



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 09:57 AM UTC

PDB ID : 7TES / pdb_00007tes
EMDB ID : EMD-25851
Title : Cryo-EM structure of GluN1b-2B NMDAR in complex with Fab5 in Non-active1 conformation
Authors : Tajima, N.; Furukawa, H.
Deposited on : 2022-01-05
Resolution : 4.70 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:

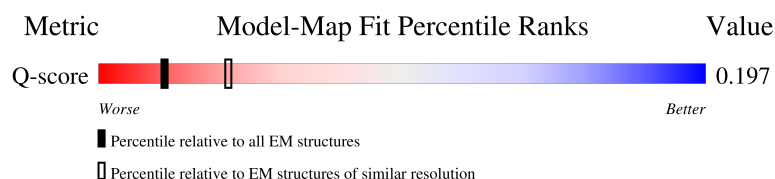
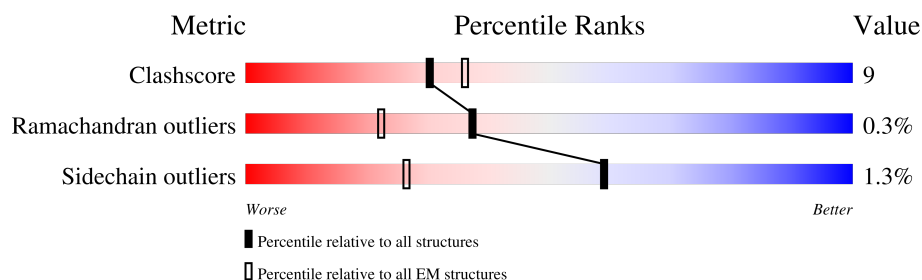
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.70 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	1989 (4.20 - 5.20)

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	
1	C	862	
2	B	883	
2	D	883	

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Mol	Chain	Length	Quality of chain
3	H	221	77% 72% 25% •
3	M	221	76% 71% 26% •
4	L	215	67% 68% 32%
4	N	215	66% 65% 34%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31306 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
1	A	789	Total	C	N	O	S	0	0
			6225	3958	1082	1148	37		
1	C	789	Total	C	N	O	S	0	0
			6225	3958	1082	1148	37		

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	774	Total	C	N	O	S	0	0
			6117	3939	984	1154	40		
2	D	774	Total	C	N	O	S	0	0
			6117	3939	984	1154	40		

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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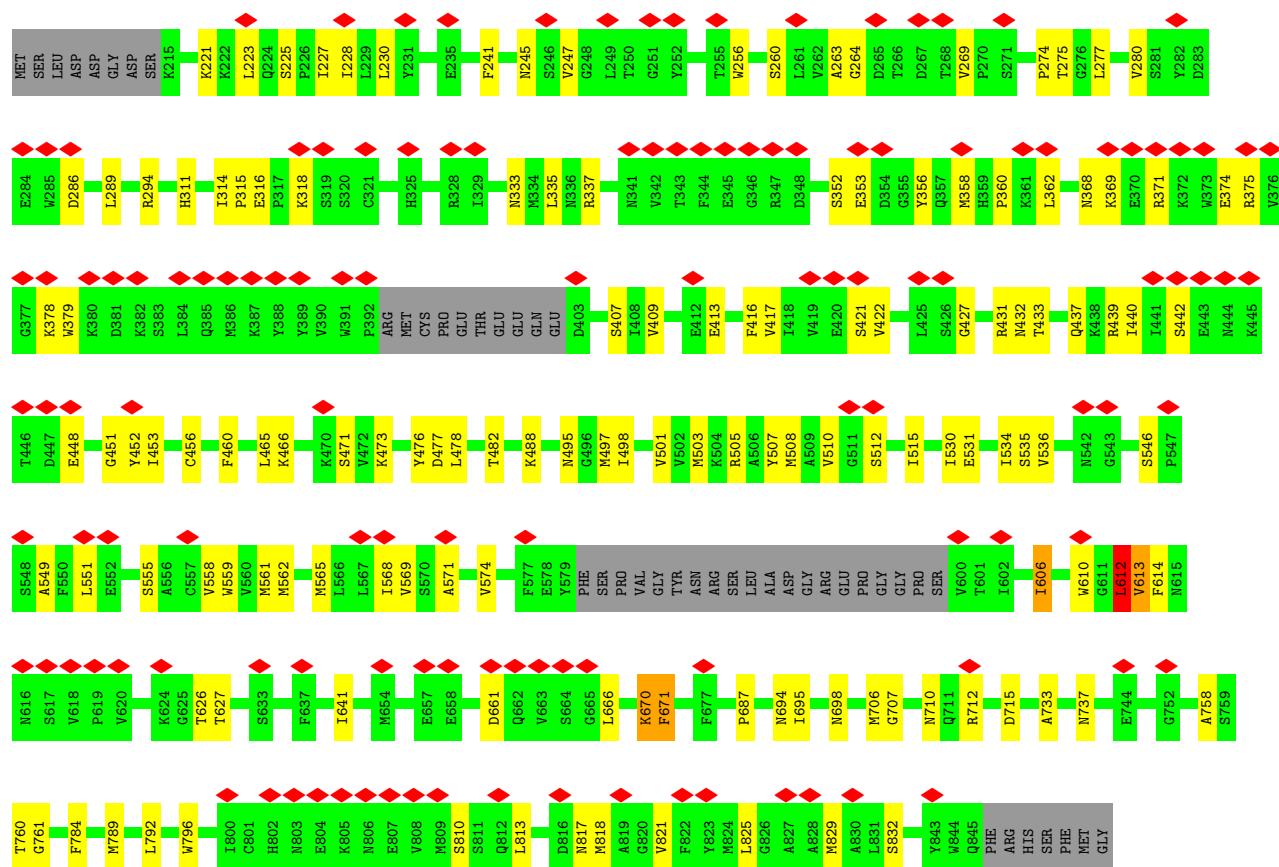
Chain	Residue	Modelled	Actual	Comment	Reference
D	17	PHE	-	expression tag	UNP Q00960
D	18	GLU	-	expression tag	UNP Q00960
D	19	LYS	-	expression tag	UNP Q00960
D	20	GLY	-	expression tag	UNP Q00960
D	21	ALA	-	expression tag	UNP Q00960
D	22	LEU	-	expression tag	UNP Q00960
D	23	VAL	-	expression tag	UNP Q00960
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 Fab5 heavy chain.

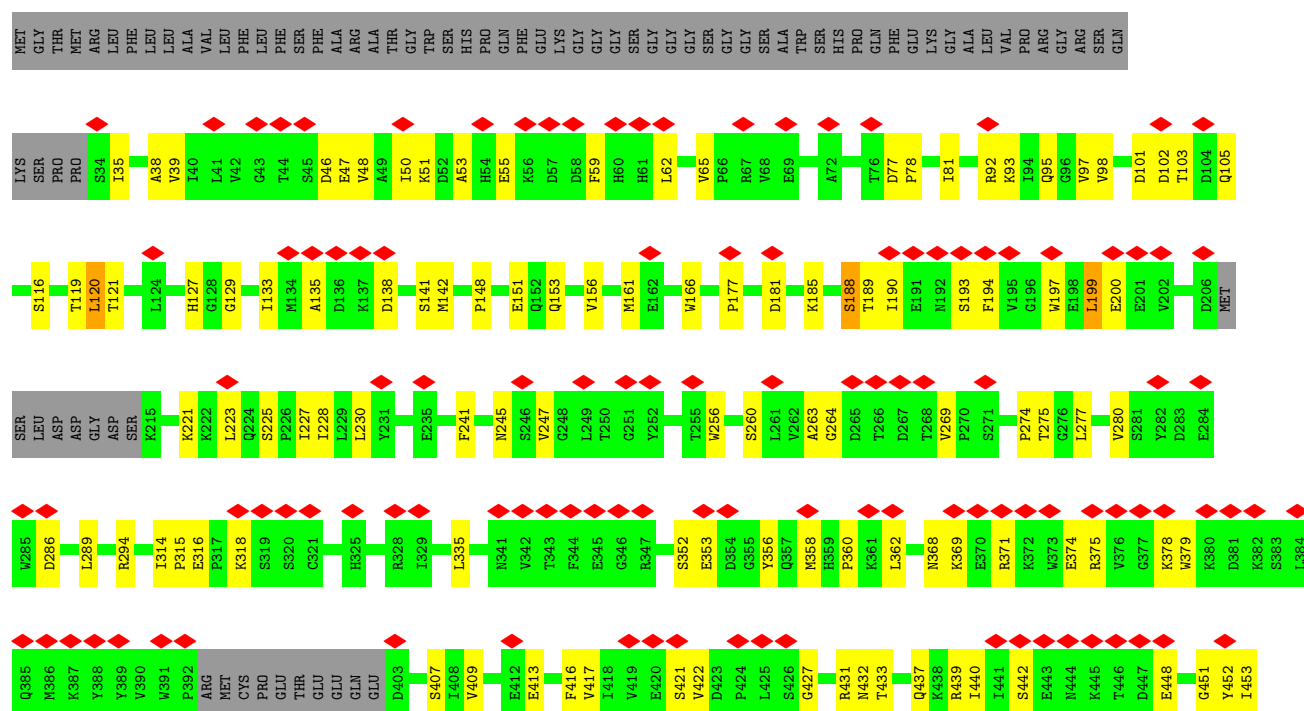
Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	215	Total	C	N	O	S	0	0
			1633	1030	269	325	9		
3	M	215	Total	C	N	O	S	0	0
			1633	1030	269	325	9		

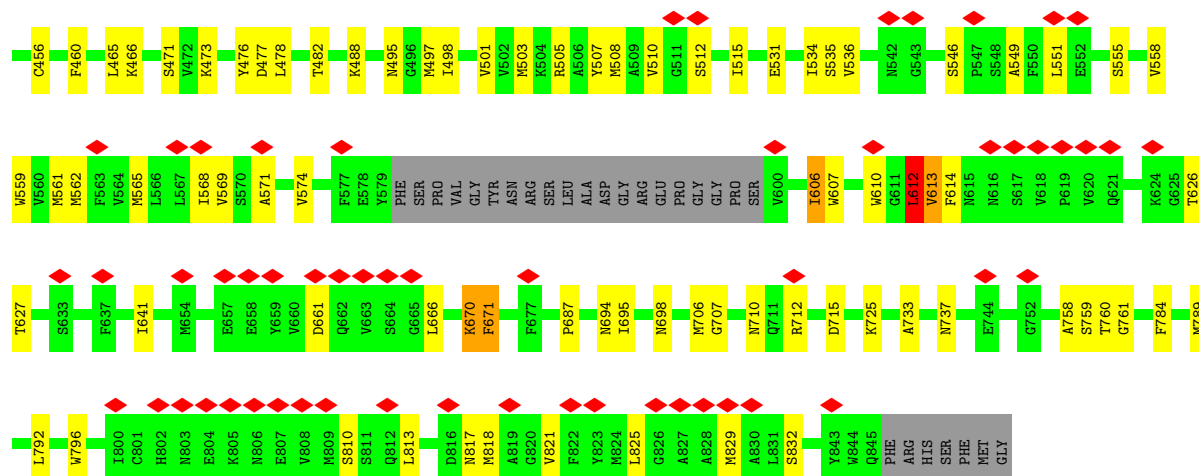
- Molecule 4 is a protein called Fab5 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	215	Total	C	N	O	S	0	0
			1678	1046	287	339	6		
4	N	215	Total	C	N	O	S	0	0
			1678	1046	287	339	6		

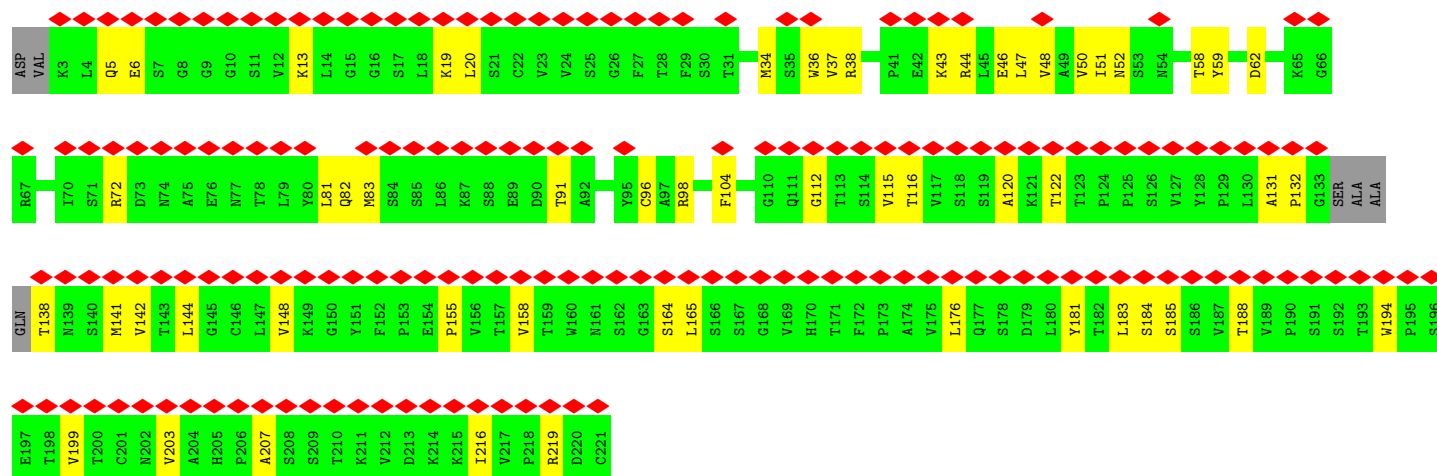
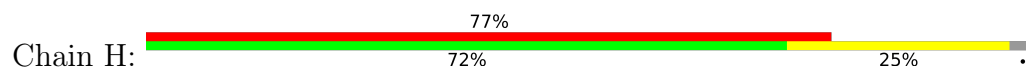


