



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:23 PM UTC

PDB ID : 7TET / pdb_00007tet
EMDB ID : EMD-25852
Title : Cryo-EM structure of GluN1b-2B NMDAR in complex with Fab5 in non-active2-like conformation
Authors : Tajima, N.; Furukawa, H.
Deposited on : 2022-01-05
Resolution : 4.45 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:

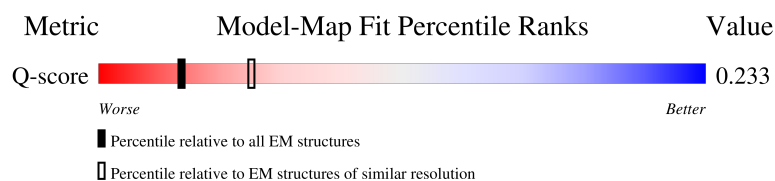
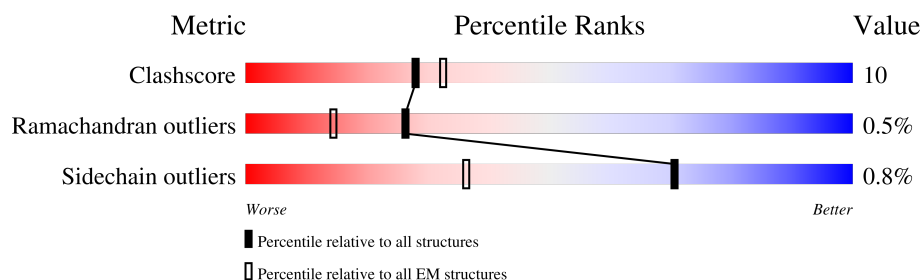
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.45 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	3027 (3.95 - 4.95)

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	27%35%15%48%
3	M	221	27%36%15%48%
4	L	209	10%33%20%46%
4	N	209	11%33%20%46%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28088 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	786	Total	C	N	O	S	0	0
			6194	3941	1071	1145	37		
1	C	786	Total	C	N	O	S	0	0
			6194	3941	1071	1145	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	769	Total	C	N	O	S	0	0
			6079	3918	980	1140	41		
2	D	770	Total	C	N	O	S	0	0
			6085	3921	981	1142	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 Fab5 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	114	Total	C	N	O	S	0	0
			893	561	150	177	5		
3	M	114	Total	C	N	O	S	0	0
			893	561	150	177	5		

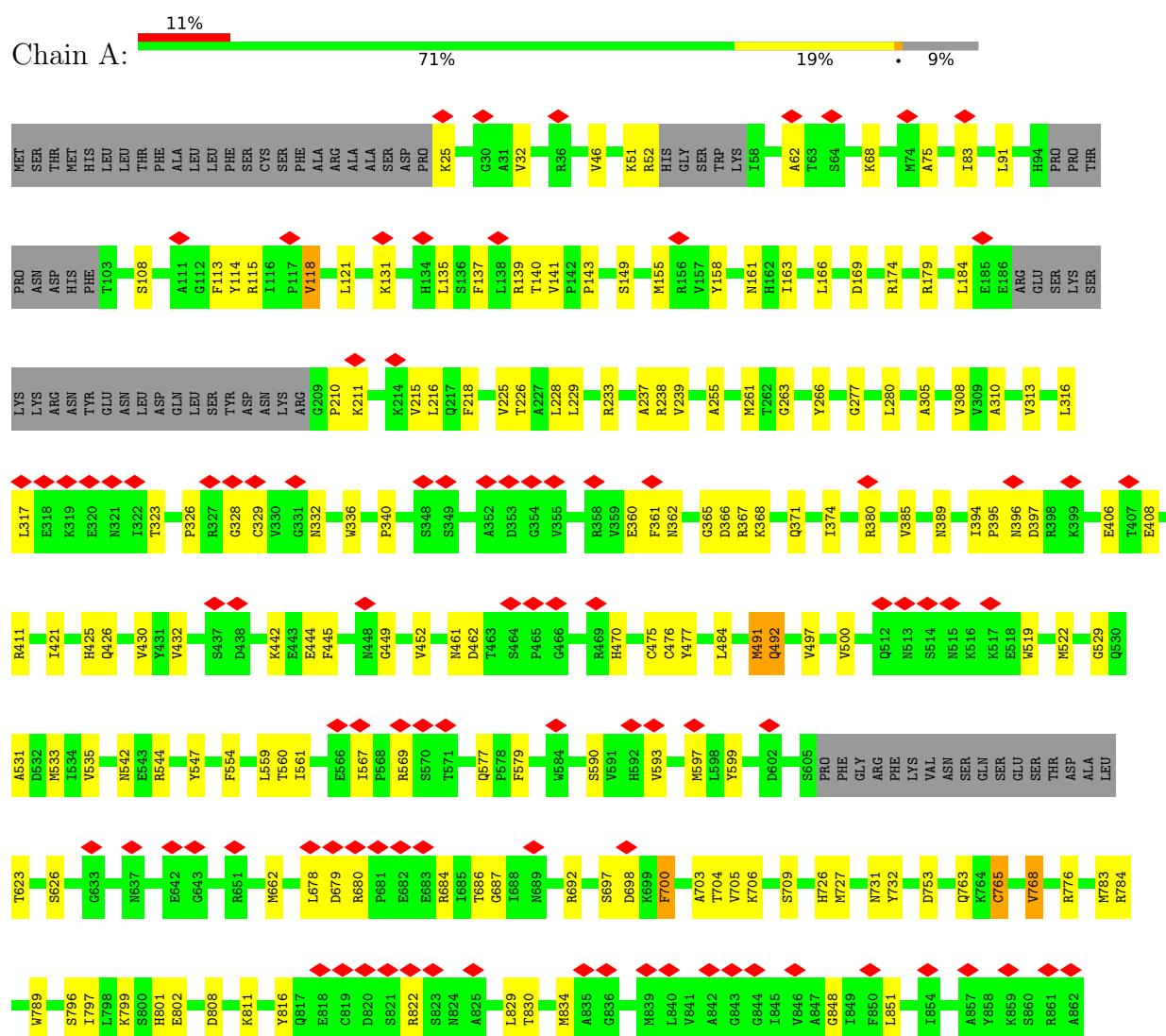
- Molecule 4 is a protein called Fab5 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	112	Total	C	N	O	S	0	0
			875	549	152	171	3		
4	N	112	Total	C	N	O	S	0	0
			875	549	152	171	3		

3 Residue-property plots

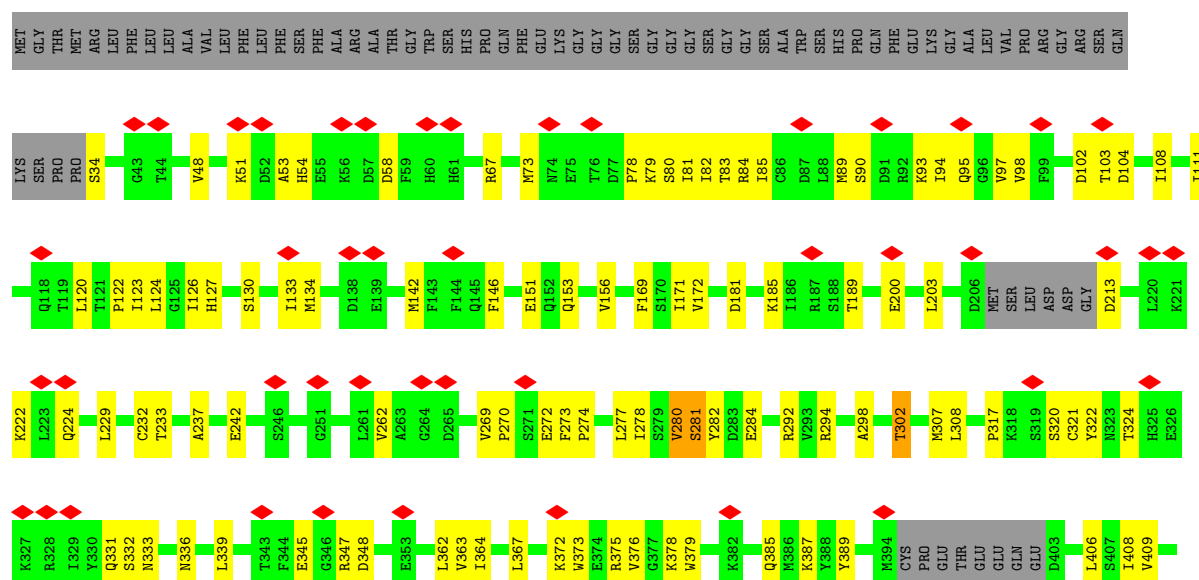
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

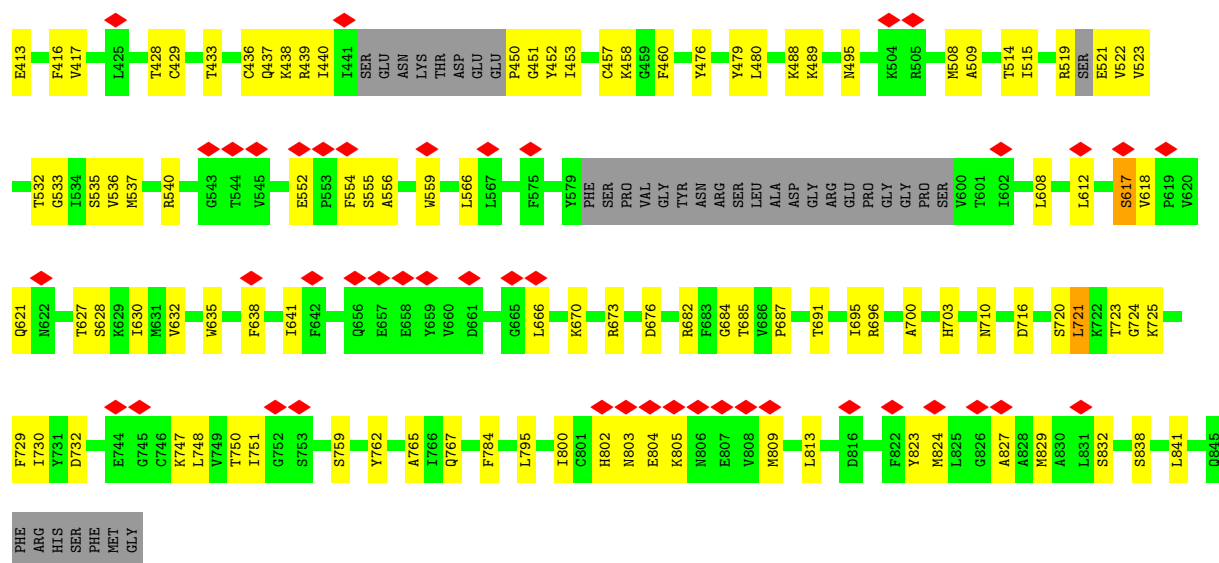
- Molecule 1: Glutamate receptor ionotropic, NMDA 1



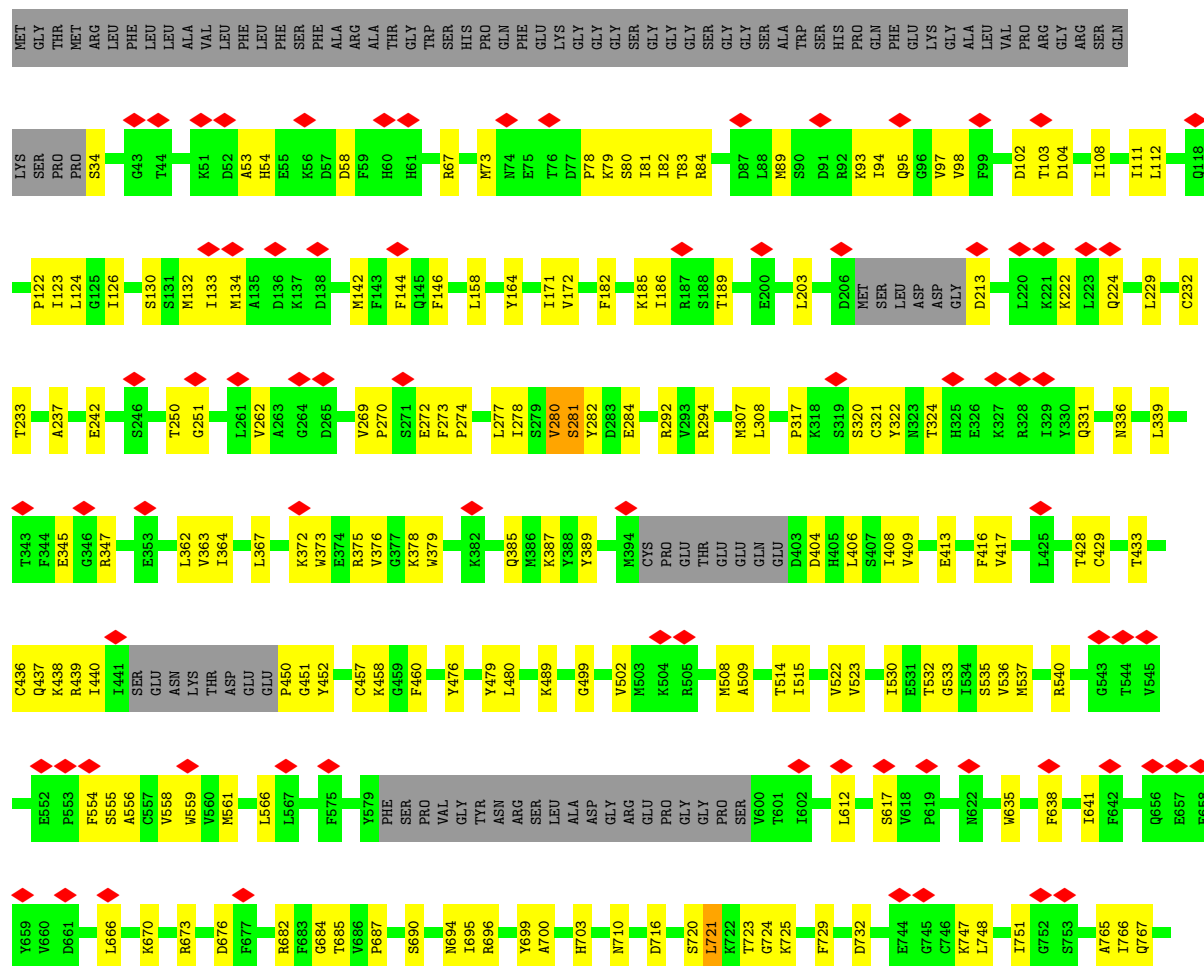
- Molecule 1: Glutamate receptor ionotropic, NMDA 1

