



Full wwPDB EM Validation Report ⓘ

Sep 9, 2024 – 09:17 AM EDT

PDB ID : 8VUS
EMDB ID : EMD-43538
Title : Human GluN1-2A with IgG 007-168
Authors : Michalski, K.; Furukawa, H.
Deposited on : 2024-01-29
Resolution : 3.99 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.dev112
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.3

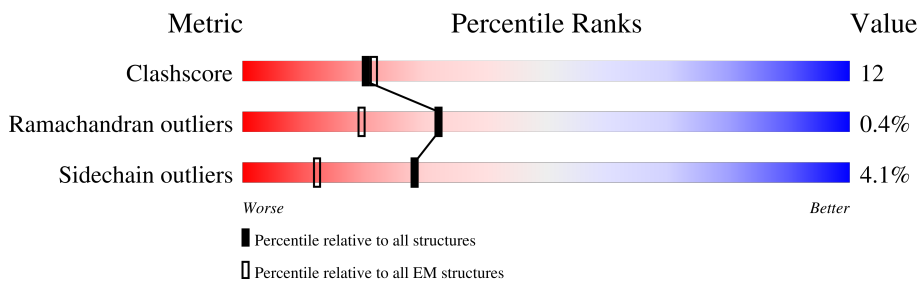
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	211	
1	H	211	
2	F	215	
2	L	215	
3	A	776	
4	B	771	
4	D	771	
5	C	776	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 25006 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 007-168 Heavy.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	207	Total	C	N	O	S	0	0
			1363	859	238	261	5		
1	H	211	Total	C	N	O	S	0	0
			1507	955	253	293	6		

- Molecule 2 is a protein called 007-168 Light.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	215	Total	C	N	O	S	0	0
			1562	974	269	314	5		
2	L	215	Total	C	N	O	S	0	0
			1513	955	261	292	5		

- Molecule 3 is a protein called Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	662	Total	C	N	O	S	0	0
			4964	3162	881	897	24		

- Molecule 4 is a protein called Glutamate receptor ionotropic, NMDA 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	654	Total	C	N	O	S	0	0
			4630	2984	794	829	23		
4	D	648	Total	C	N	O	S	0	0
			4582	2976	781	803	22		

There are 178 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	39	MET	LEU	conflict	UNP A0A6P6HB11
B	53	THR	ASN	conflict	UNP A0A6P6HB11
B	119	HIS	GLN	conflict	UNP A0A6P6HB11

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Chain	Residue	Modelled	Actual	Comment	Reference
B	122	VAL	ILE	conflict	UNP A0A6P6HB11
B	182	GLU	ASP	conflict	UNP A0A6P6HB11
B	187	VAL	ILE	conflict	UNP A0A6P6HB11
B	296	ILE	LEU	conflict	UNP A0A6P6HB11
B	304	SER	TYR	conflict	UNP A0A6P6HB11
B	324	MET	THR	conflict	UNP A0A6P6HB11
B	326	ARG	LYS	conflict	UNP A0A6P6HB11
B	329	VAL	ALA	conflict	UNP A0A6P6HB11
B	331	MET	PRO	conflict	UNP A0A6P6HB11
B	336	PRO	GLN	conflict	UNP A0A6P6HB11
B	381	HIS	GLN	conflict	UNP A0A6P6HB11
B	382	THR	SER	conflict	UNP A0A6P6HB11
B	542T	CYS	SER	conflict	UNP A0A6P6HB11
B	542W	ASP	LYS	conflict	UNP A0A6P6HB11
B	542Y	ARG	LYS	conflict	UNP A0A6P6HB11
B	543A	PRO	-	insertion	UNP A0A6P6HB11
B	543B	GLY	-	insertion	UNP A0A6P6HB11
B	543C	GLY	-	insertion	UNP A0A6P6HB11
B	543D	PRO	-	insertion	UNP A0A6P6HB11
B	543E	SER	-	insertion	UNP A0A6P6HB11
B	543F	PHE	-	insertion	UNP A0A6P6HB11
B	543G	THR	-	insertion	UNP A0A6P6HB11
B	543H	ILE	-	insertion	UNP A0A6P6HB11
B	543I	GLY	-	insertion	UNP A0A6P6HB11
B	543J	LYS	-	insertion	UNP A0A6P6HB11
B	543K	ALA	-	insertion	UNP A0A6P6HB11
B	543L	ILE	-	insertion	UNP A0A6P6HB11
B	543M	TRP	-	insertion	UNP A0A6P6HB11
B	543N	LEU	-	insertion	UNP A0A6P6HB11
B	543P	TRP	THR	conflict	UNP A0A6P6HB11
B	543R	LEU	-	insertion	UNP A0A6P6HB11
B	543S	VAL	-	insertion	UNP A0A6P6HB11
B	543T	PHE	-	insertion	UNP A0A6P6HB11
B	543U	ASN	-	insertion	UNP A0A6P6HB11
B	543V	ASN	-	insertion	UNP A0A6P6HB11
B	543W	SER	-	insertion	UNP A0A6P6HB11
B	543X	VAL	-	insertion	UNP A0A6P6HB11
B	543Y	PRO	-	insertion	UNP A0A6P6HB11
B	543Z	VAL	-	insertion	UNP A0A6P6HB11
B	544B	ASN	-	insertion	UNP A0A6P6HB11
B	544C	PRO	-	insertion	UNP A0A6P6HB11
B	544D	LYS	-	insertion	UNP A0A6P6HB11

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Chain	Residue	Modelled	Actual	Comment	Reference
B	544E	GLY	-	insertion	UNP A0A6P6HB11
B	544F	THR	-	insertion	UNP A0A6P6HB11
B	544G	THR	-	insertion	UNP A0A6P6HB11
B	544H	SER	-	insertion	UNP A0A6P6HB11
B	544I	LYS	-	insertion	UNP A0A6P6HB11
B	544J	ILE	-	insertion	UNP A0A6P6HB11
B	544K	MET	-	insertion	UNP A0A6P6HB11
B	544L	VAL	-	insertion	UNP A0A6P6HB11
B	544M	SER	-	insertion	UNP A0A6P6HB11
B	544N	VAL	-	insertion	UNP A0A6P6HB11
B	544P	ALA	-	insertion	UNP A0A6P6HB11
B	544Q	PHE	-	insertion	UNP A0A6P6HB11
B	544R	PHE	-	insertion	UNP A0A6P6HB11
B	544S	ALA	-	insertion	UNP A0A6P6HB11
B	544T	VAL	-	insertion	UNP A0A6P6HB11
B	544U	ILE	-	insertion	UNP A0A6P6HB11
B	544V	PHE	-	insertion	UNP A0A6P6HB11
B	544W	LEU	-	insertion	UNP A0A6P6HB11
B	544X	ALA	-	insertion	UNP A0A6P6HB11
B	544Y	SER	-	insertion	UNP A0A6P6HB11
B	544Z	TYR	-	insertion	UNP A0A6P6HB11
B	545A	THR	-	insertion	UNP A0A6P6HB11
B	545B	ALA	-	insertion	UNP A0A6P6HB11
B	545C	ASN	-	insertion	UNP A0A6P6HB11
B	545D	LEU	-	insertion	UNP A0A6P6HB11
B	545E	ALA	-	insertion	UNP A0A6P6HB11
B	545F	ALA	-	insertion	UNP A0A6P6HB11
B	545G	PHE	-	insertion	UNP A0A6P6HB11
B	545H	MET	-	insertion	UNP A0A6P6HB11
B	545I	ILE	-	insertion	UNP A0A6P6HB11
B	545J	GLN	-	insertion	UNP A0A6P6HB11
B	545K	GLU	-	insertion	UNP A0A6P6HB11
B	545L	GLU	-	insertion	UNP A0A6P6HB11
B	545M	PHE	-	insertion	UNP A0A6P6HB11
B	639	VAL	-	insertion	UNP A0A6P6HB11
B	640	ASP	-	insertion	UNP A0A6P6HB11
B	642	VAL	-	insertion	UNP A0A6P6HB11
B	643	THR	-	insertion	UNP A0A6P6HB11
B	644	GLY	-	insertion	UNP A0A6P6HB11
B	645	LEU	-	insertion	UNP A0A6P6HB11
B	646	SER	-	insertion	UNP A0A6P6HB11
B	647	ASP	-	insertion	UNP A0A6P6HB11

