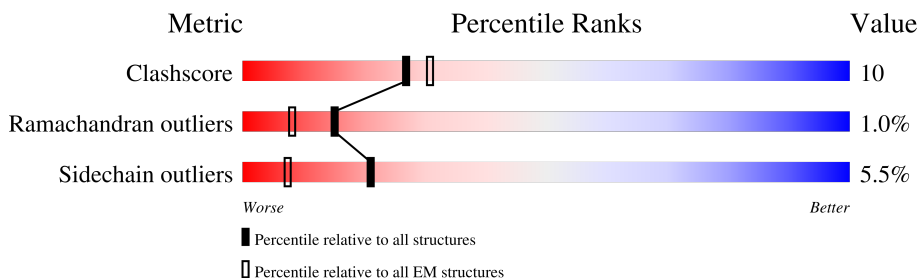
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 6.59 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.





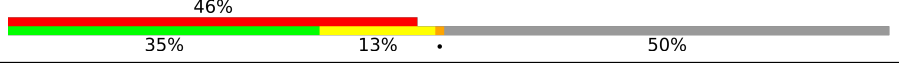
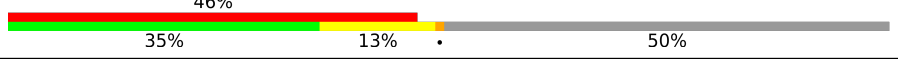
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	500 (6.09 - 7.09)

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	862	12% (red), 65% (green), 24% (yellow), 8% (grey)
1	C	862	12% (red), 65% (green), 24% (yellow), 8% (grey)
2	B	883	13% (red), 60% (green), 23% (yellow), 13% (grey)
2	D	883	13% (red), 59% (green), 24% (yellow), 13% (grey)

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Mol	Chain	Length	Quality of chain
3	H	223	 <p>42% 36% 16% 48%</p>
3	M	223	 <p>41% 36% 15% 48%</p>
4	L	213	 <p>46% 35% 13% 50%</p>
4	N	213	 <p>46% 35% 13% 50%</p>

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 28054 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, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	790	6230	3961	1081	1151	37	0	0
1	C	790	6230	3961	1081	1151	37	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	SER	CYS	conflict	UNP P35439
A	61	GLN	ASN	conflict	UNP P35439
A	260	ASP	ASN	conflict	UNP P35439
A	371	GLN	ASN	conflict	UNP P35439
A	492	GLN	ASN	conflict	UNP P35439
A	512	GLN	ASN	conflict	UNP P35439
A	615	GLN	GLU	conflict	UNP P35439
A	616	SER	GLU	conflict	UNP P35439
A	618	SER	GLU	conflict	UNP P35439
A	619	THR	GLU	conflict	UNP P35439
A	792	GLN	ASN	conflict	UNP P35439
A	831	CYS	PHE	conflict	UNP P35439
A	860	SER	-	expression tag	UNP P35439
A	861	ARG	-	expression tag	UNP P35439
A	862	ALA	-	expression tag	UNP P35439
C	22	SER	CYS	conflict	UNP P35439
C	61	GLN	ASN	conflict	UNP P35439
C	260	ASP	ASN	conflict	UNP P35439
C	371	GLN	ASN	conflict	UNP P35439
C	492	GLN	ASN	conflict	UNP P35439
C	512	GLN	ASN	conflict	UNP P35439
C	615	GLN	GLU	conflict	UNP P35439
C	616	SER	GLU	conflict	UNP P35439
C	618	SER	GLU	conflict	UNP P35439
C	619	THR	GLU	conflict	UNP P35439
C	792	GLN	ASN	conflict	UNP P35439

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Chain	Residue	Modelled	Actual	Comment	Reference
C	831	CYS	PHE	conflict	UNP P35439
C	860	SER	-	expression tag	UNP P35439
C	861	ARG	-	expression tag	UNP P35439
C	862	ALA	-	expression tag	UNP P35439

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	771	Total	C	N	O	S	0	0
			6075	3914	979	1141	41		
2	D	771	Total	C	N	O	S	0	0
			6075	3914	979	1141	41		

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-30	MET	-	expression tag	UNP Q00960
B	-29	GLY	-	expression tag	UNP Q00960
B	-28	THR	-	expression tag	UNP Q00960
B	-27	MET	-	expression tag	UNP Q00960
B	-26	ARG	-	expression tag	UNP Q00960
B	-25	LEU	-	expression tag	UNP Q00960
B	-24	PHE	-	expression tag	UNP Q00960
B	-23	LEU	-	expression tag	UNP Q00960
B	-22	LEU	-	expression tag	UNP Q00960
B	-21	ALA	-	expression tag	UNP Q00960
B	-20	VAL	-	expression tag	UNP Q00960
B	-19	LEU	-	expression tag	UNP Q00960
B	-18	PHE	-	expression tag	UNP Q00960
B	-17	LEU	-	expression tag	UNP Q00960
B	-16	PHE	-	expression tag	UNP Q00960
B	-15	SER	-	expression tag	UNP Q00960
B	-14	PHE	-	expression tag	UNP Q00960
B	-13	ALA	-	expression tag	UNP Q00960
B	-12	ARG	-	expression tag	UNP Q00960
B	-11	ALA	-	expression tag	UNP Q00960
B	-10	THR	-	expression tag	UNP Q00960
B	-9	GLY	-	expression tag	UNP Q00960
B	-8	TRP	-	expression tag	UNP Q00960
B	-7	SER	-	expression tag	UNP Q00960
B	-6	HIS	-	expression tag	UNP Q00960
B	-5	PRO	-	expression tag	UNP Q00960

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLN	-	expression tag	UNP Q00960
B	-3	PHE	-	expression tag	UNP Q00960
B	-2	GLU	-	expression tag	UNP Q00960
B	-1	LYS	-	expression tag	UNP Q00960
B	0	GLY	-	expression tag	UNP Q00960
B	1	GLY	-	expression tag	UNP Q00960
B	2	GLY	-	expression tag	UNP Q00960
B	3	SER	-	expression tag	UNP Q00960
B	4	GLY	-	expression tag	UNP Q00960
B	5	GLY	-	expression tag	UNP Q00960
B	6	GLY	-	expression tag	UNP Q00960
B	7	SER	-	expression tag	UNP Q00960
B	8	GLY	-	expression tag	UNP Q00960
B	9	GLY	-	expression tag	UNP Q00960
B	10	SER	-	expression tag	UNP Q00960
B	11	ALA	-	expression tag	UNP Q00960
B	12	TRP	-	expression tag	UNP Q00960
B	13	SER	-	expression tag	UNP Q00960
B	14	HIS	-	expression tag	UNP Q00960
B	15	PRO	-	expression tag	UNP Q00960
B	16	GLN	-	expression tag	UNP Q00960
B	17	PHE	-	expression tag	UNP Q00960
B	18	GLU	-	expression tag	UNP Q00960
B	19	LYS	-	expression tag	UNP Q00960
B	20	GLY	-	expression tag	UNP Q00960
B	21	ALA	-	expression tag	UNP Q00960
B	22	LEU	-	expression tag	UNP Q00960
B	23	VAL	-	expression tag	UNP Q00960
B	24	PRO	-	expression tag	UNP Q00960
B	25	ARG	-	expression tag	UNP Q00960
B	26	GLY	-	expression tag	UNP Q00960
B	348	ASP	ASN	conflict	UNP Q00960
B	557	CYS	ASP	conflict	UNP Q00960
B	588	SER	CYS	conflict	UNP Q00960
B	600	VAL	PHE	conflict	UNP Q00960
B	838	SER	CYS	conflict	UNP Q00960
B	849	SER	CYS	conflict	UNP Q00960
D	-30	MET	-	expression tag	UNP Q00960
D	-29	GLY	-	expression tag	UNP Q00960
D	-28	THR	-	expression tag	UNP Q00960
D	-27	MET	-	expression tag	UNP Q00960
D	-26	ARG	-	expression tag	UNP Q00960

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-25	LEU	-	expression tag	UNP Q00960
D	-24	PHE	-	expression tag	UNP Q00960
D	-23	LEU	-	expression tag	UNP Q00960
D	-22	LEU	-	expression tag	UNP Q00960
D	-21	ALA	-	expression tag	UNP Q00960
D	-20	VAL	-	expression tag	UNP Q00960
D	-19	LEU	-	expression tag	UNP Q00960
D	-18	PHE	-	expression tag	UNP Q00960
D	-17	LEU	-	expression tag	UNP Q00960
D	-16	PHE	-	expression tag	UNP Q00960
D	-15	SER	-	expression tag	UNP Q00960
D	-14	PHE	-	expression tag	UNP Q00960
D	-13	ALA	-	expression tag	UNP Q00960
D	-12	ARG	-	expression tag	UNP Q00960
D	-11	ALA	-	expression tag	UNP Q00960
D	-10	THR	-	expression tag	UNP Q00960
D	-9	GLY	-	expression tag	UNP Q00960
D	-8	TRP	-	expression tag	UNP Q00960
D	-7	SER	-	expression tag	UNP Q00960
D	-6	HIS	-	expression tag	UNP Q00960
D	-5	PRO	-	expression tag	UNP Q00960
D	-4	GLN	-	expression tag	UNP Q00960
D	-3	PHE	-	expression tag	UNP Q00960
D	-2	GLU	-	expression tag	UNP Q00960
D	-1	LYS	-	expression tag	UNP Q00960
D	0	GLY	-	expression tag	UNP Q00960
D	1	GLY	-	expression tag	UNP Q00960
D	2	GLY	-	expression tag	UNP Q00960
D	3	SER	-	expression tag	UNP Q00960
D	4	GLY	-	expression tag	UNP Q00960
D	5	GLY	-	expression tag	UNP Q00960
D	6	GLY	-	expression tag	UNP Q00960
D	7	SER	-	expression tag	UNP Q00960
D	8	GLY	-	expression tag	UNP Q00960
D	9	GLY	-	expression tag	UNP Q00960
D	10	SER	-	expression tag	UNP Q00960
D	11	ALA	-	expression tag	UNP Q00960
D	12	TRP	-	expression tag	UNP Q00960
D	13	SER	-	expression tag	UNP Q00960
D	14	HIS	-	expression tag	UNP Q00960
D	15	PRO	-	expression tag	UNP Q00960
D	16	GLN	-	expression tag	UNP Q00960

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Chain	Residue	Modelled	Actual	Comment	Reference
D	17	PHE	-	expression tag	UNP Q00960
D	18	GLU	-	expression tag	UNP Q00960
D	19	LYS	-	expression tag	UNP Q00960
D	20	GLY	-	expression tag	UNP Q00960
D	21	ALA	-	expression tag	UNP Q00960
D	22	LEU	-	expression tag	UNP Q00960
D	23	VAL	-	expression tag	UNP Q00960
D	24	PRO	-	expression tag	UNP Q00960
D	25	ARG	-	expression tag	UNP Q00960
D	26	GLY	-	expression tag	UNP Q00960
D	348	ASP	ASN	conflict	UNP Q00960
D	557	CYS	ASP	conflict	UNP Q00960
D	588	SER	CYS	conflict	UNP Q00960
D	600	VAL	PHE	conflict	UNP Q00960
D	838	SER	CYS	conflict	UNP Q00960
D	849	SER	CYS	conflict	UNP Q00960

- Molecule 3 is a protein called Fab2 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	117	905	572	153	175	5	0	0
3	M	116	899	569	152	173	5	0	0

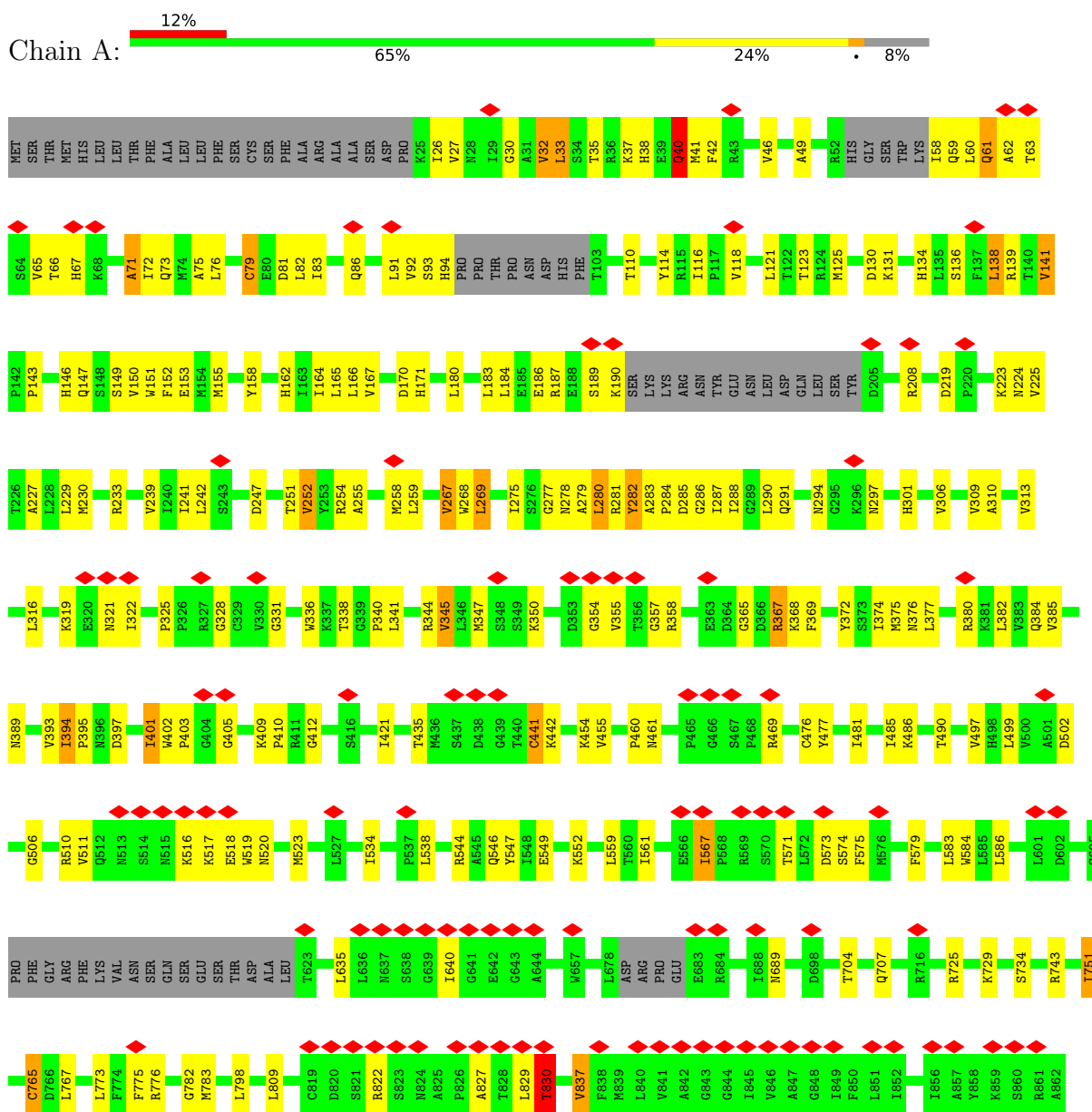
- Molecule 4 is a protein called Fab2 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	106	820	520	136	161	3	0	0
4	N	106	820	520	136	161	3	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: Glutamate receptor ionotropic, NMDA 1



- Molecule 1: Glutamate receptor ionotropic, NMDA 1

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18851	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	7.430	Depositor
Minimum map value	-1.126	Depositor
Average map value	0.054	Depositor
Map value standard deviation	0.431	Depositor
Recommended contour level	3	Depositor
Map size (\AA)	350.72, 350.72, 350.72	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.37, 1.37, 1.37	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	0.28	0/6358	0.87	20/8599 (0.2%)
1	C	0.28	0/6358	0.87	20/8599 (0.2%)
2	B	0.29	0/6209	0.91	28/8411 (0.3%)
2	D	0.29	0/6209	0.91	28/8411 (0.3%)
3	H	0.22	0/927	0.58	0/1255
3	M	0.21	0/921	0.60	0/1247
4	L	0.25	0/840	0.66	0/1136
4	N	0.25	0/840	0.66	0/1136
All	All	0.28	0/28662	0.86	96/38794 (0.2%)

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	18
1	C	0	18
2	B	0	24
2	D	0	24
3	H	0	2
3	M	0	1
4	L	0	3
4	N	0	3
All	All	0	93

There are no bond length outliers.