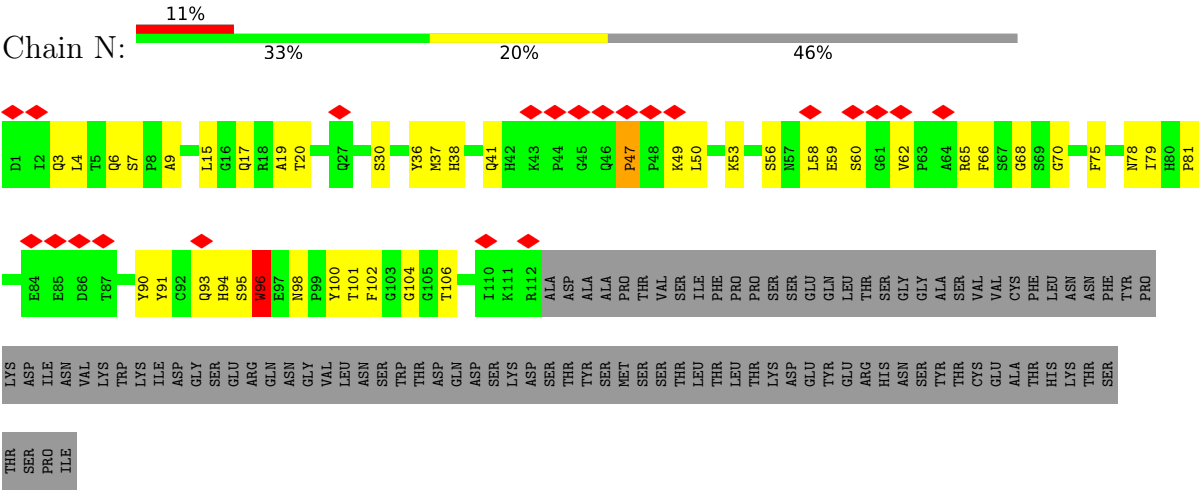






• Molecule 2: Glutamate receptor ionotropic, NMDA 2B





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74886	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	7.954	Depositor
Minimum map value	-1.591	Depositor
Average map value	0.044	Depositor
Map value standard deviation	0.420	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	0.25	0/6323	0.60	0/8556
1	C	0.25	0/6323	0.60	0/8556
2	B	0.27	0/6213	0.67	0/8413
2	D	0.27	0/6220	0.67	1/8424 (0.0%)
3	H	0.21	0/911	0.51	2/1230 (0.2%)
3	M	0.21	0/911	0.51	2/1230 (0.2%)
4	L	0.24	0/899	0.60	0/1221
4	N	0.24	0/899	0.60	0/1221
All	All	0.26	0/28699	0.63	5/38851 (0.0%)

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	10
1	C	0	10
2	B	0	7
2	D	0	8
4	L	0	4
4	N	0	4
All	All	0	43

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	800	ILE	N-CA-C	-7.87	104.08	111.48
3	M	102	ASP	CA-C-N	6.13	132.74	121.70
3	M	102	ASP	C-N-CA	6.13	132.74	121.70
3	H	102	ASP	CA-C-N	6.12	132.71	121.70
3	H	102	ASP	C-N-CA	6.12	132.71	121.70

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	367	ARG	Peptide
1	A	396	ASN	Peptide
1	A	462	ASP	Peptide
1	A	475	CYS	Peptide
1	A	491	MET	Peptide
1	A	492	GLN	Peptide
1	A	577	GLN	Peptide
1	A	700	PHE	Peptide
1	A	765	CYS	Peptide
1	A	822	ARG	Peptide
2	B	280	VAL	Peptide
2	B	281	SER	Peptide
2	B	331	GLN	Peptide
2	B	53	ALA	Peptide
2	B	617	SER	Peptide
2	B	802	HIS	Peptide
2	B	823	TYR	Peptide
1	C	367	ARG	Peptide
1	C	396	ASN	Peptide
1	C	462	ASP	Peptide
1	C	475	CYS	Peptide
1	C	491	MET	Peptide
1	C	492	GLN	Peptide
1	C	577	GLN	Peptide
1	C	700	PHE	Peptide
1	C	765	CYS	Peptide
1	C	822	ARG	Peptide
2	D	280	VAL	Peptide
2	D	281	SER	Peptide
2	D	331	GLN	Peptide
2	D	53	ALA	Peptide
2	D	617	SER	Peptide
2	D	801	CYS	Peptide
2	D	802	HIS	Peptide
2	D	823	TYR	Peptide
4	L	47	PRO	Peptide
4	L	93	GLN	Peptide
4	L	96	TRP	Peptide
4	L	98	ASN	Peptide
4	N	47	PRO	Peptide