• Molecule 2: Glutamate receptor ionotropic, NMDA 2B

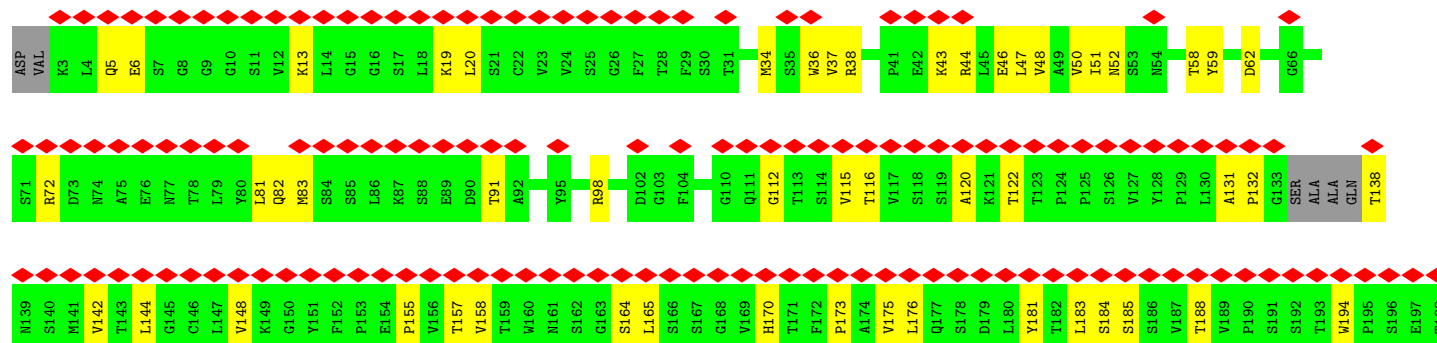
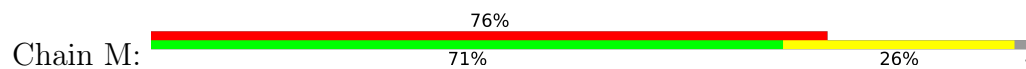


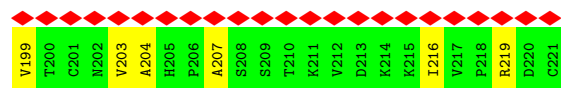


• Molecule 3: Fab5 heavy chain

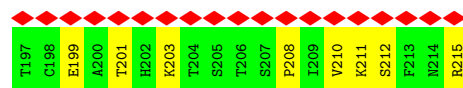
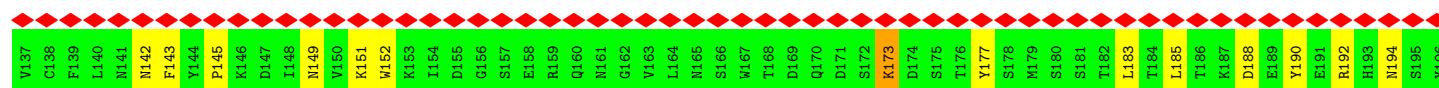
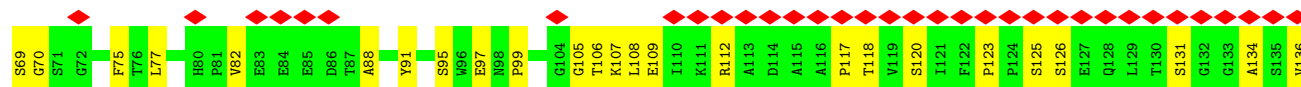
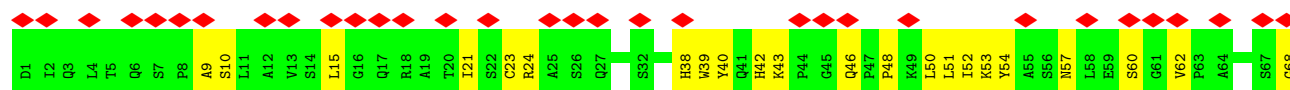


• Molecule 3: Fab5 heavy chain

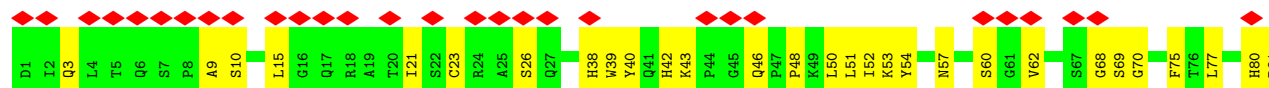




• Molecule 4: Fab5 light chain



• Molecule 4: Fab5 light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53467	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	7.087	Depositor
Minimum map value	-1.978	Depositor
Average map value	0.044	Depositor
Map value standard deviation	0.408	Depositor
Recommended contour level	3	Depositor
Map size ($\text{\AA}$)	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 ($\text{\AA}$)	1.37, 1.37, 1.37	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	0.20	0/6353	0.52	0/8590
1	C	0.20	0/6353	0.52	0/8590
2	B	0.21	0/6253	0.57	7/8472 (0.1%)
2	D	0.21	0/6253	0.57	7/8472 (0.1%)
3	H	0.22	0/1672	0.62	2/2280 (0.1%)
3	M	0.22	0/1672	0.62	2/2280 (0.1%)
4	L	0.20	0/1721	0.56	3/2340 (0.1%)
4	N	0.20	0/1721	0.56	3/2340 (0.1%)
All	All	0.20	0/31998	0.55	24/43364 (0.1%)

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	4
1	C	0	4
2	B	0	7
2	D	0	7
3	H	0	1
3	M	0	1
4	L	0	2
4	N	0	2
All	All	0	28

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	173	LYS	CB-CG-CD	8.82	131.59	111.30
4	N	173	LYS	CB-CG-CD	8.82	131.58	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	671	PHE	CA-C-N	6.26	136.69	126.86
2	D	671	PHE	C-N-CA	6.26	136.69	126.86
2	B	671	PHE	CA-C-N	6.25	136.67	126.86
2	B	671	PHE	C-N-CA	6.25	136.67	126.86
3	M	138	THR	CA-C-N	6.12	132.71	121.70
3	M	138	THR	C-N-CA	6.12	132.71	121.70
3	H	138	THR	CA-C-N	6.09	132.67	121.70
3	H	138	THR	C-N-CA	6.09	132.67	121.70
4	N	173	LYS	CG-CD-CE	6.00	125.10	111.30
4	L	173	LYS	CG-CD-CE	5.99	125.08	111.30
4	L	173	LYS	CA-CB-CG	5.77	125.64	114.10
4	N	173	LYS	CA-CB-CG	5.76	125.63	114.10
2	B	551	LEU	CA-C-N	5.49	135.19	121.80
2	B	551	LEU	C-N-CA	5.49	135.19	121.80
2	D	551	LEU	CA-C-N	5.47	135.15	121.80
2	D	551	LEU	C-N-CA	5.47	135.15	121.80
2	B	92	ARG	N-CA-CB	-5.33	108.09	114.17
2	D	92	ARG	N-CA-CB	-5.31	108.11	114.17
2	B	427	GLY	CA-C-N	5.16	128.56	120.82
2	B	427	GLY	C-N-CA	5.16	128.56	120.82
2	D	427	GLY	CA-C-N	5.14	128.54	120.82
2	D	427	GLY	C-N-CA	5.14	128.54	120.82

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	281	ARG	Peptide
1	A	282	TYR	Peptide
1	A	577	GLN	Peptide
1	A	578	PRO	Peptide
2	B	120	LEU	Peptide
2	B	199	LEU	Peptide
2	B	264	GLY	Peptide
2	B	452	TYR	Peptide
2	B	471	SER	Peptide
2	B	612	LEU	Peptide
2	B	670	LYS	Peptide
1	C	281	ARG	Peptide
1	C	282	TYR	Peptide
1	C	577	GLN	Peptide
1	C	578	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	D	120	LEU	Peptide
2	D	199	LEU	Peptide
2	D	264	GLY	Peptide
2	D	452	TYR	Peptide
2	D	471	SER	Peptide
2	D	612	LEU	Peptide
2	D	670	LYS	Peptide
3	H	194	TRP	Peptide
4	L	54	TYR	Peptide
4	L	60	SER	Peptide
3	M	194	TRP	Peptide
4	N	54	TYR	Peptide
4	N	60	SER	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6225	0	6225	107	0
1	C	6225	0	6225	111	0
2	B	6117	0	6051	110	0
2	D	6117	0	6051	111	0
3	H	1633	0	1595	32	0
3	M	1633	0	1595	33	0
4	L	1678	0	1600	43	0
4	N	1678	0	1600	46	0
All	All	31306	0	30942	563	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 9.