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	288	ILE	CA-C-N	-8.92	114.33	121.82
1	C	288	ILE	C-N-CA	-8.92	114.33	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ILE	CA-C-N	-8.86	114.38	121.82
1	A	288	ILE	C-N-CA	-8.86	114.38	121.82
2	D	125	GLY	N-CA-C	8.64	121.01	111.85
2	B	125	GLY	N-CA-C	8.62	120.99	111.85
1	C	32	VAL	N-CA-C	7.54	120.92	113.53
1	A	32	VAL	N-CA-C	7.54	120.92	113.53
1	A	357	GLY	N-CA-C	6.88	120.25	111.37
1	C	357	GLY	N-CA-C	6.88	120.24	111.37
1	C	285	ASP	N-CA-C	6.84	120.06	109.60
1	A	40	GLN	CA-C-N	6.82	134.57	121.54
1	A	40	GLN	C-N-CA	6.82	134.57	121.54
1	A	285	ASP	N-CA-C	6.82	120.03	109.60
1	C	40	GLN	CA-C-N	6.81	134.54	121.54
1	C	40	GLN	C-N-CA	6.81	134.54	121.54
2	D	358	MET	CA-C-N	-6.65	115.50	122.28
2	D	358	MET	C-N-CA	-6.65	115.50	122.28
2	D	73	MET	N-CA-C	6.62	123.96	114.16
2	B	73	MET	N-CA-C	6.61	123.94	114.16
2	B	358	MET	CA-C-N	-6.56	115.59	122.28
2	B	358	MET	C-N-CA	-6.56	115.59	122.28
2	D	250	THR	N-CA-C	-6.21	102.08	111.34
2	B	250	THR	N-CA-C	-6.18	102.13	111.34
1	A	282	TYR	CA-C-N	6.16	136.82	121.80
1	A	282	TYR	C-N-CA	6.16	136.82	121.80
1	C	282	TYR	CA-C-N	6.14	136.79	121.80
1	C	282	TYR	C-N-CA	6.14	136.79	121.80
2	D	367	LEU	CA-CB-CG	5.93	137.04	116.30
2	B	367	LEU	CA-CB-CG	5.92	137.02	116.30
2	B	199	LEU	CA-C-N	5.91	132.83	121.54
2	B	199	LEU	C-N-CA	5.91	132.83	121.54
2	D	199	LEU	CA-C-N	5.91	132.82	121.54
2	D	199	LEU	C-N-CA	5.91	132.82	121.54
2	B	356	TYR	CA-C-N	5.86	134.00	121.45
2	B	356	TYR	C-N-CA	5.86	134.00	121.45
2	D	356	TYR	CA-C-N	5.85	133.98	121.45
2	D	356	TYR	C-N-CA	5.85	133.98	121.45
2	D	107	ALA	N-CA-C	5.81	123.18	110.80
2	B	107	ALA	N-CA-C	5.79	123.12	110.80
1	A	73	GLN	N-CA-C	-5.78	105.49	113.18
1	A	401	ILE	CA-C-N	5.76	135.85	121.80
1	A	401	ILE	C-N-CA	5.76	135.85	121.80
1	C	73	GLN	N-CA-C	-5.75	105.53	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	251	GLY	N-CA-C	-5.72	104.36	112.37
1	C	401	ILE	CA-C-N	5.71	135.73	121.80
1	C	401	ILE	C-N-CA	5.71	135.73	121.80
2	D	264	GLY	CA-C-N	-5.71	114.44	123.23
2	D	264	GLY	C-N-CA	-5.71	114.44	123.23
1	A	138	LEU	CA-CB-CG	5.70	136.25	116.30
2	D	251	GLY	N-CA-C	-5.70	104.39	112.37
1	C	138	LEU	CA-CB-CG	5.69	136.22	116.30
2	B	264	GLY	CA-C-N	-5.67	114.49	123.23
2	B	264	GLY	C-N-CA	-5.67	114.49	123.23
2	B	278	ILE	CB-CA-C	-5.57	103.09	112.16
2	D	278	ILE	CB-CA-C	-5.54	103.12	112.16
2	D	96	GLY	N-CA-C	5.48	118.38	111.09
2	B	96	GLY	N-CA-C	5.47	118.36	111.09
2	B	264	GLY	N-CA-C	5.44	126.08	113.18
2	D	115	ILE	N-CA-C	-5.43	104.69	112.35
2	D	264	GLY	N-CA-C	5.43	126.05	113.18
2	B	115	ILE	N-CA-C	-5.43	104.70	112.35
2	B	89	MET	N-CA-C	5.42	122.34	110.80
2	D	89	MET	N-CA-C	5.41	122.33	110.80
1	A	279	ALA	CA-C-N	5.38	131.84	121.18
1	A	279	ALA	C-N-CA	5.38	131.84	121.18
1	C	279	ALA	CA-C-N	5.38	131.83	121.18
1	C	279	ALA	C-N-CA	5.38	131.83	121.18
2	B	221	LYS	CA-C-N	5.33	132.03	122.38
2	B	221	LYS	C-N-CA	5.33	132.03	122.38
2	D	221	LYS	CA-C-N	5.33	132.02	122.38
2	D	221	LYS	C-N-CA	5.33	132.02	122.38
1	C	283	ALA	N-CA-C	5.19	121.28	109.81
2	B	90	SER	N-CA-C	-5.19	108.71	114.62
1	A	283	ALA	N-CA-C	5.18	121.26	109.81
2	D	90	SER	N-CA-C	-5.15	108.75	114.62
2	D	352	SER	N-CA-C	5.13	119.42	111.56
1	C	367	ARG	CA-C-N	5.13	131.34	121.54
1	C	367	ARG	C-N-CA	5.13	131.34	121.54
2	B	352	SER	N-CA-C	5.12	119.40	111.56
1	A	830	THR	CA-CB-CG2	5.11	119.18	110.50
1	A	367	ARG	CA-C-N	5.09	131.26	121.54
1	A	367	ARG	C-N-CA	5.09	131.26	121.54
1	C	830	THR	CA-CB-CG2	5.09	119.15	110.50
2	D	465	LEU	CA-CB-CG	5.07	134.04	116.30
2	B	465	LEU	CA-CB-CG	5.06	134.00	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	GLY	N-CA-C	5.04	117.23	110.43
2	D	328	ARG	CA-C-N	5.03	127.09	120.60
2	D	328	ARG	C-N-CA	5.03	127.09	120.60
2	B	328	ARG	CA-C-N	5.03	127.09	120.60
2	B	328	ARG	C-N-CA	5.03	127.09	120.60
1	C	354	GLY	N-CA-C	5.02	117.21	110.43
2	B	472	VAL	CA-C-N	5.01	131.10	121.54
2	B	472	VAL	C-N-CA	5.01	131.10	121.54
2	D	472	VAL	CA-C-N	5.00	131.09	121.54
2	D	472	VAL	C-N-CA	5.00	131.09	121.54

There are no chirality outliers.

All (93) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	252	VAL	Peptide
1	A	284	PRO	Peptide
1	A	33	LEU	Peptide
1	A	35	THR	Peptide
1	A	372	TYR	Peptide
1	A	394	ILE	Peptide
1	A	40	GLN	Peptide
1	A	405	GLY	Peptide
1	A	552	LYS	Peptide
1	A	567	ILE	Peptide
1	A	61	GLN	Peptide
1	A	62	ALA	Peptide
1	A	640	ILE	Peptide
1	A	66	THR	Peptide
1	A	71	ALA	Peptide
1	A	79	CYS	Peptide
1	A	829	LEU	Peptide
1	A	830	THR	Peptide
2	B	126	ILE	Peptide
2	B	145	GLN	Peptide
2	B	193	SER	Peptide
2	B	197	TRP	Peptide
2	B	216	ILE	Mainchain
2	B	251	GLY	Peptide
2	B	255	THR	Peptide
2	B	271	SER	Peptide
2	B	278	ILE	Peptide

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Mol	Chain	Res	Type	Group
2	B	283	ASP	Peptide
2	B	285	TRP	Peptide
2	B	311	HIS	Peptide
2	B	350	SER	Peptide
2	B	354	ASP	Peptide
2	B	366	LEU	Peptide
2	B	414	ALA	Peptide
2	B	476	TYR	Peptide
2	B	506	ALA	Peptide
2	B	552	GLU	Peptide
2	B	660	VAL	Peptide
2	B	678	SER	Peptide
2	B	72	ALA	Peptide
2	B	795	LEU	Peptide
2	B	83	THR	Mainchain
1	C	252	VAL	Peptide
1	C	284	PRO	Peptide
1	C	33	LEU	Peptide
1	C	35	THR	Peptide
1	C	372	TYR	Peptide
1	C	394	ILE	Peptide
1	C	40	GLN	Peptide
1	C	405	GLY	Peptide
1	C	552	LYS	Peptide
1	C	567	ILE	Peptide
1	C	61	GLN	Peptide
1	C	62	ALA	Peptide
1	C	640	ILE	Peptide
1	C	66	THR	Peptide
1	C	71	ALA	Peptide
1	C	79	CYS	Peptide
1	C	829	LEU	Peptide
1	C	830	THR	Peptide
2	D	126	ILE	Peptide
2	D	145	GLN	Peptide
2	D	193	SER	Peptide
2	D	197	TRP	Peptide
2	D	216	ILE	Mainchain
2	D	251	GLY	Peptide
2	D	255	THR	Peptide
2	D	271	SER	Peptide
2	D	278	ILE	Peptide

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Mol	Chain	Res	Type	Group
2	D	283	ASP	Peptide
2	D	285	TRP	Peptide
2	D	311	HIS	Peptide
2	D	350	SER	Peptide
2	D	354	ASP	Peptide
2	D	366	LEU	Peptide
2	D	414	ALA	Peptide
2	D	476	TYR	Peptide
2	D	506	ALA	Peptide
2	D	552	GLU	Peptide
2	D	660	VAL	Peptide
2	D	678	SER	Peptide
2	D	72	ALA	Peptide
2	D	795	LEU	Peptide
2	D	83	THR	Mainchain
3	H	109	PHE	Peptide
3	H	36	TRP	Peptide
4	L	47	LEU	Peptide
4	L	8	PRO	Peptide
4	L	80	PRO	Peptide
3	M	109	PHE	Peptide
4	N	47	LEU	Peptide
4	N	8	PRO	Peptide
4	N	80	PRO	Peptide

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	6230	0	6230	116	0
1	C	6230	0	6230	121	0
2	B	6075	0	5994	126	0
2	D	6075	0	5994	135	0
3	H	905	0	867	22	0
3	M	899	0	862	22	0
4	L	820	0	802	19	0
4	N	820	0	802	19	0
All	All	28054	0	27781	551	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 10.