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Mol	Chain	Res	Type	Group
4	N	93	GLN	Peptide
4	N	96	TRP	Peptide
4	N	98	ASN	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	6194	0	6187	99	0
1	C	6194	0	6187	99	0
2	B	6079	0	6025	127	0
2	D	6085	0	6031	118	0
3	H	893	0	858	30	0
3	M	893	0	858	26	0
4	L	875	0	839	28	0
4	N	875	0	839	27	0
All	All	28088	0	27824	536	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 (536) 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:D:80:SER:HA	2:D:83:THR:HG22	1.68	0.76
2:B:80:SER:HA	2:B:83:THR:HG22	1.69	0.73
1:A:569:ARG:HH22	1:A:678:LEU:H	1.39	0.70
1:C:569:ARG:HH22	1:C:678:LEU:H	1.39	0.69
2:D:540:ARG:HH21	2:D:747:LYS:HA	1.59	0.68
2:D:509:ALA:HB3	2:D:765:ALA:HB3	1.76	0.68
2:B:509:ALA:HB3	2:B:765:ALA:HB3	1.78	0.66
2:D:172:VAL:HG12	2:D:203:LEU:HB2	1.78	0.66
2:B:172:VAL:HG12	2:B:203:LEU:HB2	1.78	0.66
1:A:426:GLN:H	1:A:430:VAL:HB	1.61	0.66
1:A:158:TYR:O	1:A:411:ARG:NH2	2.29	0.65
2:B:82:ILE:HD11	2:B:111:ILE:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:556:ALA:HA	2:D:559:TRP:HB3	1.77	0.65
2:B:540:ARG:HH21	2:B:747:LYS:HA	1.59	0.65
1:C:426:GLN:H	1:C:430:VAL:HB	1.61	0.65
1:C:158:TYR:O	1:C:411:ARG:NH2	2.29	0.65
2:D:282:TYR:HB3	2:D:363:VAL:HB	1.79	0.65
3:M:36:TRP:HB3	3:M:48:VAL:HB	1.79	0.64
1:C:421:ILE:HG22	1:C:533:MET:HB2	1.78	0.64
2:D:700:ALA:O	2:D:703:HIS:ND1	2.30	0.64
2:B:282:TYR:HB3	2:B:363:VAL:HB	1.79	0.64
1:C:590:SER:HA	1:C:593:VAL:HG22	1.78	0.64
3:H:36:TRP:HB3	3:H:48:VAL:HB	1.79	0.64
1:A:590:SER:HA	1:A:593:VAL:HG22	1.78	0.63
2:B:700:ALA:O	2:B:703:HIS:ND1	2.31	0.63
2:D:281:SER:H	2:D:282:TYR:HB2	1.64	0.63
1:A:421:ILE:HG22	1:A:533:MET:HB2	1.78	0.63
1:C:599:TYR:HH	1:C:623:THR:N	1.96	0.63
1:A:599:TYR:HH	1:A:623:THR:N	1.97	0.63
1:C:500:VAL:HG21	1:C:522:MET:HG2	1.82	0.62
1:A:500:VAL:HG21	1:A:522:MET:HG2	1.81	0.62
1:A:829:LEU:HD11	1:A:834:MET:HE3	1.82	0.62
2:B:281:SER:H	2:B:282:TYR:HB2	1.63	0.61
3:M:55:GLY:HA2	3:M:72:ARG:HD3	1.82	0.61
2:D:82:ILE:HD11	2:D:111:ILE:HD12	1.80	0.61
2:D:433:THR:HG22	2:D:458:LYS:HB3	1.82	0.61
2:D:278:ILE:HG23	2:D:364:ILE:HD11	1.83	0.61
1:C:233:ARG:NH1	1:C:261:MET:SD	2.72	0.61
1:C:237:ALA:O	1:C:238:ARG:NH1	2.33	0.61
1:C:829:LEU:HD11	1:C:834:MET:HE3	1.82	0.61
1:A:692:ARG:HH21	2:B:800:ILE:HG21	1.64	0.60
1:A:237:ALA:O	1:A:238:ARG:NH1	2.33	0.60
4:L:70:GLY:HA3	4:L:75:PHE:HA	1.83	0.60
4:N:38:HIS:ND1	4:N:53:LYS:O	2.34	0.60
3:H:55:GLY:HA2	3:H:72:ARG:HD3	1.82	0.60
1:A:233:ARG:NH1	1:A:261:MET:SD	2.72	0.60
2:B:278:ILE:HG23	2:B:364:ILE:HD11	1.83	0.60
1:C:313:VAL:HA	1:C:316:LEU:HB2	1.84	0.60
2:D:522:VAL:O	2:D:767:GLN:NE2	2.35	0.60
4:L:38:HIS:ND1	4:L:53:LYS:O	2.34	0.60
2:B:440:ILE:H	2:B:451:GLY:HA2	1.67	0.60
2:B:433:THR:HG22	2:B:458:LYS:HB3	1.83	0.60
1:C:280:LEU:O	1:C:380:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:440:ILE:H	2:D:451:GLY:HA2	1.67	0.60
1:A:280:LEU:O	1:A:380:ARG:NH1	2.35	0.60
1:C:362:ASN:HD22	1:C:366:ASP:HB3	1.67	0.59
4:N:70:GLY:HA3	4:N:75:PHE:HA	1.83	0.59
2:D:98:VAL:HG12	2:D:124:LEU:HB2	1.84	0.59
1:A:567:ILE:O	1:A:680:ARG:NH2	2.35	0.59
1:C:567:ILE:O	1:C:680:ARG:NH2	2.35	0.59
1:A:313:VAL:HA	1:A:316:LEU:HB2	1.84	0.59
1:A:362:ASN:HD22	1:A:366:ASP:HB3	1.67	0.59
2:B:122:PRO:HA	2:B:142:MET:HG3	1.84	0.59
2:D:277:LEU:H	2:D:367:LEU:HB2	1.67	0.59
2:B:73:MET:HE2	2:B:84:ARG:HD2	1.85	0.59
3:H:82:GLN:NE2	3:H:83:MET:O	2.35	0.59
2:D:171:ILE:HG23	2:D:229:LEU:HB2	1.85	0.59
2:D:696:ARG:HA	2:D:700:ALA:HB3	1.85	0.59
2:B:171:ILE:HG23	2:B:229:LEU:HB2	1.85	0.59
3:M:82:GLN:NE2	3:M:83:MET:O	2.35	0.59
2:B:98:VAL:HG12	2:B:124:LEU:HB2	1.85	0.58
2:B:406:LEU:H	2:B:476:TYR:HA	1.68	0.58
1:C:326:PRO:HB3	1:C:332:ASN:HD22	1.68	0.58
2:D:73:MET:HE2	2:D:84:ARG:HD2	1.84	0.58
2:D:122:PRO:HA	2:D:142:MET:HG3	1.85	0.58
2:B:277:LEU:H	2:B:367:LEU:HB2	1.67	0.58
2:D:673:ARG:HB3	2:D:676:ASP:HB2	1.86	0.58
3:M:98:ARG:NH1	3:M:99:ARG:O	2.36	0.58
2:B:673:ARG:HB3	2:B:676:ASP:HB2	1.85	0.58
1:A:326:PRO:HB3	1:A:332:ASN:HD22	1.68	0.57
3:H:98:ARG:NH1	3:H:99:ARG:O	2.36	0.57
1:A:544:ARG:HH12	1:A:709:SER:HB3	1.69	0.57
1:C:114:TYR:OH	1:C:329:CYS:O	2.22	0.57
2:D:838:SER:HA	2:D:841:LEU:HG	1.86	0.57
1:C:544:ARG:HH12	1:C:709:SER:HB3	1.69	0.57
3:H:20:LEU:HD11	3:H:113:THR:HG21	1.86	0.57
1:A:114:TYR:OH	1:A:329:CYS:O	2.22	0.57
2:D:232:CYS:H	2:D:262:VAL:HG22	1.69	0.57
4:N:49:LYS:NZ	4:N:60:SER:O	2.37	0.57
2:B:522:VAL:O	2:B:767:GLN:NE2	2.37	0.57
2:D:182:PHE:HA	2:D:185:LYS:HD2	1.85	0.56
2:B:232:CYS:H	2:B:262:VAL:HG22	1.69	0.56
1:A:706:LYS:HG3	1:A:731:ASN:HB3	1.87	0.56
2:D:89:MET:HB3	2:D:93:LYS:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:91:THR:HG23	3:M:116:THR:HA	1.88	0.56
3:H:34:MET:H	3:H:51:ILE:HD11	1.70	0.56
2:B:838:SER:HA	2:B:841:LEU:HG	1.87	0.56
3:M:34:MET:H	3:M:51:ILE:HD11	1.70	0.56
1:C:706:LYS:HG3	1:C:731:ASN:HB3	1.87	0.56
2:B:519:ARG:O	2:B:521:GLU:N	2.39	0.56
1:C:91:LEU:HD11	1:C:121:LEU:HB2	1.87	0.56
2:D:406:LEU:H	2:D:476:TYR:HA	1.71	0.56
2:D:685:THR:HG23	2:D:687:PRO:HD3	1.87	0.56
1:C:484:LEU:HD11	1:C:535:VAL:HG11	1.88	0.56
3:M:20:LEU:HD11	3:M:113:THR:HG21	1.86	0.56
1:A:91:LEU:HD11	1:A:121:LEU:HB2	1.87	0.55
2:D:536:VAL:H	2:D:751:ILE:HD12	1.71	0.55
2:B:536:VAL:H	2:B:751:ILE:HD12	1.72	0.55
2:B:824:MET:HB2	2:B:827:ALA:HB3	1.89	0.55
1:A:484:LEU:HD11	1:A:535:VAL:HG11	1.88	0.55
3:H:51:ILE:HG22	3:H:70:ILE:HG21	1.89	0.55
2:B:89:MET:HB3	2:B:93:LYS:HB3	1.89	0.55
4:N:3:GLN:NE2	4:N:102:PHE:O	2.38	0.55
2:B:67:ARG:HE	2:B:93:LYS:HD3	1.71	0.55
2:D:378:LYS:HG2	2:D:385:GLN:HB2	1.89	0.55
4:L:49:LYS:NZ	4:L:60:SER:O	2.37	0.55
3:H:91:THR:HG23	3:H:116:THR:HA	1.88	0.54
2:D:685:THR:HG21	2:D:710:ASN:HA	1.89	0.54
2:B:685:THR:HG23	2:B:687:PRO:HD3	1.89	0.54
2:D:540:ARG:HE	2:D:748:LEU:H	1.54	0.54
2:D:684:GLY:HA3	2:D:729:PHE:HA	1.90	0.54
2:B:540:ARG:HE	2:B:748:LEU:H	1.55	0.54
1:C:32:VAL:N	1:C:91:LEU:O	2.38	0.54
2:D:824:MET:HB2	2:D:827:ALA:HB3	1.90	0.54
4:L:3:GLN:NE2	4:L:4:LEU:O	2.38	0.54
3:M:51:ILE:HG22	3:M:70:ILE:HG21	1.89	0.54
1:A:140:THR:OG1	1:A:141:VAL:N	2.41	0.54
2:B:684:GLY:HA3	2:B:729:PHE:HA	1.90	0.54
2:D:67:ARG:HE	2:D:93:LYS:HD3	1.71	0.54
2:D:409:VAL:HG22	2:D:479:TYR:HD2	1.73	0.54
2:D:666:LEU:HD22	2:D:670:LYS:HG2	1.89	0.54
4:L:65:ARG:HD3	4:L:81:PRO:HG2	1.90	0.54
2:D:95:GLN:HE21	2:D:317:PRO:HD3	1.72	0.54
3:H:52:ASN:O	3:H:72:ARG:NH1	2.41	0.54
2:B:682:ARG:NH2	2:B:724:GLY:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:GLU:HG3	1:A:408:GLU:H	1.73	0.53
2:B:440:ILE:HD12	2:B:450:PRO:HG2	1.90	0.53
2:D:682:ARG:NH2	2:D:724:GLY:O	2.42	0.53
1:A:118:VAL:HG23	1:A:137:PHE:HB3	1.91	0.53
1:A:491:MET:HB3	1:A:492:GLN:HE21	1.74	0.53
2:B:151:GLU:HG3	2:B:185:LYS:HE2	1.90	0.53
3:M:52:ASN:O	3:M:72:ARG:NH1	2.41	0.53
1:A:83:ILE:HD13	1:A:328:GLY:HA2	1.91	0.53
2:D:436:CYS:SG	2:D:457:CYS:N	2.82	0.53
2:B:409:VAL:HG22	2:B:479:TYR:HD2	1.73	0.53
2:B:436:CYS:SG	2:B:457:CYS:N	2.82	0.53
1:C:491:MET:HB3	1:C:492:GLN:HE21	1.74	0.53
1:C:118:VAL:HG23	1:C:137:PHE:HB3	1.91	0.53
1:C:140:THR:OG1	1:C:141:VAL:N	2.41	0.53
1:A:113:PHE:O	1:A:115:ARG:NH1	2.42	0.53
3:H:62:ASP:OD1	3:H:62:ASP:N	2.42	0.53
2:B:685:THR:HG21	2:B:710:ASN:HA	1.91	0.52
1:C:25:LYS:HD2	1:C:317:LEU:HD22	1.91	0.52
2:D:34:SER:OG	2:D:67:ARG:NH1	2.42	0.52
3:H:36:TRP:HB2	3:H:49:ALA:HB3	1.92	0.52
2:B:95:GLN:HE21	2:B:317:PRO:HD3	1.74	0.52
2:B:696:ARG:HA	2:B:700:ALA:HB3	1.91	0.52
2:D:284:GLU:O	2:D:292:ARG:NH1	2.42	0.52
4:N:58:LEU:HB2	4:N:62:VAL:HG21	1.91	0.52
2:B:34:SER:OG	2:B:67:ARG:NH1	2.42	0.52
1:C:277:GLY:HA2	1:C:280:LEU:HB2	1.91	0.52
1:C:406:GLU:HG3	1:C:408:GLU:H	1.73	0.52
2:D:362:LEU:O	2:D:379:TRP:N	2.43	0.52
4:N:65:ARG:HD3	4:N:81:PRO:HG2	1.90	0.52
2:B:284:GLU:O	2:B:292:ARG:NH1	2.42	0.52
2:B:378:LYS:HG2	2:B:385:GLN:HB2	1.91	0.52
1:A:277:GLY:HA2	1:A:280:LEU:HB2	1.91	0.52
4:L:58:LEU:HB2	4:L:62:VAL:HG21	1.91	0.52
4:L:94:HIS:HE1	4:L:96:TRP:HE3	1.58	0.52
3:M:36:TRP:HB2	3:M:49:ALA:HB3	1.92	0.52
1:C:83:ILE:HD13	1:C:328:GLY:HA2	1.91	0.52
1:C:445:PHE:HB3	1:C:449:GLY:HA2	1.92	0.52
3:M:52:ASN:ND2	3:M:57:ASN:OD1	2.43	0.52
1:C:113:PHE:O	1:C:115:ARG:NH1	2.42	0.52
2:D:440:ILE:HD12	2:D:450:PRO:HG2	1.91	0.52
3:H:12:VAL:HG21	3:H:86:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:612:LEU:HB2	2:B:635:TRP:HZ3	1.75	0.52
2:B:723:THR:HG23	2:B:725:LYS:HG2	1.91	0.52
2:D:723:THR:HG23	2:D:725:LYS:HG2	1.91	0.52
3:H:111:GLN:NE2	4:L:45:GLY:O	2.43	0.52
4:N:94:HIS:HE1	4:N:96:TRP:HE3	1.58	0.52
2:B:416:PHE:HA	2:B:460:PHE:HB3	1.92	0.51
3:H:52:ASN:ND2	3:H:57:ASN:OD1	2.43	0.51
1:C:684:ARG:HH22	1:C:768:VAL:HG21	1.75	0.51
3:M:68:PHE:HA	3:M:83:MET:HA	1.92	0.51
1:A:698:ASP:OD1	1:A:698:ASP:N	2.44	0.51
4:L:56:SER:OG	4:L:68:GLY:O	2.29	0.51
2:B:108:ILE:HB	2:B:133:ILE:HD11	1.93	0.51
3:H:68:PHE:HA	3:H:83:MET:HA	1.92	0.51
4:N:3:GLN:NE2	4:N:4:LEU:O	2.38	0.51
2:B:269:VAL:HG13	2:B:273:PHE:HB2	1.93	0.51
2:B:375:ARG:HE	2:B:387:LYS:HD2	1.76	0.51
3:M:12:VAL:HG21	3:M:86:LEU:HD12	1.92	0.51
1:A:216:LEU:HD13	1:A:229:LEU:HD22	1.93	0.51
1:A:684:ARG:HH22	1:A:768:VAL:HG21	1.75	0.51
2:D:108:ILE:HB	2:D:133:ILE:HD11	1.92	0.51
1:A:25:LYS:HD2	1:A:317:LEU:HD22	1.92	0.50
2:B:556:ALA:HA	2:B:559:TRP:HB3	1.92	0.50
2:D:269:VAL:HG13	2:D:273:PHE:HB2	1.93	0.50
1:A:623:THR:HB	1:A:626:SER:HB2	1.93	0.50
1:A:700:PHE:O	1:A:726:HIS:NE2	2.40	0.50
1:C:529:GLY:HA2	1:C:784:ARG:HH21	1.77	0.50
3:H:99:ARG:HA	3:H:106:MET:HA	1.93	0.50
4:L:3:GLN:NE2	4:L:102:PHE:O	2.38	0.50
2:B:784:PHE:HZ	1:C:776:ARG:H	1.60	0.50
1:C:698:ASP:OD1	1:C:698:ASP:N	2.44	0.50
3:M:62:ASP:OD1	3:M:62:ASP:N	2.42	0.50
2:B:320:SER:O	2:B:324:THR:OG1	2.23	0.50
1:A:569:ARG:NH1	1:A:679:ASP:O	2.45	0.50
1:A:115:ARG:HG2	1:A:340:PRO:HG3	1.94	0.49
1:A:445:PHE:HB3	1:A:449:GLY:HA2	1.92	0.49
1:A:461:ASN:O	1:A:470:HIS:N	2.44	0.49
1:A:529:GLY:HA2	1:A:784:ARG:HH21	1.77	0.49
2:D:274:PRO:HD2	2:D:277:LEU:HD11	1.93	0.49
4:N:56:SER:OG	4:N:68:GLY:O	2.29	0.49
2:B:336:ASN:HA	2:B:339:LEU:HB2	1.94	0.49
2:B:413:GLU:H	2:B:417:VAL:HB	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:307:MET:HE3	2:D:308:LEU:HG	1.94	0.49
2:D:375:ARG:HE	2:D:387:LYS:HD2	1.77	0.49
1:A:704:THR:OG1	1:A:705:VAL:N	2.43	0.49
1:C:115:ARG:HG2	1:C:340:PRO:HG3	1.94	0.49
1:C:569:ARG:NH1	1:C:679:ASP:O	2.45	0.49
2:D:213:ASP:N	2:D:213:ASP:OD1	2.45	0.49
2:D:413:GLU:H	2:D:417:VAL:HB	1.77	0.49
3:H:98:ARG:NH1	3:H:107:ASP:OD2	2.46	0.49
4:L:41:GLN:HB2	4:L:90:TYR:HD1	1.77	0.49
3:M:99:ARG:HA	3:M:106:MET:HA	1.93	0.49
1:A:848:GLY:HA2	1:A:851:LEU:HB2	1.94	0.49
2:B:537:MET:HE2	2:B:721:LEU:HD21	1.94	0.49
1:C:692:ARG:HH21	2:D:800:ILE:HG12	1.77	0.49
3:M:98:ARG:NH1	3:M:107:ASP:OD2	2.46	0.49
2:B:213:ASP:OD1	2:B:213:ASP:N	2.46	0.49
2:B:274:PRO:HD2	2:B:277:LEU:HD11	1.94	0.49
2:B:362:LEU:O	2:B:379:TRP:N	2.44	0.49
1:C:542:ASN:OD1	1:C:542:ASN:N	2.46	0.49
1:C:216:LEU:HD13	1:C:229:LEU:HD22	1.93	0.49
1:A:225:VAL:HG13	1:A:229:LEU:HD12	1.95	0.49
1:C:461:ASN:O	1:C:470:HIS:N	2.44	0.49
2:D:537:MET:HE2	2:D:721:LEU:HD21	1.95	0.49
2:D:612:LEU:HB2	2:D:635:TRP:HZ3	1.78	0.49
2:B:535:SER:OG	2:B:536:VAL:N	2.46	0.49
1:C:848:GLY:HA2	1:C:851:LEU:HB2	1.94	0.49
1:A:51:LYS:HG3	1:A:52:ARG:HG3	1.95	0.49
1:A:131:LYS:NZ	1:A:137:PHE:O	2.42	0.49
2:B:514:THR:OG1	2:B:515:ILE:N	2.46	0.49
1:C:531:ALA:O	1:C:784:ARG:NH2	2.46	0.49
2:D:416:PHE:HA	2:D:460:PHE:HB3	1.94	0.49
4:N:66:PHE:HB3	4:N:79:ILE:HG12	1.95	0.49
2:B:185:LYS:O	2:B:189:THR:OG1	2.27	0.48
2:D:320:SER:O	2:D:324:THR:OG1	2.23	0.48
2:D:695:ILE:O	2:D:699:TYR:N	2.42	0.48
1:A:32:VAL:N	1:A:91:LEU:O	2.38	0.48
2:D:242:GLU:HG3	2:D:272:GLU:HG3	1.95	0.48
1:C:623:THR:HB	1:C:626:SER:HB2	1.93	0.48
1:A:305:ALA:HA	1:A:308:VAL:HG22	1.95	0.48
1:A:531:ALA:O	1:A:784:ARG:NH2	2.46	0.48
1:C:149:SER:OG	1:C:179:ARG:NH2	2.47	0.48
1:A:542:ASN:N	1:A:542:ASN:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:ARG:H	2:D:784:PHE:HZ	1.60	0.48
2:D:102:ASP:OD1	2:D:102:ASP:N	2.46	0.48
4:N:41:GLN:HB2	4:N:90:TYR:HD1	1.77	0.48
2:D:89:MET:HB2	2:D:94:ILE:HG12	1.94	0.48
4:L:95:SER:HB2	4:L:100:TYR:HA	1.95	0.48
2:B:102:ASP:OD1	2:B:102:ASP:N	2.46	0.48
2:D:535:SER:OG	2:D:536:VAL:N	2.46	0.48
1:C:225:VAL:HG13	1:C:229:LEU:HD12	1.95	0.48
1:C:305:ALA:HA	1:C:308:VAL:HG22	1.95	0.48
1:A:559:LEU:HA	1:A:753:ASP:HA	1.96	0.48