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Chain	Residue	Modelled	Actual	Comment	Reference
B	648	LYS	-	insertion	UNP A0A6P6HB11
B	649	LYS	-	insertion	UNP A0A6P6HB11
D	39	MET	LEU	conflict	UNP A0A6P6HB11
D	53	THR	ASN	conflict	UNP A0A6P6HB11
D	119	HIS	GLN	conflict	UNP A0A6P6HB11
D	122	VAL	ILE	conflict	UNP A0A6P6HB11
D	182	GLU	ASP	conflict	UNP A0A6P6HB11
D	187	VAL	ILE	conflict	UNP A0A6P6HB11
D	296	ILE	LEU	conflict	UNP A0A6P6HB11
D	304	SER	TYR	conflict	UNP A0A6P6HB11
D	324	MET	THR	conflict	UNP A0A6P6HB11
D	326	ARG	LYS	conflict	UNP A0A6P6HB11
D	329	VAL	ALA	conflict	UNP A0A6P6HB11
D	331	MET	PRO	conflict	UNP A0A6P6HB11
D	336	PRO	GLN	conflict	UNP A0A6P6HB11
D	381	HIS	GLN	conflict	UNP A0A6P6HB11
D	382	THR	SER	conflict	UNP A0A6P6HB11
D	542T	CYS	SER	conflict	UNP A0A6P6HB11
D	542W	ASP	LYS	conflict	UNP A0A6P6HB11
D	542Y	ARG	LYS	conflict	UNP A0A6P6HB11
D	543A	PRO	-	insertion	UNP A0A6P6HB11
D	543B	GLY	-	insertion	UNP A0A6P6HB11
D	543C	GLY	-	insertion	UNP A0A6P6HB11
D	543D	PRO	-	insertion	UNP A0A6P6HB11
D	543E	SER	-	insertion	UNP A0A6P6HB11
D	543F	PHE	-	insertion	UNP A0A6P6HB11
D	543G	THR	-	insertion	UNP A0A6P6HB11
D	543H	ILE	-	insertion	UNP A0A6P6HB11
D	543I	GLY	-	insertion	UNP A0A6P6HB11
D	543J	LYS	-	insertion	UNP A0A6P6HB11
D	543K	ALA	-	insertion	UNP A0A6P6HB11
D	543L	ILE	-	insertion	UNP A0A6P6HB11
D	543M	TRP	-	insertion	UNP A0A6P6HB11
D	543N	LEU	-	insertion	UNP A0A6P6HB11
D	543P	TRP	THR	conflict	UNP A0A6P6HB11
D	543R	LEU	-	insertion	UNP A0A6P6HB11
D	543S	VAL	-	insertion	UNP A0A6P6HB11
D	543T	PHE	-	insertion	UNP A0A6P6HB11
D	543U	ASN	-	insertion	UNP A0A6P6HB11
D	543V	ASN	-	insertion	UNP A0A6P6HB11
D	543W	SER	-	insertion	UNP A0A6P6HB11
D	543X	VAL	-	insertion	UNP A0A6P6HB11

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Chain	Residue	Modelled	Actual	Comment	Reference
D	543Y	PRO	-	insertion	UNP A0A6P6HB11
D	543Z	VAL	-	insertion	UNP A0A6P6HB11
D	544B	ASN	-	insertion	UNP A0A6P6HB11
D	544C	PRO	-	insertion	UNP A0A6P6HB11
D	544D	LYS	-	insertion	UNP A0A6P6HB11
D	544E	GLY	-	insertion	UNP A0A6P6HB11
D	544F	THR	-	insertion	UNP A0A6P6HB11
D	544G	THR	-	insertion	UNP A0A6P6HB11
D	544H	SER	-	insertion	UNP A0A6P6HB11
D	544I	LYS	-	insertion	UNP A0A6P6HB11
D	544J	ILE	-	insertion	UNP A0A6P6HB11
D	544K	MET	-	insertion	UNP A0A6P6HB11
D	544L	VAL	-	insertion	UNP A0A6P6HB11
D	544M	SER	-	insertion	UNP A0A6P6HB11
D	544N	VAL	-	insertion	UNP A0A6P6HB11
D	544P	ALA	-	insertion	UNP A0A6P6HB11
D	544Q	PHE	-	insertion	UNP A0A6P6HB11
D	544R	PHE	-	insertion	UNP A0A6P6HB11
D	544S	ALA	-	insertion	UNP A0A6P6HB11
D	544T	VAL	-	insertion	UNP A0A6P6HB11
D	544U	ILE	-	insertion	UNP A0A6P6HB11
D	544V	PHE	-	insertion	UNP A0A6P6HB11
D	544W	LEU	-	insertion	UNP A0A6P6HB11
D	544X	ALA	-	insertion	UNP A0A6P6HB11
D	544Y	SER	-	insertion	UNP A0A6P6HB11
D	544Z	TYR	-	insertion	UNP A0A6P6HB11
D	545A	THR	-	insertion	UNP A0A6P6HB11
D	545B	ALA	-	insertion	UNP A0A6P6HB11
D	545C	ASN	-	insertion	UNP A0A6P6HB11
D	545D	LEU	-	insertion	UNP A0A6P6HB11
D	545E	ALA	-	insertion	UNP A0A6P6HB11
D	545F	ALA	-	insertion	UNP A0A6P6HB11
D	545G	PHE	-	insertion	UNP A0A6P6HB11
D	545H	MET	-	insertion	UNP A0A6P6HB11
D	545I	ILE	-	insertion	UNP A0A6P6HB11
D	545J	GLN	-	insertion	UNP A0A6P6HB11
D	545K	GLU	-	insertion	UNP A0A6P6HB11
D	545L	GLU	-	insertion	UNP A0A6P6HB11
D	545M	PHE	-	insertion	UNP A0A6P6HB11
D	639	VAL	-	insertion	UNP A0A6P6HB11
D	640	ASP	-	insertion	UNP A0A6P6HB11
D	642	VAL	-	insertion	UNP A0A6P6HB11