All (551) 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:B:83:THR:O	2:B:87:ASP:HB2	1.71	0.90
2:D:83:THR:O	2:D:87:ASP:HB2	1.71	0.88
2:B:615:ASN:HD21	2:D:615:ASN:HD21	1.33	0.75
3:M:15:GLY:H	3:M:87:LYS:HE3	1.54	0.72
4:L:29:ILE:HG12	4:L:69:ARG:HA	1.76	0.68
2:B:65:VAL:HG23	2:B:67:ARG:HH12	1.60	0.67
2:D:65:VAL:HG23	2:D:67:ARG:HH12	1.60	0.67
4:N:29:ILE:HG12	4:N:69:ARG:HA	1.76	0.67
1:A:79:CYS:HA	1:A:82:LEU:HB2	1.77	0.67
1:A:319:LYS:HB2	1:A:322:ILE:HD11	1.78	0.66
1:C:319:LYS:HB2	1:C:322:ILE:HD11	1.78	0.66
1:C:79:CYS:HA	1:C:82:LEU:HB2	1.77	0.66
2:B:462:ILE:HA	2:B:465:LEU:HG	1.79	0.65
3:H:53:ASN:O	3:H:74:ASN:ND2	2.29	0.65
2:D:88:LEU:O	2:D:90:SER:N	2.29	0.65
1:A:546:GLN:O	2:D:774:ARG:NH2	2.30	0.65
2:D:462:ILE:HA	2:D:465:LEU:HG	1.79	0.65
2:B:88:LEU:O	2:B:90:SER:N	2.29	0.65
1:A:725:ARG:HH12	1:A:729:LYS:HE3	1.62	0.65
2:D:555:SER:HA	2:D:559:TRP:HB2	1.78	0.64
2:B:555:SER:HA	2:B:559:TRP:HB2	1.78	0.63
3:M:110:ASP:OD2	4:N:55:GLN:NE2	2.32	0.63
1:A:230:MET:SD	1:A:233:ARG:NH2	2.72	0.62
1:C:86:GLN:NE2	1:C:328:GLY:O	2.33	0.62
4:N:11:LEU:HB2	4:N:103:LEU:HA	1.81	0.62
1:C:331:GLY:H	2:D:77:ASP:HB2	1.64	0.62
1:C:230:MET:SD	1:C:233:ARG:NH2	2.72	0.62
1:C:725:ARG:HH12	1:C:729:LYS:HE3	1.62	0.62
4:L:11:LEU:HB2	4:L:103:LEU:HA	1.81	0.62
2:D:410:THR:OG1	2:D:411:LEU:N	2.33	0.62
1:A:86:GLN:NE2	1:A:328:GLY:O	2.33	0.61
1:C:634:VAL:O	2:D:616:ASN:ND2	2.29	0.61
3:M:19:LYS:HE2	3:M:80:TYR:HB3	1.82	0.61
3:H:4:LEU:HB2	3:H:113:GLY:HA2	1.84	0.60
3:M:53:ASN:O	3:M:74:ASN:ND2	2.34	0.60
4:N:49:HIS:HB2	4:N:53:SER:HB3	1.83	0.60
2:D:271:SER:O	2:D:273:PHE:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:49:HIS:HB2	4:L:53:SER:HB3	1.83	0.60
2:B:653:PHE:HA	1:C:827:ALA:HB1	1.84	0.59
1:C:38:HIS:O	1:C:42:PHE:HB3	2.02	0.59
1:A:38:HIS:O	1:A:42:PHE:HB3	2.02	0.59
2:B:250:THR:OG1	2:B:251:GLY:N	2.35	0.59
2:D:250:THR:OG1	2:D:251:GLY:N	2.35	0.59
2:B:438:LYS:HB2	2:B:480:LEU:HD12	1.85	0.59
1:C:350:LYS:HE3	1:C:358:ARG:HH12	1.68	0.59
2:D:220:LEU:HD13	2:D:223:LEU:HD13	1.84	0.59
3:H:6:GLU:HA	3:H:22:CYS:HA	1.84	0.59
2:B:223:LEU:HD12	2:B:249:LEU:HD13	1.85	0.59
1:C:38:HIS:O	1:C:42:PHE:CB	2.51	0.59
2:D:145:GLN:H	2:D:355:GLY:HA3	1.68	0.59
1:A:46:VAL:HA	1:A:60:LEU:HD12	1.85	0.59
1:A:162:HIS:NE2	1:A:412:GLY:O	2.36	0.59
2:B:271:SER:O	2:B:273:PHE:N	2.34	0.59
2:B:539:SER:HA	2:B:721:LEU:HD21	1.85	0.59
2:D:438:LYS:HB2	2:D:480:LEU:HD12	1.85	0.59
1:A:38:HIS:O	1:A:42:PHE:CB	2.51	0.59
1:C:46:VAL:HA	1:C:60:LEU:HD12	1.85	0.58
2:B:145:GLN:H	2:B:355:GLY:HA3	1.68	0.58
3:H:19:LYS:HE2	3:H:80:TYR:HB3	1.85	0.58
3:M:93:MET:HA	3:M:117:THR:HA	1.85	0.58
1:A:58:ILE:HG13	1:A:59:GLN:HE21	1.68	0.58
1:C:58:ILE:HG13	1:C:59:GLN:HE21	1.68	0.58
2:B:682:ARG:NH2	2:B:724:GLY:O	2.37	0.58
1:C:162:HIS:NE2	1:C:412:GLY:O	2.36	0.58
2:B:220:LEU:HD13	2:B:223:LEU:HD13	1.85	0.58
1:A:350:LYS:HE3	1:A:358:ARG:HH12	1.68	0.58
2:D:539:SER:HA	2:D:721:LEU:HD21	1.85	0.57
1:A:519:TRP:NE1	1:A:547:TYR:OH	2.37	0.57
1:C:519:TRP:NE1	1:C:547:TYR:OH	2.37	0.57
2:D:223:LEU:HD12	2:D:249:LEU:HD13	1.85	0.57
1:A:579:PHE:O	1:A:583:LEU:N	2.36	0.57
1:A:72:ILE:HG23	1:A:75:ALA:HB3	1.87	0.57
2:D:245:ASN:ND2	2:D:272:GLU:O	2.37	0.57
2:B:245:ASN:ND2	2:B:272:GLU:O	2.37	0.57
1:C:114:TYR:HB2	1:C:116:ILE:HD11	1.87	0.57
1:C:579:PHE:O	1:C:583:LEU:N	2.36	0.56
2:D:682:ARG:NH2	2:D:724:GLY:O	2.37	0.56
3:M:16:GLY:O	3:M:84:ASN:ND2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:51:ILE:HD12	3:H:72:ARG:HD2	1.87	0.56
1:C:72:ILE:HG23	1:C:75:ALA:HB3	1.87	0.56
1:C:316:LEU:HG	1:C:345:VAL:HG11	1.87	0.56
3:M:4:LEU:HB2	3:M:113:GLY:HA2	1.86	0.56
1:A:441:CYS:SG	1:A:442:LYS:N	2.79	0.56
1:C:82:LEU:HD22	1:C:86:GLN:HB3	1.87	0.56
1:C:441:CYS:SG	1:C:442:LYS:N	2.79	0.56
1:A:239:VAL:HA	1:A:267:VAL:HG23	1.88	0.56
1:A:316:LEU:HG	1:A:345:VAL:HG11	1.87	0.56
2:B:319:SER:H	2:B:327:LYS:HE2	1.71	0.56
2:D:319:SER:H	2:D:327:LYS:HE2	1.71	0.56
1:A:114:TYR:HB2	1:A:116:ILE:HD11	1.87	0.56
2:B:66:PRO:O	2:B:67:ARG:NH1	2.39	0.56
3:H:52:SER:O	3:H:72:ARG:NH1	2.38	0.56
1:A:82:LEU:HD22	1:A:86:GLN:HB3	1.87	0.56
1:C:743:ARG:HG2	1:C:767:LEU:HD21	1.88	0.55
2:B:789:MET:SD	2:B:789:MET:N	2.72	0.55
2:D:483:ASN:HD21	2:D:496:GLY:H	1.55	0.55
2:D:66:PRO:O	2:D:67:ARG:NH1	2.39	0.55
1:C:239:VAL:HA	1:C:267:VAL:HG23	1.88	0.55
2:B:253:GLY:HA2	2:B:394:MET:HB3	1.89	0.55
2:D:41:LEU:HA	2:D:100:ALA:HB2	1.89	0.55
4:N:4:MET:HA	4:N:25:ALA:HA	1.89	0.55
2:B:497:MET:HE3	2:B:509:ALA:HB1	1.89	0.55
4:L:4:MET:HA	4:L:25:ALA:HA	1.89	0.55
3:M:50:TYR:HE1	4:N:95:TYR:HB2	1.72	0.55
2:D:366:LEU:HB3	2:D:376:VAL:HB	1.89	0.54
2:B:41:LEU:HA	2:B:100:ALA:HB2	1.89	0.54
2:B:86:CYS:HA	2:B:89:MET:HB2	1.90	0.54
2:B:288:GLY:O	2:B:292:ARG:N	2.37	0.54
1:A:37:LYS:NZ	1:A:40:GLN:OE1	2.40	0.54
2:B:252:TYR:O	2:B:393:ARG:NH2	2.41	0.54
2:D:252:TYR:O	2:D:393:ARG:NH2	2.41	0.54
1:C:83:ILE:HA	1:C:328:GLY:HA2	1.90	0.54
2:D:437:GLN:NE2	2:D:452:TYR:O	2.34	0.54
2:D:497:MET:HE3	2:D:509:ALA:HB1	1.89	0.54
1:A:375:MET:HE3	1:A:382:LEU:HD13	1.89	0.54
1:A:743:ARG:HG2	1:A:767:LEU:HD21	1.88	0.54
2:B:353:GLU:O	2:B:356:TYR:N	2.41	0.54
2:B:483:ASN:HD21	2:B:496:GLY:H	1.55	0.54
1:C:37:LYS:NZ	1:C:40:GLN:OE1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:93:MET:HA	3:H:117:THR:HA	1.90	0.54
4:L:25:ALA:O	4:L:69:ARG:NH2	2.40	0.54
1:A:83:ILE:HA	1:A:328:GLY:HA2	1.90	0.54
2:B:366:LEU:HB3	2:B:376:VAL:HB	1.89	0.54
2:B:437:GLN:NE2	2:B:452:TYR:O	2.34	0.53
1:C:421:ILE:HB	1:C:497:VAL:HG22	1.89	0.53
2:D:488:LYS:NZ	2:D:688:ASN:OD1	2.42	0.53
4:N:25:ALA:O	4:N:69:ARG:NH2	2.40	0.53
1:C:375:MET:HE3	1:C:382:LEU:HD13	1.89	0.53
2:D:253:GLY:HA2	2:D:394:MET:HB3	1.89	0.53
2:B:364:ILE:HB	2:B:377:GLY:HA3	1.91	0.53
2:D:669:LYS:NZ	2:D:673:ARG:O	2.41	0.53
2:B:316:GLU:OE1	2:B:328:ARG:NH2	2.42	0.53
2:B:488:LYS:NZ	2:B:688:ASN:OD1	2.42	0.53
2:D:86:CYS:HA	2:D:89:MET:HB2	1.90	0.53
3:H:107:TRP:O	4:L:95:TYR:OH	2.26	0.53
4:N:48:ILE:HG23	4:N:52:SER:HA	1.91	0.53
1:C:294:ASN:O	1:C:301:HIS:NE2	2.41	0.53
1:A:421:ILE:HB	1:A:497:VAL:HG22	1.89	0.52
2:D:364:ILE:HB	2:D:377:GLY:HA3	1.91	0.52
3:H:50:TYR:HE1	4:L:95:TYR:HB2	1.74	0.52
1:A:306:VAL:HA	1:A:309:VAL:HG12	1.92	0.52
2:D:230:LEU:HD11	2:D:255:THR:HG22	1.92	0.52
2:D:316:GLU:OE1	2:D:328:ARG:NH2	2.42	0.52
1:C:306:VAL:HA	1:C:309:VAL:HG12	1.92	0.52
1:C:186:GLU:O	1:C:208:ARG:NH2	2.43	0.52
3:M:38:ARG:HD3	3:M:86:LEU:HD22	1.92	0.52
2:B:410:THR:OG1	2:B:411:LEU:N	2.33	0.52
3:H:109:PHE:O	4:L:36:TYR:OH	2.18	0.52
4:L:48:ILE:HG23	4:L:52:SER:HA	1.91	0.52
1:C:123:THR:HG21	1:C:125:MET:HE3	1.92	0.52
2:D:291:ALA:HA	2:D:294:ARG:HG2	1.91	0.51
2:B:291:ALA:HA	2:B:294:ARG:HG2	1.91	0.51
2:D:353:GLU:O	2:D:356:TYR:N	2.41	0.51
1:A:331:GLY:H	2:B:77:ASP:HB2	1.75	0.51
2:B:230:LEU:HD11	2:B:255:THR:HG22	1.92	0.51
2:B:669:LYS:NZ	2:B:673:ARG:O	2.41	0.51
1:C:384:GLN:NE2	1:C:385:VAL:O	2.44	0.51
1:C:506:GLY:O	1:C:544:ARG:NH1	2.44	0.51
2:D:216:ILE:O	2:D:220:LEU:HG	2.11	0.51
1:A:294:ASN:O	1:A:301:HIS:NE2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:410:THR:HG23	2:D:480:LEU:HD23	1.93	0.51
1:A:186:GLU:O	1:A:208:ARG:NH2	2.43	0.51
1:A:506:GLY:O	1:A:544:ARG:NH1	2.44	0.51
1:C:510:ARG:HD3	2:D:190:ILE:HG12	1.93	0.51
2:D:789:MET:SD	2:D:789:MET:N	2.72	0.51
1:A:123:THR:HG21	1:A:125:MET:HE3	1.92	0.51
2:B:216:ILE:O	2:B:220:LEU:HG	2.11	0.51
2:B:407:SER:HA	2:B:477:ASP:HB2	1.92	0.51
1:A:384:GLN:NE2	1:A:385:VAL:O	2.44	0.51
2:D:288:GLY:O	2:D:292:ARG:N	2.37	0.51
4:N:34:ALA:HB3	4:N:89:LEU:HB2	1.93	0.51
1:A:139:ARG:N	1:A:365:GLY:O	2.44	0.51
2:D:407:SER:HA	2:D:477:ASP:HB2	1.92	0.51
2:B:214:SER:O	2:B:218:ASN:ND2	2.44	0.50
2:B:468:ILE:HD11	2:B:783:LEU:HD11	1.93	0.50
3:H:68:PHE:HB3	3:H:81:LEU:HD11	1.94	0.50
3:M:68:PHE:HB3	3:M:81:LEU:HD11	1.92	0.50
2:D:214:SER:O	2:D:218:ASN:ND2	2.44	0.50
2:D:75:GLU:OE1	2:D:84:ARG:NH1	2.44	0.50
1:A:229:LEU:HG	1:A:259:LEU:HD22	1.94	0.50
2:B:104:ASP:OD1	2:B:104:ASP:N	2.45	0.50
2:B:107:ALA:O	2:B:110:GLN:NE2	2.37	0.50
2:B:271:SER:N	2:B:272:GLU:OE1	2.45	0.50
2:B:217:GLN:HE22	2:B:247:VAL:HB	1.77	0.50
1:C:152:PHE:HB2	1:C:183:LEU:HD13	1.93	0.50
1:C:229:LEU:HG	1:C:259:LEU:HD22	1.94	0.50
1:A:139:ARG:HH21	1:A:141:VAL:HG12	1.77	0.50
2:B:537:MET:HE3	2:B:721:LEU:HD13	1.93	0.50
2:D:537:MET:HE3	2:D:721:LEU:HD13	1.93	0.50
2:D:468:ILE:HD11	2:D:783:LEU:HD11	1.93	0.50
3:M:29:PHE:HA	3:M:32:TYR:HB2	1.94	0.50
1:A:152:PHE:HB2	1:A:183:LEU:HD13	1.93	0.50
2:B:75:GLU:OE1	2:B:84:ARG:NH1	2.45	0.50
2:D:126:ILE:HD13	2:D:292:ARG:HG2	1.94	0.50
2:D:271:SER:N	2:D:272:GLU:OE1	2.45	0.50
2:B:675:ASN:OD1	2:B:675:ASN:N	2.44	0.49
1:C:139:ARG:HH21	1:C:141:VAL:HG12	1.77	0.49
2:B:410:THR:HG23	2:B:480:LEU:HD23	1.93	0.49
2:D:105:GLN:HB2	2:D:130:SER:H	1.77	0.49
2:D:137:LYS:HG3	2:D:143:PHE:HZ	1.77	0.49
2:D:104:ASP:N	2:D:104:ASP:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:VAL:HG23	1:A:121:LEU:HG	1.94	0.49
2:D:217:GLN:HE22	2:D:247:VAL:HB	1.77	0.49
2:D:253:GLY:HA3	2:D:393:ARG:HH21	1.78	0.49
2:D:277:LEU:HD13	2:D:369:LYS:HG2	1.94	0.49
2:D:393:ARG:HE	2:D:393:ARG:HA	1.78	0.49
4:L:34:ALA:HB3	4:L:89:LEU:HB2	1.93	0.49
3:M:6:GLU:HA	3:M:22:CYS:HA	1.93	0.49
2:D:244:ALA:HB1	2:D:249:LEU:HB3	1.95	0.49
4:N:92:ASP:OD1	4:N:92:ASP:N	2.41	0.49
2:B:105:GLN:HB2	2:B:130:SER:H	1.77	0.49
2:B:253:GLY:HA3	2:B:393:ARG:HH21	1.78	0.49
2:B:431:ARG:NH1	2:B:431:ARG:O	2.43	0.49
1:A:338:THR:HG23	1:A:341:LEU:HD23	1.95	0.49
2:B:77:ASP:OD2	2:B:80:SER:N	2.37	0.49
2:B:349:LEU:HD22	2:B:359:HIS:H	1.77	0.49
1:C:92:VAL:HG23	1:C:121:LEU:HG	1.94	0.49
2:D:414:ALA:O	2:D:416:PHE:N	2.45	0.49
1:A:71:ALA:HB1	2:B:118:GLN:HE21	1.78	0.49
2:B:323:ASN:OD1	2:B:323:ASN:N	2.46	0.49
2:B:414:ALA:O	2:B:416:PHE:N	2.45	0.49
1:C:139:ARG:N	1:C:365:GLY:O	2.44	0.49
2:D:349:LEU:HD22	2:D:359:HIS:H	1.77	0.49
2:B:126:ILE:HD13	2:B:292:ARG:HG2	1.93	0.49
2:D:431:ARG:O	2:D:431:ARG:NH1	2.43	0.49
2:B:393:ARG:HA	2:B:393:ARG:HE	1.78	0.48
3:H:101:ARG:HH22	3:H:108:TYR:HB2	1.76	0.48
1:A:166:LEU:N	1:A:241:ILE:O	2.44	0.48
2:B:137:LYS:HG3	2:B:143:PHE:HZ	1.77	0.48
2:B:465:LEU:HD23	2:B:510:VAL:HG21	1.96	0.48
2:D:465:LEU:HD23	2:D:510:VAL:HG21	1.96	0.48
2:B:304:ALA:HA	2:B:307:MET:HE2	1.96	0.48
1:A:340:PRO:HB3	1:A:344:ARG:HH21	1.78	0.48
2:B:273:PHE:CD2	2:B:274:PRO:HD2	2.49	0.48
2:B:437:GLN:OE1	2:B:454:LYS:NZ	2.39	0.48
1:C:573:ASP:OD1	1:C:573:ASP:N	2.45	0.48
1:A:189:SER:HA	1:A:190:LYS:HA	1.64	0.48
2:D:94:ILE:HG22	2:D:96:GLY:H	1.79	0.48
2:D:323:ASN:OD1	2:D:323:ASN:N	2.46	0.48
1:A:510:ARG:HD3	2:B:190:ILE:HG12	1.95	0.48
2:D:304:ALA:HA	2:D:307:MET:HE2	1.96	0.48
2:B:94:ILE:HG22	2:B:96:GLY:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:LEU:HD13	2:B:369:LYS:HG2	1.95	0.48
1:C:438:ASP:OD1	1:C:438:ASP:N	2.46	0.48
3:M:50:TYR:CE1	4:N:95:TYR:HB2	2.49	0.48
2:B:244:ALA:HB1	2:B:249:LEU:HB3	1.95	0.48
1:C:165:LEU:HA	1:C:241:ILE:HB	1.95	0.48
2:D:77:ASP:OD2	2:D:80:SER:N	2.37	0.48
1:A:367:ARG:HG3	1:A:369:PHE:H	1.78	0.48
2:B:379:TRP:HD1	2:B:384:LEU:HG	1.79	0.48
2:D:273:PHE:CD2	2:D:274:PRO:HD2	2.49	0.48
1:A:118:VAL:HG22	1:A:138:LEU:HB2	1.96	0.48
2:D:600:VAL:HA	2:D:604:LYS:HD2	1.96	0.48
2:B:280:VAL:HG22	2:B:364:ILE:HG13	1.96	0.47
2:B:286:ASP:HB3	2:B:289:LEU:HB2	1.96	0.47
1:C:189:SER:HA	1:C:190:LYS:HA	1.64	0.47
1:C:251:THR:HG23	1:C:254:ARG:HE	1.79	0.47
1:C:338:THR:HG23	1:C:341:LEU:HD23	1.95	0.47
2:D:379:TRP:HD1	2:D:384:LEU:HG	1.79	0.47
1:A:183:LEU:O	1:A:187:ARG:NH1	2.47	0.47
1:C:367:ARG:HG3	1:C:369:PHE:H	1.78	0.47
1:A:165:LEU:HA	1:A:241:ILE:HB	1.95	0.47
2:D:40:ILE:HG23	2:D:99:PHE:HA	1.96	0.47
1:C:520:ASN:ND2	1:C:707:GLN:OE1	2.48	0.47
1:A:573:ASP:N	1:A:573:ASP:OD1	2.45	0.47
1:C:118:VAL:HG22	1:C:138:LEU:HB2	1.96	0.47
1:C:138:LEU:HD12	1:C:365:GLY:HA2	1.96	0.47
1:C:344:ARG:HA	1:C:347:MET:HG2	1.97	0.47
2:D:437:GLN:OE1	2:D:454:LYS:NZ	2.39	0.47
1:A:143:PRO:HD2	1:A:146:HIS:HB2	1.97	0.47
1:A:520:ASN:ND2	1:A:707:GLN:OE1	2.48	0.47
2:B:86:CYS:HB2	2:B:321:CYS:HB3	1.66	0.47
2:B:105:GLN:HB2	2:B:130:SER:N	2.30	0.47
2:B:774:ARG:NH2	1:C:546:GLN:O	2.47	0.47
1:C:183:LEU:O	1:C:187:ARG:NH1	2.47	0.47
1:C:340:PRO:HB3	1:C:344:ARG:HH21	1.78	0.47
3:H:96:CYS:O	3:H:113:GLY:N	2.48	0.47
1:A:344:ARG:HA	1:A:347:MET:HG2	1.96	0.47
1:A:486:LYS:O	1:A:490:THR:OG1	2.29	0.47
2:B:600:VAL:HA	2:B:604:LYS:HD2	1.96	0.47
1:C:143:PRO:HD2	1:C:146:HIS:HB2	1.97	0.47
3:H:16:GLY:O	3:H:84:ASN:ND2	2.48	0.47
3:H:31:SER:O	3:H:103:GLY:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:92:ASP:OD1	4:L:92:ASP:N	2.41	0.47