2:D:132:MET:HB3	2:D:132:MET:HE3	1.75	0.48
2:D:499:GLY:HA2	2:D:502:VAL:HG12	1.95	0.48
2:D:555:SER:O	2:D:559:TRP:N	2.46	0.48
2:B:242:GLU:HG3	2:B:272:GLU:HG3	1.95	0.48
1:C:51:LYS:HG3	1:C:52:ARG:HG3	1.95	0.48
4:L:37:MET:HE3	4:L:37:MET:HB2	1.70	0.48
2:B:345:GLU:OE1	2:B:347:ARG:NH2	2.47	0.47
2:D:336:ASN:HA	2:D:339:LEU:HB2	1.95	0.47
2:D:438:LYS:HB2	2:D:480:LEU:HD12	1.97	0.47
2:B:307:MET:HE3	2:B:308:LEU:HG	1.95	0.47
2:B:348:ASP:OD1	2:B:348:ASP:N	2.46	0.47
1:C:559:LEU:HA	1:C:753:ASP:HA	1.96	0.47
2:D:345:GLU:OE1	2:D:347:ARG:NH2	2.46	0.47
2:D:514:THR:OG1	2:D:515:ILE:N	2.47	0.47
4:N:95:SER:HB2	4:N:100:TYR:HA	1.95	0.47
1:A:149:SER:OG	1:A:179:ARG:NH2	2.47	0.47
2:B:332:SER:OG	3:H:102:ASP:OD1	2.30	0.47
3:M:52:ASN:HD22	3:M:57:ASN:H	1.62	0.47
1:C:169:ASP:OD1	1:C:174:ARG:NH1	2.47	0.47
2:D:428:THR:OG1	2:D:429:CYS:N	2.47	0.47
1:A:801:HIS:ND1	1:A:802:GLU:OE2	2.40	0.47
1:C:452:VAL:HG21	1:C:477:TYR:HE1	1.79	0.47
4:L:66:PHE:HB3	4:L:79:ILE:HG12	1.95	0.47
3:M:47:LEU:HD21	4:N:100:TYR:HB2	1.96	0.47
1:A:452:VAL:HG21	1:A:477:TYR:HE1	1.79	0.47
2:B:321:CYS:SG	2:B:322:TYR:N	2.88	0.47
2:D:367:LEU:HA	2:D:373:TRP:HA	1.96	0.47
4:L:30:SER:HA	4:L:36:TYR:HD1	1.80	0.47
4:N:30:SER:HA	4:N:36:TYR:HD1	1.80	0.47
1:A:519:TRP:HE1	1:A:547:TYR:HE2	1.63	0.47
2:B:58:ASP:OD2	2:B:294:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:6:GLU:HB3	3:H:113:THR:HB	1.97	0.47
3:H:52:ASN:HD22	3:H:57:ASN:H	1.62	0.47
1:A:169:ASP:OD1	1:A:174:ARG:NH1	2.47	0.47
2:B:428:THR:OG1	2:B:429:CYS:N	2.47	0.47
4:L:50:LEU:HG	4:L:59:GLU:HG3	1.96	0.47
2:B:367:LEU:HA	2:B:373:TRP:HA	1.97	0.46
1:C:700:PHE:O	1:C:726:HIS:NE2	2.40	0.46
2:B:515:ILE:HG22	2:B:519:ARG:HB3	1.96	0.46
1:C:79:CYS:HB2	1:C:329:CYS:HB3	1.46	0.46
4:N:95:SER:OG	4:N:96:TRP:N	2.47	0.46
2:B:438:LYS:HB2	2:B:480:LEU:HD12	1.97	0.46
1:A:155:MET:HG2	1:A:210:PRO:HB3	1.97	0.46
1:A:703:ALA:HA	1:A:727:MET:HB2	1.97	0.46
1:C:155:MET:HG2	1:C:210:PRO:HB3	1.97	0.46
1:A:238:ARG:HA	1:A:238:ARG:HD3	1.79	0.46
1:C:783:MET:HB3	1:C:783:MET:HE2	1.85	0.46
1:C:560:THR:OG1	1:C:561:ILE:N	2.45	0.46
1:C:706:LYS:N	1:C:732:TYR:O	2.48	0.46
1:A:579:PHE:HB3	2:B:813:LEU:HB2	1.98	0.46
1:C:139:ARG:HB3	1:C:366:ASP:HA	1.98	0.46
1:C:163:ILE:HA	1:C:239:VAL:HB	1.98	0.46
1:C:184:LEU:HD11	1:C:211:LYS:HA	1.98	0.46
1:C:697:SER:OG	1:C:698:ASP:N	2.49	0.46
1:C:808:ASP:HA	1:C:811:LYS:HE2	1.98	0.46
2:D:89:MET:O	2:D:93:LYS:N	2.48	0.46
4:L:9:ALA:HA	4:L:106:THR:HG22	1.98	0.46
3:M:6:GLU:HB3	3:M:113:THR:HB	1.97	0.46
1:A:163:ILE:HA	1:A:239:VAL:HB	1.98	0.46
2:D:307:MET:HE2	2:D:307:MET:HB3	1.85	0.46
1:A:184:LEU:HD11	1:A:211:LYS:HA	1.98	0.45
1:A:360:GLU:OE1	1:A:368:LYS:NZ	2.46	0.45
2:B:666:LEU:HD22	2:B:670:LYS:HG2	1.98	0.45
1:C:579:PHE:HB3	2:D:813:LEU:HB2	1.98	0.45
2:D:185:LYS:O	2:D:189:THR:OG1	2.27	0.45
2:D:408:ILE:HG12	2:D:508:MET:HB3	1.97	0.45
1:A:425:HIS:CD2	1:A:432:VAL:HG22	2.52	0.45
1:A:361:PHE:HB3	1:A:365:GLY:HA2	1.99	0.45
1:A:808:ASP:HA	1:A:811:LYS:HE2	1.98	0.45
2:B:552:GLU:O	2:B:556:ALA:HB2	2.15	0.45
2:D:134:MET:HG2	2:D:146:PHE:HZ	1.81	0.45
2:D:321:CYS:SG	2:D:322:TYR:N	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:42:GLU:O	3:M:44:ARG:NH1	2.49	0.45
2:B:555:SER:O	2:B:559:TRP:N	2.49	0.45
1:C:238:ARG:HD3	1:C:238:ARG:HA	1.80	0.45
2:D:690:SER:O	2:D:694:ASN:ND2	2.49	0.45
4:N:50:LEU:HG	4:N:59:GLU:HG3	1.97	0.45
1:C:75:ALA:O	2:D:79:LYS:NZ	2.50	0.45
1:C:360:GLU:OE1	1:C:368:LYS:NZ	2.46	0.45
1:C:361:PHE:HB3	1:C:365:GLY:HA2	1.99	0.45
1:C:519:TRP:HE1	1:C:547:TYR:HE2	1.63	0.45
1:C:704:THR:OG1	1:C:705:VAL:N	2.43	0.45
2:D:58:ASP:OD2	2:D:294:ARG:NH2	2.48	0.45
2:D:98:VAL:HB	2:D:126:ILE:HD11	1.98	0.45
2:B:829:MET:SD	2:B:832:SER:OG	2.75	0.45
2:D:103:THR:OG1	2:D:104:ASP:N	2.50	0.45
2:D:378:LYS:HE2	2:D:378:LYS:HB3	1.82	0.45
3:H:105:ALA:HB2	4:L:38:HIS:CE1	2.51	0.45
2:D:720:SER:O	2:D:725:LYS:N	2.46	0.45
2:B:169:PHE:O	2:B:200:GLU:N	2.44	0.45
2:B:181:ASP:N	2:B:181:ASP:OD1	2.50	0.45
2:D:164:TYR:HE1	2:D:389:TYR:HA	1.83	0.45
2:D:638:PHE:HA	2:D:641:ILE:HG22	1.99	0.45
3:H:42:GLU:O	3:H:44:ARG:NH1	2.49	0.45
1:A:374:ILE:O	1:A:385:VAL:N	2.44	0.44
1:A:697:SER:OG	1:A:698:ASP:N	2.49	0.44
2:D:566:LEU:HD21	2:D:635:TRP:CE2	2.53	0.44
4:L:65:ARG:HH11	4:L:81:PRO:HG2	1.83	0.44
1:C:425:HIS:CD2	1:C:432:VAL:HG22	2.52	0.44
1:C:703:ALA:HA	1:C:727:MET:HB2	1.97	0.44
1:A:139:ARG:HB3	1:A:366:ASP:HA	1.98	0.44
2:B:98:VAL:HB	2:B:126:ILE:HD11	1.98	0.44
1:C:126:SER:O	1:C:129:SER:OG	2.30	0.44
1:C:374:ILE:O	1:C:385:VAL:N	2.44	0.44
2:B:222:LYS:O	2:B:224:GLN:NE2	2.50	0.44
2:B:691:THR:O	2:B:695:ILE:HG12	2.17	0.44
1:C:281:ARG:HE	1:C:281:ARG:HB2	1.68	0.44
2:D:489:LYS:HE2	2:D:489:LYS:HB3	1.78	0.44
2:B:720:SER:O	2:B:725:LYS:N	2.46	0.44
2:D:78:PRO:HA	2:D:81:ILE:HB	1.99	0.44
4:L:19:ALA:HB3	4:L:79:ILE:HB	2.00	0.44
3:M:85:SER:O	3:M:85:SER:OG	2.24	0.44
2:D:523:VAL:HA	2:D:767:GLN:HE22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:98:ARG:HB3	3:M:108:TYR:HB2	1.99	0.44
1:C:374:ILE:HG13	1:C:394:ILE:HD11	2.00	0.44
1:C:649:SER:HB2	2:D:832:SER:HB2	2.00	0.44
4:N:65:ARG:HH11	4:N:81:PRO:HG2	1.83	0.44
1:C:686:THR:OG1	1:C:687:GLY:N	2.51	0.44
3:H:98:ARG:HB3	3:H:108:TYR:HB2	1.99	0.44
4:N:9:ALA:HA	4:N:106:THR:HG22	1.98	0.44
1:A:686:THR:OG1	1:A:687:GLY:N	2.51	0.44
2:B:298:ALA:O	2:B:302:THR:OG1	2.24	0.43
4:L:95:SER:HA	4:L:101:THR:H	1.83	0.43
2:B:89:MET:O	2:B:94:ILE:N	2.51	0.43
2:B:532:THR:OG1	2:B:533:GLY:N	2.51	0.43
2:B:554:PHE:HA	1:C:830:THR:HG23	2.00	0.43
2:B:566:LEU:HD21	2:B:635:TRP:CE2	2.53	0.43
1:C:597:MET:HB2	1:C:597:MET:HE2	1.74	0.43
1:A:560:THR:OG1	1:A:561:ILE:N	2.45	0.43
2:B:78:PRO:HA	2:B:81:ILE:HB	2.00	0.43
2:B:89:MET:O	2:B:93:LYS:N	2.51	0.43
2:B:638:PHE:HA	2:B:641:ILE:HG22	1.99	0.43
4:N:19:ALA:HB3	4:N:79:ILE:HB	2.00	0.43
2:B:458:LYS:HE3	2:B:458:LYS:HB2	1.86	0.43
1:A:374:ILE:HG13	1:A:394:ILE:HD11	2.00	0.43
2:D:439:ARG:HA	2:D:451:GLY:HA2	2.00	0.43
2:D:532:THR:OG1	2:D:732:ASP:OD1	2.32	0.43
3:H:111:GLN:HE22	4:L:46:GLN:HA	1.82	0.43
2:B:437:GLN:NE2	2:B:451:GLY:O	2.52	0.43
2:B:732:ASP:OD2	2:B:762:TYR:OH	2.33	0.43
3:H:58:THR:HG21	3:H:70:ILE:HB	2.01	0.43
4:N:37:MET:HB2	4:N:37:MET:HE3	1.70	0.43
2:D:720:SER:HB2	2:D:725:LYS:HB2	2.01	0.43
2:B:48:VAL:HA	2:B:51:LYS:HD3	2.00	0.43
2:B:759:SER:O	2:B:759:SER:OG	2.33	0.43
2:D:437:GLN:NE2	2:D:451:GLY:O	2.52	0.43
2:B:103:THR:OG1	2:B:104:ASP:N	2.50	0.43
1:C:421:ILE:HG13	1:C:497:VAL:HG22	2.01	0.43
4:L:6:GLN:HG3	4:L:104:GLY:H	1.84	0.43
4:N:36:TYR:HB3	4:N:94:HIS:CD2	2.54	0.43
4:N:95:SER:HA	4:N:101:THR:H	1.83	0.43
1:A:706:LYS:N	1:A:732:TYR:O	2.48	0.42
2:B:89:MET:HB2	2:B:94:ILE:HG12	2.01	0.42
2:D:158:LEU:HD11	2:D:186:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:222:LYS:O	2:D:224:GLN:NE2	2.52	0.42
2:D:530:ILE:HD12	2:D:530:ILE:HA	1.95	0.42
2:B:617:SER:OG	2:B:618:VAL:N	2.42	0.42
1:A:421:ILE:HG13	1:A:497:VAL:HG22	2.01	0.42
1:A:662:MET:HE2	1:A:662:MET:HB2	1.89	0.42
2:B:627:THR:HA	2:B:630:ILE:HD12	2.01	0.42
2:B:408:ILE:HG12	2:B:508:MET:HB3	2.01	0.42
2:B:489:LYS:HB3	2:B:489:LYS:HE2	1.78	0.42
3:H:34:MET:O	3:H:99:ARG:NH1	2.53	0.42
4:L:107:LYS:HA	4:L:107:LYS:HD2	1.94	0.42
1:A:783:MET:HE1	1:A:789:TRP:HB2	2.02	0.42
2:B:364:ILE:HG13	2:B:376:VAL:HB	2.01	0.42
2:B:523:VAL:HA	2:B:767:GLN:HE22	1.83	0.42
1:C:161:ASN:OD1	1:C:161:ASN:N	2.52	0.42
1:C:226:THR:HG23	1:C:255:ALA:HB1	2.02	0.42
2:D:364:ILE:HG13	2:D:376:VAL:HB	2.01	0.42
4:L:36:TYR:HB3	4:L:94:HIS:CD2	2.54	0.42
1:A:226:THR:HG23	1:A:255:ALA:HB1	2.02	0.42
2:B:134:MET:HG2	2:B:146:PHE:HZ	1.83	0.42
1:C:108:SER:OG	1:C:135:LEU:O	2.38	0.42
1:C:801:HIS:ND1	1:C:802:GLU:OE2	2.40	0.42
3:H:19:LYS:HE3	3:H:19:LYS:HB2	1.89	0.42
1:A:68:LYS:HD3	1:A:68:LYS:HA	1.85	0.42
1:A:108:SER:OG	1:A:135:LEU:O	2.38	0.42
1:A:796:SER:HA	1:A:799:LYS:HD3	2.02	0.42
2:D:122:PRO:HB3	2:D:142:MET:HE3	2.00	0.42
4:N:6:GLN:HG3	4:N:104:GLY:H	1.84	0.42
1:A:75:ALA:O	2:B:79:LYS:NZ	2.53	0.42
2:B:439:ARG:HA	2:B:451:GLY:HA2	2.01	0.42
1:C:426:GLN:O	1:C:430:VAL:N	2.48	0.42
1:C:644:ALA:HA	1:C:645:PRO:HD3	1.91	0.42
3:M:34:MET:O	3:M:99:ARG:NH1	2.53	0.42
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.93	0.42
1:A:426:GLN:O	1:A:430:VAL:N	2.48	0.42
2:D:126:ILE:N	2:D:130:SER:OG	2.53	0.42
4:N:15:LEU:O	4:N:17:GLN:NE2	2.42	0.42
1:A:310:ALA:HA	1:A:313:VAL:HG12	2.02	0.41
1:A:554:PHE:HD1	1:A:797:ILE:HG23	1.85	0.41
1:A:678:LEU:HD23	2:B:809:MET:HG3	2.02	0.41
2:D:404:ASP:OD1	2:D:404:ASP:N	2.53	0.41
2:B:720:SER:HB2	2:B:725:LYS:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:233:THR:O	2:D:237:ALA:N	2.51	0.41
3:M:58:THR:HG21	3:M:70:ILE:HB	2.01	0.41
1:A:161:ASN:OD1	1:A:161:ASN:N	2.53	0.41
2:B:378:LYS:HE2	2:B:378:LYS:HB3	1.82	0.41
2:D:345:GLU:HB2	2:D:347:ARG:HH21	1.86	0.41
2:D:829:MET:SD	2:D:832:SER:OG	2.78	0.41
3:H:85:SER:O	3:H:85:SER:OG	2.24	0.41
1:C:131:LYS:NZ	1:C:137:PHE:O	2.42	0.41
1:C:310:ALA:HA	1:C:313:VAL:HG12	2.02	0.41
2:B:608:LEU:HD13	2:B:621:GLN:H	1.86	0.41
2:B:750:THR:OG1	2:B:751:ILE:N	2.52	0.41
2:D:97:VAL:HG13	2:D:123:ILE:HG22	2.03	0.41
2:D:532:THR:OG1	2:D:533:GLY:N	2.51	0.41
2:B:628:SER:O	2:B:632:VAL:HG23	2.20	0.41
1:C:783:MET:HE1	1:C:789:TRP:HB2	2.02	0.41
2:B:153:GLN:HA	2:B:156:VAL:HG12	2.02	0.41
2:B:280:VAL:HG11	2:B:362:LEU:HD23	2.02	0.41
2:D:797:LEU:HD12	2:D:797:LEU:HA	1.84	0.41
3:H:6:GLU:OE1	3:H:112:GLY:N	2.53	0.41
3:M:6:GLU:OE1	3:M:112:GLY:N	2.53	0.41
4:N:20:THR:HA	4:N:78:ASN:HA	2.03	0.41
1:A:700:PHE:HD1	1:A:700:PHE:HA	1.77	0.41
1:A:783:MET:HB3	1:A:783:MET:HE2	1.85	0.41
2:B:233:THR:O	2:B:237:ALA:N	2.50	0.41
1:C:281:ARG:HA	1:C:380:ARG:HH12	1.86	0.41
2:D:280:VAL:HG11	2:D:362:LEU:HD23	2.01	0.41
3:H:20:LEU:HD12	3:H:20:LEU:HA	1.86	0.41
1:A:166:LEU:HD11	1:A:218:PHE:HB2	2.03	0.41
1:A:371:GLN:NE2	1:A:389:ASN:OD1	2.47	0.41
1:A:442:LYS:NZ	1:A:444:GLU:OE1	2.53	0.41
1:A:597:MET:HE2	1:A:597:MET:HB2	1.74	0.41
1:A:830:THR:HA	2:D:554:PHE:HB3	2.02	0.41
2:B:97:VAL:HG13	2:B:123:ILE:HG22	2.03	0.41
2:B:120:LEU:HD13	2:B:333:ASN:HB2	2.03	0.41
1:C:36:ARG:HA	1:C:36:ARG:HD3	1.98	0.41
1:C:491:MET:HB3	1:C:491:MET:HE3	1.84	0.41
1:C:554:PHE:HD1	1:C:797:ILE:HG23	1.85	0.41
1:C:796:SER:HA	1:C:799:LYS:HD3	2.01	0.41
2:D:108:ILE:HG22	2:D:144:PHE:HE2	1.86	0.41
2:D:558:VAL:HA	2:D:561:MET:HB2	2.02	0.41
2:B:85:ILE:O	2:B:90:SER:OG	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:VAL:HG21	1:C:62:ALA:HB2	2.03	0.41
1:C:323:THR:O	1:C:336:TRP:NE1	2.31	0.41
2:D:389:TYR:HB2	2:D:452:TYR:CZ	2.55	0.41
2:B:389:TYR:HB2	2:B:452:TYR:CZ	2.56	0.40
2:B:536:VAL:HA	2:B:730:ILE:HA	2.03	0.40
1:C:166:LEU:HD11	1:C:218:PHE:HB2	2.03	0.40
4:L:66:PHE:HA	4:L:79:ILE:HA	2.03	0.40
3:M:105:ALA:HB2	4:N:38:HIS:CE1	2.56	0.40
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.87	0.40
2:D:439:ARG:HA	2:D:439:ARG:HD2	1.92	0.40
1:A:323:THR:O	1:A:336:TRP:NE1	2.30	0.40
1:A:763:GLN:NE2	1:A:816:TYR:O	2.54	0.40
2:B:127:HIS:N	2:B:130:SER:OG	2.54	0.40
2:B:345:GLU:HB2	2:B:347:ARG:HH21	1.86	0.40
1:C:263:GLY:H	1:C:266:TYR:HD2	1.69	0.40
1:C:485:ILE:HD13	1:C:485:ILE:HA	1.90	0.40
4:L:18:ARG:HG3	4:L:78:ASN:HD21	1.86	0.40
1:A:397:ASP:OD1	1:A:397:ASP:N	2.53	0.40
2:B:440:ILE:HG12	2:B:453:ILE:HB	2.03	0.40
2:D:250:THR:OG1	2:D:251:GLY:N	2.47	0.40
2:D:372:LYS:HG3	2:D:373:TRP:CD1	2.56	0.40
4:N:6:GLN:HE22	4:N:91:TYR:HA	1.86	0.40
1:A:46:VAL:HG21	1:A:62:ALA:HB2	2.03	0.40
1:A:263:GLY:H	1:A:266:TYR:HD2	1.69	0.40
2:B:126:ILE:N	2:B:130:SER:OG	2.54	0.40
2:B:372:LYS:H	2:B:372:LYS:HG2	1.55	0.40
2:B:372:LYS:HG3	2:B:373:TRP:CD1	2.57	0.40
2:B:488:LYS:HB3	2:B:495:ASN:HD21	1.87	0.40
1:C:763:GLN:NE2	1:C:816:TYR:O	2.54	0.40
2:D:89:MET:O	2:D:94:ILE:N	2.53	0.40
2:D:112:LEU:HD13	2:D:144:PHE:CD1	2.57	0.40
4:L:6:GLN:HE22	4:L:91:TYR:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	774/862 (90%)	693 (90%)	79 (10%)	2 (0%)	36	71
1	C	774/862 (90%)	694 (90%)	78 (10%)	2 (0%)	36	71
2	B	757/883 (86%)	669 (88%)	83 (11%)	5 (1%)	18	55
2	D	760/883 (86%)	672 (88%)	85 (11%)	3 (0%)	30	67
3	H	112/221 (51%)	105 (94%)	7 (6%)	0	100	100
3	M	112/221 (51%)	105 (94%)	7 (6%)	0	100	100
4	L	110/209 (53%)	91 (83%)	17 (16%)	2 (2%)	6	33
4	N	110/209 (53%)	91 (83%)	17 (16%)	2 (2%)	6	33
All	All	3509/4350 (81%)	3120 (89%)	373 (11%)	16 (0%)	26	63