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Chain	Residue	Modelled	Actual	Comment	Reference
D	643	THR	-	insertion	UNP A0A6P6HB11
D	644	GLY	-	insertion	UNP A0A6P6HB11
D	645	LEU	-	insertion	UNP A0A6P6HB11
D	646	SER	-	insertion	UNP A0A6P6HB11
D	647	ASP	-	insertion	UNP A0A6P6HB11
D	648	LYS	-	insertion	UNP A0A6P6HB11
D	649	LYS	-	insertion	UNP A0A6P6HB11

- Molecule 5 is a protein called Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	663	4885	3114	873	875	23	0	0


There are 2 discrepancies between the modelled and reference sequences:

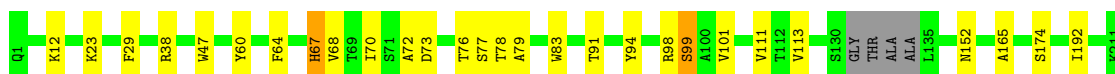
Chain	Residue	Modelled	Actual	Comment	Reference
C	54	ALA	GLY	conflict	UNP Q05586
C	358	ARG	ASN	conflict	UNP Q05586

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

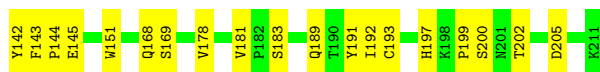
- Molecule 1: 007-168 Heavy

Chain E: 



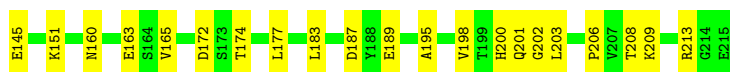
- Molecule 1: 007-168 Heavy

Chain H: 




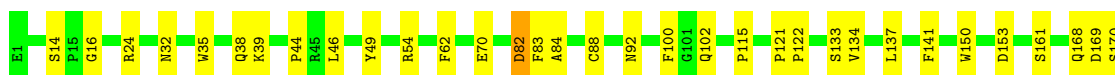
- Molecule 2: 007-168 Light

Chain F: 

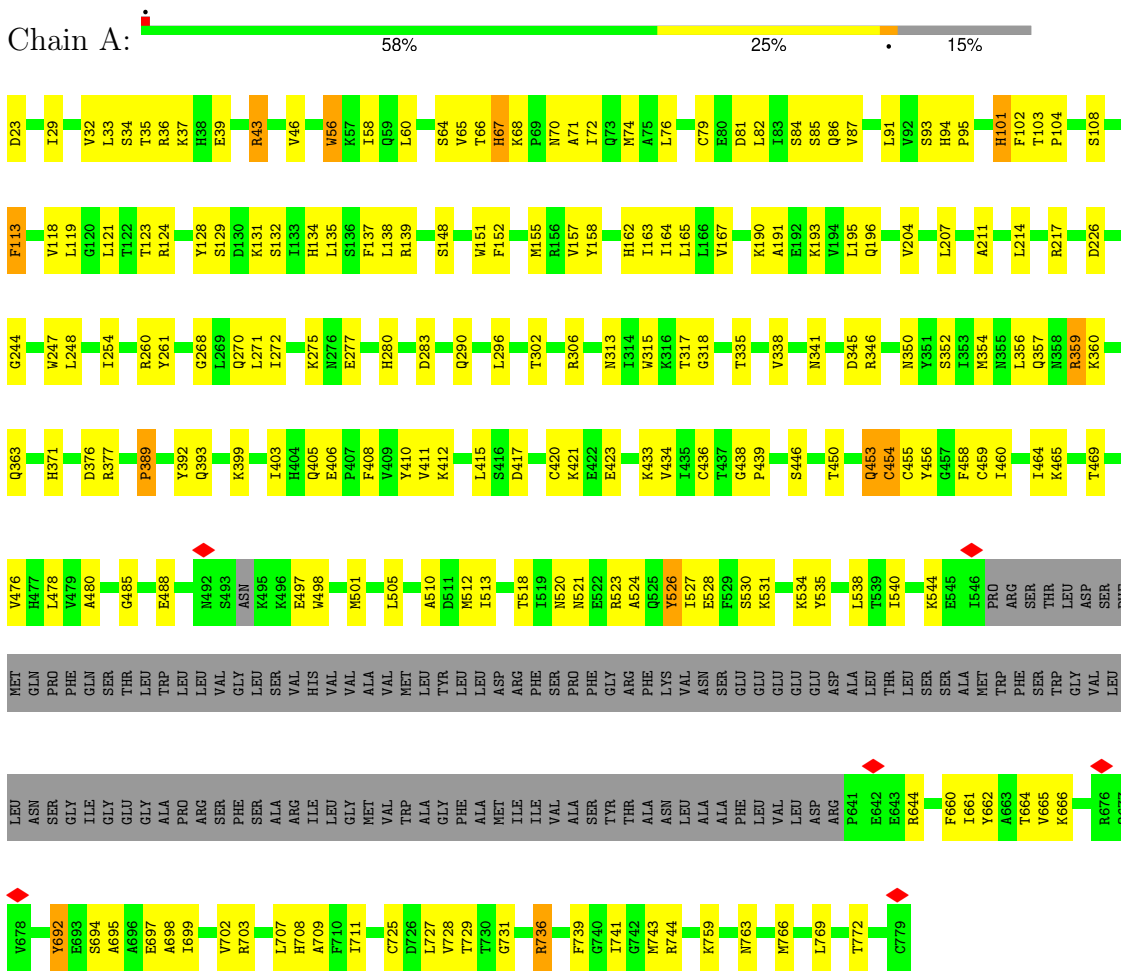


- Molecule 2: 007-168 Light

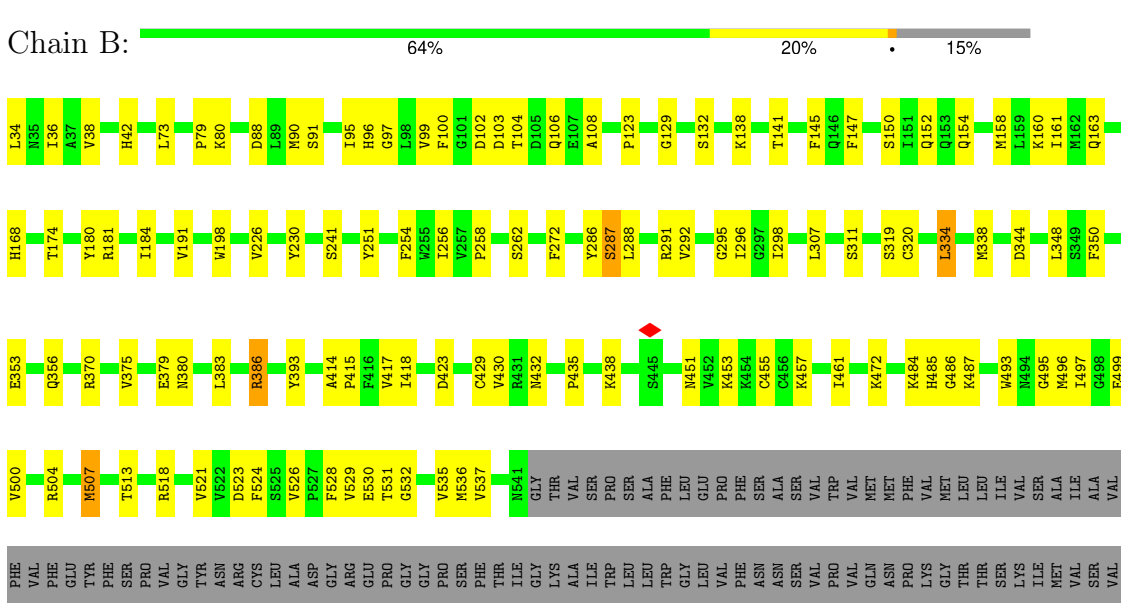
Chain L: 