1:A:275:ILE:O	1:A:278:ASN:ND2	2.48	0.47
2:D:286:ASP:HB3	2:D:289:LEU:HB2	1.96	0.47
2:D:428:THR:OG1	2:D:429:CYS:N	2.48	0.47
2:D:538:VAL:N	2:D:749:VAL:O	2.47	0.47
2:D:280:VAL:HG22	2:D:364:ILE:HG13	1.96	0.47
2:B:353:GLU:HB3	2:B:356:TYR:HB2	1.97	0.46
1:C:275:ILE:O	1:C:278:ASN:ND2	2.48	0.46
1:C:282:TYR:O	1:C:380:ARG:NH1	2.42	0.46
2:D:172:VAL:HG12	2:D:203:LEU:HB2	1.97	0.46
2:D:637:PHE:HA	2:D:640:VAL:HG22	1.96	0.46
1:A:251:THR:HG23	1:A:254:ARG:HE	1.79	0.46
1:A:389:ASN:OD1	1:A:389:ASN:N	2.49	0.46
1:C:460:PRO:HD3	1:C:499:LEU:HD12	1.98	0.46
1:C:225:VAL:HG11	1:C:252:VAL:HG12	1.97	0.46
2:B:226:PRO:HA	2:B:252:TYR:HE1	1.80	0.46
2:B:637:PHE:HA	2:B:640:VAL:HG22	1.96	0.46
2:D:353:GLU:HB3	2:D:356:TYR:HB2	1.98	0.46
1:A:184:LEU:O	1:A:187:ARG:NH2	2.48	0.46
2:B:40:ILE:HG23	2:B:99:PHE:HA	1.96	0.46
1:C:170:ASP:OD1	1:C:171:HIS:ND1	2.49	0.46
2:D:105:GLN:HB2	2:D:130:SER:N	2.30	0.46
1:A:138:LEU:HD12	1:A:365:GLY:HA2	1.96	0.46
1:C:131:LYS:HB2	2:D:177:PRO:HG3	1.96	0.46
1:A:460:PRO:HD3	1:A:499:LEU:HD12	1.98	0.46
2:B:172:VAL:HG12	2:B:203:LEU:HB2	1.98	0.46
1:C:584:TRP:HB3	1:C:586:LEU:H	1.80	0.46
1:A:225:VAL:HG11	1:A:252:VAL:HG12	1.97	0.46
1:A:584:TRP:HB3	1:A:586:LEU:H	1.80	0.46
1:A:773:LEU:HD12	1:A:776:ARG:HE	1.80	0.46
1:A:827:ALA:HB1	2:D:653:PHE:HA	1.97	0.46
2:B:175:TYR:CZ	2:B:204:LEU:HB3	2.51	0.46
2:B:540:ARG:HD3	2:B:747:LYS:HE3	1.98	0.46
2:D:226:PRO:HA	2:D:252:TYR:HE1	1.80	0.46
4:N:39:LYS:HD2	4:N:42:LYS:HD3	1.98	0.46
1:A:170:ASP:OD1	1:A:171:HIS:ND1	2.49	0.46
2:B:349:LEU:HD22	2:B:358:MET:HG3	1.98	0.46
2:B:428:THR:OG1	2:B:429:CYS:N	2.48	0.46
1:C:773:LEU:HD12	1:C:776:ARG:HE	1.80	0.46
2:D:540:ARG:HD3	2:D:747:LYS:HE3	1.98	0.46
3:M:109:PHE:O	4:N:36:TYR:OH	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:374:GLU:HG3	2:B:375:ARG:HE	1.81	0.45
2:D:107:ALA:O	2:D:110:GLN:NE2	2.37	0.45
4:L:39:LYS:HD2	4:L:42:LYS:HD3	1.98	0.45
2:D:349:LEU:HD22	2:D:358:MET:HG3	1.98	0.45
3:M:31:SER:O	3:M:103:GLY:N	2.49	0.45
3:M:99:PRO:HA	3:M:109:PHE:HB3	1.98	0.45
1:C:184:LEU:O	1:C:187:ARG:NH2	2.48	0.45
2:D:133:ILE:O	2:D:356:TYR:OH	2.34	0.45
2:D:374:GLU:HG3	2:D:375:ARG:HE	1.81	0.45
2:D:175:TYR:CZ	2:D:204:LEU:HB3	2.51	0.45
3:M:94:TYR:N	3:M:116:THR:O	2.45	0.45
2:B:434:VAL:HG21	2:B:457:CYS:HB2	1.98	0.45
2:B:460:PHE:HE1	2:B:792:LEU:HB3	1.82	0.45
2:B:493:THR:OG1	2:B:494:TRP:N	2.50	0.45
1:C:389:ASN:OD1	1:C:389:ASN:N	2.49	0.45
2:D:408:ILE:HG12	2:D:508:MET:HB2	1.98	0.45
2:D:493:THR:OG1	2:D:494:TRP:N	2.50	0.45
2:D:654:MET:HE2	2:D:654:MET:HB2	1.73	0.45
1:A:151:TRP:CG	1:A:269:LEU:HD21	2.52	0.45
2:B:420:GLU:OE2	2:B:432:ASN:ND2	2.50	0.45
2:D:222:LYS:HD2	2:D:222:LYS:HA	1.87	0.45
1:C:704:THR:HB	1:C:751:ILE:HG23	1.99	0.45
2:D:152:GLN:NE2	2:D:358:MET:HA	2.32	0.45
2:D:420:GLU:OE2	2:D:432:ASN:ND2	2.50	0.45
1:C:71:ALA:HB1	2:D:118:GLN:HE21	1.81	0.45
1:A:310:ALA:HA	1:A:313:VAL:HG22	1.98	0.45
1:C:397:ASP:OD1	1:C:397:ASP:N	2.49	0.45
2:D:125:GLY:HA3	2:D:127:HIS:NE2	2.31	0.44
1:A:93:SER:OG	1:A:94:HIS:N	2.47	0.44
2:B:133:ILE:O	2:B:356:TYR:OH	2.34	0.44
2:B:152:GLN:NE2	2:B:358:MET:HA	2.32	0.44
2:B:408:ILE:HG12	2:B:508:MET:HB2	1.98	0.44
1:C:310:ALA:HA	1:C:313:VAL:HG22	1.98	0.44
3:H:50:TYR:CE1	4:L:95:TYR:HB2	2.52	0.44
3:H:112:TRP:CH2	4:L:43:GLY:HA3	2.53	0.44
1:A:49:ALA:HB3	1:A:60:LEU:HD11	1.99	0.44
1:A:571:THR:HG22	1:A:574:SER:HB3	2.00	0.44
2:B:125:GLY:HA3	2:B:127:HIS:NE2	2.31	0.44
1:C:38:HIS:O	1:C:42:PHE:HB2	2.18	0.44
1:C:519:TRP:NE1	1:C:547:TYR:HH	2.13	0.44
2:D:434:VAL:HG21	2:D:457:CYS:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:LYS:HG2	1:A:477:TYR:HB3	1.98	0.44
2:B:93:LYS:HD2	2:B:317:PRO:HG2	2.00	0.44
2:B:124:LEU:HD22	2:B:300:ILE:HD11	2.00	0.44
1:C:454:LYS:HG2	1:C:477:TYR:HB3	1.98	0.44
2:D:431:ARG:HA	2:D:431:ARG:HD2	1.66	0.44
2:D:509:ALA:HB3	2:D:765:ALA:HB3	1.99	0.44
3:H:110:ASP:OD1	3:H:110:ASP:N	2.41	0.44
2:B:44:THR:O	2:B:45:SER:OG	2.32	0.44
2:D:460:PHE:HE1	2:D:792:LEU:HB3	1.82	0.44
2:D:537:MET:HB2	2:D:736:LEU:HD22	1.99	0.44
1:A:223:LYS:HE2	1:A:223:LYS:HB2	1.83	0.44
2:B:99:PHE:HZ	2:B:112:LEU:HD22	1.82	0.44
2:B:509:ALA:HB3	2:B:765:ALA:HB3	1.99	0.44
1:C:151:TRP:CG	1:C:269:LEU:HD21	2.52	0.44
1:C:811:LYS:HA	1:C:811:LYS:HD2	1.73	0.44
2:D:99:PHE:HZ	2:D:112:LEU:HD22	1.82	0.44
1:C:149:SER:HA	1:C:152:PHE:HB3	2.00	0.44
1:C:33:LEU:O	1:C:38:HIS:NE2	2.51	0.44
2:D:675:ASN:OD1	2:D:675:ASN:N	2.44	0.44
1:A:149:SER:HA	1:A:152:PHE:HB3	2.00	0.44
1:A:290:LEU:HD23	1:A:374:ILE:HG12	2.00	0.44
1:A:397:ASP:OD1	1:A:397:ASP:N	2.49	0.44
1:A:523:MET:HE1	1:A:544:ARG:HA	1.99	0.44
2:B:831:LEU:HD23	2:B:834:ILE:HD12	2.00	0.44
1:C:290:LEU:HD23	1:C:374:ILE:HG12	2.00	0.44
1:C:765:CYS:O	1:C:822:ARG:NH2	2.51	0.44
1:A:33:LEU:O	1:A:38:HIS:NE2	2.51	0.43
1:A:224:ASN:HD21	1:A:227:ALA:HB3	1.83	0.43
1:A:516:LYS:HA	1:A:516:LYS:HD3	1.79	0.43
2:D:365:ILE:HA	2:D:375:ARG:HA	2.00	0.43
1:A:502:ASP:OD1	1:A:502:ASP:N	2.50	0.43
1:C:166:LEU:N	1:C:241:ILE:O	2.44	0.43
1:C:571:THR:HG22	1:C:574:SER:HB3	2.00	0.43
1:A:38:HIS:O	1:A:42:PHE:HB2	2.18	0.43
2:B:537:MET:HB2	2:B:736:LEU:HD22	1.99	0.43
1:C:523:MET:HE1	1:C:544:ARG:HA	1.99	0.43
2:D:366:LEU:HG	2:D:373:TRP:HB3	2.00	0.43
1:A:286:GLY:HA3	1:A:403:PRO:HA	1.99	0.43
1:A:294:ASN:HD22	1:A:297:ASN:HB3	1.84	0.43
1:C:49:ALA:HB3	1:C:60:LEU:HD11	2.00	0.43
2:D:405:HIS:HA	2:D:475:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:112:TRP:CH2	4:N:43:GLY:HA3	2.53	0.43
1:A:704:THR:HB	1:A:751:ILE:HG23	1.99	0.43
1:C:435:THR:HG22	1:C:441:CYS:HB2	2.01	0.43
4:N:47:LEU:HB3	4:N:48:ILE:HG12	2.00	0.43
1:A:75:ALA:HB1	1:A:110:THR:HG21	2.01	0.43
2:B:405:HIS:HA	2:B:475:THR:HB	1.99	0.43
2:D:201:GLU:HG3	2:D:203:LEU:HG	2.01	0.43
2:B:693:ARG:HD2	2:B:693:ARG:HA	1.92	0.43
1:C:75:ALA:HB1	1:C:110:THR:HG21	2.01	0.43
1:C:534:ILE:N	1:C:782:GLY:O	2.47	0.43
1:A:765:CYS:O	1:A:822:ARG:NH2	2.51	0.43
1:A:131:LYS:HB2	2:B:177:PRO:HG3	1.99	0.43
2:B:184:ASN:OD1	2:B:187:ARG:NH1	2.52	0.43
1:C:72:ILE:HG13	2:D:118:GLN:NE2	2.34	0.43
1:C:268:TRP:HB2	1:C:287:ILE:HG23	2.01	0.43
1:C:499:LEU:HD23	1:C:499:LEU:HA	1.91	0.43
3:H:3:LYS:HD3	3:H:3:LYS:HA	1.84	0.43
1:C:72:ILE:HG13	2:D:118:GLN:HE22	1.84	0.43
2:D:86:CYS:HB2	2:D:321:CYS:HB3	1.66	0.43
1:A:116:ILE:O	1:A:136:SER:OG	2.31	0.42
1:A:158:TYR:HD1	1:A:409:LYS:HE3	1.84	0.42
1:A:375:MET:HE2	1:A:375:MET:HB2	1.60	0.42
1:C:286:GLY:HA3	1:C:403:PRO:HA	1.99	0.42
2:D:35:ILE:HG23	2:D:64:VAL:HG21	2.01	0.42
2:D:124:LEU:HD22	2:D:300:ILE:HD11	2.00	0.42
2:D:831:LEU:HD23	2:D:834:ILE:HD12	2.00	0.42
1:A:574:SER:O	1:A:574:SER:OG	2.26	0.42
2:B:365:ILE:HA	2:B:375:ARG:HA	2.00	0.42
2:D:93:LYS:HD2	2:D:317:PRO:HG2	2.00	0.42
2:D:453:ILE:HD12	2:D:453:ILE:HA	1.90	0.42
1:C:277:GLY:HA2	1:C:280:LEU:HB2	2.02	0.42
1:C:294:ASN:HD22	1:C:297:ASN:HB3	1.84	0.42
1:A:534:ILE:N	1:A:782:GLY:O	2.46	0.42
2:B:164:TYR:HB2	2:B:166:TRP:CD1	2.55	0.42
2:B:181:ASP:N	2:B:181:ASP:OD1	2.52	0.42
1:C:224:ASN:HD21	1:C:227:ALA:HB3	1.83	0.42
3:H:15:GLY:H	3:H:87:LYS:HE2	1.84	0.42
3:H:97:ALA:HA	3:H:112:TRP:HA	2.01	0.42
2:D:181:ASP:OD1	2:D:181:ASP:N	2.52	0.42
2:D:184:ASN:OD1	2:D:187:ARG:NH1	2.52	0.42
4:L:47:LEU:HB3	4:L:48:ILE:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:TYR:O	1:A:380:ARG:NH1	2.43	0.42
1:A:376:ASN:HD21	1:A:385:VAL:HG11	1.85	0.42
2:B:366:LEU:HG	2:B:373:TRP:HB3	2.00	0.42
2:D:404:ASP:N	2:D:404:ASP:OD1	2.53	0.42
2:D:703:HIS:HA	2:D:706:MET:HB2	2.01	0.42
1:C:113:PHE:CE2	2:D:78:PRO:HG3	2.55	0.42
1:C:255:ALA:HA	1:C:258:MET:HE2	2.02	0.42
2:D:299:ILE:HD13	2:D:299:ILE:HA	1.91	0.42
2:B:201:GLU:HG3	2:B:203:LEU:HG	2.01	0.42
1:A:58:ILE:HG13	1:A:59:GLN:NE2	2.35	0.42
1:A:325:PRO:HG3	1:A:336:TRP:CD2	2.55	0.42
1:A:435:THR:HG22	1:A:441:CYS:HB2	2.01	0.42
2:B:116:SER:O	2:B:120:LEU:N	2.51	0.42
2:B:703:HIS:HA	2:B:706:MET:HB2	2.01	0.42
1:C:275:ILE:HG21	1:C:291:GLN:HE21	1.85	0.42
1:C:477:TYR:C	1:C:481:ILE:HD13	2.45	0.42
2:D:254:TYR:CZ	2:D:278:ILE:HG23	2.55	0.42
2:D:669:LYS:HA	2:D:669:LYS:HD2	1.90	0.42
3:M:24:ALA:HB3	3:M:77:ASN:HB3	2.01	0.42
4:N:6:GLN:HB2	4:N:100:GLY:H	1.85	0.42
1:A:130:ASP:H	1:A:134:HIS:CE1	2.37	0.42
1:A:255:ALA:HA	1:A:258:MET:HE2	2.02	0.42
2:B:674:PRO:HB2	2:B:680:PRO:HB2	2.02	0.42
1:C:30:GLY:HA3	1:C:91:LEU:HA	2.02	0.42
1:C:321:ASN:OD1	1:C:321:ASN:N	2.38	0.42
1:C:559:LEU:HG	1:C:775:PHE:HB3	2.02	0.42
2:D:742:ARG:HD2	2:D:742:ARG:HA	1.91	0.42
3:M:3:LYS:HD3	3:M:3:LYS:HA	1.84	0.42
1:A:268:TRP:HB2	1:A:287:ILE:HG23	2.01	0.41
2:B:538:VAL:N	2:B:749:VAL:O	2.47	0.41
1:C:32:VAL:HG22	1:C:91:LEU:HB3	2.02	0.41
1:C:517:LYS:HE2	2:D:190:ILE:HD13	2.01	0.41
1:C:561:ILE:HD11	1:C:774:PHE:HZ	1.85	0.41
4:L:46:LEU:HD21	4:L:49:HIS:CE1	2.55	0.41
1:A:147:GLN:HE21	1:A:290:LEU:HB2	1.84	0.41
1:A:517:LYS:HE2	2:B:190:ILE:HD13	2.02	0.41
2:D:164:TYR:HB2	2:D:166:TRP:CD1	2.55	0.41
4:N:23:CYS:HB3	4:N:90:GLN:HE22	1.86	0.41
1:C:130:ASP:H	1:C:134:HIS:CE1	2.37	0.41
1:C:376:ASN:HD21	1:C:385:VAL:HG11	1.85	0.41
2:D:504:LYS:HA	2:D:507:TYR:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:46:LEU:HD21	4:N:49:HIS:CE1	2.55	0.41
2:B:35:ILE:HG23	2:B:64:VAL:HG21	2.01	0.41
2:B:429:CYS:HB3	2:B:432:ASN:HD22	1.85	0.41
1:C:147:GLN:HE21	1:C:290:LEU:HB2	1.84	0.41
1:C:158:TYR:HD1	1:C:409:LYS:HE3	1.84	0.41
1:C:325:PRO:HG3	1:C:336:TRP:CD2	2.55	0.41
1:C:369:PHE:HD2	1:C:371:GLN:HE22	1.68	0.41
2:D:116:SER:O	2:D:120:LEU:N	2.51	0.41
1:A:559:LEU:HG	1:A:775:PHE:HB3	2.02	0.41
2:B:515:ILE:HD11	2:B:763:GLY:HA3	2.03	0.41
1:C:223:LYS:HB2	1:C:223:LYS:HE2	1.84	0.41
2:D:515:ILE:HD11	2:D:763:GLY:HA3	2.03	0.41
3:M:70:ILE:HD13	3:M:81:LEU:HD13	2.03	0.41
1:A:277:GLY:HA2	1:A:280:LEU:HB2	2.01	0.41
1:A:409:LYS:HA	1:A:410:PRO:HD3	1.85	0.41
1:A:477:TYR:C	1:A:481:ILE:HD13	2.45	0.41
2:B:474:PHE:HD1	2:B:474:PHE:HA	1.78	0.41
4:L:29:ILE:HG21	4:L:90:GLN:HG2	2.02	0.41
1:A:219:ASP:OD1	1:A:219:ASP:N	2.52	0.41
2:B:366:LEU:HD12	2:B:367:LEU:H	1.86	0.41
2:B:490:ILE:HD13	2:B:495:ASN:HD21	1.86	0.41
1:C:461:ASN:HB3	1:C:469:ARG:HD2	2.03	0.41
1:C:486:LYS:O	1:C:490:THR:OG1	2.29	0.41
1:C:511:VAL:HG21	1:C:518:GLU:HG2	2.03	0.41
2:D:267:ASP:OD1	2:D:267:ASP:N	2.52	0.41
2:D:524:ASP:HB2	2:D:768:LYS:HA	2.03	0.41
1:A:485:ILE:HD13	1:A:485:ILE:HA	1.96	0.41
1:A:809:LEU:HD12	1:A:809:LEU:HA	1.94	0.41
2:B:230:LEU:H	2:B:257:ILE:HG22	1.86	0.41
2:B:254:TYR:CZ	2:B:278:ILE:HG23	2.55	0.41
1:C:33:LEU:HA	1:C:66:THR:HG23	2.02	0.41
1:C:393:VAL:O	1:C:395:PRO:HD3	2.21	0.41
1:A:164:ILE:HD13	1:A:164:ILE:HA	1.89	0.41
1:C:516:LYS:HD3	1:C:516:LYS:HA	1.79	0.41
2:D:490:ILE:HD13	2:D:495:ASN:HD21	1.85	0.41
2:D:674:PRO:HB2	2:D:680:PRO:HB2	2.02	0.41
1:A:30:GLY:HA3	1:A:91:LEU:HA	2.02	0.40
1:A:32:VAL:HG22	1:A:91:LEU:HB3	2.02	0.40
1:A:461:ASN:HB3	1:A:469:ARG:HD2	2.03	0.40
1:C:219:ASP:OD1	1:C:219:ASP:N	2.52	0.40
4:N:29:ILE:HG21	4:N:90:GLN:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:673:ARG:HA	2:B:674:PRO:HD3	1.93	0.40
2:D:532:THR:OG1	2:D:533:GLY:N	2.55	0.40
3:M:13:GLN:HB3	3:M:16:GLY:HA3	2.02	0.40
1:A:511:VAL:HG21	1:A:518:GLU:HG2	2.03	0.40
2:B:504:LYS:HA	2:B:507:TYR:HE2	1.86	0.40
1:C:350:LYS:HA	1:C:350:LYS:HD2	1.90	0.40
2:D:366:LEU:HD12	2:D:367:LEU:H	1.86	0.40
4:L:85:THR:OG1	4:L:101:THR:O	2.29	0.40
1:A:393:VAL:O	1:A:395:PRO:HD3	2.21	0.40
1:A:575:PHE:HB3	1:A:837:VAL:HG13	2.03	0.40
2:B:105:GLN:HG3	2:B:129:GLY:H	1.86	0.40
2:D:254:TYR:CZ	2:D:276:GLY:HA2	2.57	0.40
2:D:429:CYS:HB3	2:D:432:ASN:HD22	1.85	0.40
1:A:275:ILE:HG21	1:A:291:GLN:HE21	1.85	0.40
1:A:549:GLU:HG3	1:A:783:MET:HB2	2.03	0.40
2:B:552:GLU:HB3	2:B:553:PRO:HD3	2.04	0.40
1:C:58:ILE:HG13	1:C:59:GLN:NE2	2.35	0.40
1:C:93:SER:OG	1:C:94:HIS:N	2.47	0.40
1:C:575:PHE:HB3	1:C:837:VAL:HG13	2.03	0.40
1:C:829:LEU:HD13	1:C:831:CYS:SG	2.62	0.40
3:H:17:SER:OG	3:H:84:ASN:ND2	2.46	0.40
4:L:6:GLN:HB2	4:L:100:GLY:H	1.85	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	778/862 (90%)	688 (88%)	81 (10%)	9 (1%)	10	44
1	C	778/862 (90%)	688 (88%)	81 (10%)	9 (1%)	10	44
2	B	759/883 (86%)	647 (85%)	104 (14%)	8 (1%)	11	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	759/883 (86%)	647 (85%)	104 (14%)	8 (1%)	11	46
3	H	113/223 (51%)	107 (95%)	6 (5%)	0	100	100
3	M	112/223 (50%)	109 (97%)	3 (3%)	0	100	100
4	L	104/213 (49%)	90 (86%)	13 (12%)	1 (1%)	12	48
4	N	104/213 (49%)	90 (86%)	13 (12%)	1 (1%)	12	48
All	All	3507/4362 (80%)	3066 (87%)	405 (12%)	36 (1%)	15	48