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	803	ASN
2	B	54	HIS
2	B	804	GLU
2	D	54	HIS
1	A	395	PRO
1	C	395	PRO
4	L	96	TRP
4	N	96	TRP
1	A	143	PRO
1	C	143	PRO
2	B	803	ASN
2	B	805	LYS
4	L	47	PRO
4	N	47	PRO
2	B	270	PRO
2	D	270	PRO

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	675/744 (91%)	670 (99%)	5 (1%)	76	79
1	C	675/744 (91%)	670 (99%)	5 (1%)	76	79
2	B	672/762 (88%)	668 (99%)	4 (1%)	78	80
2	D	673/762 (88%)	669 (99%)	4 (1%)	78	80
3	H	97/192 (50%)	95 (98%)	2 (2%)	47	65
3	M	97/192 (50%)	95 (98%)	2 (2%)	47	65
4	L	96/184 (52%)	95 (99%)	1 (1%)	68	76
4	N	96/184 (52%)	95 (99%)	1 (1%)	68	76
All	All	3081/3764 (82%)	3057 (99%)	24 (1%)	70	77

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	VAL
1	A	215	VAL
1	A	476	CYS
1	A	765	CYS
1	A	768	VAL
2	B	302	THR
2	B	716	ASP
2	B	721	LEU
2	B	795	LEU
1	C	118	VAL
1	C	215	VAL
1	C	476	CYS
1	C	765	CYS
1	C	768	VAL
2	D	716	ASP
2	D	721	LEU
2	D	766	ILE
2	D	795	LEU
3	H	85	SER
3	H	88	SER
4	L	7	SER
3	M	85	SER
3	M	88	SER
4	N	7	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	59	GLN
1	A	70	ASN
1	A	86	GLN
1	A	217	GLN
1	A	362	ASN
1	A	376	ASN
1	A	384	GLN
1	A	425	HIS
1	A	492	GLN
1	A	515	ASN
1	A	730	HIS
1	A	731	ASN
1	A	763	GLN
1	A	833	ASN
2	B	60	HIS
2	B	61	HIS
2	B	95	GLN
2	B	105	GLN
2	B	192	ASN
2	B	224	GLN
2	B	336	ASN
2	B	437	GLN
2	B	710	ASN
2	B	711	GLN
2	B	782	GLN
2	B	812	GLN
2	B	840	HIS
1	C	59	GLN
1	C	70	ASN
1	C	86	GLN
1	C	217	GLN
1	C	362	ASN
1	C	376	ASN
1	C	384	GLN
1	C	425	HIS
1	C	492	GLN
1	C	515	ASN
1	C	730	HIS
1	C	763	GLN
1	C	833	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	60	HIS
2	D	61	HIS
2	D	95	GLN
2	D	105	GLN
2	D	192	ASN
2	D	224	GLN
2	D	245	ASN
2	D	336	ASN
2	D	437	GLN
2	D	711	GLN
2	D	782	GLN
2	D	803	ASN
2	D	812	GLN
3	H	5	GLN
3	H	77	ASN
3	H	111	GLN
4	L	78	ASN
4	L	94	HIS
3	M	5	GLN
3	M	77	ASN
3	M	111	GLN
4	N	78	ASN
4	N	94	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
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	4.40
1	C	824:ASN	C	825:ALA	N	4.40

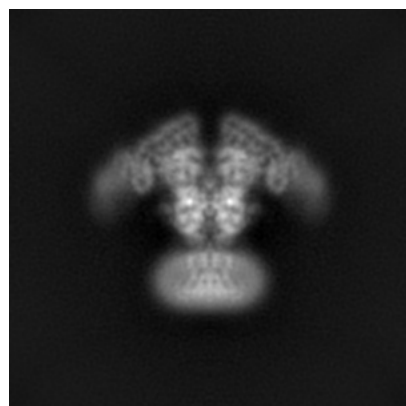
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25852. These allow visual inspection of the internal detail of the map and identification of artifacts.