• Molecule 3: Glutamate receptor ionotropic, NMDA 1



• Molecule 4: Glutamate receptor ionotropic, NMDA 2A



T402	I403	H404	Q405	E406	P407	F408	V411	K412	K421	K433	V434	I435	D441	V451	P452	Q453	C454	F458	L466	T469	K483	F484	G485	V490	S493	G500	E504	L505	A510	D511	M512	I513	V514	I519	R523	E528	F529	F533	R534	Y535	Q536							
G537	L538	I546	PRO	ARG	SER	THR	LEU	ASP	SER	PHE	MET	GLN	PRO	PHE	GLY	ILE	GLN	SER	THR	LEU	TRP	P452	LEU	VAL	GLY	LEU	ASP	ARG	PHE	SER	PRO	PHE	GLY	ARG	PHE	LYS	VAL	ASN	SER	GLU	GLU	GLU	GLU	ASP	ALA	LEU	THR	
LEU	SER	SER	ALA	MET	TRP	PHE	SER	TRP	GLY	VAL	LEU	LEU	ASN	SER	GLY	ILE	GLY	GLU	GLY	GLY	ALA	PRO	ARG	SER	PHE	SER	ALA	ARG	ILE	ILE	VAL	ALA	SER	TYR	THR	ALA	ASN	LEU	ALA	PHE	ALA	VAL	LEU	LEU	ASP	ARG	P641	E642
S657	I661	V665	K666	D671	F674	S681	Y684	R685	H686	E693	L707	F710	I711	W712	V716	L717	E718	F719	F735	R736	S737	G738	I741	G742	M743	W749	S756	I757	H761	F765	M766	E767	D768	L769	T772	C779												

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	119725	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.634	Depositor
Minimum map value	-0.321	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.0508	Depositor
Map size (\AA)	376.64, 376.64, 376.64	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.856, 0.856, 0.856	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	E	0.31	0/1394	0.48	0/1913
1	H	0.32	0/1550	0.52	0/2125
2	F	0.32	0/1597	0.53	1/2181 (0.0%)
2	L	0.31	0/1548	0.52	0/2120
3	A	0.30	0/5075	0.52	0/6904
4	B	0.26	0/4740	0.48	0/6490
4	D	0.26	0/4689	0.50	0/6421
5	C	0.30	0/4993	0.54	1/6803 (0.0%)
All	All	0.29	0/25586	0.51	2/34957 (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	H	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	60	LEU	CA-CB-CG	5.56	128.09	115.30
2	F	93	ASN	C-N-CA	-5.10	108.96	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	101	VAL	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1363	0	1089	19	0
1	H	1507	0	1358	44	0
2	F	1562	0	1410	39	0
2	L	1513	0	1338	28	0
3	A	4964	0	4747	126	0
4	B	4630	0	4175	102	0
4	D	4582	0	4107	102	0
5	C	4885	0	4624	123	0
All	All	25006	0	22848	572	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 12.