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	41	MET
1	A	402	TRP
2	B	89	MET
2	B	272	GLU
1	C	40	GLN
1	C	41	MET
1	C	402	TRP
2	D	89	MET
2	D	272	GLU
1	A	394	ILE
1	A	830	THR
2	B	351	PHE
1	C	394	ILE
1	C	830	THR
2	D	351	PHE
1	A	281	ARG
1	A	401	ILE
2	B	88	LEU
2	B	220	LEU
2	B	252	TYR
1	C	281	ARG
1	C	401	ILE
2	D	88	LEU
2	D	220	LEU
2	D	252	TYR
1	A	67	HIS
1	A	368	LYS
1	C	67	HIS
1	C	368	LYS

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Mol	Chain	Res	Type
2	B	200	GLU
2	D	200	GLU
2	B	679	PRO
2	D	679	PRO
4	L	8	PRO
4	N	8	PRO

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	679/744 (91%)	644 (95%)	35 (5%)	21	42
1	C	679/744 (91%)	644 (95%)	35 (5%)	21	42
2	B	668/762 (88%)	626 (94%)	42 (6%)	16	37
2	D	668/762 (88%)	626 (94%)	42 (6%)	16	37
3	H	96/189 (51%)	92 (96%)	4 (4%)	26	48
3	M	95/189 (50%)	93 (98%)	2 (2%)	47	65
4	L	91/189 (48%)	86 (94%)	5 (6%)	19	41
4	N	91/189 (48%)	86 (94%)	5 (6%)	19	41
All	All	3067/3768 (81%)	2897 (94%)	170 (6%)	21	41

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ILE
1	A	27	VAL
1	A	61	GLN
1	A	63	THR
1	A	65	VAL
1	A	76	LEU
1	A	81	ASP
1	A	141	VAL
1	A	150	VAL

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Mol	Chain	Res	Type
1	A	153	GLU
1	A	155	MET
1	A	167	VAL
1	A	180	LEU
1	A	242	LEU
1	A	247	ASP
1	A	267	VAL
1	A	269	LEU
1	A	280	LEU
1	A	321	ASN
1	A	345	VAL
1	A	355	VAL
1	A	377	LEU
1	A	441	CYS
1	A	455	VAL
1	A	476	CYS
1	A	538	LEU
1	A	561	ILE
1	A	567	ILE
1	A	635	LEU
1	A	689	ASN
1	A	734	SER
1	A	751	ILE
1	A	765	CYS
1	A	798	LEU
1	A	837	VAL
2	B	40	ILE
2	B	41	LEU
2	B	67	ARG
2	B	71	VAL
2	B	77	ASP
2	B	97	VAL
2	B	104	ASP
2	B	111	ILE
2	B	112	LEU
2	B	113	ASP
2	B	123	ILE
2	B	126	ILE
2	B	127	HIS
2	B	162	GLU
2	B	173	THR
2	B	207	MET