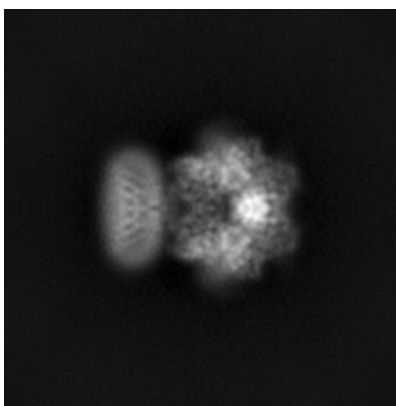
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

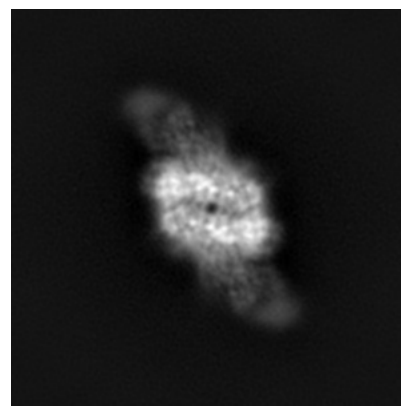
6.1.1 Primary map



X

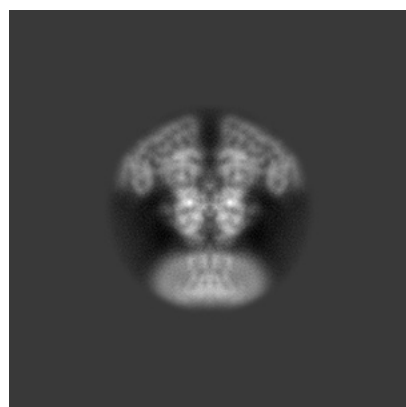


Y

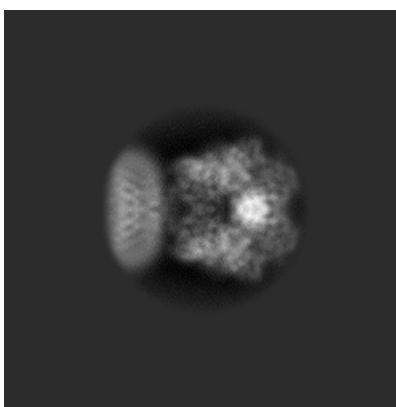


Z

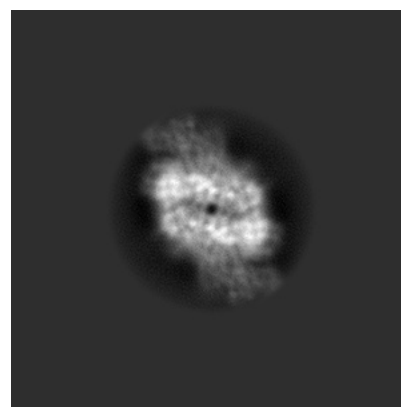
6.1.2 Raw map



X



Y

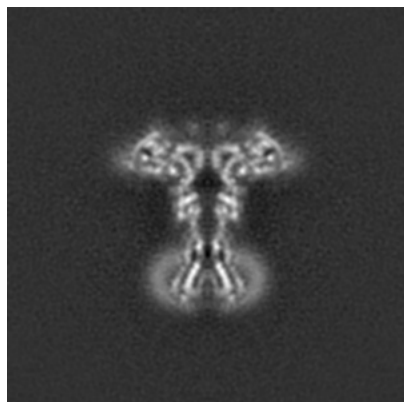


Z

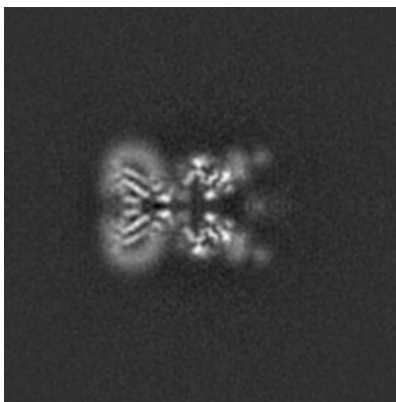
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

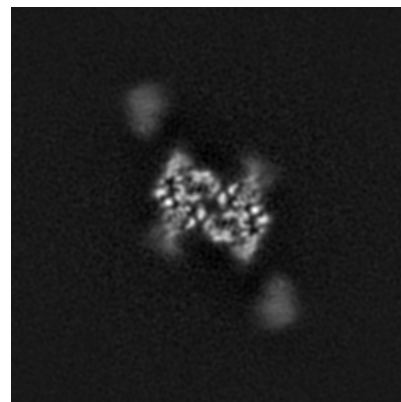
6.2.1 Primary map



X Index: 128

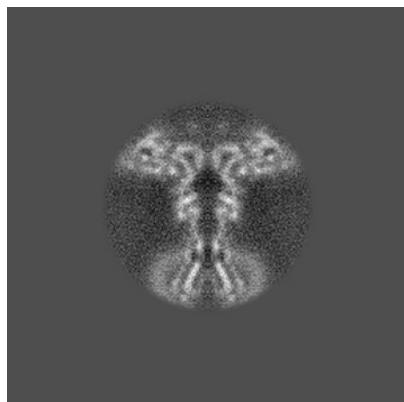


Y Index: 128

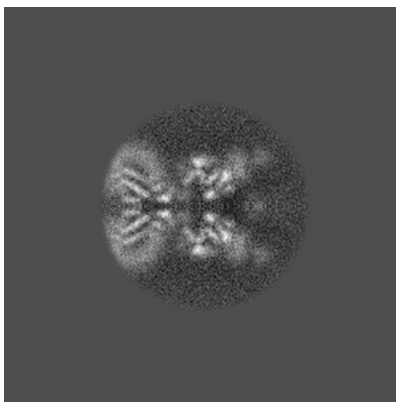


Z Index: 128

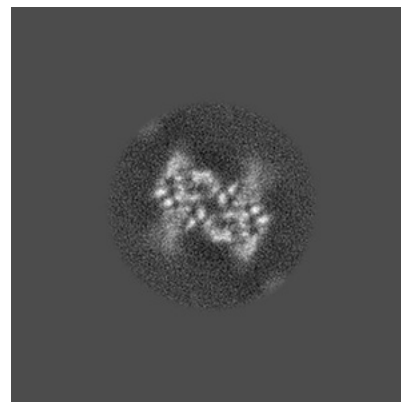
6.2.2 Raw map



X Index: 128



Y Index: 128

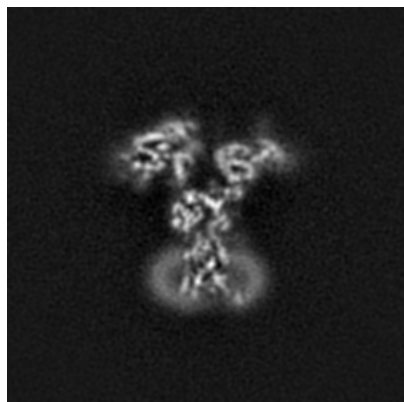


Z Index: 128

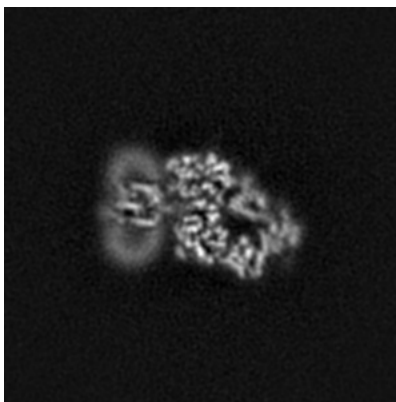
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

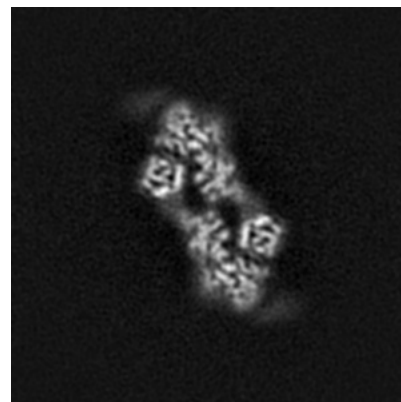
6.3.1 Primary map



X Index: 135

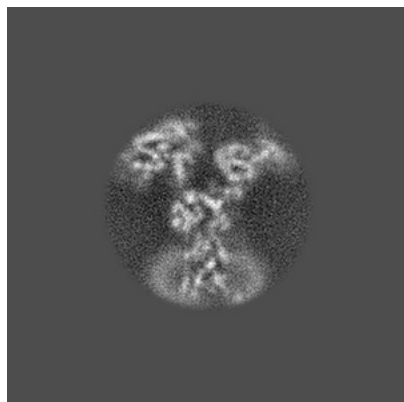


Y Index: 139

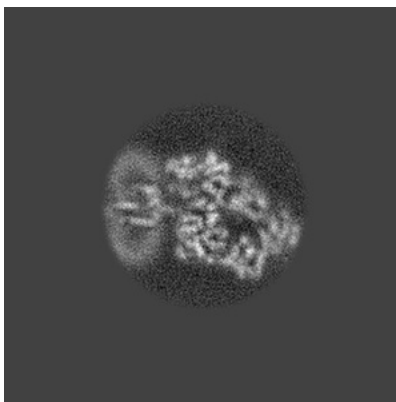


Z Index: 155

6.3.2 Raw map



X Index: 135



Y Index: 140

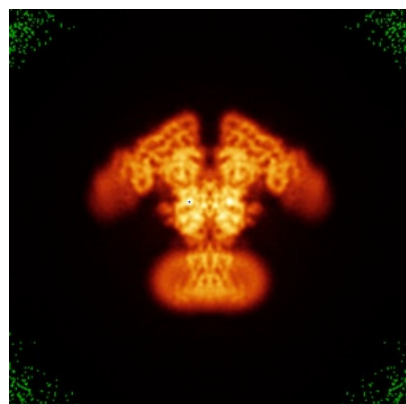


Z Index: 155

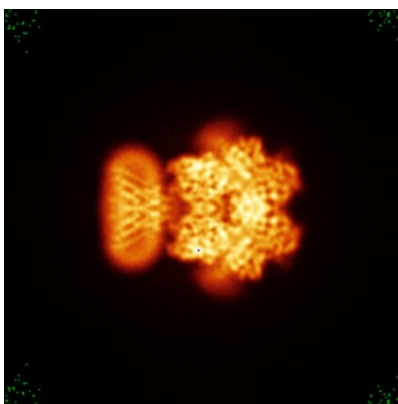
The images above show the largest variance slices of the map in three orthogonal directions.