All (563) 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:555:SER:HB3	1:C:831:CYS:H	1.52	0.74
2:B:531:GLU:H	1:C:776:ARG:HH22	1.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:534:ILE:H	2:D:758:ALA:HB3	1.59	0.68
2:B:534:ILE:H	2:B:758:ALA:HB3	1.59	0.66
3:H:6:GLU:HB2	3:H:112:GLY:HA2	1.80	0.64
1:C:459:GLY:HA2	1:C:499:LEU:HB2	1.81	0.63
3:H:37:VAL:HA	3:H:47:LEU:HA	1.81	0.63
3:M:6:GLU:HB2	3:M:112:GLY:HA2	1.80	0.63
2:D:47:GLU:HA	2:D:50:ILE:HD12	1.81	0.63
3:M:37:VAL:HA	3:M:47:LEU:HA	1.81	0.63
1:A:459:GLY:HA2	1:A:499:LEU:HB2	1.81	0.62
1:C:256:ALA:HB1	1:C:261:MET:HB2	1.82	0.62
2:B:47:GLU:HA	2:B:50:ILE:HD12	1.81	0.62
1:A:256:ALA:HB1	1:A:261:MET:HB2	1.82	0.61
3:M:47:LEU:HD21	4:N:100:TYR:HA	1.83	0.61
2:D:558:VAL:HA	2:D:561:MET:HB2	1.82	0.60
2:B:558:VAL:HA	2:B:561:MET:HB2	1.82	0.60
1:A:362:ASN:HB2	1:A:366:ASP:HB3	1.84	0.60
1:C:372:TYR:H	1:C:388:TYR:HB3	1.67	0.60
4:L:199:GLU:HG2	4:L:210:VAL:HG22	1.83	0.60
4:N:199:GLU:HG2	4:N:210:VAL:HG22	1.83	0.60
1:C:362:ASN:HB2	1:C:366:ASP:HB3	1.84	0.60
4:L:151:LYS:HB2	4:L:199:GLU:HB2	1.83	0.59
1:A:292:LEU:HD12	1:A:372:TYR:HB3	1.84	0.59
1:C:292:LEU:HD12	1:C:372:TYR:HB3	1.84	0.59
2:D:437:GLN:HB2	2:D:451:GLY:HA2	1.85	0.59
3:H:34:MET:HE3	3:H:72:ARG:HH12	1.67	0.59
3:M:34:MET:HE3	3:M:72:ARG:HH12	1.67	0.59
4:N:151:LYS:HB2	4:N:199:GLU:HB2	1.83	0.59
2:D:440:ILE:HG12	2:D:453:ILE:HG12	1.85	0.58
4:N:15:LEU:O	4:N:112:ARG:NH2	2.36	0.58
1:A:372:TYR:H	1:A:388:TYR:HB3	1.67	0.58
1:A:460:PRO:HG2	1:A:462:ASP:HB2	1.85	0.58
2:B:437:GLN:HB2	2:B:451:GLY:HA2	1.85	0.58
2:D:507:TYR:HB3	2:D:508:MET:HE2	1.85	0.58
2:D:256:TRP:HB2	2:D:277:LEU:HD22	1.86	0.58
2:B:256:TRP:HB2	2:B:277:LEU:HD22	1.86	0.58
1:C:460:PRO:HG2	1:C:462:ASP:HB2	1.86	0.58
4:L:40:TYR:HA	4:L:51:LEU:HB2	1.86	0.58
1:A:645:PRO:O	1:A:651:ARG:NH2	2.36	0.58
1:C:402:TRP:NE1	1:C:408:GLU:O	2.37	0.58
2:B:440:ILE:HG12	2:B:453:ILE:HG12	1.84	0.58
4:L:15:LEU:O	4:L:112:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:40:TYR:HA	4:N:51:LEU:HB2	1.86	0.58
3:M:52:ASN:O	3:M:72:ARG:NH1	2.37	0.57
2:B:507:TYR:HB3	2:B:508:MET:HE2	1.85	0.57
1:A:402:TRP:NE1	1:A:408:GLU:O	2.37	0.57
1:A:776:ARG:HH22	2:D:531:GLU:H	1.52	0.57
2:B:568:ILE:HG13	2:B:569:VAL:HG13	1.86	0.57
1:C:645:PRO:O	1:C:651:ARG:NH2	2.36	0.57
2:D:241:PHE:O	2:D:245:ASN:ND2	2.38	0.57
4:L:117:PRO:HB3	4:L:142:ASN:H	1.68	0.57
1:A:660:PHE:HE2	2:B:825:LEU:HB2	1.70	0.57
2:B:275:THR:HG22	2:B:371:ARG:HH22	1.70	0.57
4:N:117:PRO:HB3	4:N:142:ASN:H	1.68	0.57
2:B:48:VAL:HA	2:B:51:LYS:HD2	1.87	0.57
2:B:241:PHE:O	2:B:245:ASN:ND2	2.38	0.57
2:D:274:PRO:HG2	2:D:277:LEU:HD21	1.87	0.57
1:A:811:LYS:HG3	1:A:815:ARG:HH11	1.70	0.57
1:A:451:PRO:O	1:A:453:LYS:NZ	2.38	0.56
1:A:791:GLN:HE21	1:A:792:GLN:HG2	1.70	0.56
2:B:337:ARG:NE	4:L:97:GLU:OE2	2.38	0.56
2:B:559:TRP:HA	2:B:562:MET:HE3	1.87	0.56
1:C:158:TYR:HB3	1:C:411:ARG:HH21	1.70	0.56
3:M:131:ALA:HB2	3:M:216:ILE:HG22	1.87	0.56
1:A:166:LEU:HB3	1:A:242:LEU:HD13	1.87	0.56
2:D:48:VAL:HA	2:D:51:LYS:HD2	1.87	0.56
2:D:568:ILE:HG13	2:D:569:VAL:HG13	1.86	0.56
3:H:51:ILE:HG13	3:H:58:THR:HG22	1.86	0.56
4:L:68:GLY:HA2	4:L:77:LEU:HA	1.87	0.56
3:M:51:ILE:HG13	3:M:58:THR:HG22	1.86	0.56
1:A:158:TYR:HB3	1:A:411:ARG:HH21	1.70	0.56
3:H:141:MET:HE1	4:L:211:LYS:HD2	1.88	0.56
2:B:274:PRO:HG2	2:B:277:LEU:HD21	1.87	0.56
1:C:791:GLN:HE21	1:C:792:GLN:HG2	1.69	0.56
1:C:811:LYS:HG3	1:C:815:ARG:HH11	1.70	0.56
2:D:95:GLN:NE2	2:D:315:PRO:O	2.39	0.56
3:H:52:ASN:O	3:H:72:ARG:NH1	2.37	0.56
1:C:169:ASP:HB2	1:C:219:ASP:HB3	1.88	0.56
4:N:70:GLY:HA3	4:N:75:PHE:HA	1.88	0.56
1:C:422:VAL:HG12	1:C:498:HIS:HB3	1.88	0.56
2:D:275:THR:HG22	2:D:371:ARG:HH22	1.70	0.56
2:D:352:SER:OG	2:D:353:GLU:N	2.39	0.56
2:B:95:GLN:NE2	2:B:315:PRO:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:131:ALA:HB2	3:H:216:ILE:HG22	1.87	0.55
4:L:42:HIS:HB3	4:L:48:PRO:HA	1.87	0.55
4:L:70:GLY:HA3	4:L:75:PHE:HA	1.88	0.55
1:C:166:LEU:HB3	1:C:242:LEU:HD13	1.87	0.55
2:D:559:TRP:HA	2:D:562:MET:HE3	1.87	0.55
4:N:42:HIS:HB3	4:N:48:PRO:HA	1.87	0.55
1:A:740:GLN:OE1	1:A:743:ARG:NH1	2.40	0.55
4:N:68:GLY:HA2	4:N:77:LEU:HA	1.87	0.55
1:A:489:ARG:O	1:A:492:GLN:NE2	2.40	0.55
1:A:422:VAL:HG12	1:A:498:HIS:HB3	1.88	0.55
1:C:489:ARG:O	1:C:492:GLN:NE2	2.40	0.55
1:C:740:GLN:OE1	1:C:743:ARG:NH1	2.40	0.55
1:A:169:ASP:HB2	1:A:219:ASP:HB3	1.88	0.54
1:A:590:SER:HA	1:A:593:VAL:HG22	1.90	0.54
1:C:451:PRO:O	1:C:453:LYS:NZ	2.38	0.54
2:B:286:ASP:OD1	2:B:286:ASP:N	2.40	0.54
2:B:142:MET:HE2	2:B:335:LEU:HD23	1.90	0.54
2:B:333:ASN:HD22	3:H:104:PHE:H	1.55	0.54
2:B:352:SER:OG	2:B:353:GLU:N	2.39	0.54
1:C:590:SER:HA	1:C:593:VAL:HG22	1.89	0.54
2:B:181:ASP:N	2:B:181:ASP:OD1	2.41	0.54
1:C:644:ALA:HB1	1:C:651:ARG:HE	1.73	0.54
2:D:733:ALA:O	2:D:737:ASN:ND2	2.41	0.54
4:N:40:TYR:HB3	4:N:50:LEU:HD12	1.90	0.54
3:M:175:VAL:HG22	4:N:164:LEU:HD21	1.90	0.53
2:D:142:MET:HE2	2:D:335:LEU:HD23	1.90	0.53
2:D:707:GLY:O	2:D:710:ASN:ND2	2.40	0.53
1:A:246:GLU:HG3	1:A:278:ASN:HB2	1.91	0.53
2:B:133:ILE:O	2:B:356:TYR:OH	2.26	0.53
2:B:733:ALA:O	2:B:737:ASN:ND2	2.41	0.53
2:D:465:LEU:O	2:D:476:TYR:OH	2.27	0.53
1:C:807:GLU:O	1:C:815:ARG:NH1	2.41	0.53
4:N:199:GLU:HB3	4:N:208:PRO:HB2	1.91	0.53
1:A:807:GLU:O	1:A:815:ARG:NH1	2.41	0.53
2:B:102:ASP:OD1	2:B:127:HIS:NE2	2.42	0.53
2:B:465:LEU:O	2:B:476:TYR:OH	2.27	0.53
2:D:535:SER:OG	2:D:536:VAL:N	2.41	0.53
2:B:535:SER:OG	2:B:536:VAL:N	2.41	0.53
4:L:40:TYR:HB3	4:L:50:LEU:HD12	1.90	0.53
1:A:644:ALA:HB1	1:A:651:ARG:HE	1.73	0.53
2:B:437:GLN:NE2	2:B:478:LEU:O	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:515:ILE:HD13	1:C:552:LYS:HE2	1.90	0.53
1:C:416:SER:OG	1:C:417:THR:N	2.42	0.53
2:D:133:ILE:O	2:D:356:TYR:OH	2.26	0.53
4:L:199:GLU:HB3	4:L:208:PRO:HB2	1.91	0.53
1:A:777:SER:OG	1:A:778:GLY:N	2.42	0.52
2:B:707:GLY:O	2:B:710:ASN:ND2	2.40	0.52
3:H:38:ARG:HB2	3:H:46:GLU:HB2	1.92	0.52
1:C:225:VAL:HG21	1:C:252:VAL:HG12	1.90	0.52
1:C:386:GLY:HA3	1:C:395:PRO:HA	1.92	0.52
1:C:777:SER:OG	1:C:778:GLY:N	2.42	0.52
3:M:132:PRO:HG2	3:M:142:VAL:HA	1.92	0.52
1:A:416:SER:OG	1:A:417:THR:N	2.42	0.52
2:D:102:ASP:OD1	2:D:127:HIS:NE2	2.42	0.52
2:D:269:VAL:HB	2:D:371:ARG:HB3	1.92	0.52
2:B:269:VAL:HB	2:B:371:ARG:HB3	1.92	0.52
1:C:389:ASN:HD22	1:C:394:ILE:HD12	1.75	0.52
1:A:225:VAL:HG21	1:A:252:VAL:HG12	1.90	0.52
1:A:831:CYS:H	2:D:555:SER:HB3	1.75	0.52
1:C:246:GLU:HG3	1:C:278:ASN:HB2	1.91	0.52
1:C:811:LYS:HA	1:C:815:ARG:HB2	1.91	0.52
3:M:219:ARG:HH21	4:N:122:PHE:HE1	1.58	0.52
2:D:813:LEU:HD21	2:D:817:ASN:HD21	1.75	0.52
3:H:132:PRO:HG2	3:H:142:VAL:HA	1.92	0.52
4:N:15:LEU:HA	4:N:82:VAL:HB	1.92	0.52
4:N:38:HIS:HB2	4:N:50:LEU:HD11	1.92	0.52
4:L:23:CYS:HB3	4:L:75:PHE:HB2	1.92	0.51
1:C:331:GLY:H	2:D:77:ASP:HB2	1.74	0.51
3:M:38:ARG:HB2	3:M:46:GLU:HB2	1.92	0.51
2:D:181:ASP:N	2:D:181:ASP:OD1	2.41	0.51
1:A:566:GLU:OE2	1:A:569:ARG:NH1	2.44	0.51
1:A:811:LYS:HA	1:A:815:ARG:HB2	1.91	0.51
2:B:565:MET:HA	2:B:568:ILE:HG12	1.92	0.51
4:L:15:LEU:HA	4:L:82:VAL:HB	1.92	0.51
2:B:55:GLU:OE1	2:B:294:ARG:NH2	2.44	0.51
1:A:263:GLY:H	1:A:266:TYR:HD2	1.59	0.51
1:A:386:GLY:HA3	1:A:395:PRO:HA	1.92	0.51
2:B:813:LEU:HD21	2:B:817:ASN:HD21	1.75	0.51
2:D:55:GLU:OE1	2:D:294:ARG:NH2	2.44	0.51
2:D:59:PHE:HB3	2:D:62:LEU:HG	1.93	0.51
2:B:151:GLU:HG2	2:B:185:LYS:HD2	1.93	0.51
1:C:263:GLY:H	1:C:266:TYR:HD2	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:38:HIS:HB2	4:L:50:LEU:HD11	1.92	0.51
1:A:443:GLU:OE2	1:A:454:LYS:NZ	2.44	0.51
2:B:368:ASN:OD1	2:B:369:LYS:NZ	2.44	0.51
2:B:626:THR:OG1	2:B:627:THR:N	2.44	0.51
4:N:23:CYS:HB3	4:N:75:PHE:HB2	1.92	0.51
1:A:389:ASN:HD22	1:A:394:ILE:HD12	1.75	0.50
2:B:546:SER:OG	2:B:549:ALA:O	2.28	0.50
1:A:31:ALA:HA	1:A:91:LEU:H	1.76	0.50
1:A:817:GLN:NE2	1:A:819:CYS:O	2.44	0.50
2:B:661:ASP:OD1	2:B:661:ASP:N	2.44	0.50
2:D:286:ASP:N	2:D:286:ASP:OD1	2.40	0.50
1:C:31:ALA:HA	1:C:91:LEU:H	1.76	0.50
1:C:443:GLU:OE2	1:C:454:LYS:NZ	2.44	0.50
2:D:53:ALA:O	2:D:294:ARG:NH1	2.39	0.50
2:B:59:PHE:HB3	2:B:62:LEU:HG	1.93	0.50
2:D:116:SER:HB2	2:D:121:THR:HB	1.93	0.50
2:D:439:ARG:HB3	2:D:482:THR:HG21	1.94	0.50
2:D:565:MET:HA	2:D:568:ILE:HG12	1.92	0.50
1:A:35:THR:HG21	1:A:37:LYS:HE3	1.93	0.50
1:C:566:GLU:OE2	1:C:569:ARG:NH1	2.44	0.50
1:C:817:GLN:NE2	1:C:819:CYS:O	2.44	0.50
3:M:19:LYS:HE2	3:M:82:GLN:HE21	1.77	0.50
2:D:148:PRO:O	2:D:153:GLN:NE2	2.45	0.50
1:A:510:ARG:HA	1:A:517:LYS:HA	1.94	0.50
2:B:116:SER:HB2	2:B:121:THR:HB	1.94	0.50
1:C:510:ARG:HA	1:C:517:LYS:HA	1.94	0.50
2:D:432:ASN:O	2:D:466:LYS:NZ	2.38	0.50
2:D:46:ASP:HB3	2:D:289:LEU:HD22	1.94	0.49
1:A:426:GLN:NE2	1:A:427:GLU:O	2.44	0.49
1:C:35:THR:HG21	1:C:37:LYS:HE3	1.93	0.49
1:C:120:GLY:N	1:C:138:LEU:O	2.46	0.49
1:C:421:ILE:HD13	1:C:484:LEU:HD21	1.94	0.49
2:D:546:SER:OG	2:D:549:ALA:O	2.29	0.49
2:B:148:PRO:O	2:B:153:GLN:NE2	2.45	0.49
2:D:626:THR:OG1	2:D:627:THR:N	2.44	0.49
1:A:120:GLY:N	1:A:138:LEU:O	2.46	0.49
2:B:439:ARG:HB3	2:B:482:THR:HG21	1.94	0.49
1:C:425:HIS:CD2	1:C:432:VAL:H	2.31	0.49
4:N:53:LYS:HB3	4:N:57:ASN:HB3	1.95	0.49
2:B:535:SER:HB3	2:B:733:ALA:HB2	1.94	0.49
2:D:535:SER:HB3	2:D:733:ALA:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:69:SER:OG	4:N:70:GLY:N	2.46	0.49
2:B:53:ALA:O	2:B:294:ARG:NH1	2.39	0.49
2:B:200:GLU:HB3	2:B:223:LEU:HD22	1.95	0.49
4:L:53:LYS:HB3	4:L:57:ASN:HB3	1.95	0.49
4:N:188:ASP:O	4:N:192:ARG:NE	2.44	0.49
2:D:151:GLU:HG2	2:D:185:LYS:HD2	1.93	0.49
1:A:801:HIS:CE1	2:D:759:SER:H	2.31	0.49
2:B:375:ARG:HH21	2:B:378:LYS:HB2	1.78	0.49
2:D:225:SER:HB3	2:D:228:ILE:HG12	1.95	0.49
4:N:134:ALA:HB3	4:N:185:LEU:HB2	1.95	0.48
1:A:421:ILE:HD13	1:A:484:LEU:HD21	1.94	0.48
2:B:225:SER:HB3	2:B:228:ILE:HG12	1.95	0.48
2:D:661:ASP:OD1	2:D:661:ASP:N	2.44	0.48
1:A:683:GLU:OE1	1:A:822:ARG:NH2	2.46	0.48
2:B:138:ASP:HB3	2:B:141:SER:HB2	1.95	0.48
1:C:32:VAL:HB	1:C:92:VAL:HA	1.95	0.48
2:B:694:ASN:O	2:B:698:ASN:ND2	2.47	0.48
1:C:43:ARG:NH1	1:C:62:ALA:O	2.45	0.48
1:C:655:MET:HG2	2:D:610:TRP:CD2	2.49	0.48
2:B:46:ASP:HB3	2:B:289:LEU:HD22	1.94	0.48
1:C:327:ARG:HH11	1:C:330:VAL:HG21	1.78	0.48
3:H:19:LYS:HE2	3:H:82:GLN:HE21	1.77	0.48
3:H:43:LYS:O	3:H:44:ARG:NH1	2.45	0.48
1:A:116:ILE:O	1:A:136:SER:OG	2.31	0.48
1:A:768:VAL:HG11	1:A:822:ARG:HD2	1.96	0.48
2:D:375:ARG:HH21	2:D:378:LYS:HB2	1.78	0.48
3:M:13:LYS:NZ	3:M:120:ALA:O	2.46	0.48
1:A:32:VAL:HB	1:A:92:VAL:HA	1.96	0.48
2:B:432:ASN:O	2:B:466:LYS:NZ	2.38	0.48
2:D:437:GLN:NE2	2:D:478:LEU:O	2.38	0.48
1:C:431:TYR:N	1:C:477:TYR:O	2.47	0.48
2:D:200:GLU:HB3	2:D:223:LEU:HD22	1.95	0.48
2:D:35:ILE:N	2:D:65:VAL:O	2.44	0.48
3:H:13:LYS:NZ	3:H:120:ALA:O	2.46	0.48
1:A:327:ARG:HH11	1:A:330:VAL:HG21	1.78	0.47
1:A:431:TYR:N	1:A:477:TYR:O	2.47	0.47
1:A:698:ASP:OD1	1:A:698:ASP:N	2.46	0.47
1:C:426:GLN:NE2	1:C:427:GLU:O	2.44	0.47
2:D:221:LYS:HG3	2:D:247:VAL:HB	1.96	0.47
3:M:50:VAL:HB	3:M:59:TYR:HB3	1.95	0.47
1:A:79:CYS:HA	1:A:82:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ILE:O	1:C:136:SER:OG	2.31	0.47
2:D:694:ASN:O	2:D:698:ASN:ND2	2.47	0.47
2:D:818:MET:HA	2:D:821:VAL:HB	1.96	0.47
2:B:715:ASP:N	2:B:715:ASP:OD1	2.47	0.47
1:A:425:HIS:CD2	1:A:432:VAL:H	2.31	0.47
2:B:35:ILE:N	2:B:65:VAL:O	2.44	0.47
2:B:194:PHE:O	2:B:431:ARG:NH1	2.47	0.47
2:B:221:LYS:HG3	2:B:247:VAL:HB	1.96	0.47
1:C:768:VAL:HG11	1:C:822:ARG:HD2	1.96	0.47
2:D:138:ASP:HB3	2:D:141:SER:HB2	1.95	0.47
2:D:488:LYS:N	2:D:495:ASN:OD1	2.46	0.47
1:C:698:ASP:OD1	1:C:698:ASP:N	2.46	0.47
2:D:148:PRO:HG2	2:D:153:GLN:HE21	1.80	0.47
2:D:194:PHE:O	2:D:431:ARG:NH1	2.47	0.47
1:A:423:THR:HA	1:A:522:MET:HE2	1.95	0.47
4:L:188:ASP:O	4:L:192:ARG:NE	2.44	0.47
1:C:423:THR:HA	1:C:522:MET:HE2	1.95	0.47
3:H:50:VAL:HB	3:H:59:TYR:HB3	1.95	0.47
1:A:126:SER:O	1:A:129:SER:OG	2.33	0.47
1:A:331:GLY:H	2:B:77:ASP:HB2	1.80	0.46
1:A:835:ALA:HB1	1:A:838:PHE:HB3	1.97	0.46
1:C:690:ASP:OD2	1:C:692:ARG:NH1	2.44	0.46
4:L:134:ALA:HB3	4:L:185:LEU:HB2	1.95	0.46
3:M:170:HIS:CE1	4:N:178:SER:HB3	2.51	0.46
2:B:818:MET:HA	2:B:821:VAL:HB	1.96	0.46
2:B:190:ILE:HD12	2:B:197:TRP:H	1.80	0.46
1:C:79:CYS:HA	1:C:82:LEU:HB2	1.96	0.46
2:D:360:PRO:HG2	2:D:379:TRP:HZ3	1.81	0.46
2:D:725:LYS:HA	2:D:725:LYS:HD3	1.84	0.46
1:A:187:ARG:HH12	1:A:210:PRO:HD2	1.80	0.46
1:A:842:ALA:HA	1:A:845:ILE:HD12	1.97	0.46
1:C:731:ASN:OD1	1:C:731:ASN:N	2.49	0.46
2:D:368:ASN:OD1	2:D:369:LYS:NZ	2.44	0.46
1:A:161:ASN:N	1:A:161:ASN:OD1	2.49	0.46
2:B:148:PRO:HG2	2:B:153:GLN:HE21	1.80	0.46
1:C:835:ALA:HB1	1:C:838:PHE:HB3	1.97	0.46
2:B:260:SER:HA	2:B:263:ALA:HB3	1.98	0.46
1:C:126:SER:O	1:C:129:SER:OG	2.33	0.46
1:C:486:LYS:O	1:C:490:THR:OG1	2.30	0.46