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Mol	Chain	Res	Type
2	B	219	GLN
2	B	227	ILE
2	B	230	LEU
2	B	258	VAL
2	B	261	LEU
2	B	266	THR
2	B	267	ASP
2	B	271	SER
2	B	292	ARG
2	B	328	ARG
2	B	329	ILE
2	B	335	LEU
2	B	349	LEU
2	B	363	VAL
2	B	366	LEU
2	B	378	LYS
2	B	393	ARG
2	B	462	ILE
2	B	465	LEU
2	B	486	HIS
2	B	527	VAL
2	B	618	VAL
2	B	632	VAL
2	B	660	VAL
2	B	714	VAL
2	B	786	ASP
1	C	26	ILE
1	C	27	VAL
1	C	61	GLN
1	C	63	THR
1	C	65	VAL
1	C	76	LEU
1	C	81	ASP
1	C	141	VAL
1	C	150	VAL
1	C	153	GLU
1	C	155	MET
1	C	167	VAL
1	C	180	LEU
1	C	242	LEU
1	C	247	ASP
1	C	267	VAL

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Mol	Chain	Res	Type
1	C	269	LEU
1	C	280	LEU
1	C	321	ASN
1	C	345	VAL
1	C	355	VAL
1	C	377	LEU
1	C	441	CYS
1	C	455	VAL
1	C	476	CYS
1	C	538	LEU
1	C	561	ILE
1	C	567	ILE
1	C	635	LEU
1	C	689	ASN
1	C	734	SER
1	C	751	ILE
1	C	765	CYS
1	C	798	LEU
1	C	837	VAL
2	D	40	ILE
2	D	41	LEU
2	D	67	ARG
2	D	71	VAL
2	D	77	ASP
2	D	97	VAL
2	D	104	ASP
2	D	111	ILE
2	D	112	LEU
2	D	113	ASP
2	D	123	ILE
2	D	126	ILE
2	D	127	HIS
2	D	162	GLU
2	D	173	THR
2	D	207	MET
2	D	219	GLN
2	D	227	ILE
2	D	230	LEU
2	D	258	VAL
2	D	261	LEU
2	D	266	THR
2	D	267	ASP

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Mol	Chain	Res	Type
2	D	271	SER
2	D	292	ARG
2	D	328	ARG
2	D	329	ILE
2	D	335	LEU
2	D	349	LEU
2	D	363	VAL
2	D	366	LEU
2	D	378	LYS
2	D	393	ARG
2	D	462	ILE
2	D	465	LEU
2	D	486	HIS
2	D	527	VAL
2	D	618	VAL
2	D	632	VAL
2	D	660	VAL
2	D	714	VAL
2	D	786	ASP
3	H	28	THR
3	H	37	VAL
3	H	116	THR
3	H	118	VAL
4	L	5	THR
4	L	15	LEU
4	L	19	VAL
4	L	22	THR
4	L	92	ASP
3	M	117	THR
3	M	118	VAL
4	N	5	THR
4	N	15	LEU
4	N	19	VAL
4	N	22	THR
4	N	92	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	59	GLN
1	A	147	GLN

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Mol	Chain	Res	Type
1	A	217	GLN
1	A	224	ASN
1	A	291	GLN
1	A	311	GLN
1	A	470	HIS
1	A	498	HIS
1	A	515	ASN
1	A	542	ASN
1	A	763	GLN
2	B	118	GLN
2	B	152	GLN
2	B	217	GLN
2	B	218	ASN
2	B	325	HIS
2	B	357	GLN
2	B	432	ASN
2	B	491	ASN
2	B	495	ASN
2	B	615	ASN
2	B	616	ASN
2	B	656	GLN
2	B	698	ASN
2	B	711	GLN
1	C	47	ASN
1	C	59	GLN
1	C	147	GLN
1	C	217	GLN
1	C	291	GLN
1	C	311	GLN
1	C	384	GLN
1	C	515	ASN
1	C	542	ASN
1	C	763	GLN
2	D	152	GLN
2	D	217	GLN
2	D	218	ASN
2	D	357	GLN
2	D	432	ASN
2	D	491	ASN
2	D	495	ASN
2	D	656	GLN
2	D	698	ASN

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Mol	Chain	Res	Type
2	D	711	GLN
2	D	782	GLN
3	H	84	ASN
4	L	3	GLN
4	L	38	HIS
3	M	13	GLN
3	M	84	ASN
4	N	3	GLN
4	N	38	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	44:THR	C	45:SER	N	5.82
1	D	44:THR	C	45:SER	N	5.82

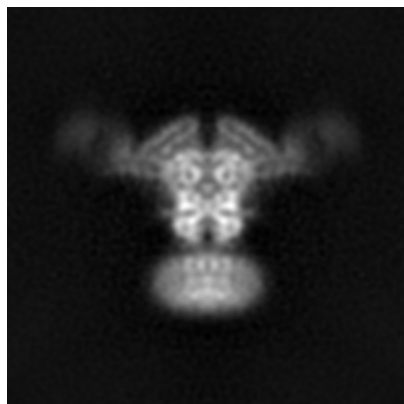
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25845. These allow visual inspection of the internal detail of the map and identification of artifacts.

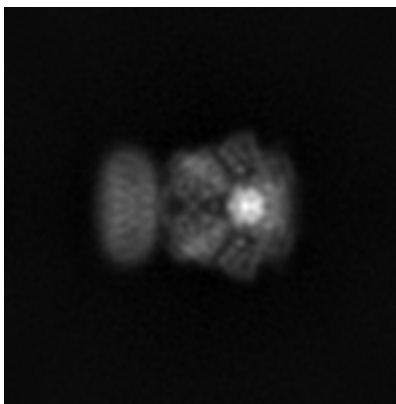
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

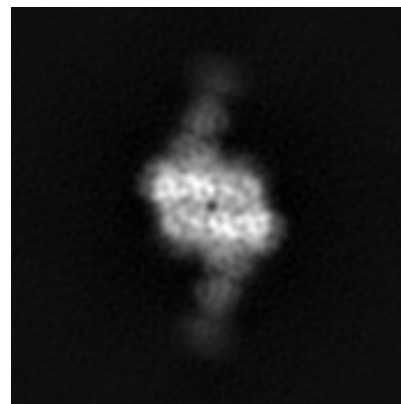
6.1.1 Primary map



X

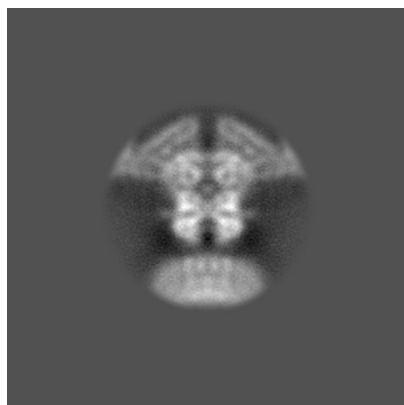


Y

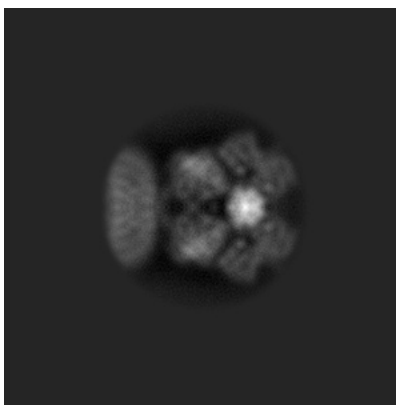


Z

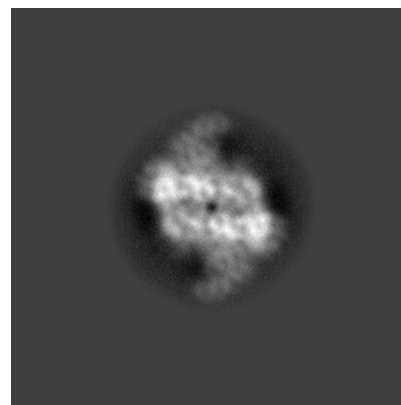
6.1.2 Raw map



X



Y

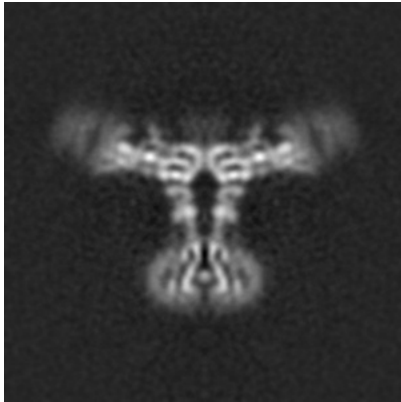


Z

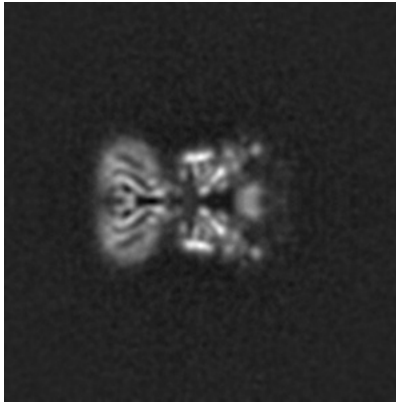
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

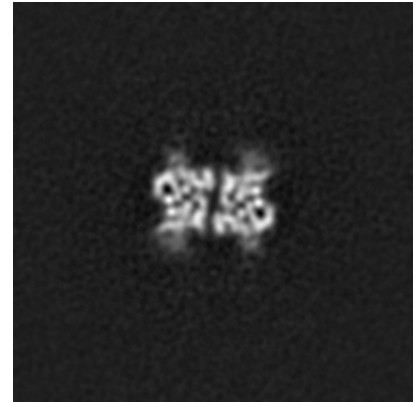
6.2.1 Primary map



X Index: 128

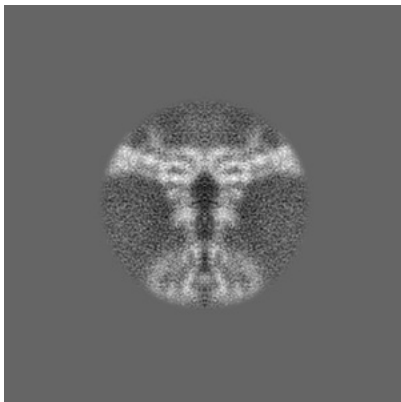


Y Index: 128

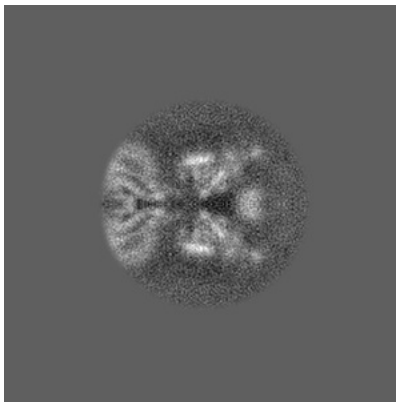


Z Index: 128

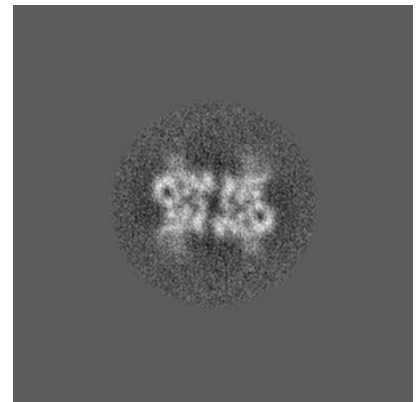
6.2.2 Raw map



X Index: 128



Y Index: 128

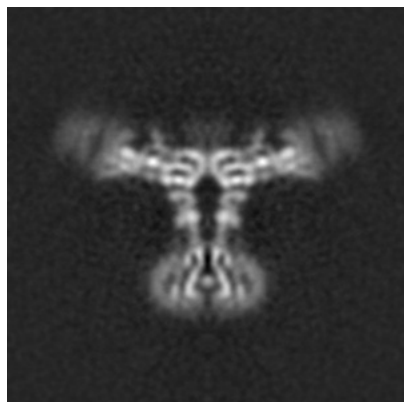


Z Index: 128

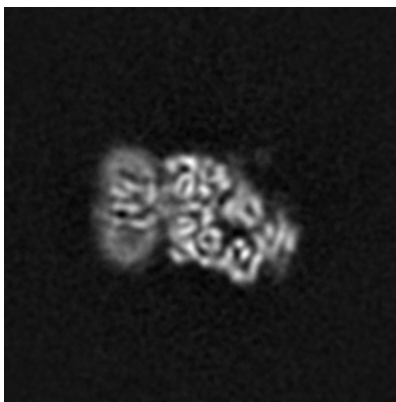
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

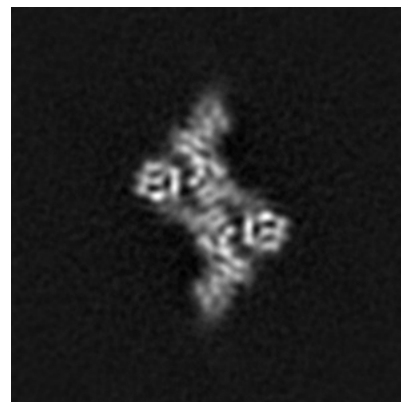
6.3.1 Primary map



X Index: 128

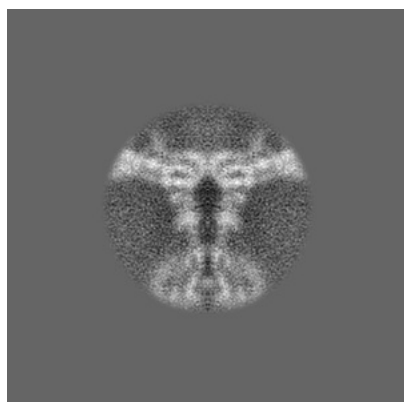


Y Index: 138

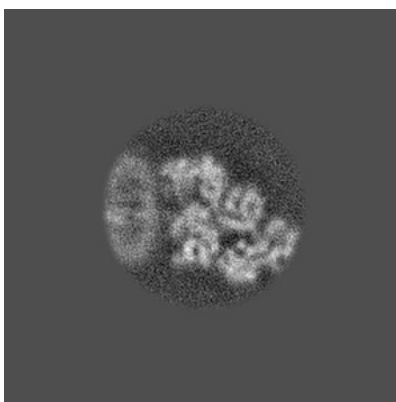


Z Index: 151

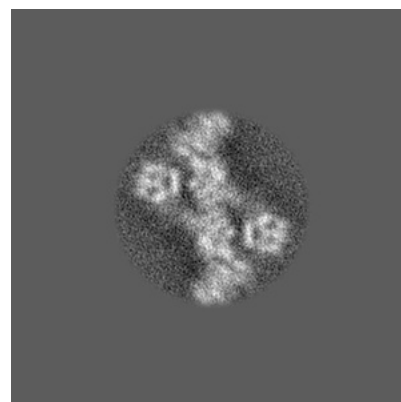
6.3.2 Raw map



X Index: 128



Y Index: 143

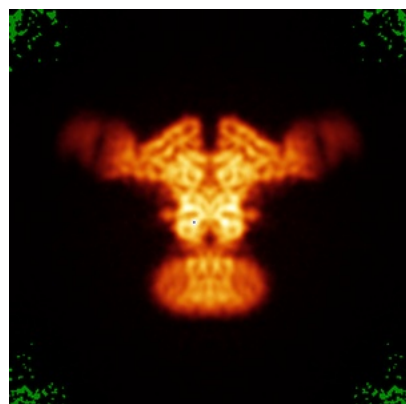


Z Index: 152

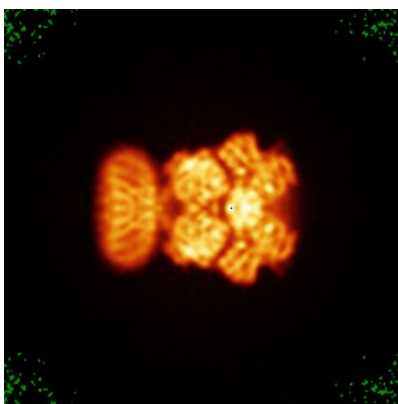
The images above show the largest variance slices of the map in three orthogonal directions.