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

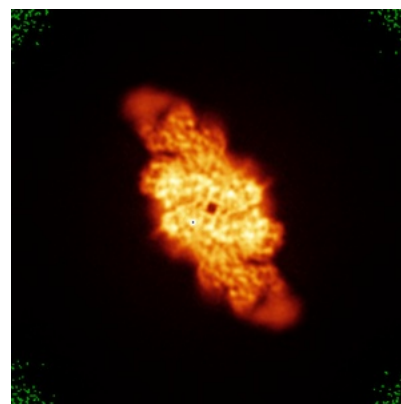
6.4.1 Primary map



X

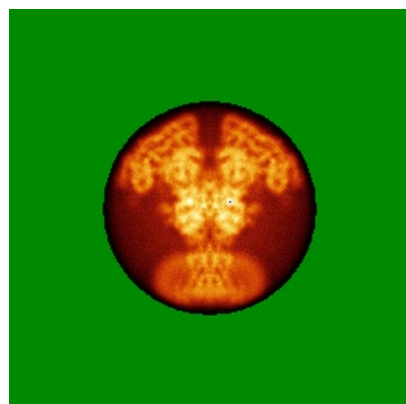


Y

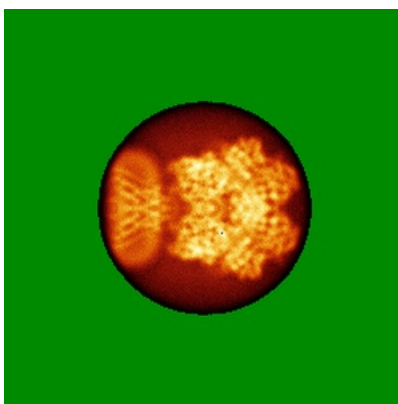


Z

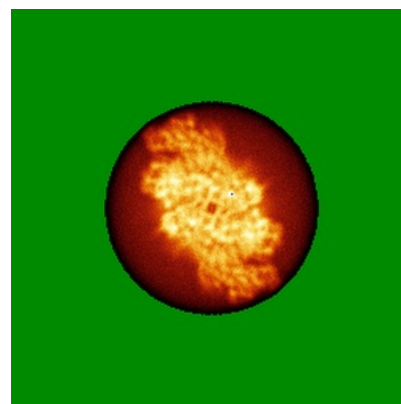
6.4.2 Raw map



X



Y

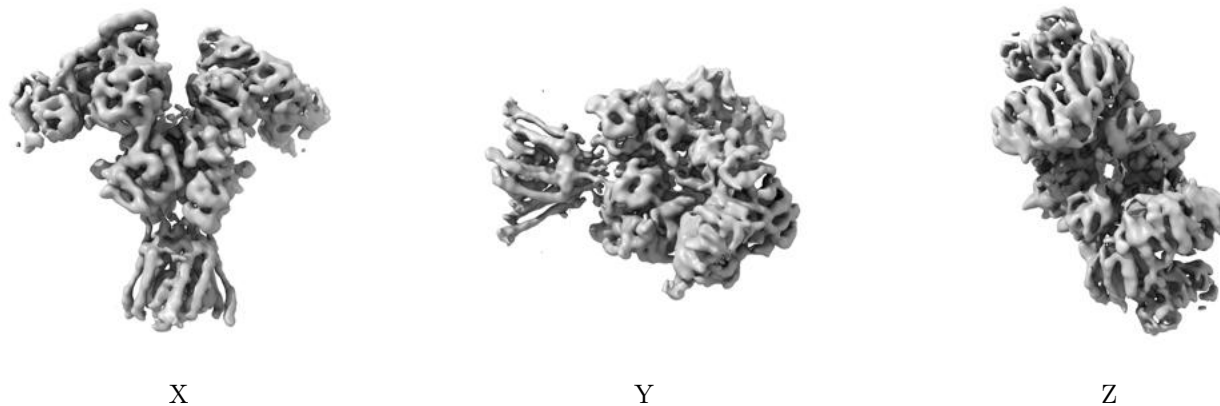


Z

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.

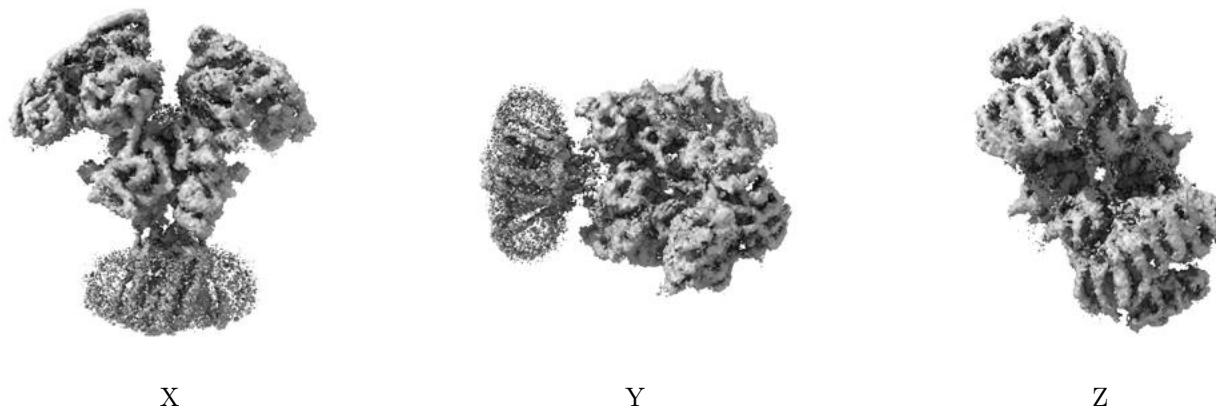
6.5 Orthogonal surface views [i](#)

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.

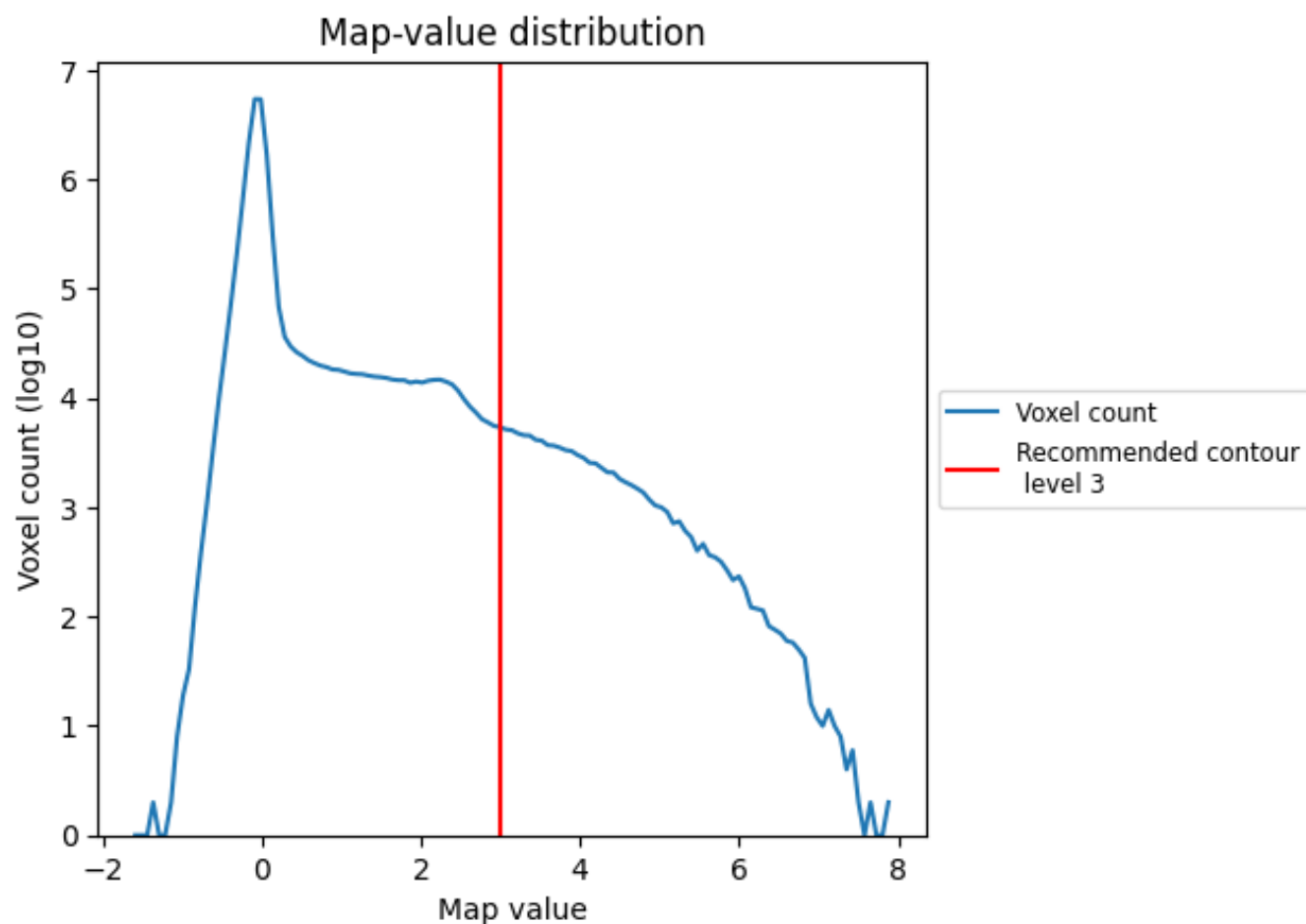
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

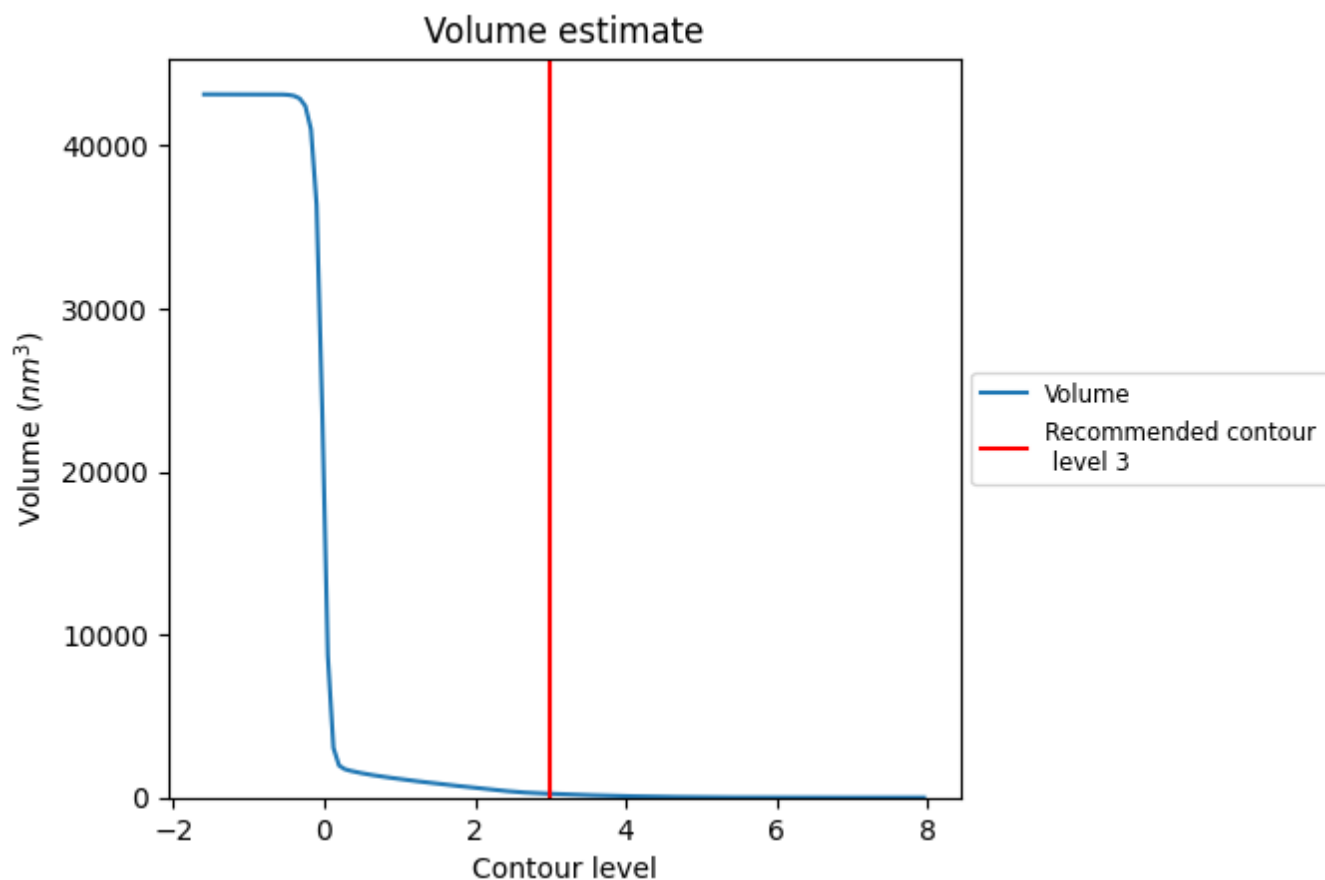
This section contains the results of statistical analysis of the map.

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.