2:D:314:ILE:HD12	2:D:315:PRO:HD2	1.98	0.46
2:D:715:ASP:N	2:D:715:ASP:OD1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:155:PRO:HD2	3:M:207:ALA:HB2	1.98	0.46
2:B:314:ILE:HD12	2:B:315:PRO:HD2	1.98	0.46
1:C:187:ARG:HH12	1:C:210:PRO:HD2	1.80	0.46
2:D:421:SER:OG	2:D:422:VAL:N	2.49	0.46
3:H:158:VAL:HG22	3:H:203:VAL:HG13	1.97	0.46
3:M:38:ARG:N	3:M:46:GLU:O	2.48	0.46
1:A:470:HIS:HB3	1:A:472:VAL:HG23	1.97	0.46
1:C:500:VAL:HG12	1:C:502:ASP:H	1.81	0.46
3:M:148:VAL:HG13	3:M:183:LEU:HB2	1.98	0.46
1:A:124:ARG:NH1	1:A:142:PRO:O	2.46	0.46
2:B:360:PRO:HG2	2:B:379:TRP:HZ3	1.81	0.46
1:C:574:SER:HA	1:C:577:GLN:HB2	1.97	0.46
3:H:155:PRO:HD2	3:H:207:ALA:HB2	1.98	0.46
4:L:143:PHE:O	4:L:177:TYR:N	2.47	0.46
3:M:158:VAL:HG22	3:M:203:VAL:HG13	1.97	0.46
1:C:683:GLU:OE1	1:C:822:ARG:NH2	2.46	0.46
3:M:173:PRO:HD2	4:N:166:SER:HA	1.98	0.46
2:B:421:SER:OG	2:B:422:VAL:N	2.49	0.45
1:C:470:HIS:HB3	1:C:472:VAL:HG23	1.97	0.45
4:L:51:LEU:HG	4:L:62:VAL:HG21	1.98	0.45
4:N:149:ASN:ND2	4:N:201:THR:OG1	2.49	0.45
1:A:574:SER:HA	1:A:577:GLN:HB2	1.97	0.45
1:C:842:ALA:HA	1:C:845:ILE:HD12	1.97	0.45
3:H:34:MET:HA	3:H:98:ARG:HG2	1.97	0.45
1:A:510:ARG:NH1	2:B:188:SER:OG	2.49	0.45
2:B:119:THR:OG1	2:B:120:LEU:N	2.50	0.45
4:L:149:ASN:ND2	4:L:201:THR:OG1	2.49	0.45
3:M:157:THR:OG1	3:M:204:ALA:O	2.34	0.45
1:C:567:ILE:O	1:C:569:ARG:NH1	2.50	0.45
3:H:144:LEU:HD21	3:H:199:VAL:HG21	1.98	0.45
4:N:117:PRO:HD3	4:N:143:PHE:HB3	1.98	0.45
1:A:677:VAL:HA	1:A:680:ARG:HH21	1.82	0.45
1:A:731:ASN:OD1	1:A:731:ASN:N	2.49	0.45
1:C:579:PHE:HZ	1:C:668:TYR:HA	1.82	0.45
2:D:197:TRP:HB3	2:D:199:LEU:HD23	1.99	0.45
3:H:83:MET:HE1	3:H:115:VAL:HG11	1.99	0.45
3:M:62:ASP:OD1	3:M:62:ASP:N	2.50	0.45
4:N:3:GLN:H	4:N:26:SER:HG	1.62	0.45
2:D:792:LEU:O	2:D:796:TRP:N	2.49	0.45
3:H:20:LEU:HD12	3:H:81:LEU:HD23	1.99	0.45
4:L:39:TRP:HB3	4:L:52:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:NH1	1:A:62:ALA:O	2.45	0.45
2:B:666:LEU:HB2	2:B:670:LYS:HB2	1.99	0.45
1:C:429:PHE:HD2	1:C:537:PRO:HG3	1.82	0.45
2:D:818:MET:HE3	2:D:818:MET:HB2	1.84	0.45
3:H:36:TRP:O	3:H:48:VAL:N	2.38	0.45
3:H:148:VAL:HG13	3:H:183:LEU:HB2	1.98	0.45
3:M:34:MET:HA	3:M:98:ARG:HG2	1.97	0.45
4:N:143:PHE:O	4:N:177:TYR:N	2.47	0.45
2:B:38:ALA:HB3	2:B:97:VAL:HG12	1.99	0.45
2:D:190:ILE:HD12	2:D:197:TRP:H	1.81	0.45
2:D:606:ILE:HD12	2:D:606:ILE:HA	1.90	0.45
3:H:184:SER:OG	3:H:185:SER:N	2.50	0.45
1:A:567:ILE:O	1:A:569:ARG:NH1	2.50	0.44
1:A:579:PHE:HZ	1:A:668:TYR:HA	1.82	0.44
2:B:311:HIS:NE2	4:L:99:PRO:HD3	2.33	0.44
2:D:666:LEU:HB2	2:D:670:LYS:HB2	1.99	0.44
1:C:283:ALA:HB1	1:C:287:ILE:HG21	1.98	0.44
2:D:260:SER:HA	2:D:263:ALA:HB3	1.98	0.44
3:H:62:ASP:OD1	3:H:62:ASP:N	2.50	0.44
4:L:117:PRO:HD3	4:L:143:PHE:HB3	1.98	0.44
2:B:433:THR:HB	2:B:456:CYS:HB3	1.99	0.44
2:D:105:GLN:H	2:D:129:GLY:HA3	1.82	0.44
2:D:416:PHE:HD1	2:D:460:PHE:HB3	1.83	0.44
4:L:23:CYS:N	4:L:75:PHE:O	2.49	0.44
1:A:163:ILE:H	1:A:212:ALA:HB3	1.82	0.44
2:B:612:LEU:O	2:B:614:PHE:N	2.51	0.44
1:C:161:ASN:N	1:C:161:ASN:OD1	2.49	0.44
1:C:560:THR:OG1	1:C:561:ILE:N	2.50	0.44
1:C:658:ALA:HB3	2:D:610:TRP:HH2	1.82	0.44
2:B:230:LEU:HD22	2:B:256:TRP:HE3	1.83	0.44
1:C:189:SER:HA	1:C:190:LYS:HA	1.71	0.44
2:D:38:ALA:HB3	2:D:97:VAL:HG12	2.00	0.44
2:D:119:THR:OG1	2:D:120:LEU:N	2.50	0.44
4:L:69:SER:OG	4:L:70:GLY:N	2.46	0.44
4:L:145:PRO:HD3	4:L:203:LYS:HG3	1.99	0.44
1:A:560:THR:HG23	1:A:757:LEU:HD12	2.00	0.44
2:B:784:PHE:HD1	2:B:789:MET:HE2	1.83	0.44
1:C:414:GLN:NE2	1:C:415:MET:O	2.48	0.44
3:M:144:LEU:HD21	3:M:199:VAL:HG21	1.98	0.44
4:N:39:TRP:HB3	4:N:52:ILE:HB	1.99	0.44
1:A:429:PHE:HD2	1:A:537:PRO:HG3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:695:ILE:HG12	2:B:706:MET:HE1	2.00	0.44
4:L:152:TRP:HB3	4:L:183:LEU:HD22	2.00	0.44
3:M:20:LEU:HD12	3:M:81:LEU:HD23	1.99	0.44
3:M:91:THR:HG23	3:M:116:THR:HA	1.99	0.44
1:A:106:PRO:HA	1:A:109:TYR:HB2	2.00	0.44
1:A:522:MET:HB3	1:A:534:ILE:HD13	1.99	0.44
3:M:83:MET:HE1	3:M:115:VAL:HG11	1.99	0.44
4:N:51:LEU:HG	4:N:62:VAL:HG21	1.98	0.44
1:A:500:VAL:HG12	1:A:502:ASP:H	1.81	0.44
4:L:107:LYS:HA	4:L:107:LYS:HD3	1.87	0.44
3:M:184:SER:OG	3:M:185:SER:N	2.50	0.44
2:B:105:GLN:H	2:B:129:GLY:HA3	1.83	0.43
2:B:416:PHE:HD1	2:B:460:PHE:HB3	1.83	0.43
2:D:695:ILE:HG12	2:D:706:MET:HE1	2.00	0.43
3:H:91:THR:HG23	3:H:116:THR:HA	1.99	0.43
3:M:34:MET:HE2	3:M:34:MET:HB2	1.89	0.43
2:B:39:VAL:HG12	2:B:98:VAL:HG23	2.00	0.43
1:C:163:ILE:H	1:C:212:ALA:HB3	1.82	0.43
1:C:431:TYR:HB2	1:C:477:TYR:HB2	2.00	0.43
1:C:677:VAL:HA	1:C:680:ARG:HH21	1.82	0.43
2:D:687:PRO:HG3	2:D:712:ARG:HG2	2.00	0.43
4:N:145:PRO:HD3	4:N:203:LYS:HG3	1.99	0.43
1:A:658:ALA:HB3	2:B:610:TRP:HH2	1.83	0.43
2:B:197:TRP:HB3	2:B:199:LEU:HD23	1.99	0.43
3:M:36:TRP:O	3:M:48:VAL:N	2.38	0.43
4:N:95:SER:HA	4:N:99:PRO:HA	2.00	0.43
4:N:152:TRP:HB3	4:N:183:LEU:HD22	2.00	0.43
1:A:283:ALA:HB1	1:A:287:ILE:HG21	1.98	0.43
1:A:560:THR:OG1	1:A:561:ILE:N	2.50	0.43
2:D:612:LEU:HD23	2:D:613:VAL:H	1.83	0.43
2:D:784:PHE:HD1	2:D:789:MET:HE2	1.83	0.43
3:H:5:GLN:NE2	3:H:6:GLU:O	2.51	0.43
1:A:486:LYS:O	1:A:490:THR:OG1	2.30	0.43
1:A:552:LYS:HE2	2:D:515:ILE:HD13	2.00	0.43
1:C:353:ASP:OD1	1:C:353:ASP:N	2.52	0.43
2:D:316:GLU:O	2:D:318:LYS:NZ	2.42	0.43
4:L:21:ILE:HD12	4:L:77:LEU:HD23	2.01	0.43
4:L:123:PRO:HB2	4:L:190:TYR:HE1	1.83	0.43
4:N:10:SER:OG	4:N:109:GLU:OE2	2.37	0.43
4:N:145:PRO:HD3	4:N:203:LYS:HE3	2.00	0.43
1:C:522:MET:HB3	1:C:534:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:TYR:HB2	1:A:477:TYR:HB2	2.00	0.43
2:B:488:LYS:N	2:B:495:ASN:OD1	2.46	0.43
1:C:795:LEU:HA	1:C:798:LEU:HD12	2.01	0.43
4:N:123:PRO:HB2	4:N:190:TYR:HE1	1.83	0.43
1:A:558:GLY:HA3	1:A:773:LEU:HD22	2.01	0.43
1:C:580:GLN:HB3	1:C:583:LEU:HB3	2.01	0.43
1:C:651:ARG:HD3	2:D:607:TRP:CG	2.54	0.43
2:D:368:ASN:ND2	2:D:374:GLU:OE2	2.52	0.43
4:L:10:SER:OG	4:L:109:GLU:OE2	2.37	0.43
4:N:138:CYS:N	4:N:181:SER:O	2.46	0.43
1:A:690:ASP:HB3	1:A:693:LEU:HB2	2.01	0.43
1:C:510:ARG:NH1	2:D:188:SER:OG	2.52	0.43
1:C:560:THR:HG23	1:C:757:LEU:HD12	2.00	0.43
2:D:39:VAL:HG12	2:D:98:VAL:HG23	2.00	0.43
1:A:580:GLN:HB3	1:A:583:LEU:HB3	2.01	0.42
1:A:795:LEU:HA	1:A:798:LEU:HD12	2.01	0.42
2:B:687:PRO:HG3	2:B:712:ARG:HG2	2.00	0.42
1:C:124:ARG:NH1	1:C:142:PRO:O	2.46	0.42
1:C:690:ASP:HB3	1:C:693:LEU:HB2	2.01	0.42
2:D:612:LEU:O	2:D:614:PHE:N	2.51	0.42
4:L:145:PRO:HD3	4:L:203:LYS:HE3	2.00	0.42
3:M:5:GLN:NE2	3:M:6:GLU:O	2.51	0.42
3:M:43:LYS:O	3:M:44:ARG:NH1	2.45	0.42
1:A:794:SER:HA	1:A:797:ILE:HD12	2.01	0.42
2:B:166:TRP:HB3	2:B:227:ILE:HG13	2.02	0.42
1:C:106:PRO:HA	1:C:109:TYR:HB2	2.00	0.42
2:D:135:ALA:HA	2:D:177:PRO:HG2	2.01	0.42
2:D:148:PRO:HG3	2:D:362:LEU:HD11	2.01	0.42
2:D:230:LEU:HD22	2:D:256:TRP:HE3	1.83	0.42
1:A:453:LYS:HA	1:A:453:LYS:HD3	1.88	0.42
2:B:102:ASP:HA	2:B:127:HIS:CD2	2.54	0.42
2:B:368:ASN:ND2	2:B:374:GLU:OE2	2.52	0.42
1:C:504:LYS:HB3	1:C:707:GLN:HB2	2.02	0.42
4:N:194:ASN:HA	4:N:215:ARG:HB3	2.02	0.42
2:B:612:LEU:HD23	2:B:613:VAL:H	1.83	0.42
2:B:760:THR:OG1	2:B:761:GLY:N	2.52	0.42
4:L:88:ALA:H	4:L:108:LEU:HD12	1.84	0.42
4:L:194:ASN:HA	4:L:215:ARG:HB3	2.02	0.42
1:A:353:ASP:OD1	1:A:353:ASP:N	2.52	0.42
1:A:732:TYR:HE2	1:A:747:LEU:HD22	1.85	0.42
2:B:407:SER:HA	2:B:477:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:446:THR:N	1:C:450:ASP:O	2.50	0.42
1:C:836:GLY:O	1:C:840:LEU:HG	2.19	0.42
2:D:93:LYS:HB3	2:D:93:LYS:HE2	1.87	0.42
2:D:225:SER:OG	2:D:227:ILE:O	2.35	0.42
2:D:433:THR:HB	2:D:456:CYS:HB3	1.99	0.42
1:A:298:GLU:HA	1:A:301:HIS:HB2	2.01	0.42
1:A:579:PHE:CZ	1:A:671:ASN:HB3	2.55	0.42
2:B:316:GLU:O	2:B:318:LYS:NZ	2.42	0.42
1:C:558:GLY:HA3	1:C:773:LEU:HD22	2.00	0.42
4:L:95:SER:HA	4:L:99:PRO:HA	2.00	0.42
4:N:88:ALA:H	4:N:108:LEU:HD12	1.84	0.42
2:B:571:ALA:HA	2:B:574:VAL:HG12	2.02	0.42
1:C:399:LYS:HA	1:C:399:LYS:HD2	1.89	0.42
1:C:461:ASN:HB3	1:C:471:THR:HG22	2.02	0.42
2:D:102:ASP:HA	2:D:127:HIS:CD2	2.54	0.42
3:H:38:ARG:N	3:H:46:GLU:O	2.47	0.42
3:H:176:LEU:HG	3:H:181:TYR:HB3	2.02	0.42
1:A:340:PRO:O	1:A:344:ARG:NH1	2.53	0.42
1:A:461:ASN:HB3	1:A:471:THR:HG22	2.02	0.42
2:B:148:PRO:HG3	2:B:362:LEU:HD11	2.01	0.42
1:C:340:PRO:O	1:C:344:ARG:NH1	2.53	0.42
2:D:161:MET:HB3	2:D:161:MET:HE2	1.80	0.42
2:D:166:TRP:HB3	2:D:227:ILE:HG13	2.02	0.42
2:D:407:SER:HA	2:D:477:ASP:HB3	2.01	0.42
3:H:34:MET:HE2	3:H:34:MET:HB2	1.89	0.42
4:N:21:ILE:HD12	4:N:77:LEU:HD23	2.01	0.42
4:N:23:CYS:N	4:N:75:PHE:O	2.49	0.42
1:A:446:THR:N	1:A:450:ASP:O	2.50	0.42
2:B:135:ALA:HA	2:B:177:PRO:HG2	2.01	0.42
1:C:732:TYR:HE2	1:C:747:LEU:HD22	1.85	0.42
2:D:101:ASP:OD2	2:D:103:THR:OG1	2.38	0.42
2:D:156:VAL:HG11	2:D:280:VAL:HG11	2.02	0.42
2:D:413:GLU:H	2:D:417:VAL:HG11	1.85	0.42
2:D:760:THR:OG1	2:D:761:GLY:N	2.52	0.42
4:L:91:TYR:HB3	4:L:105:GLY:HA2	2.02	0.42
3:M:176:LEU:HG	3:M:181:TYR:HB3	2.02	0.42
1:A:504:LYS:HB3	1:A:707:GLN:HB2	2.01	0.41
1:A:690:ASP:OD2	1:A:692:ARG:NH1	2.44	0.41
2:B:409:VAL:HG13	2:B:497:MET:HE3	2.02	0.41
1:C:313:VAL:HA	1:C:316:LEU:HB2	2.02	0.41
1:A:46:VAL:HG21	1:A:62:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:VAL:HA	1:A:316:LEU:HB2	2.02	0.41
1:A:836:GLY:O	1:A:840:LEU:HG	2.20	0.41
1:C:74:MET:HE3	1:C:74:MET:HB3	1.95	0.41
4:L:9:ALA:HA	4:L:106:THR:HG22	2.02	0.41
1:C:298:GLU:HA	1:C:301:HIS:HB2	2.01	0.41
1:C:458:THR:O	1:C:458:THR:OG1	2.34	0.41
1:C:579:PHE:CZ	1:C:671:ASN:HB3	2.55	0.41
1:A:479:PHE:HE1	1:A:813:TRP:HB2	1.85	0.41
2:B:101:ASP:OD2	2:B:103:THR:OG1	2.38	0.41
2:B:503:MET:HE2	2:B:505:ARG:HE	1.86	0.41
2:D:498:ILE:HA	2:D:501:VAL:HG12	2.03	0.41
4:N:53:LYS:N	4:N:57:ASN:O	2.50	0.41
1:A:626:SER:HB3	1:A:642:GLU:HB2	2.03	0.41
1:C:453:LYS:HA	1:C:453:LYS:HD3	1.88	0.41
2:D:78:PRO:HA	2:D:81:ILE:HD12	2.02	0.41
2:D:571:ALA:HA	2:D:574:VAL:HG12	2.02	0.41
1:A:31:ALA:HB3	1:A:65:VAL:HG11	2.02	0.41
2:B:792:LEU:O	2:B:796:TRP:N	2.49	0.41
2:D:190:ILE:O	2:D:193:SER:OG	2.39	0.41
2:D:409:VAL:HG13	2:D:497:MET:HE3	2.02	0.41
1:C:29:ILE:HD13	1:C:29:ILE:HA	1.95	0.41
1:C:223:LYS:HA	1:C:223:LYS:HD3	1.94	0.41
1:C:696:PRO:HG3	1:C:722:THR:HG22	2.03	0.41
4:N:80:HIS:HA	4:N:81:PRO:HA	1.95	0.41
4:N:91:TYR:HB3	4:N:105:GLY:HA2	2.02	0.41
1:A:85:SER:O	1:A:86:GLN:NE2	2.54	0.41
1:A:538:LEU:HD23	1:A:538:LEU:HA	1.87	0.41
1:A:696:PRO:HG3	1:A:722:THR:HG22	2.03	0.41
2:B:442:SER:H	2:B:448:GLU:HG2	1.86	0.41
2:B:473:LYS:HE2	2:B:473:LYS:HB2	1.83	0.41
1:C:46:VAL:HG21	1:C:62:ALA:HB2	2.02	0.41
1:C:85:SER:O	1:C:86:GLN:NE2	2.54	0.41
1:C:694:ARG:NH2	1:C:719:GLU:O	2.42	0.41
1:C:794:SER:HA	1:C:797:ILE:HD12	2.01	0.41
2:D:442:SER:H	2:D:448:GLU:HG2	1.86	0.41
4:N:9:ALA:HA	4:N:106:THR:HG22	2.02	0.41
1:A:223:LYS:HA	1:A:223:LYS:HD3	1.94	0.41
2:B:79:LYS:HE3	2:B:79:LYS:HB3	1.91	0.41
2:B:156:VAL:HG11	2:B:280:VAL:HG11	2.02	0.41
2:B:333:ASN:HB2	3:H:104:PHE:HD2	1.86	0.41
2:B:565:MET:HB3	1:C:838:PHE:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:829:MET:O	2:B:832:SER:OG	2.39	0.41
3:H:96:CYS:SG	3:H:98:ARG:NH1	2.91	0.41
1:A:223:LYS:HG3	4:L:69:SER:HB2	2.02	0.40
2:B:80:SER:OG	2:B:84:ARG:NH2	2.51	0.40
2:B:413:GLU:H	2:B:417:VAL:HG11	1.85	0.40
1:C:289:GLY:N	1:C:375:MET:O	2.46	0.40
2:D:829:MET:O	2:D:832:SER:OG	2.39	0.40
4:N:123:PRO:HA	4:N:136:VAL:HG22	2.02	0.40
1:A:441:CYS:HB2	1:A:454:LYS:HD3	2.03	0.40
2:B:185:LYS:HE2	2:B:185:LYS:HB2	1.93	0.40
1:C:626:SER:HB3	1:C:642:GLU:HB2	2.03	0.40
1:C:660:PHE:HE2	2:D:825:LEU:HB2	1.86	0.40
2:D:473:LYS:HB2	2:D:473:LYS:HE2	1.83	0.40
4:N:166:SER:O	4:N:166:SER:OG	2.39	0.40
2:B:530:ILE:HD13	2:B:530:ILE:HA	1.93	0.40
2:B:606:ILE:HD12	2:B:606:ILE:HA	1.90	0.40
2:D:503:MET:HE2	2:D:505:ARG:HE	1.86	0.40
4:L:24:ARG:HA	4:L:24:ARG:HD3	1.89	0.40
1:A:516:LYS:HA	1:A:516:LYS:HD2	1.82	0.40
2:B:161:MET:HE2	2:B:161:MET:HB3	1.80	0.40
2:B:498:ILE:HA	2:B:501:VAL:HG12	2.03	0.40
1:C:479:PHE:HE1	1:C:813:TRP:HB2	1.85	0.40
2:D:185:LYS:O	2:D:189:THR:OG1	2.33	0.40
3:H:219:ARG:HD3	4:L:125:SER:HA	2.02	0.40
4:L:123:PRO:HA	4:L:136:VAL:HG22	2.02	0.40
1:A:324:ASP:HA	1:A:325:PRO:HD3	1.90	0.40
4:L:43:LYS:HB2	4:L:46:GLN:HB2	2.03	0.40
4:N:43:LYS:HB2	4:N:46:GLN:HB2	2.03	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	775/862 (90%)	706 (91%)	67 (9%)	2 (0%)	36	72
1	C	775/862 (90%)	706 (91%)	67 (9%)	2 (0%)	36	72
2	B	766/883 (87%)	694 (91%)	69 (9%)	3 (0%)	30	67
2	D	766/883 (87%)	694 (91%)	69 (9%)	3 (0%)	30	67
3	H	211/221 (96%)	193 (92%)	18 (8%)	0	100	100
3	M	211/221 (96%)	193 (92%)	18 (8%)	0	100	100
4	L	213/215 (99%)	193 (91%)	20 (9%)	0	100	100
4	N	213/215 (99%)	193 (91%)	20 (9%)	0	100	100
All	All	3930/4362 (90%)	3572 (91%)	348 (9%)	10 (0%)	37	72