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

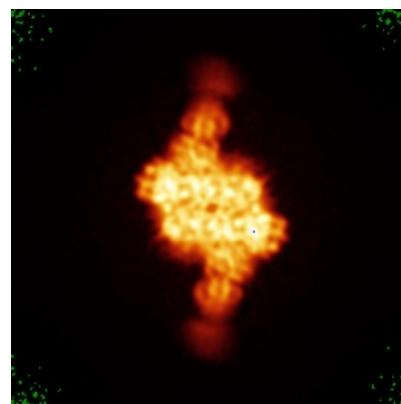
6.4.1 Primary map



X

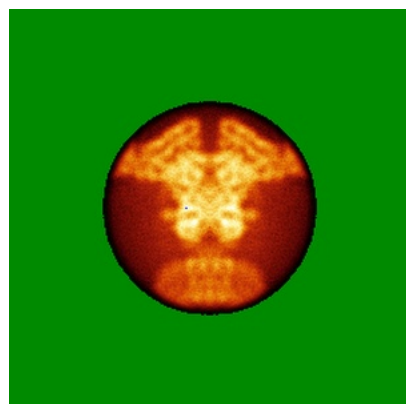


Y

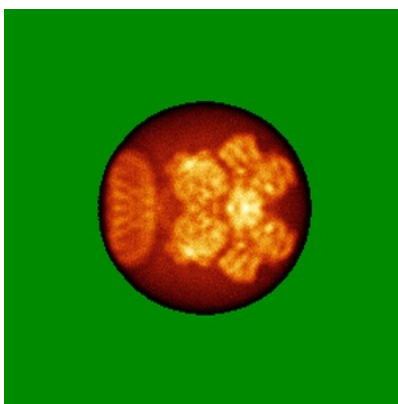


Z

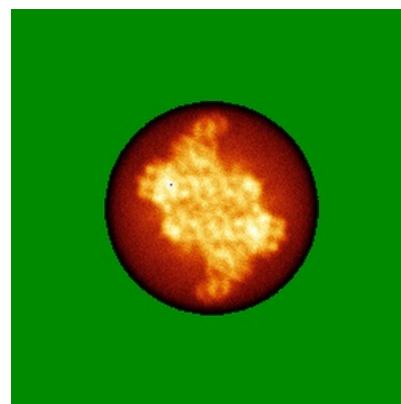
6.4.2 Raw map



X



Y

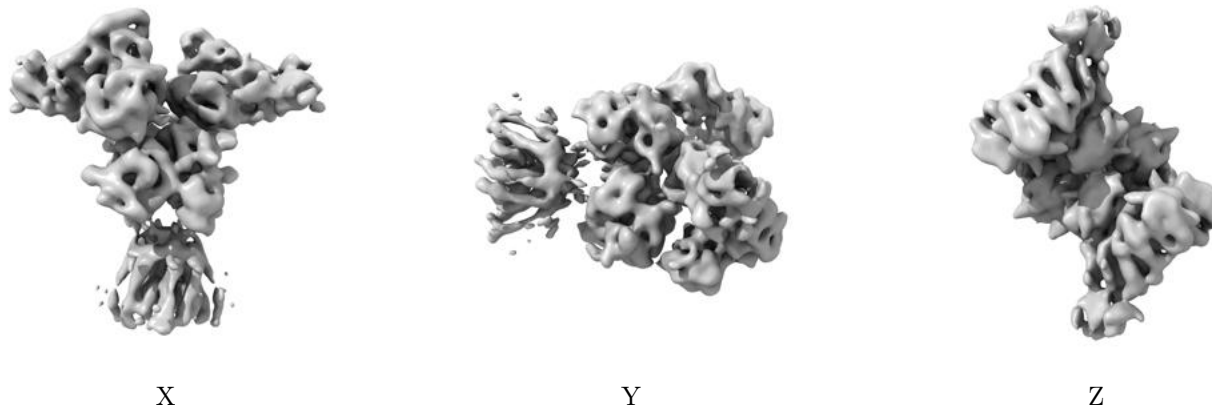


Z

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.

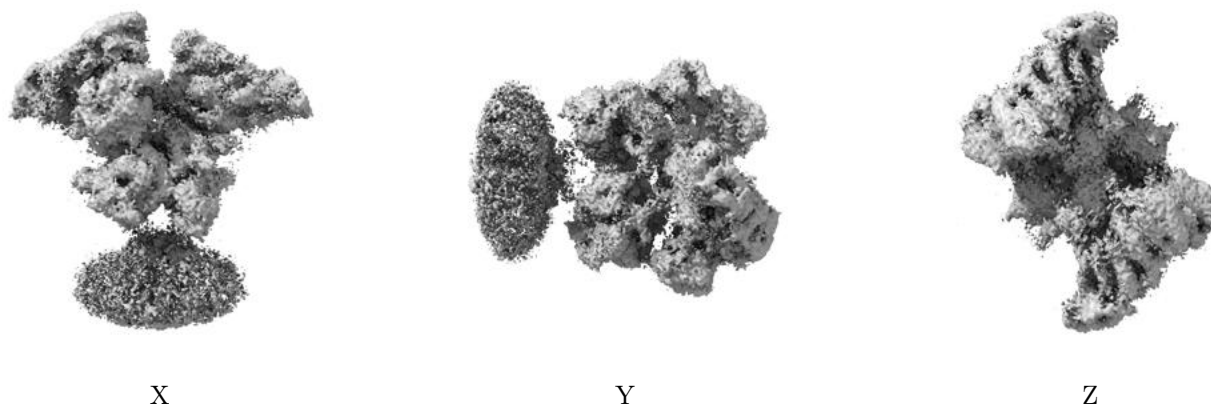
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. 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.

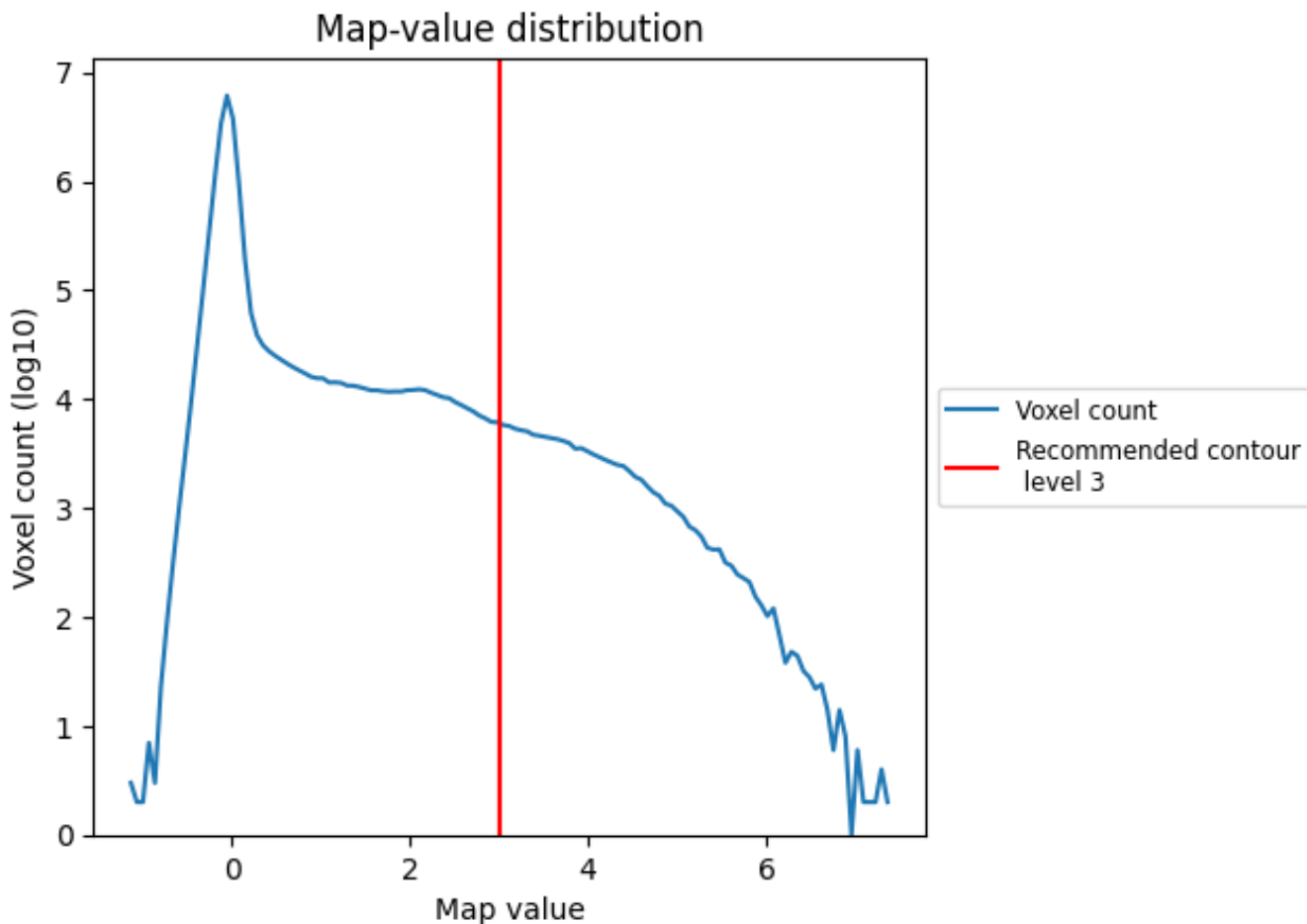
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

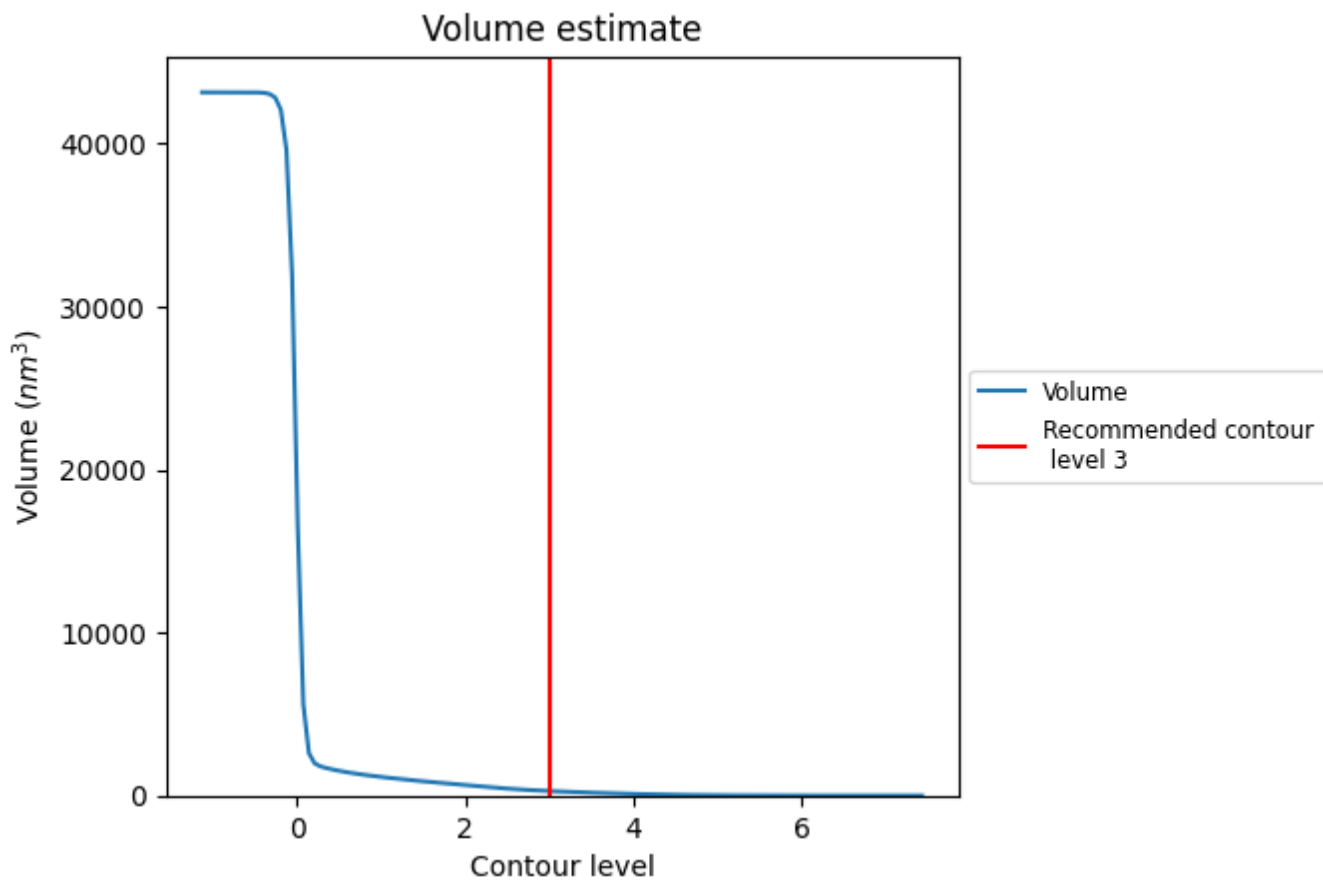
This section contains the results of statistical analysis of the map.

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.