All (572) 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)
3:A:36:ARG:O	3:A:39:GLU:HB2	1.60	0.98
5:C:338:VAL:HG23	5:C:346:ARG:HE	1.45	0.81
5:C:125:MET:H	5:C:139:ARG:HH22	1.29	0.80
3:A:436:CYS:N	3:A:455:CYS:SG	2.50	0.79
5:C:104:PRO:HG3	5:C:123:THR:HG21	1.66	0.78
5:C:254:ILE:HD13	5:C:268:GLY:HA3	1.65	0.77
3:A:498:TRP:HE1	3:A:526:TYR:HH	1.31	0.76
4:B:536:MET:HB3	4:B:708:PHE:HB3	1.66	0.76
2:F:115:PRO:HB3	2:F:141:PHE:HB3	1.66	0.75
4:B:429:CYS:SG	4:B:430:VAL:N	2.60	0.74
4:B:417:VAL:HG12	4:B:461:ILE:HD11	1.69	0.74
5:C:435:ILE:HD11	5:C:452:PRO:HB2	1.70	0.74
3:A:439:PRO:HG3	3:A:480:ALA:HA	1.70	0.73
5:C:458:PHE:HE1	5:C:769:LEU:HD13	1.51	0.73
3:A:23:ASP:N	3:A:56:TRP:O	2.22	0.72
4:B:295:GLY:HA2	4:B:298:ILE:HD12	1.70	0.72
5:C:31:ALA:HB3	5:C:91:LEU:H	1.55	0.72
3:A:131:LYS:NZ	3:A:137:PHE:O	2.23	0.71
3:A:534:LYS:HB3	3:A:739:PHE:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:123:THR:O	5:C:139:ARG:NH2	2.23	0.71
4:B:500:VAL:O	4:B:746:GLN:NE2	2.23	0.70
4:B:100:PHE:HE1	4:B:102:ASP:HB2	1.57	0.70
1:H:40:MET:SD	1:H:43:SER:OG	2.50	0.70
5:C:136:SER:HA	5:C:322:LYS:HZ1	1.58	0.69
4:D:466:LYS:HB2	4:D:469:ARG:HH21	1.57	0.68
3:A:104:PRO:HG2	3:A:123:THR:HG21	1.75	0.68
4:B:160:LYS:HB3	4:B:383:LEU:HD11	1.74	0.67
1:H:97:ALA:HB1	1:H:102:PHE:HB3	1.76	0.67
2:F:183:LEU:HD12	2:F:187:ASP:HB3	1.77	0.67
5:C:483:LYS:NZ	5:C:666:LYS:O	2.27	0.67
2:F:110:ARG:NH1	2:F:111:THR:O	2.28	0.67
4:B:679:PRO:O	4:B:683:GLN:N	2.27	0.67
4:B:513:THR:O	4:B:518:ARG:NH1	2.29	0.66
4:B:721:ARG:NH2	4:B:775:TRP:O	2.28	0.66
5:C:671:ASP:OD1	5:C:684:TYR:OH	2.13	0.66
5:C:743:MET:HE1	5:C:749:TRP:HB2	1.77	0.66
3:A:68:LYS:H	3:A:74:MET:HE1	1.59	0.66
5:C:533:PHE:HB3	5:C:757:ILE:HD11	1.76	0.66
2:F:90:GLN:NE2	2:F:99:THR:OG1	2.27	0.66
4:B:163:GLN:HB3	4:B:198:TRP:HH2	1.61	0.66
3:A:510:ALA:O	3:A:744:ARG:NH2	2.29	0.66
5:C:100:ASP:O	5:C:101:HIS:ND1	2.30	0.65
3:A:439:PRO:HA	3:A:450:THR:HA	1.79	0.65
4:B:38:VAL:HG22	4:B:99:VAL:HB	1.76	0.65
5:C:451:VAL:O	5:C:453:GLN:NE2	2.29	0.65
3:A:354:MET:HA	3:A:363:GLN:HA	1.79	0.65
1:E:99:SER:OG	1:E:99:SER:O	2.10	0.64
3:A:544:LYS:H	3:A:727:LEU:HA	1.62	0.64
4:D:410:THR:HG22	4:D:477:LEU:HD11	1.78	0.64
4:B:226:VAL:HG22	4:B:254:PHE:HB2	1.78	0.64
4:B:461:ILE:HD12	4:B:461:ILE:H	1.61	0.64
3:A:415:LEU:HG	3:A:417:ASP:H	1.63	0.64
1:H:2:VAL:HB	1:H:104:TYR:HD2	1.62	0.64
3:A:403:ILE:O	3:A:405:GLN:NE2	2.30	0.63
1:H:141:ASP:OD1	1:H:168:GLN:NE2	2.31	0.63
5:C:403:ILE:HG12	5:C:484:PHE:HE1	1.62	0.63
3:A:501:MET:HG3	3:A:513:ILE:HD11	1.79	0.63
3:A:94:HIS:ND1	3:A:95:PRO:O	2.30	0.63
3:A:535:TYR:HD1	3:A:736:ARG:HH12	1.48	0.62
3:A:702:VAL:HG12	3:A:707:LEU:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:475:TYR:HD2	4:D:477:LEU:H	1.46	0.62
2:F:24:ARG:HH11	2:F:70:GLU:HB3	1.64	0.62
2:F:172:ASP:OD2	2:F:174:THR:OG1	2.18	0.62
3:A:530:SER:HB3	3:A:741:ILE:HB	1.82	0.62
2:L:115:PRO:HB3	2:L:141:PHE:HB3	1.82	0.62
5:C:93:SER:HB2	5:C:121:LEU:HD12	1.82	0.62
4:D:270:LYS:N	4:D:270:LYS:HD3	2.16	0.61
3:A:465:LYS:NZ	3:A:469:THR:OG1	2.30	0.61
4:D:35:ASN:N	4:D:68:ASN:OD1	2.33	0.61
4:D:72:LEU:HD13	4:D:89:LEU:HD21	1.80	0.61
4:D:54:LEU:HG	4:D:293:ARG:HH22	1.66	0.61
3:A:190:LYS:NZ	3:A:191:ALA:O	2.33	0.61
4:D:500:VAL:O	4:D:747:LYS:NZ	2.34	0.61
3:A:121:LEU:HD22	3:A:280:HIS:HB3	1.83	0.61
3:A:411:VAL:HG13	3:A:453:GLN:HG3	1.83	0.61
4:B:292:VAL:O	4:B:296:ILE:HG12	2.01	0.61
1:H:140:LYS:NZ	1:H:141:ASP:OD1	2.33	0.61
3:A:101:HIS:O	3:A:104:PRO:HD2	2.01	0.61
4:B:780:CYS:SG	4:B:781:HIS:N	2.74	0.60
3:A:436:CYS:HB3	3:A:476:VAL:HG22	1.82	0.60
4:B:181:ARG:HA	4:B:181:ARG:HH11	1.66	0.60
1:E:23:LYS:HG3	1:E:78:THR:HG22	1.82	0.60
4:B:430:VAL:HG12	4:B:432:ASN:H	1.66	0.60
4:B:451:ASN:O	4:B:453:LYS:NZ	2.34	0.60
3:A:39:GLU:OE1	3:A:64:SER:OG	2.11	0.60
4:D:39:MET:HG2	4:D:98:LEU:HD11	1.83	0.60
5:C:761:HIS:HA	5:C:766:MET:HG3	1.83	0.60
3:A:505:LEU:HB2	3:A:513:ILE:HD13	1.83	0.60
4:D:270:LYS:HD3	4:D:270:LYS:H	1.67	0.60
4:D:462:ASP:OD1	4:D:462:ASP:N	2.35	0.59
3:A:163:ILE:HG22	3:A:165:LEU:H	1.67	0.59
3:A:335:THR:HG22	3:A:346:ARG:HH22	1.67	0.59
2:L:153:ASP:HA	2:L:193:VAL:HB	1.85	0.58
5:C:68:LYS:HG2	5:C:69:PRO:HD2	1.84	0.58
5:C:126:SER:O	5:C:129:SER:OG	2.21	0.58