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	613	VAL
2	B	613	VAL
2	B	671	PHE
2	D	671	PHE
1	A	462	ASP
1	A	579	PHE
1	C	462	ASP
1	C	579	PHE
2	B	612	LEU
2	D	612	LEU

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	678/744 (91%)	673 (99%)	5 (1%)	76	79
1	C	678/744 (91%)	673 (99%)	5 (1%)	76	79
2	B	677/762 (89%)	670 (99%)	7 (1%)	68	76
2	D	677/762 (89%)	670 (99%)	7 (1%)	68	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	188/192 (98%)	184 (98%)	4 (2%)	47	65
3	M	188/192 (98%)	184 (98%)	4 (2%)	47	65
4	L	190/190 (100%)	184 (97%)	6 (3%)	34	56
4	N	190/190 (100%)	184 (97%)	6 (3%)	34	56
All	All	3466/3776 (92%)	3422 (99%)	44 (1%)	59	72

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	VAL
1	A	338	THR
1	A	458	THR
1	A	467	SER
1	A	851	LEU
2	B	188	SER
2	B	358	MET
2	B	510	VAL
2	B	512	SER
2	B	606	ILE
2	B	641	ILE
2	B	810	SER
1	C	270	VAL
1	C	338	THR
1	C	458	THR
1	C	467	SER
1	C	851	LEU
2	D	188	SER
2	D	358	MET
2	D	510	VAL
2	D	512	SER
2	D	606	ILE
2	D	641	ILE
2	D	810	SER
3	H	122	THR
3	H	164	SER
3	H	165	LEU
3	H	188	THR
4	L	118	THR
4	L	120	SER
4	L	126	SER
4	L	131	SER

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Mol	Chain	Res	Type
4	L	173	LYS
4	L	212	SER
3	M	122	THR
3	M	164	SER
3	M	165	LEU
3	M	188	THR
4	N	118	THR
4	N	120	SER
4	N	126	SER
4	N	131	SER
4	N	173	LYS
4	N	212	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	67	HIS
1	A	86	GLN
1	A	291	GLN
1	A	334	ASN
1	A	389	ASN
1	A	425	HIS
1	A	557	GLN
1	A	763	GLN
1	A	791	GLN
1	A	792	GLN
1	A	801	HIS
1	A	817	GLN
2	B	153	GLN
2	B	159	ASN
2	B	333	ASN
2	B	385	GLN
2	B	698	ASN
2	B	803	ASN
1	C	38	HIS
1	C	67	HIS
1	C	73	GLN
1	C	86	GLN
1	C	171	HIS
1	C	291	GLN
1	C	334	ASN

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Mol	Chain	Res	Type
1	C	389	ASN
1	C	425	HIS
1	C	557	GLN
1	C	791	GLN
1	C	792	GLN
1	C	817	GLN
2	D	153	GLN
2	D	159	ASN
2	D	218	ASN
2	D	385	GLN
2	D	444	ASN
2	D	698	ASN
2	D	803	ASN
3	H	5	GLN
3	H	82	GLN
4	L	3	GLN
4	L	6	GLN
4	L	46	GLN
4	L	57	ASN
4	L	94	HIS
4	L	128	GLN
4	L	149	ASN
4	L	161	ASN
3	M	5	GLN
3	M	82	GLN
3	M	170	HIS
4	N	3	GLN
4	N	6	GLN
4	N	46	GLN
4	N	57	ASN
4	N	94	HIS
4	N	128	GLN
4	N	149	ASN
4	N	161	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	A	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	824:ASN	C	825:ALA	N	5.58
1	C	824:ASN	C	825:ALA	N	5.58

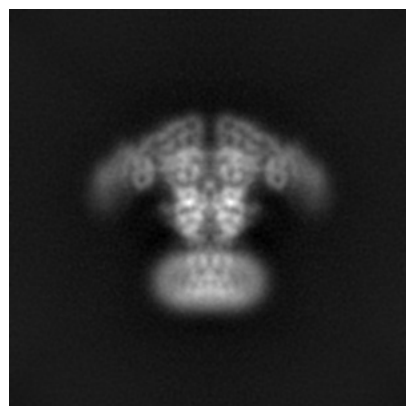
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25851. These allow visual inspection of the internal detail of the map and identification of artifacts.