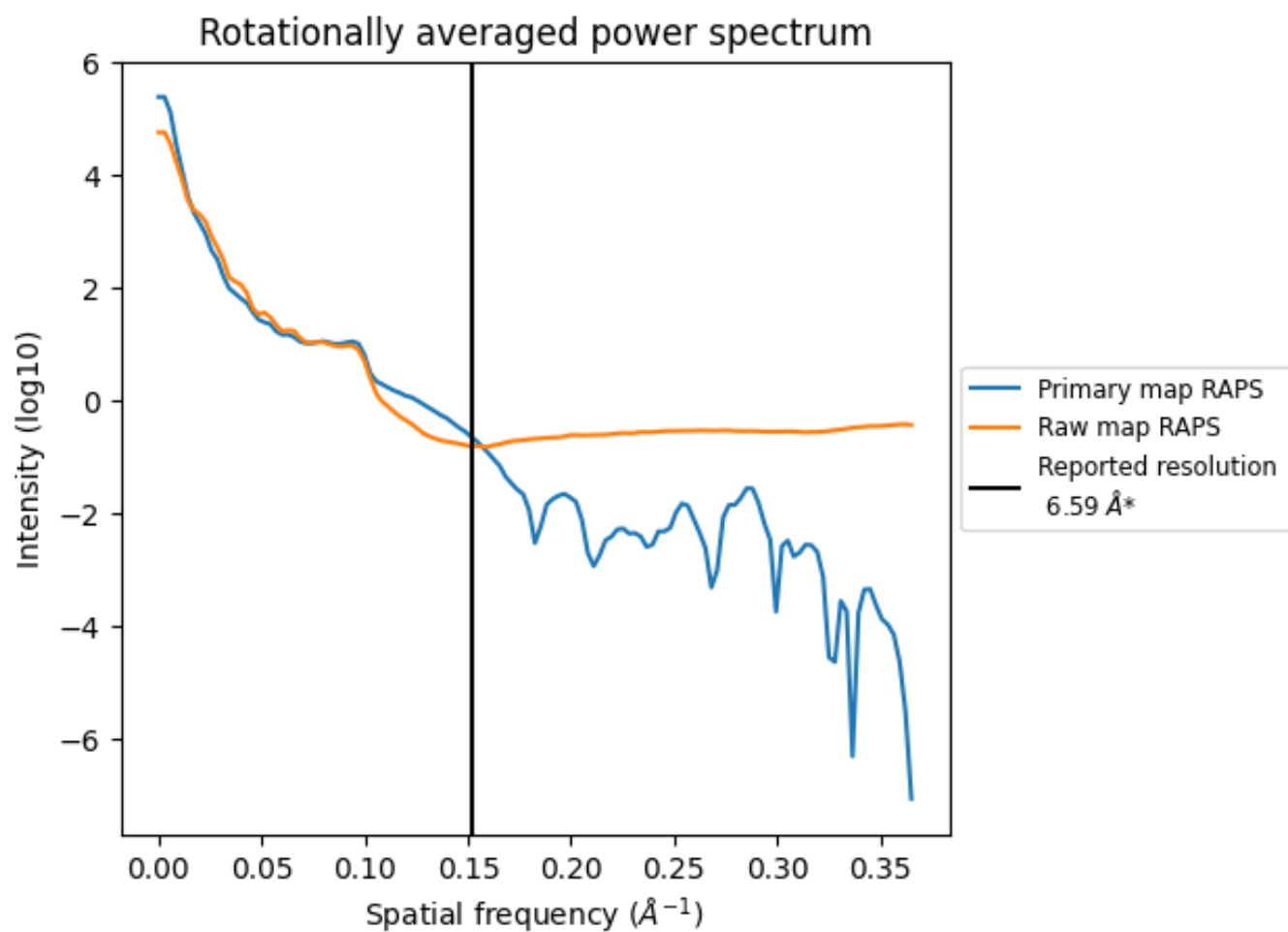
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 279 nm³; this corresponds to an approximate mass of 252 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

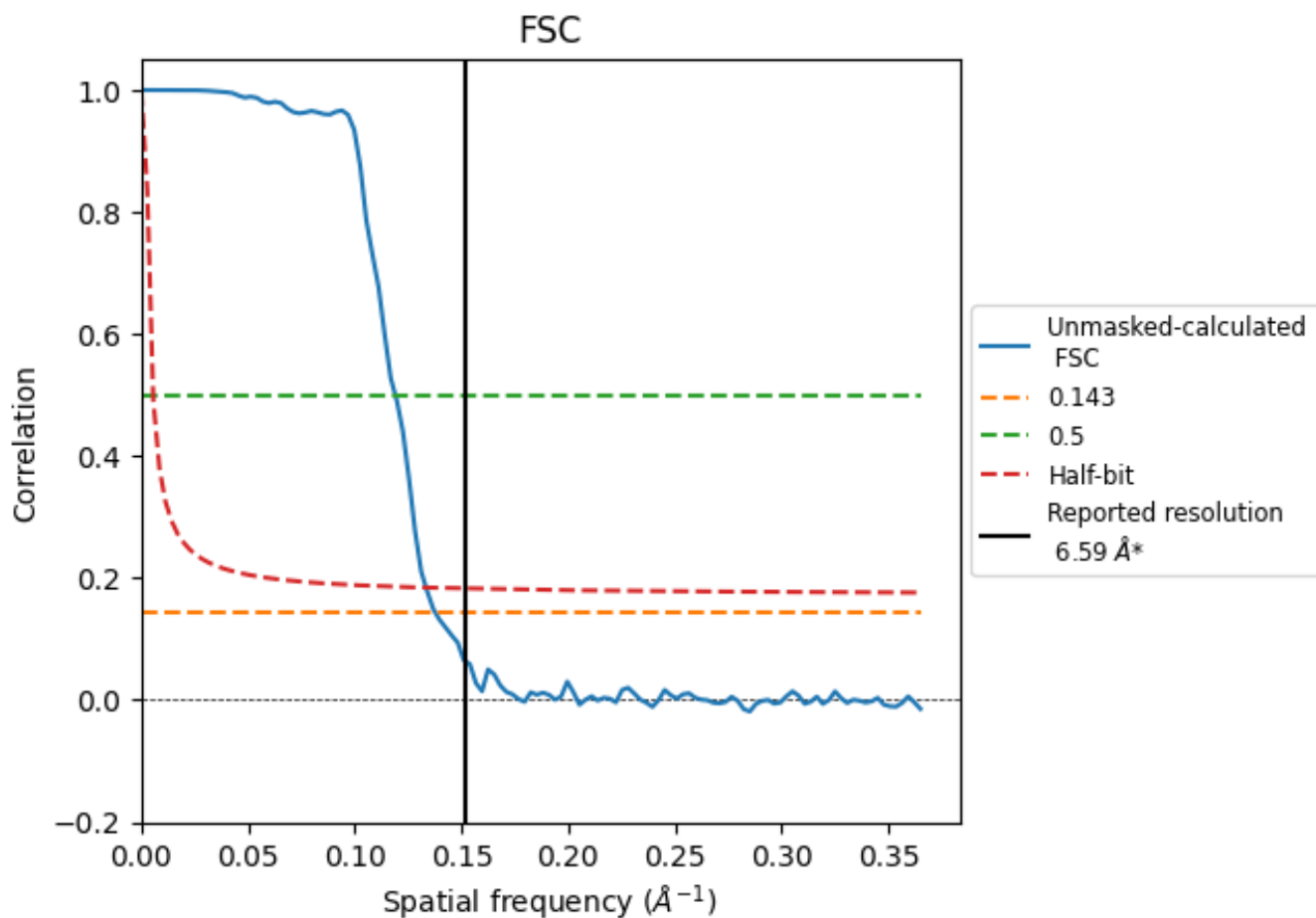


*Reported resolution corresponds to spatial frequency of 0.152 Å⁻¹

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 0.152 Å⁻¹

8.2 Resolution estimates [i](#)

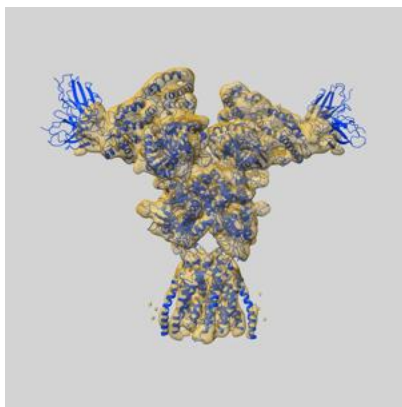
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.59	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.26	8.40	7.49

*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 7.26 differs from the reported value 6.59 by more than 10 %

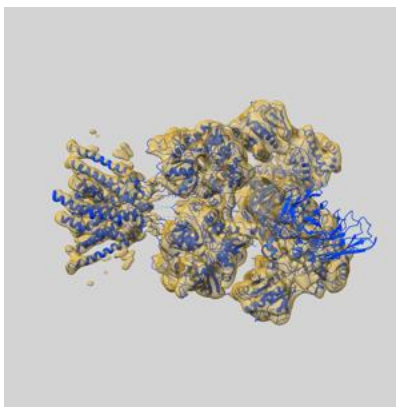
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25845 and PDB model 7TEE. Per-residue inclusion information can be found in section 3 on page 9.

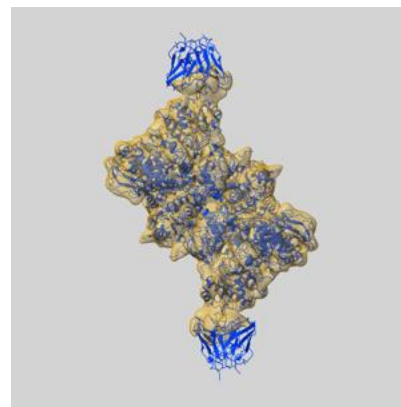
9.1 Map-model overlay [i](#)



X



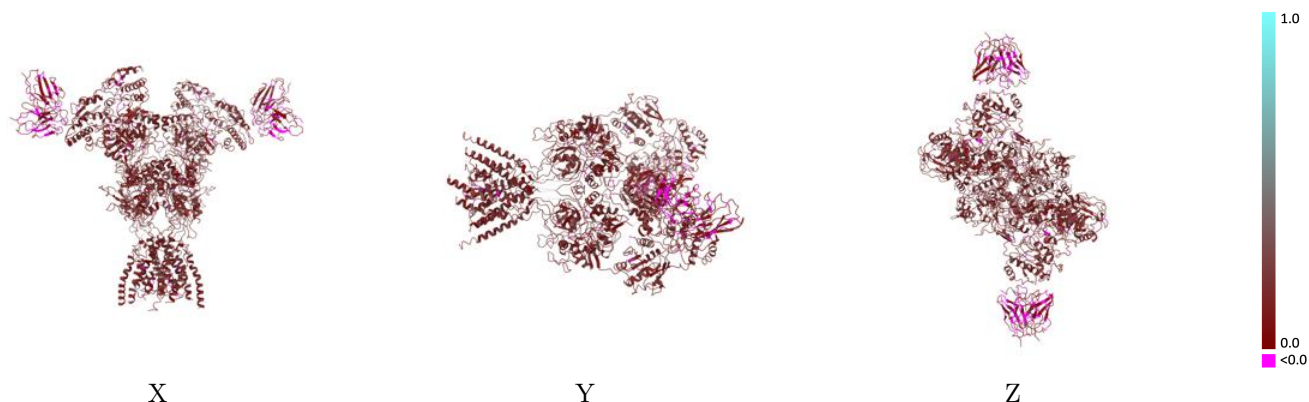
Y



Z

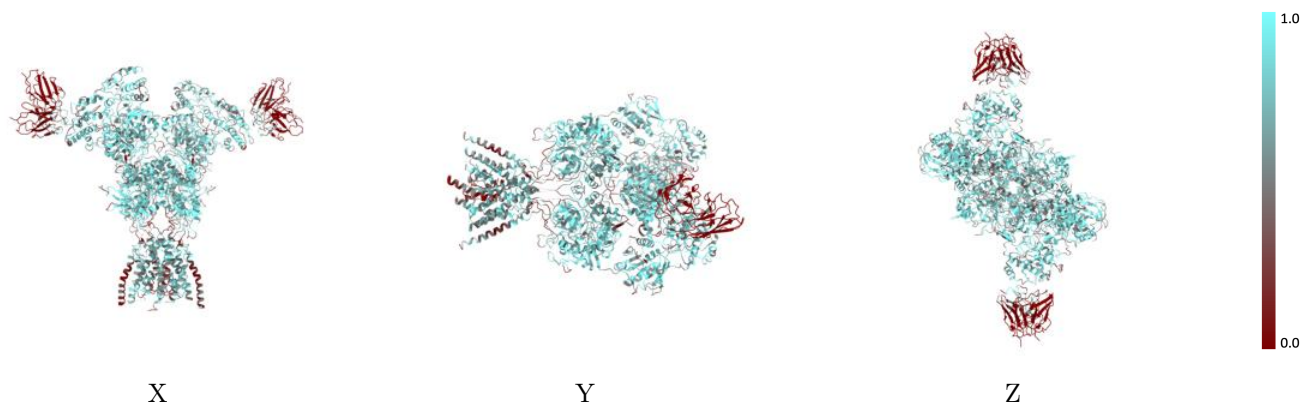
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



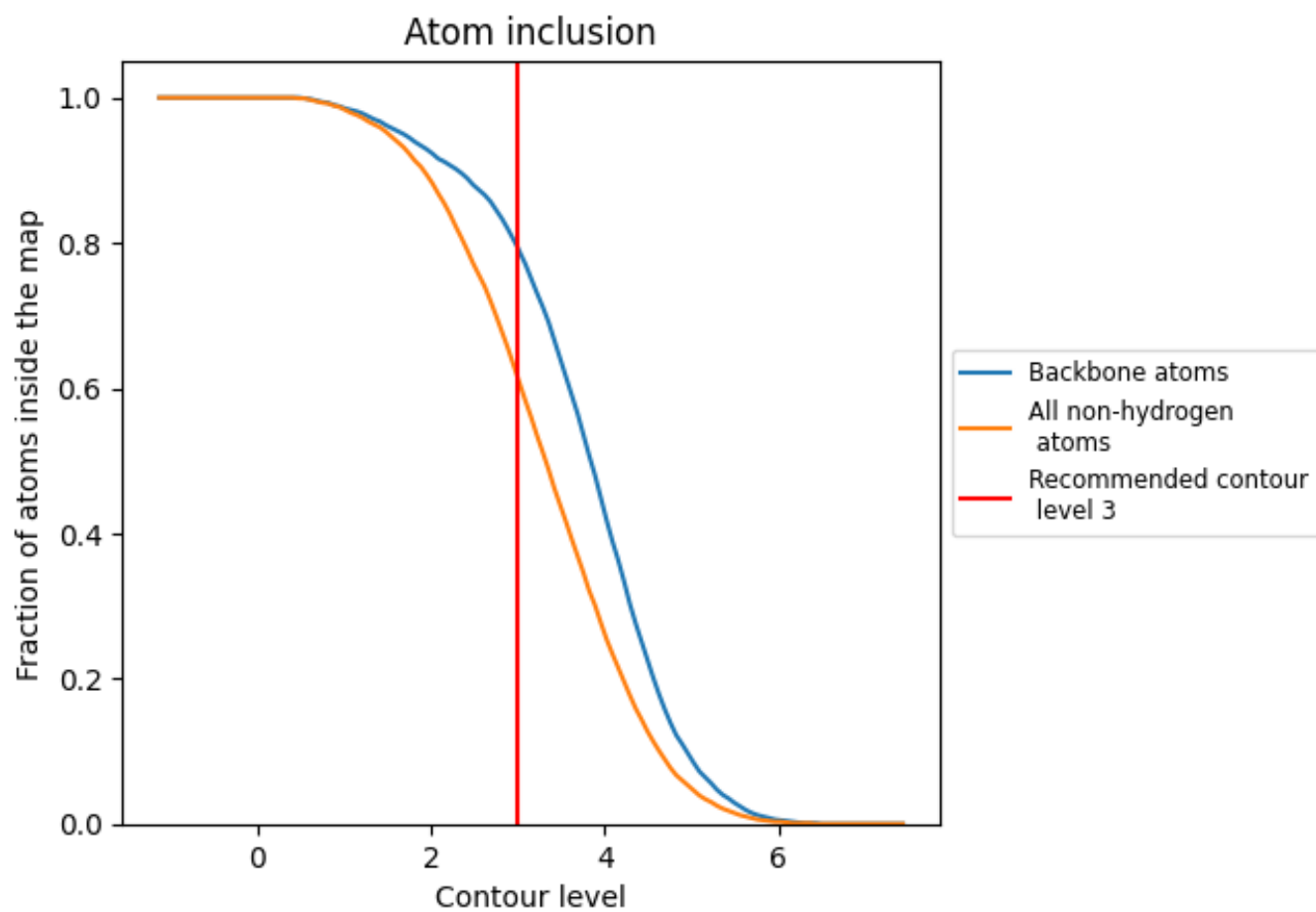
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 61% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6130	 0.1570
A	 0.6820	 0.1740
B	 0.6740	 0.1680
C	 0.6840	 0.1740
D	 0.6750	 0.1700
H	 0.1850	 0.0260
L	 0.0910	 0.0730
M	 0.1840	 0.0280
N	 0.0940	 0.0950