1:H:197:HIS:CD2	1:H:199:PRO:HD2	2.38	0.58
3:A:244:GLY:HA2	3:A:389:PRO:HB3	1.85	0.58
3:A:408:PHE:HA	3:A:458:PHE:HB3	1.85	0.58
4:D:292:VAL:O	4:D:296:ILE:HG12	2.04	0.58
3:A:70:ASN:O	3:A:72:ILE:N	2.37	0.58
5:C:90:ILE:HB	5:C:118:VAL:HG12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:509:VAL:HG23	4:D:743:ILE:HG13	1.86	0.58
4:D:435:PRO:O	4:D:437:ARG:NH1	2.36	0.57
2:L:32:ASN:ND2	2:L:92:ASN:OD1	2.38	0.57
5:C:135:LEU:HD23	5:C:135:LEU:H	1.68	0.57
5:C:505:LEU:HD22	5:C:510:ALA:HA	1.86	0.57
2:L:122:PRO:HD3	2:L:134:VAL:HG12	1.86	0.57
5:C:681:SER:HA	5:C:684:TYR:HB2	1.85	0.57
1:H:45:LEU:HD12	2:L:100:PHE:HE2	1.70	0.56
5:C:105:THR:HG23	5:C:106:PRO:HD3	1.87	0.56
4:D:470:THR:HG23	4:D:471:VAL:HG23	1.87	0.56
1:E:165:ALA:HA	1:E:174:SER:O	2.06	0.56
2:L:54:ARG:NH1	2:L:62:PHE:O	2.37	0.56
4:B:435:PRO:HA	4:B:455:CYS:HA	1.88	0.56
5:C:58:ILE:HD12	5:C:293:HIS:ND1	2.20	0.56
3:A:528:GLU:HG3	3:A:743:MET:HB2	1.86	0.56
4:B:102:ASP:OD2	4:B:104:THR:N	2.37	0.56
3:A:79:CYS:SG	4:B:80:LYS:HB2	2.46	0.56
5:C:264:ASP:OD1	5:C:359:ARG:NH2	2.39	0.56
1:E:91:THR:HA	1:E:111:VAL:O	2.05	0.56
1:E:152:ASN:HA	1:E:192:ILE:HB	1.86	0.56
3:A:664:THR:HG23	3:A:665:VAL:H	1.70	0.56
5:C:514:VAL:HG12	5:C:741:ILE:HD12	1.87	0.56
2:F:34:ALA:HB1	2:F:36:TYR:HE2	1.71	0.55
4:B:721:ARG:HG3	4:B:778:GLY:HA2	1.88	0.55
3:A:66:THR:HG22	3:A:67:HIS:H	1.72	0.55
3:A:354:MET:HG3	3:A:363:GLN:HB3	1.87	0.55
5:C:178:LYS:O	5:C:182:THR:OG1	2.21	0.55
1:H:15:GLY:H	1:H:86:LEU:HA	1.70	0.55
3:A:644:ARG:NH2	3:A:731:GLY:O	2.39	0.55
5:C:27:VAL:O	5:C:60:LEU:HA	2.06	0.55
3:A:104:PRO:O	3:A:108:SER:HB3	2.06	0.55
3:A:151:TRP:CZ3	3:A:248:LEU:HB3	2.41	0.55
4:B:102:ASP:OD2	4:B:103:ASP:N	2.39	0.55
3:A:148:SER:HA	3:A:151:TRP:CD1	2.42	0.55
4:B:781:HIS:CD2	4:B:782:ASN:H	2.25	0.55
4:D:177:PHE:CG	4:D:178:PRO:HD2	2.41	0.55
4:B:672:ARG:O	4:B:676:ASN:ND2	2.40	0.55
4:D:152:GLN:N	4:D:152:GLN:OE1	2.39	0.55
3:A:119:LEU:HA	3:A:138:LEU:O	2.07	0.54
4:D:171:SER:OG	4:D:202:ASN:O	2.16	0.54
4:B:487:LYS:HA	4:B:672:ARG:HH12	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:538:LEU:HD23	5:C:711:ILE:HG22	1.90	0.54
4:D:690:GLN:HG2	4:D:696:ALA:HA	1.90	0.54
5:C:712:TRP:HD1	5:C:716:VAL:HG11	1.73	0.54
4:D:167:TRP:HB3	4:D:226:VAL:HG21	1.90	0.54
3:A:152:PHE:O	3:A:155:MET:HG3	2.08	0.54
3:A:699:ILE:HA	3:A:702:VAL:HG22	1.90	0.54
4:D:767:GLU:HA	4:D:770:GLU:HG3	1.90	0.54
1:H:40:MET:SD	1:H:40:MET:N	2.66	0.53
3:A:341:ASN:HD21	3:A:345:ASP:HB2	1.73	0.53
4:D:117:SER:HB2	4:D:124:ILE:HD11	1.90	0.53
4:D:436:CYS:HB2	4:D:477:LEU:HG	1.90	0.53
4:D:40:LEU:O	4:D:74:MET:N	2.41	0.53
3:A:32:VAL:HG22	3:A:65:VAL:HG12	1.90	0.53
4:B:163:GLN:HB3	4:B:198:TRP:CH2	2.43	0.53
3:A:270:GLN:OE1	3:A:271:LEU:N	2.42	0.53
5:C:269:LEU:HD12	5:C:353:ILE:HG22	1.91	0.53
3:A:211:ALA:HA	3:A:214:LEU:HD12	1.90	0.53
3:A:412:LYS:O	3:A:454:CYS:N	2.23	0.53
3:A:759:LYS:O	3:A:763:ASN:ND2	2.42	0.53
5:C:136:SER:HA	5:C:322:LYS:NZ	2.23	0.52
5:C:148:SER:HA	5:C:151:TRP:HD1	1.74	0.52
4:D:356:GLN:O	4:D:358:HIS:N	2.36	0.52
1:H:135:LEU:HD11	1:H:191:TYR:HD1	1.74	0.52
3:A:524:ALA:HA	3:A:527:ILE:HG22	1.92	0.52
4:B:97:GLY:HA2	4:B:123:PRO:O	2.08	0.52
4:B:288:LEU:HA	4:B:291:ARG:HD2	1.90	0.52
5:C:402:THR:OG1	5:C:403:ILE:N	2.42	0.52
5:C:765:PHE:CZ	5:C:769:LEU:HD23	2.45	0.52
4:D:158:MET:HE1	4:D:258:PRO:HA	1.91	0.52
4:D:215:THR:OG1	4:D:216:GLN:OE1	2.28	0.52
5:C:295:LEU:HD23	5:C:296:LEU:HD12	1.91	0.52
4:D:374:LYS:O	4:D:386:ARG:NH2	2.43	0.52
4:B:745:LEU:HD12	4:B:746:GLN:H	1.74	0.52
2:F:5:THR:O	2:F:24:ARG:N	2.37	0.52
2:F:200:HIS:CD2	2:F:202:GLY:H	2.27	0.52
1:H:140:LYS:HG3	1:H:141:ASP:H	1.75	0.52
1:H:84:SER:OG	1:H:85:SER:N	2.42	0.51
1:H:192:ILE:HD11	1:H:205:ASP:HB3	1.92	0.51
3:A:86:GLN:HB3	3:A:306:ARG:HG2	1.91	0.51
4:B:174:THR:HG21	4:B:184:ILE:HD11	1.92	0.51
5:C:301:ILE:HG23	5:C:317:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:746:GLN:O	4:D:752:LYS:NZ	2.32	0.51
1:E:60:TYR:CZ	1:E:70:ILE:HG22	2.45	0.51
2:F:208:THR:O	2:F:209:LYS:NZ	2.39	0.51
3:A:356:LEU:HD12	3:A:357:GLN:H	1.75	0.51
5:C:519:ILE:HG23	5:C:529:PHE:HD2	1.76	0.51
4:D:83:ILE:HD13	4:D:116:ILE:HD11	1.91	0.51
4:D:294:ASP:O	4:D:298:ILE:HG12	2.11	0.51
4:D:147:PHE:O	4:D:356:GLN:NE2	2.43	0.51