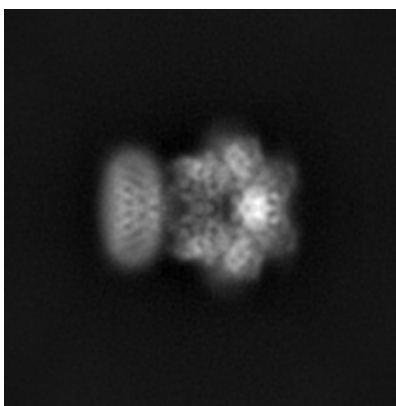
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

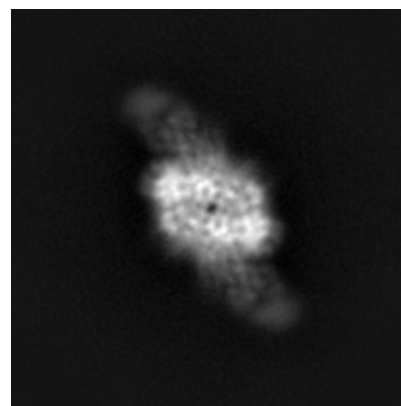
6.1.1 Primary map



X

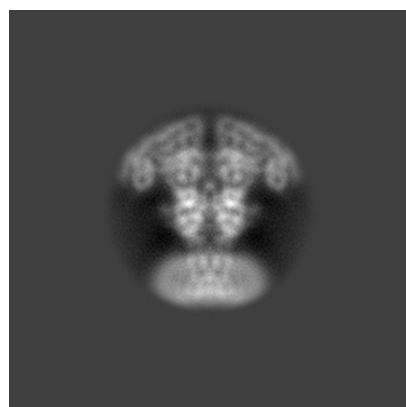


Y

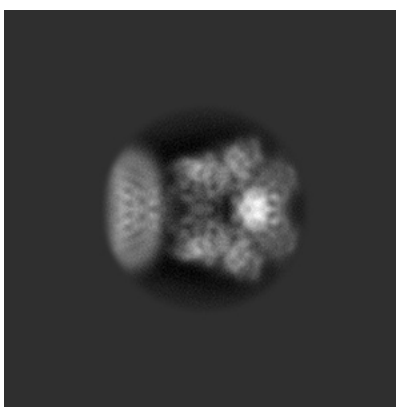


Z

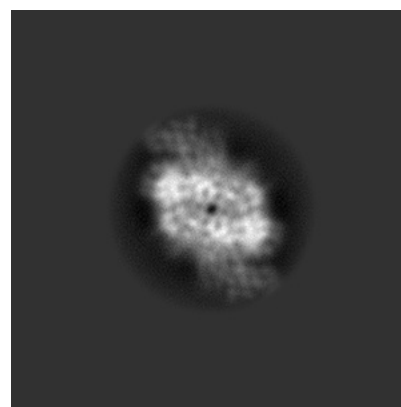
6.1.2 Raw map



X



Y

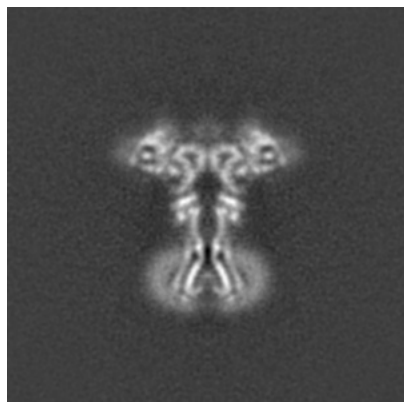


Z

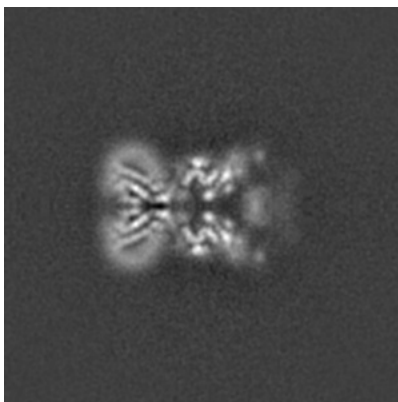
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

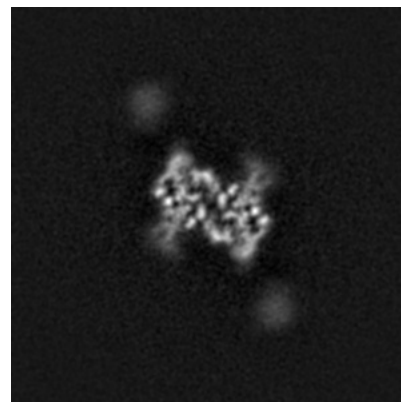
6.2.1 Primary map



X Index: 128

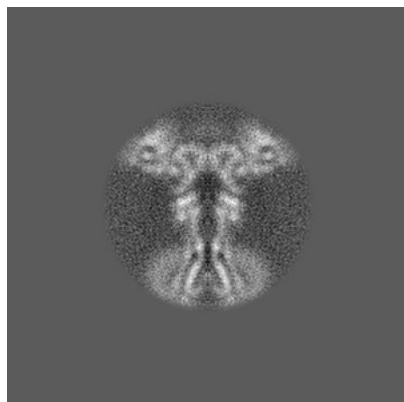


Y Index: 128

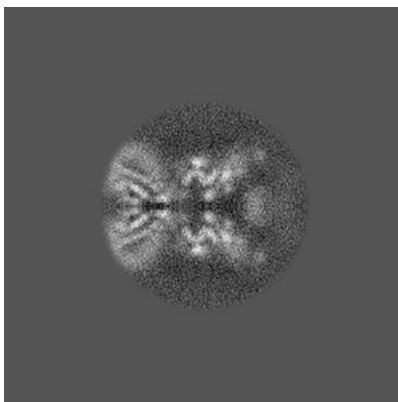


Z Index: 128

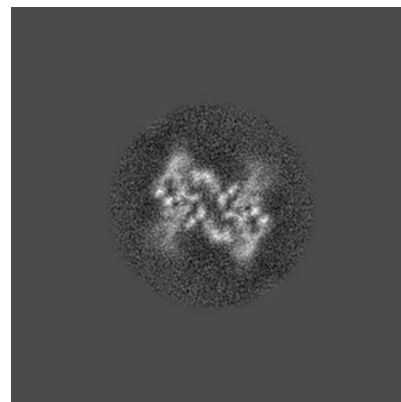
6.2.2 Raw map



X Index: 128



Y Index: 128

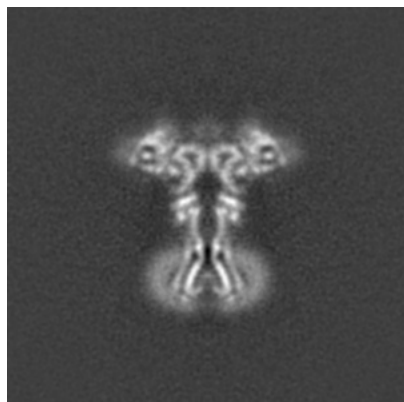


Z Index: 128

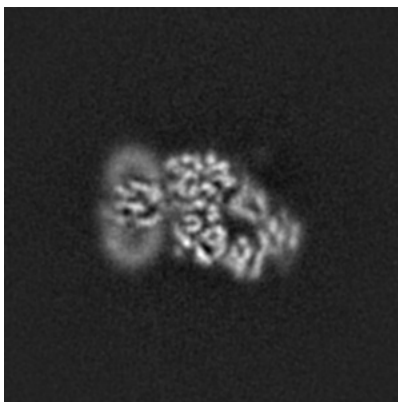
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

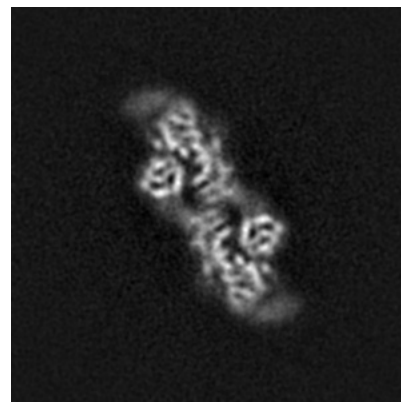
6.3.1 Primary map



X Index: 128

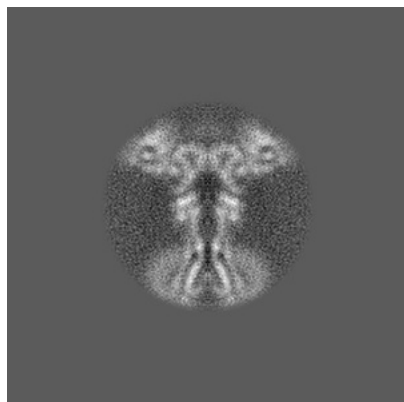


Y Index: 138

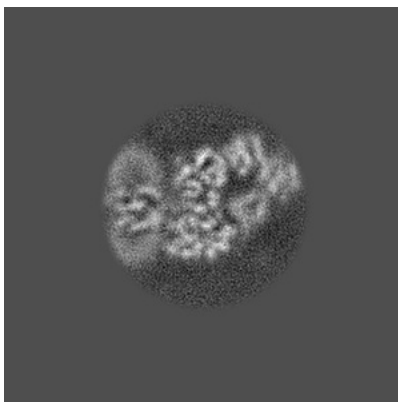


Z Index: 154

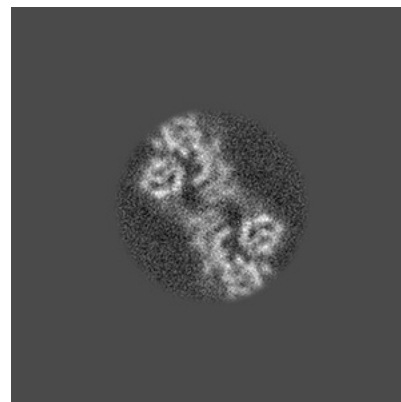
6.3.2 Raw map



X Index: 128



Y Index: 118

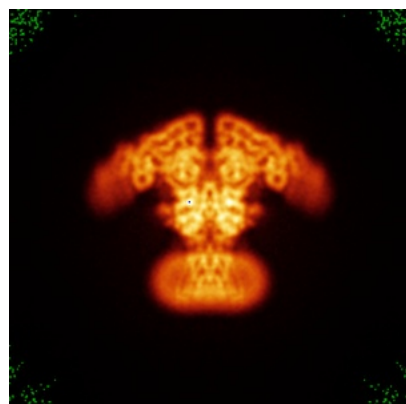


Z Index: 154

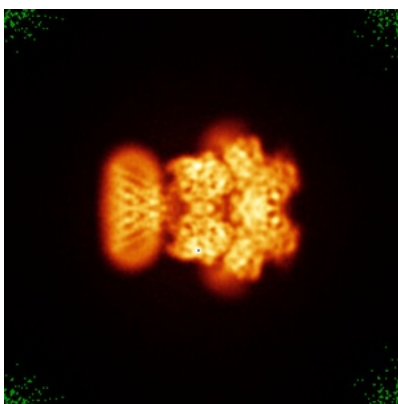
The images above show the largest variance slices of the map in three orthogonal directions.