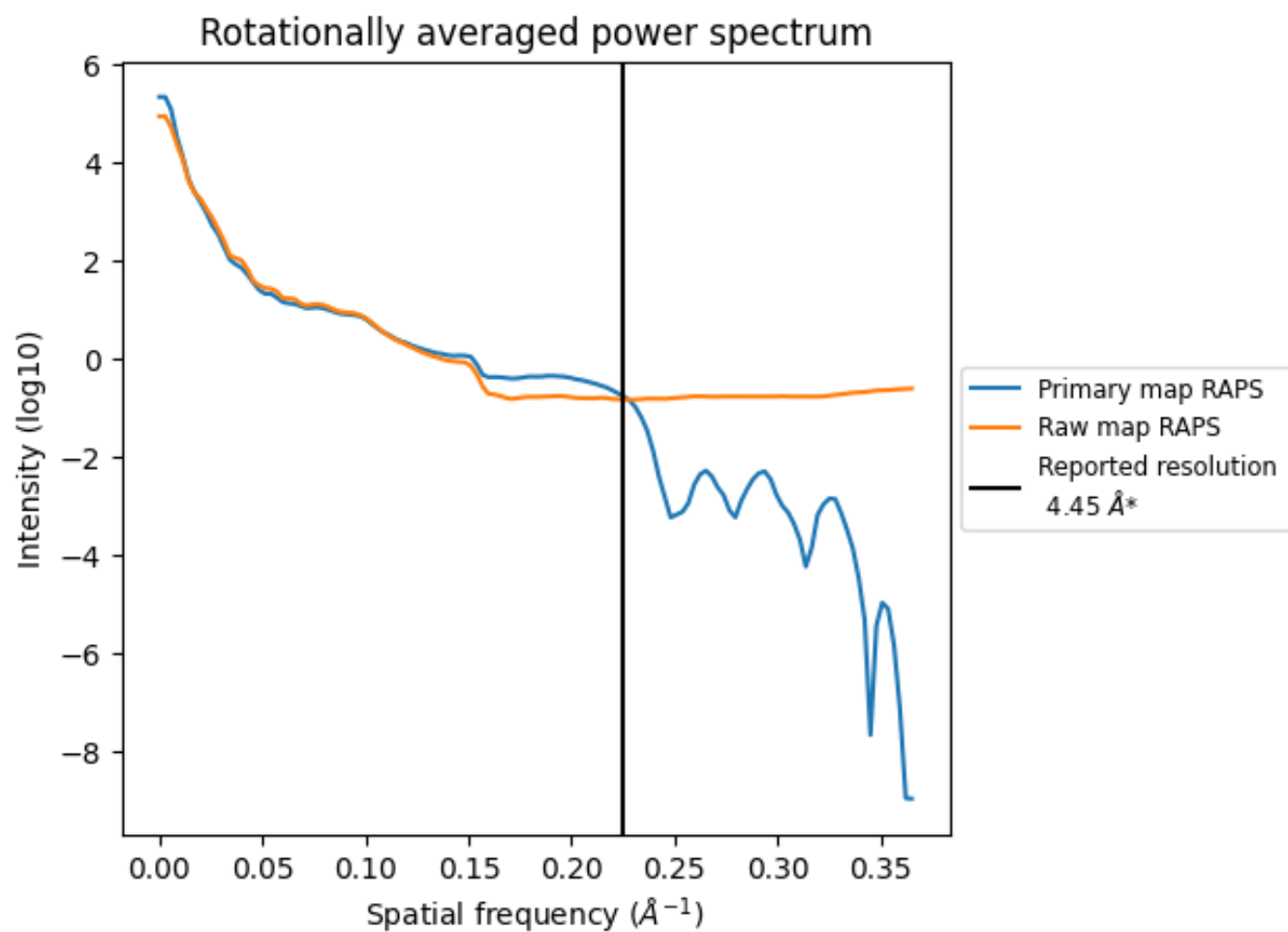
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 233 nm³; this corresponds to an approximate mass of 210 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 ⓘ

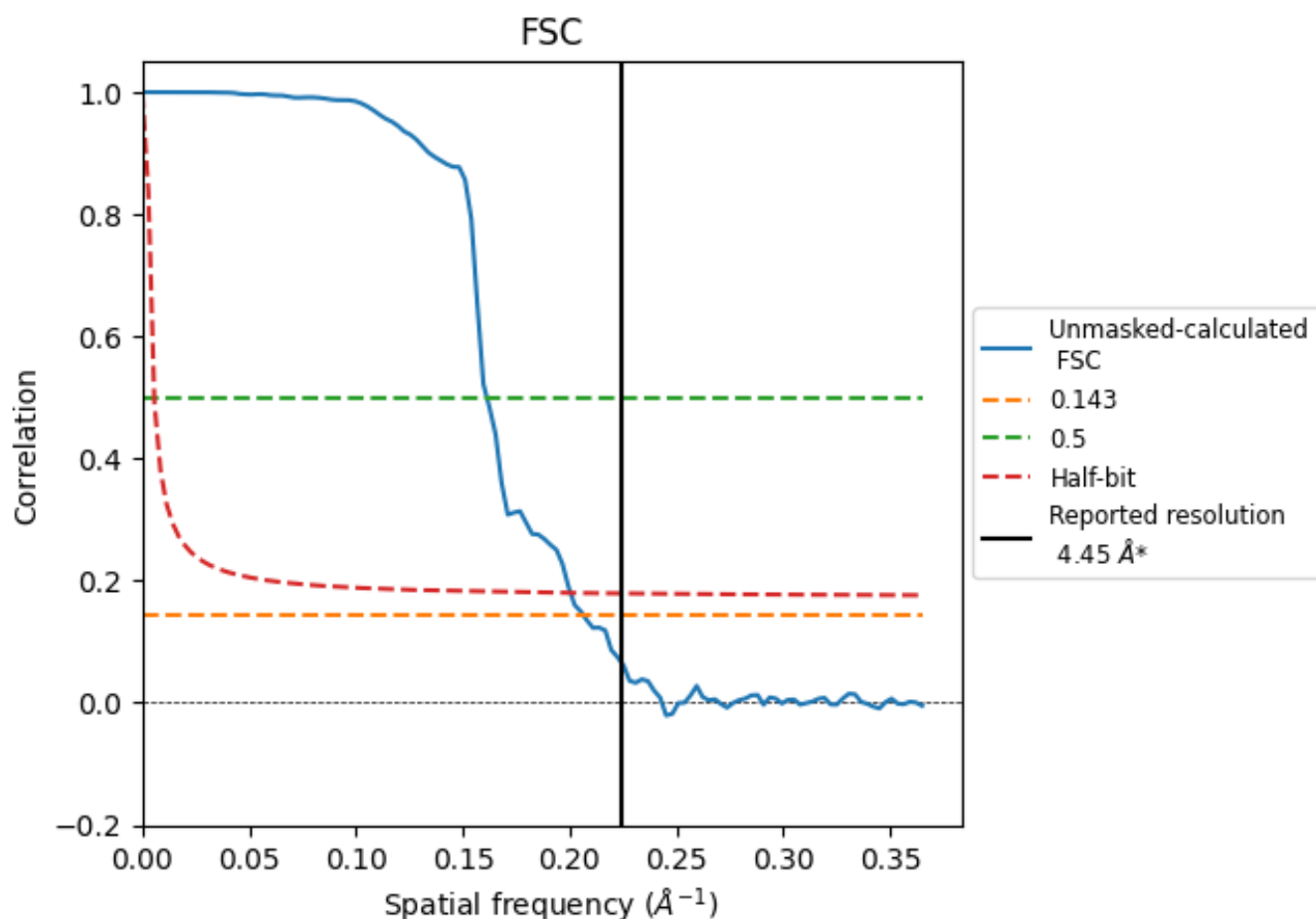


*Reported resolution corresponds to spatial frequency of $0.225 \text{ \AA}^{-1}$

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 0.225 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.45	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.84	6.20	4.99

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

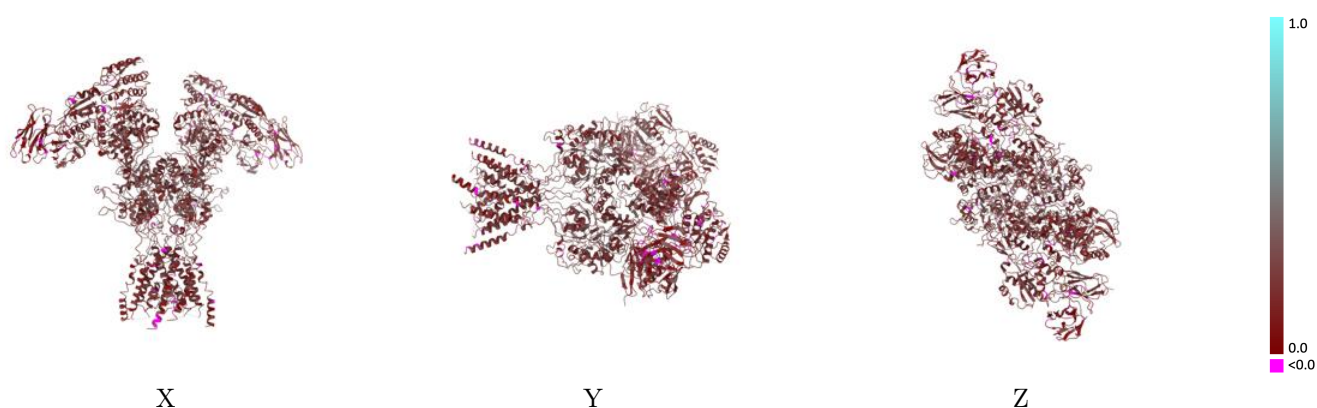
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25852 and PDB model 7TET. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

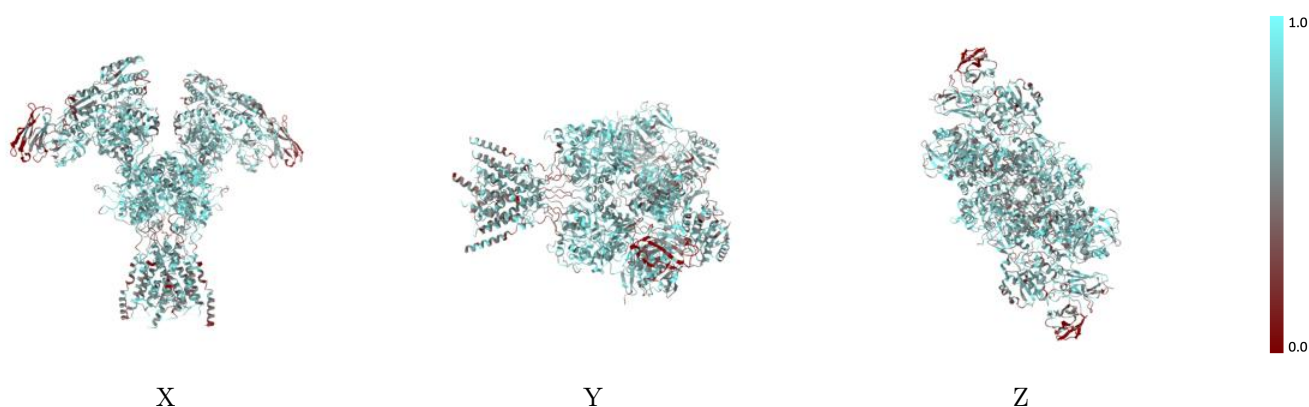
This section was not generated.

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



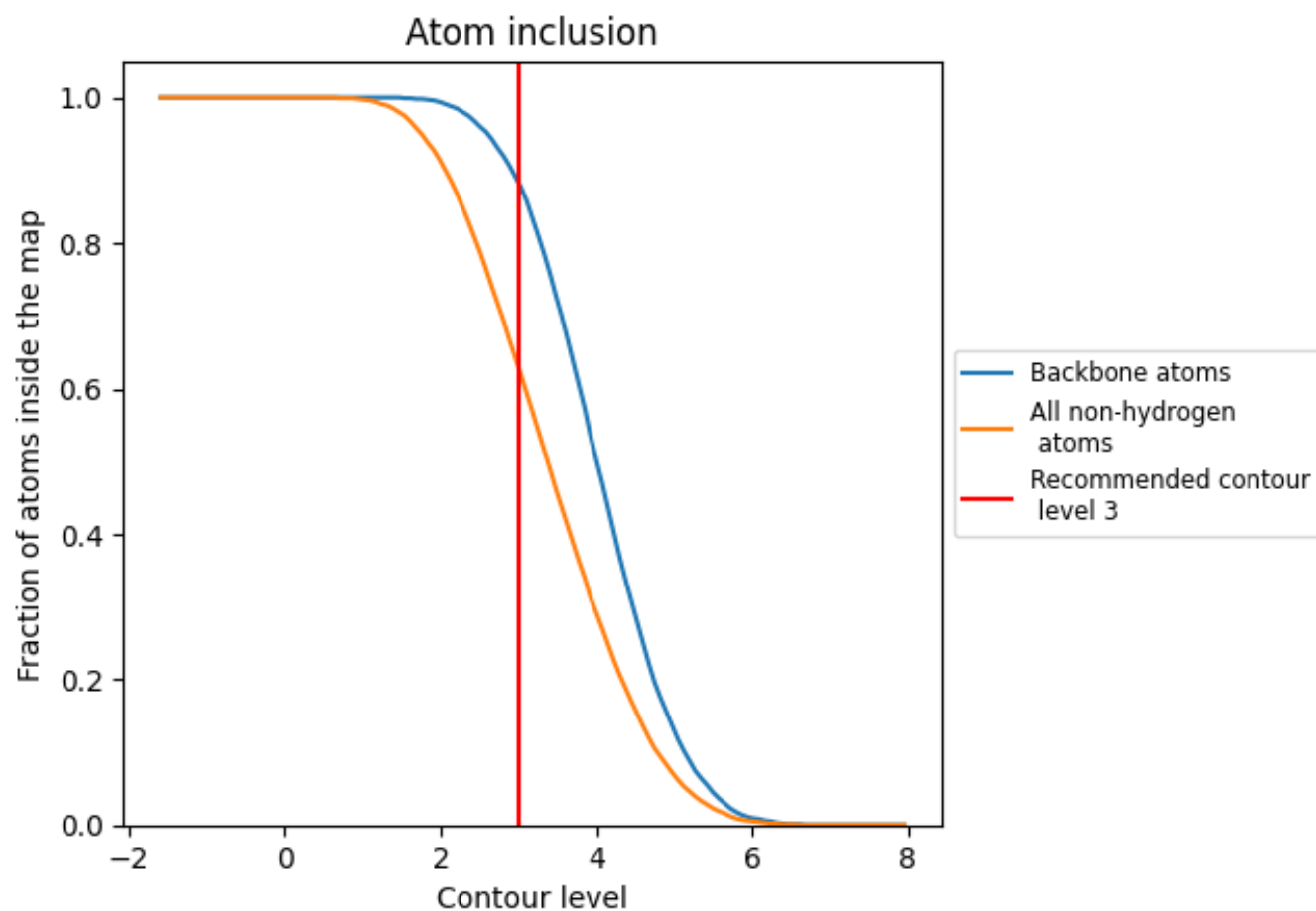
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 88% of all backbone atoms, 63% 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	0.6300	0.2330
A	0.6540	0.2450
B	0.6430	0.2350
C	0.6550	0.2440
D	0.6430	0.2350
H	0.3750	0.1570
L	0.6280	0.2150
M	0.3630	0.1560
N	0.6180	0.2170

1.0

0.0

<0.0