4:D:98:LEU:HG	4:D:100:PHE:H	1.76	0.51
4:B:671:GLU:N	4:B:671:GLU:OE1	2.43	0.51
5:C:504:GLU:OE1	5:C:504:GLU:N	2.42	0.51
4:D:362:VAL:HG12	4:D:377:LYS:HG2	1.92	0.51
3:A:728:VAL:HG22	3:A:729:THR:H	1.76	0.51
5:C:31:ALA:HB3	5:C:91:LEU:N	2.24	0.51
5:C:490:VAL:HG23	5:C:493:SER:HB2	1.93	0.51
5:C:681:SER:HA	5:C:684:TYR:HD2	1.76	0.51
5:C:108:SER:O	5:C:112:GLY:N	2.44	0.51
1:H:38:ARG:HB2	1:H:94:TYR:CE1	2.46	0.50
5:C:710:PHE:CE2	5:C:717:LEU:HD21	2.47	0.50
1:H:168:GLN:HG2	1:H:169:SER:H	1.76	0.50
5:C:400:ILE:HG21	5:C:514:VAL:HG22	1.93	0.50
4:D:415:PRO:HG3	4:D:717:TYR:CD2	2.46	0.50
2:F:39:LYS:HA	2:F:84:ALA:HB1	1.93	0.50
2:F:64:GLY:HA2	2:F:73:LEU:HA	1.93	0.50
3:A:434:VAL:HG22	3:A:460:ILE:HD12	1.93	0.50
5:C:154:MET:O	5:C:158:TYR:HB2	2.11	0.50
4:D:99:VAL:HG12	4:D:99:VAL:O	2.11	0.50
1:H:145:GLU:OE1	1:H:145:GLU:N	2.42	0.50
3:A:769:LEU:HA	3:A:772:THR:HG22	1.93	0.50
5:C:215:GLU:HA	5:C:393:GLN:NE2	2.27	0.50
5:C:512:MET:O	5:C:512:MET:HG3	2.12	0.50
1:H:133:ALA:HB2	1:H:183:SER:HA	1.93	0.50
2:L:38:GLN:HG3	2:L:44:PRO:HD3	1.93	0.50
3:A:485:GLY:O	3:A:523:ARG:NH1	2.44	0.50
4:B:90:MET:HA	4:B:95:ILE:HG21	1.92	0.50
4:D:416:PHE:O	4:D:459:PHE:N	2.44	0.50
2:L:183:LEU:HD13	2:L:187:ASP:HB3	1.93	0.50
4:B:486:GLY:HA3	4:B:497:ILE:HD12	1.93	0.50
1:H:43:SER:O	2:L:102:GLN:NE2	2.45	0.50
2:L:82:ASP:O	2:L:83:PHE:HB3	2.11	0.50
3:A:315:TRP:O	3:A:318:GLY:N	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:38:VAL:HG22	4:D:99:VAL:HB	1.94	0.49
1:E:60:TYR:CE2	1:E:68:VAL:HG23	2.47	0.49
2:L:133:SER:HA	2:L:181:LEU:O	2.12	0.49
2:L:161:SER:HA	2:L:180:THR:O	2.12	0.49
4:B:532:GLY:O	4:B:712:ALA:N	2.43	0.49
5:C:58:ILE:HD12	5:C:293:HIS:CE1	2.48	0.49
4:B:100:PHE:CE1	4:B:102:ASP:HB2	2.44	0.49
4:D:139:ASP:OD1	4:D:141:THR:OG1	2.23	0.49
4:B:743:ILE:HD11	4:B:755:ILE:HD13	1.93	0.49
5:C:271:LEU:HD12	5:C:272:ILE:N	2.27	0.49
3:A:164:ILE:O	3:A:164:ILE:HG13	2.13	0.49
4:B:129:GLY:O	4:B:132:SER:OG	2.21	0.49
4:D:57:PRO:HB3	4:D:300:THR:HG21	1.94	0.49
1:E:47:TRP:CE3	2:F:98:TRP:HB2	2.47	0.49
2:L:169:ASP:OD1	2:L:170:SER:N	2.44	0.49
3:A:217:ARG:CZ	3:A:393:GLN:HG3	2.42	0.49
2:F:38:GLN:HB2	2:F:44:PRO:HG3	1.94	0.49
2:F:126:GLN:NE2	2:F:133:SER:OG	2.42	0.49
3:A:520:ASN:HD22	3:A:523:ARG:HG3	1.78	0.49
4:D:468:SER:OG	4:D:473:PHE:O	2.29	0.49
4:B:755:ILE:O	4:B:759:LEU:HG	2.13	0.49
4:D:375:VAL:HG12	4:D:386:ARG:HE	1.78	0.49
2:F:120:PHE:HB2	2:F:135:VAL:HB	1.95	0.49
4:B:700:LEU:HB2	4:B:705:LEU:HD23	1.95	0.49
5:C:34:SER:OG	5:C:35:THR:N	2.45	0.49
5:C:519:ILE:HG23	5:C:529:PHE:CD2	2.48	0.49
4:D:438:LYS:HA	4:D:479:LEU:HB3	1.95	0.49
4:B:526:VAL:HG21	4:B:760:LEU:HD21	1.95	0.48
1:E:73:ASP:OD2	1:E:76:THR:N	2.40	0.48
4:D:298:ILE:HD11	4:D:348:LEU:HD11	1.94	0.48
2:L:134:VAL:HG23	2:L:150:TRP:CH2	2.49	0.48
4:D:266:GLU:N	4:D:266:GLU:OE1	2.46	0.48
1:H:122:SER:OG	1:H:140:LYS:HB3	2.14	0.48
5:C:393:GLN:OE1	5:C:393:GLN:N	2.46	0.48
3:A:436:CYS:HA	3:A:476:VAL:HG13	1.95	0.48
1:E:29:PHE:CD1	1:E:77:SER:HB3	2.49	0.48
3:A:661:ILE:O	3:A:708:HIS:N	2.44	0.48
4:B:535:VAL:HG12	4:B:537:VAL:HG23	1.95	0.47
5:C:458:PHE:CE1	5:C:769:LEU:HD13	2.39	0.47
4:D:123:PRO:HG2	4:D:334:LEU:HG	1.96	0.47
4:B:145:PHE:CE2	4:B:338:MET:HG2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:150:SER:O	4:B:154:GLN:NE2	2.47	0.47
4:B:230:TYR:HD1	4:B:258:PRO:HG3	1.79	0.47
5:C:31:ALA:HB2	5:C:90:ILE:HD13	1.96	0.47
5:C:113:PHE:CD2	4:D:79:PRO:HG3	2.50	0.47
4:D:162:MET:HG2	4:D:198:TRP:CZ3	2.50	0.47
3:A:420:CYS:HB3	3:A:433:LYS:HE2	1.95	0.47
4:B:141:THR:O	4:B:141:THR:OG1	2.31	0.47
5:C:407:PRO:HB3	5:C:719:PHE:CD2	2.49	0.47
5:C:674:PHE:HB3	5:C:684:TYR:CE2	2.48	0.47
4:D:127:ILE:HA	4:D:147:PHE:CZ	2.49	0.47
5:C:768:ASP:O	5:C:772:THR:HG23	2.14	0.47
4:D:120:THR:HB	4:D:122:VAL:HG22	1.96	0.47
3:A:666:LYS:N	3:A:692:TYR:O	2.33	0.47
4:D:512:LEU:HD12	4:D:512:LEU:H	1.79	0.47
4:B:453:LYS:HA	4:B:453:LYS:HD3	1.54	0.47
5:C:404:HIS:CE1	5:C:411:VAL:HG22	2.49	0.47
4:D:177:PHE:CD1	4:D:178:PRO:HD2	2.50	0.47
2:F:209:LYS:HD3	2:F:209:LYS:HA	1.71	0.47
1:H:168:GLN:OE1	1:H:168:GLN:N	2.45	0.47
2:L:24:ARG:HG3	2:L:70:GLU:H	1.80	0.47
3:A:662:TYR:HB3	3:A:709:ALA:HB3	1.95	0.47
3:A:694:SER:N	3:A:697:GLU:OE2	2.48	0.47