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

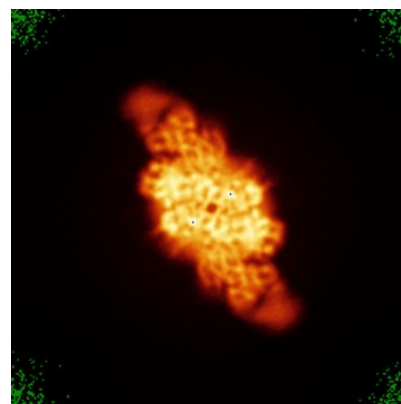
6.4.1 Primary map



X

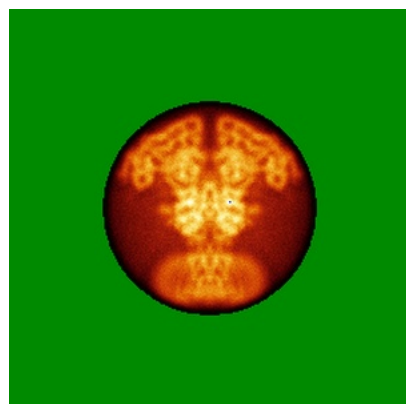


Y

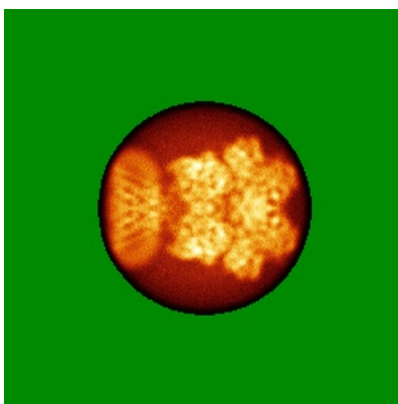


Z

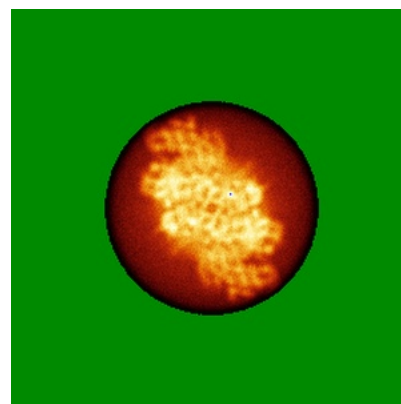
6.4.2 Raw map



X



Y

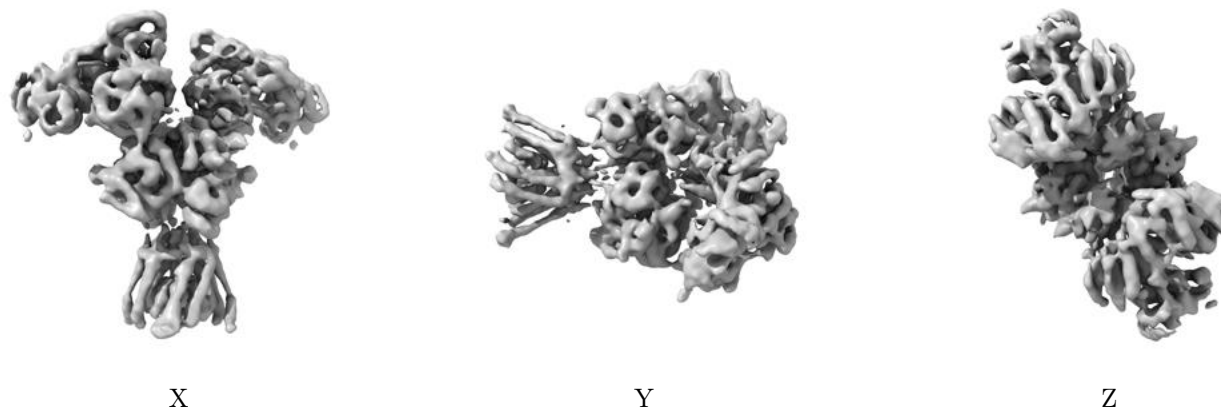


Z

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.

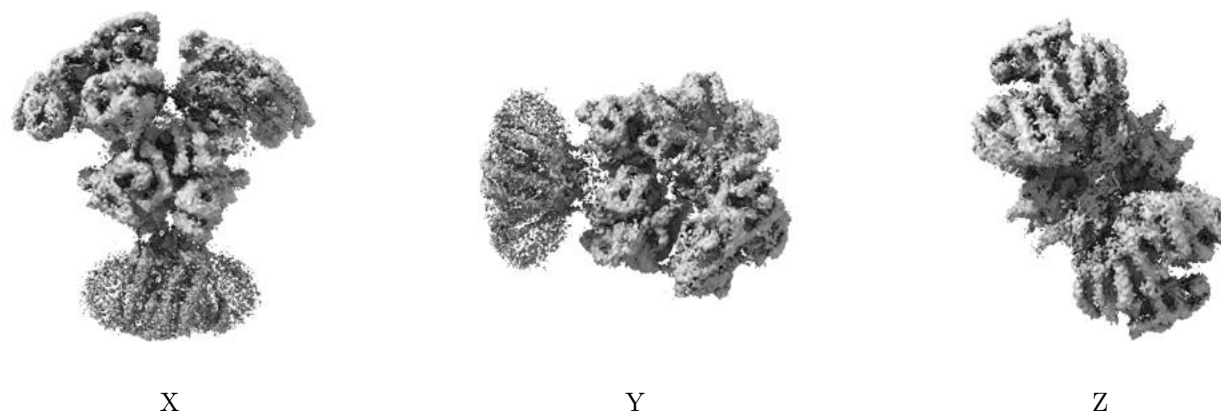
6.5 Orthogonal surface views [i](#)

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.

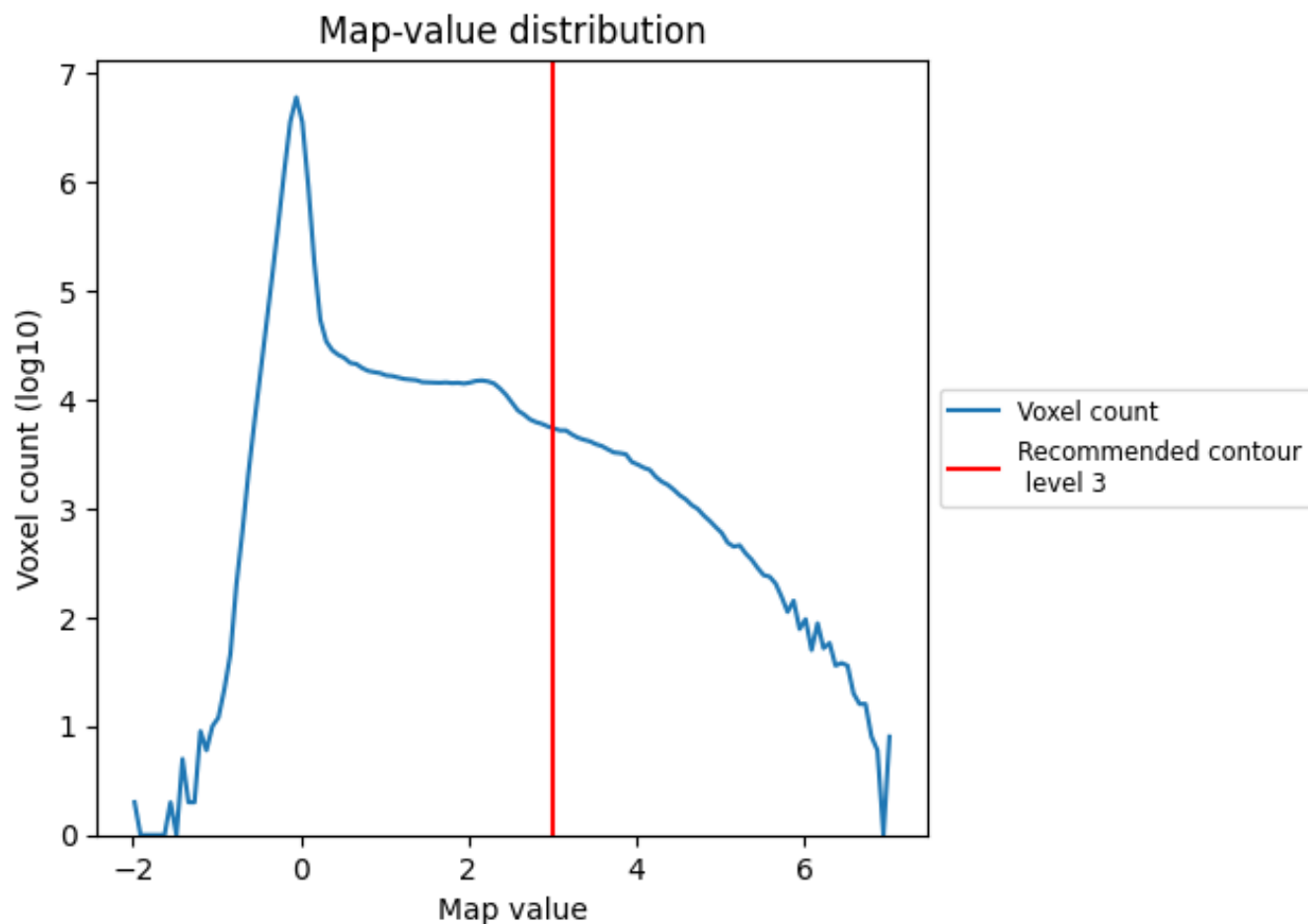
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

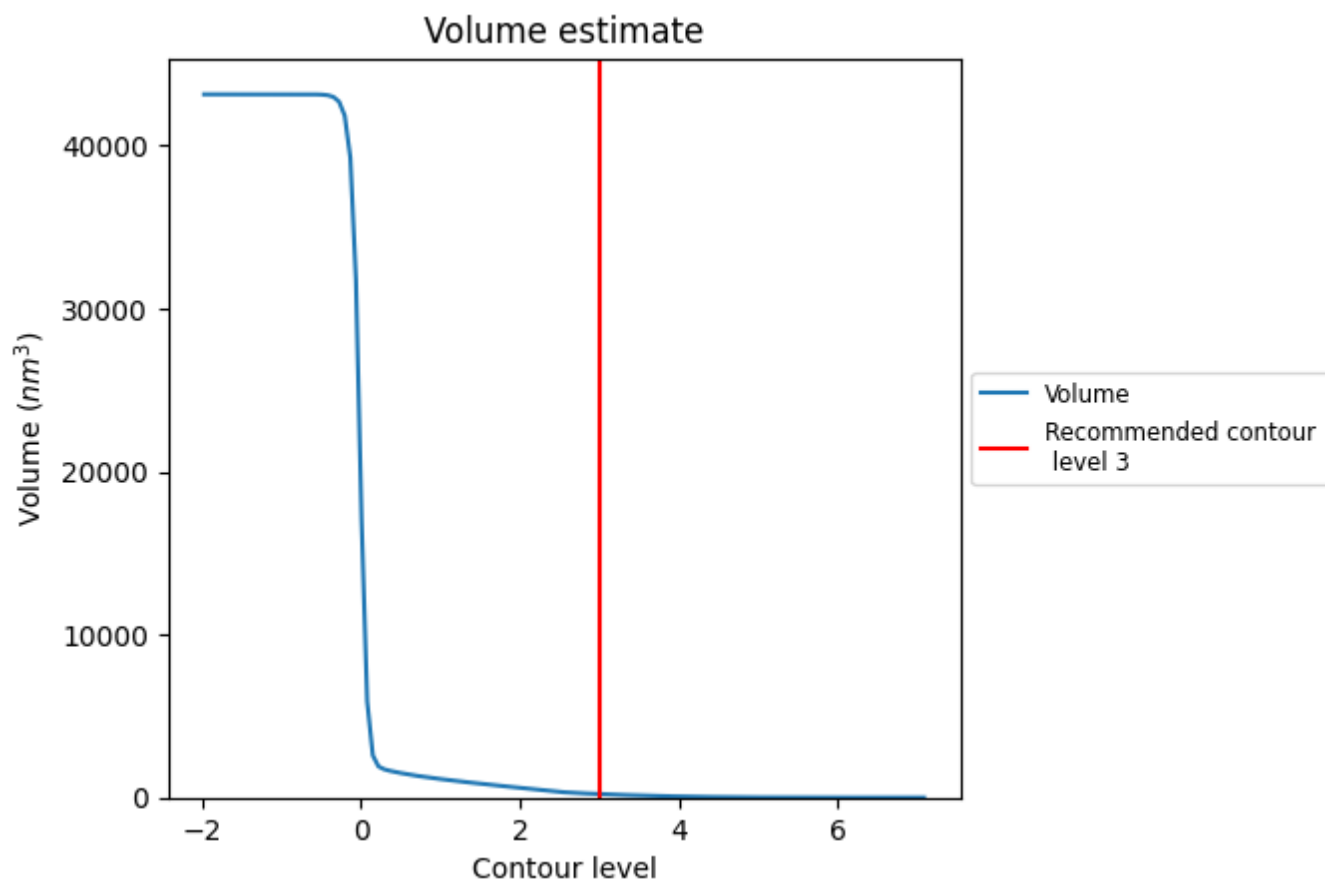
This section contains the results of statistical analysis of the map.

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.

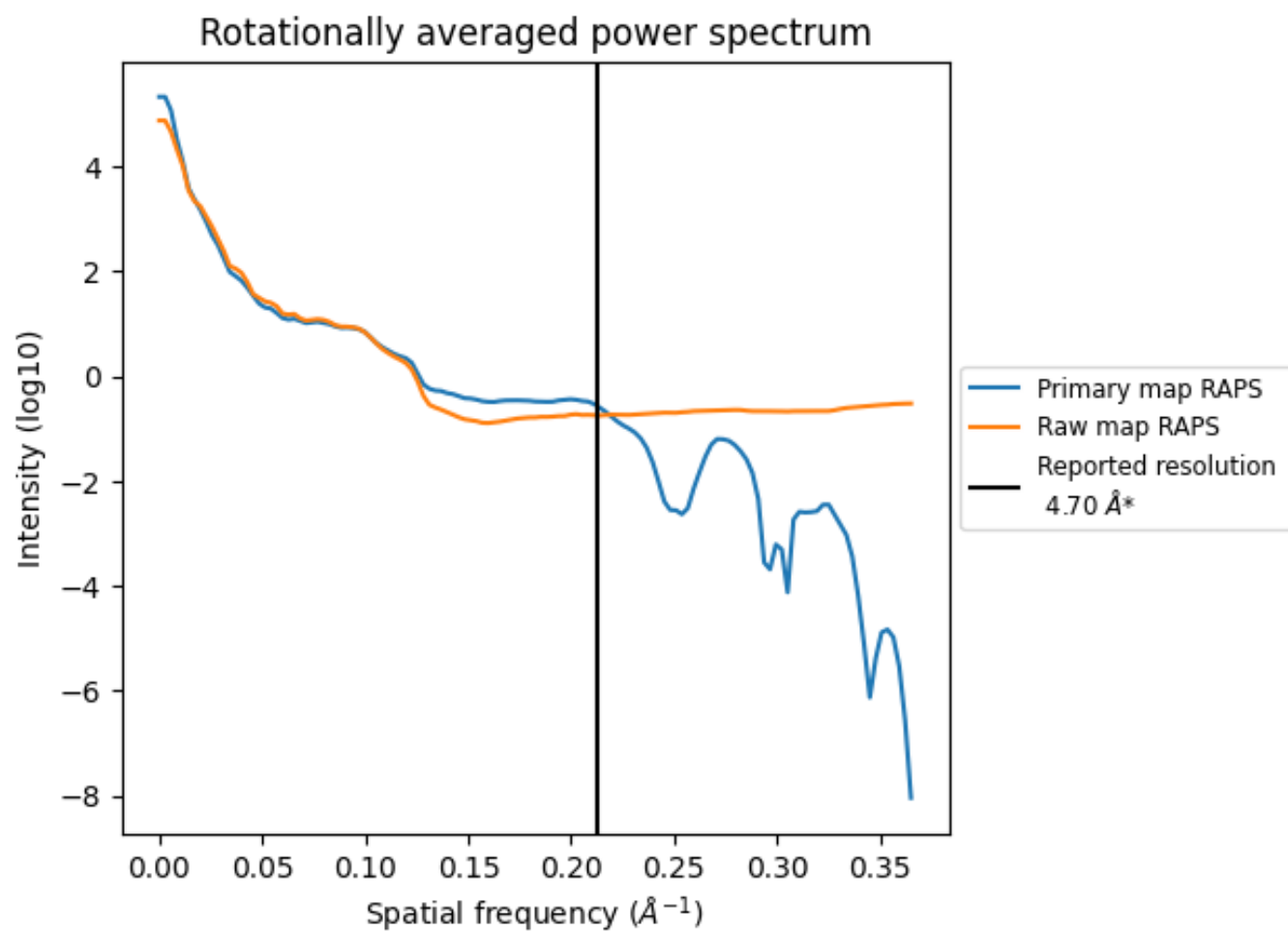
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 216 nm³; this corresponds to an approximate mass of 195 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 ⓘ

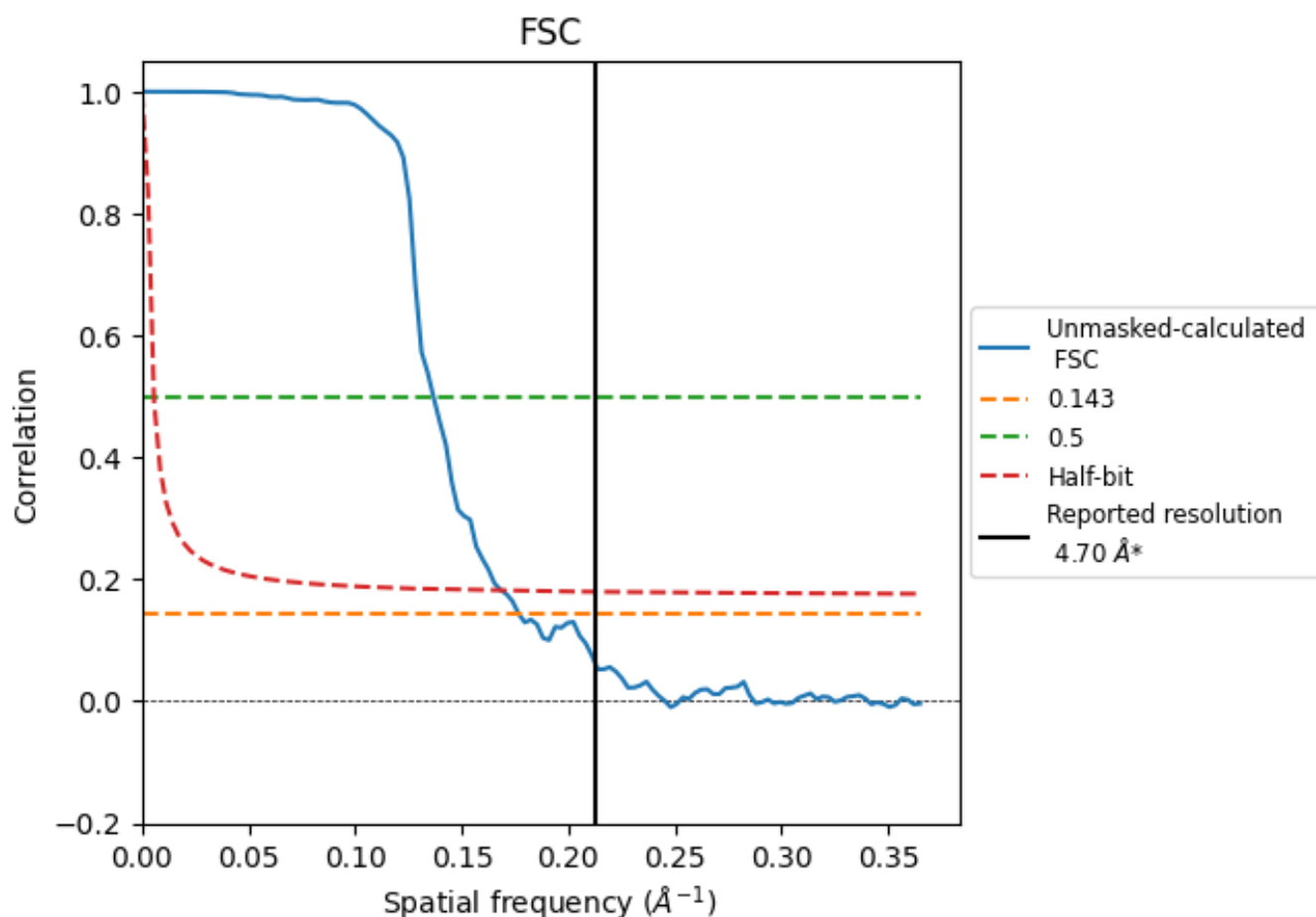


*Reported resolution corresponds to spatial frequency of $0.213 \text{ \AA}^{-1}$

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 0.213 Å⁻¹

8.2 Resolution estimates [i](#)

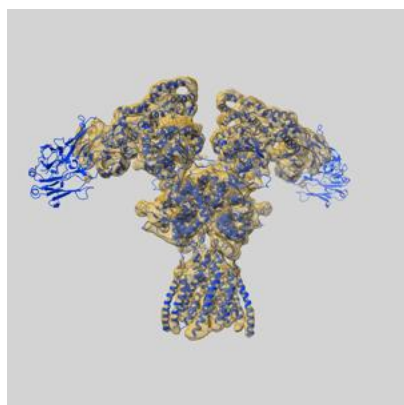
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.66	7.32	5.93

*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 5.66 differs from the reported value 4.7 by more than 10 %

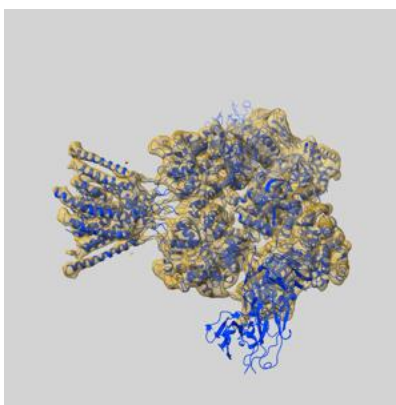
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25851 and PDB model 7TES. Per-residue inclusion information can be found in section [3](#) on page [9](#).

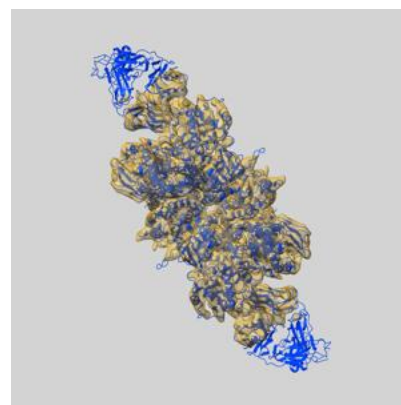
9.1 Map-model overlay [i](#)



X



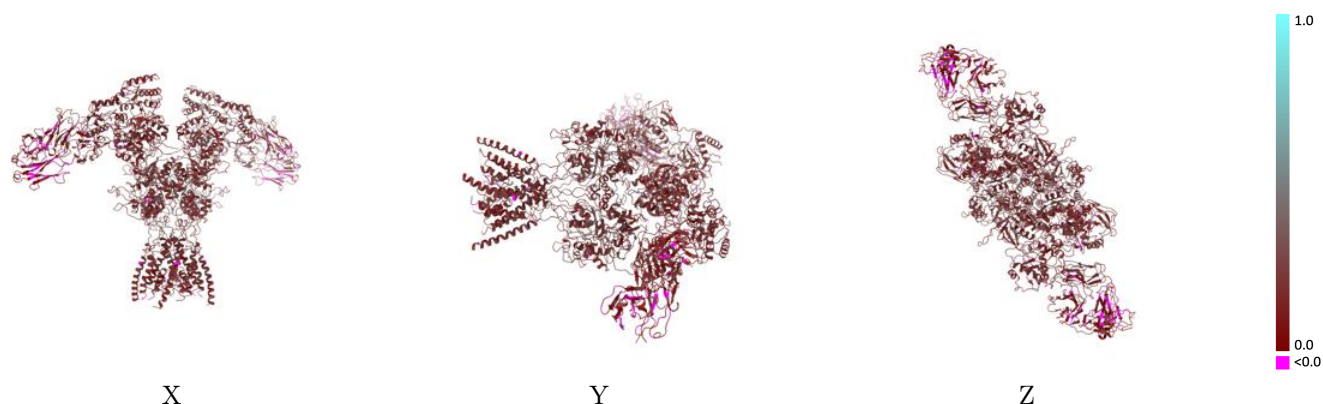
Y



Z

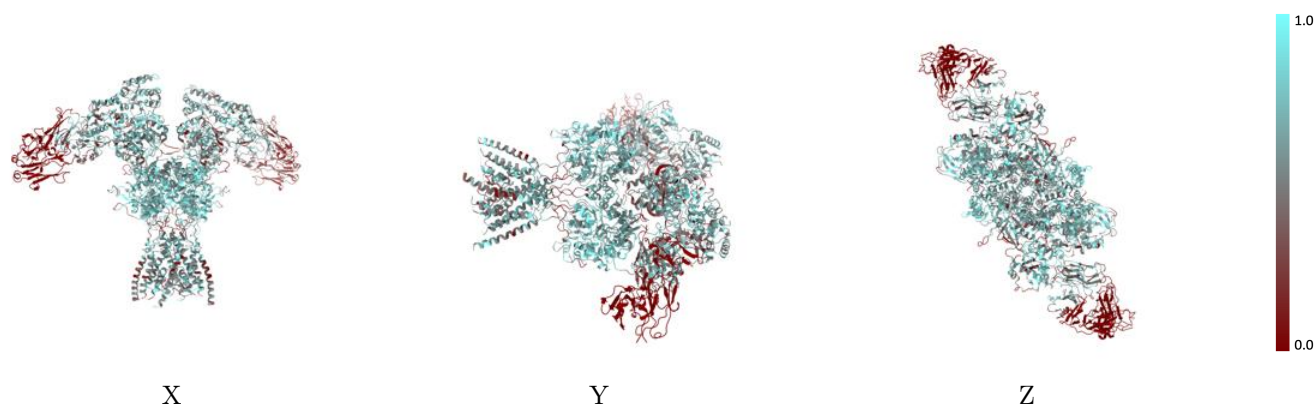
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



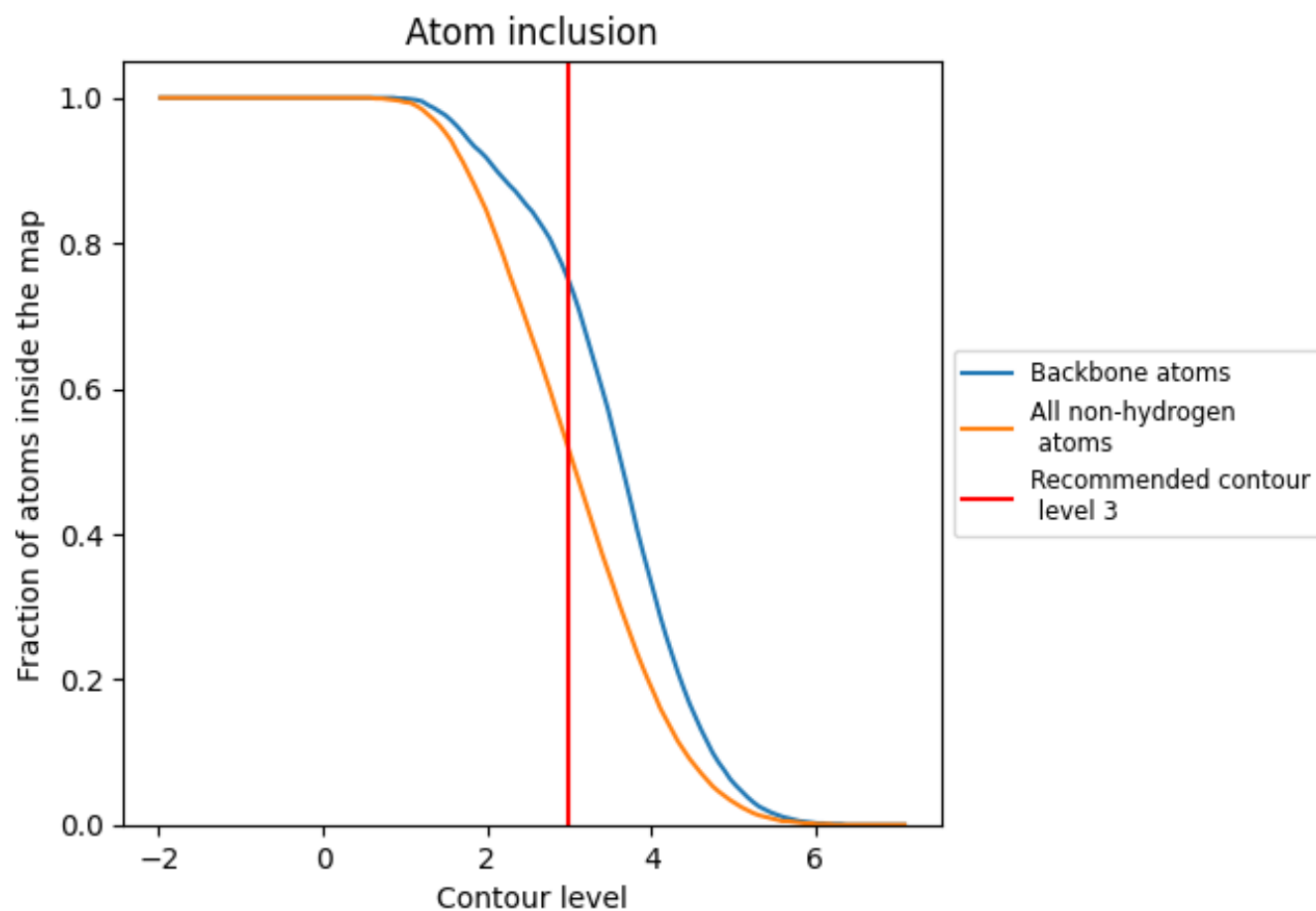
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 75% of all backbone atoms, 52% 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	0.5150	0.1970
A	0.6170	0.2170
B	0.5690	0.2110
C	0.6170	0.2170
D	0.5690	0.2130
H	0.1830	0.1340
L	0.2570	0.1280
M	0.1880	0.1320
N	0.2610	0.1310

1.0

0.0

<0.0