5:C:144:TYR:O	5:C:147:GLN:HB2	2.14	0.47
5:C:271:LEU:HD12	5:C:272:ILE:H	1.78	0.47
3:A:104:PRO:CG	3:A:123:THR:HG21	2.42	0.47
3:A:204:VAL:HG12	3:A:207:LEU:HB2	1.97	0.47
5:C:224:SER:O	5:C:224:SER:OG	2.31	0.47
5:C:717:LEU:HD23	5:C:717:LEU:HA	1.68	0.47
1:H:23:LYS:HB3	1:H:23:LYS:HE2	1.63	0.47
5:C:27:VAL:HG23	5:C:88:TYR:CD1	2.50	0.47
4:D:499:GLU:HB3	4:D:504:ARG:HB3	1.97	0.47
3:A:421:LYS:HD2	3:A:423:GLU:HG3	1.97	0.47
3:A:530:SER:OG	3:A:531:LYS:N	2.48	0.47
4:B:42:HIS:CE1	4:B:73:LEU:HD21	2.50	0.47
4:D:277:ILE:HD12	4:D:390:TRP:HZ2	1.79	0.47
4:D:718:LYS:HB3	4:D:718:LYS:HE2	1.82	0.47
3:A:438:GLY:HA3	3:A:478:LEU:HB2	1.97	0.46
5:C:148:SER:HA	5:C:151:TRP:CD1	2.50	0.46
4:D:167:TRP:O	4:D:169:VAL:N	2.47	0.46
4:D:405:HIS:NE2	4:D:475:TYR:O	2.48	0.46
1:E:38:ARG:HB2	1:E:94:TYR:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:138:LEU:HD21	2:F:198:VAL:HG21	1.96	0.46
2:F:145:GLU:OE1	2:F:145:GLU:N	2.36	0.46
1:H:143:PHE:CE2	1:H:144:PRO:HB3	2.50	0.46
2:L:183:LEU:HD23	2:L:183:LEU:HA	1.80	0.46
4:B:375:VAL:HG23	4:B:386:ARG:HB3	1.97	0.46
4:D:268:ILE:HD11	4:D:370:ARG:HH11	1.80	0.46
1:E:152:ASN:N	1:E:192:ILE:O	2.48	0.46
4:B:781:HIS:CG	4:B:782:ASN:H	2.33	0.46
5:C:403:ILE:HG12	5:C:484:PHE:CE1	2.48	0.46
4:D:40:LEU:HD12	4:D:40:LEU:HA	1.81	0.46
4:B:530:GLU:H	4:B:530:GLU:CD	2.18	0.46
5:C:485:GLY:HA2	5:C:500:GLY:HA3	1.97	0.46
2:F:145:GLU:H	2:F:145:GLU:CD	2.17	0.46
5:C:505:LEU:HA	5:C:510:ALA:HA	1.98	0.46
5:C:528:GLU:N	5:C:528:GLU:OE1	2.46	0.46
3:A:699:ILE:HG23	3:A:703:ARG:HH22	1.80	0.46
5:C:138:LEU:HD11	5:C:326:MET:SD	2.56	0.46
5:C:217:ARG:HA	5:C:245:TYR:HD1	1.81	0.46
4:D:37:ALA:O	4:D:98:LEU:HA	2.15	0.46
4:D:259:SER:O	4:D:261:VAL:N	2.48	0.46
4:D:466:LYS:HD3	4:D:762:PHE:CE2	2.50	0.46
1:E:67:HIS:O	1:E:67:HIS:ND1	2.48	0.46
1:H:181:VAL:HG21	1:H:191:TYR:OH	2.16	0.46
5:C:355:ASN:OD1	5:C:356:LEU:N	2.48	0.46
4:D:408:ILE:HD13	4:D:507:MET:HB2	1.98	0.46
2:F:90:GLN:HE21	2:F:99:THR:HG1	1.61	0.46
1:H:200:SER:OG	1:H:202:THR:OG1	2.22	0.46
3:A:694:SER:OG	3:A:695:ALA:N	2.49	0.46
4:B:530:GLU:OE2	4:B:530:GLU:N	2.34	0.46
5:C:183:LEU:HD23	5:C:183:LEU:HA	1.80	0.46
4:D:229:LEU:O	4:D:258:PRO:HD3	2.15	0.46
2:F:160:ASN:OD1	2:F:160:ASN:N	2.49	0.46
4:B:91:SER:O	4:B:91:SER:OG	2.28	0.46
3:A:121:LEU:HD23	3:A:121:LEU:HA	1.78	0.45
4:B:438:LYS:HB2	4:B:438:LYS:HE3	1.78	0.45
5:C:405:GLN:HB3	5:C:408:PHE:HB2	1.98	0.45
4:D:462:ASP:HA	4:D:465:LYS:HG2	1.97	0.45
2:F:151:LYS:HB2	2:F:195:ALA:HB3	1.97	0.45
2:F:203:LEU:HD23	2:F:203:LEU:HA	1.78	0.45
4:B:123:PRO:HG2	4:B:334:LEU:HD11	1.98	0.45
1:E:60:TYR:OH	1:E:70:ILE:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:198:VAL:O	2:F:206:PRO:HA	2.17	0.45
3:A:540:ILE:HD12	3:A:711:ILE:HB	1.98	0.45
3:A:666:LYS:HA	3:A:666:LYS:HD2	1.84	0.45
4:B:95:ILE:HD12	4:B:96:HIS:H	1.81	0.45
5:C:657:SER:O	5:C:686:HIS:NE2	2.50	0.45
4:D:174:THR:OG1	4:D:175:THR:N	2.50	0.45
3:A:81:ASP:O	3:A:84:SER:OG	2.35	0.45
4:D:356:GLN:HE21	4:D:359:PRO:HB3	1.81	0.45
4:D:433:THR:HA	4:D:457:LYS:HG2	1.97	0.45
5:C:666:LYS:HA	5:C:693:GLU:HA	1.98	0.45
4:D:158:MET:HE3	4:D:258:PRO:HB3	1.99	0.45
3:A:128:TYR:HA	3:A:134:HIS:HD2	1.82	0.45
4:B:106:GLN:O	4:B:108:ALA:N	2.48	0.45
5:C:223:ALA:HB3	5:C:228:ALA:HB2	1.99	0.45
5:C:378:LYS:HD2	5:C:378:LYS:HA	1.62	0.45
1:H:151:TRP:CZ3	1:H:193:CYS:HB3	2.51	0.45
3:A:352:SER:OG	3:A:354:MET:SD	2.74	0.45
5:C:355:ASN:HB3	5:C:364:VAL:HG21	1.99	0.45
5:C:535:TYR:HA	5:C:738:GLY:HA2	1.98	0.45
5:C:765:PHE:O	5:C:769:LEU:HG	2.17	0.45
1:H:89:SER:O	1:H:89:SER:OG	2.31	0.45
4:B:160:LYS:HD3	4:B:160:LYS:HA	1.84	0.45
4:B:756:ASP:O	4:B:760:LEU:HD23	2.17	0.45
4:B:34:LEU:HA	4:B:96:HIS:HD2	1.81	0.44
4:B:661:ARG:HA	4:B:688:PHE:CE2	2.53	0.44
4:D:464:LEU:HD13	4:D:509:VAL:HG11	1.98	0.44
4:D:751:TRP:O	4:D:755:ILE:HG12	2.17	0.44
5:C:92:VAL:HG13	5:C:92:VAL:O	2.18	0.44
1:H:48:ILE:HG22	1:H:64:PHE:CE2	2.52	0.44
4:B:507:MET:SD	4:B:745:LEU:HD13	2.57	0.44
5:C:161:ASN:N	5:C:161:ASN:OD1	2.50	0.44
5:C:421:LYS:O	5:C:433:LYS:NZ	2.51	0.44
5:C:537:GLY:HA2	5:C:736:ARG:HA	1.99	0.44
4:D:498:GLY:HA2	4:D:501:VAL:HG22	2.00	0.44
2:F:35:TRP:CD2	2:F:73:LEU:HD23	2.51	0.44
4:B:418:ILE:HG12	4:B:457:LYS:O	2.17	0.44
5:C:710:PHE:CE2	5:C:712:TRP:HB2	2.52	0.44
4:D:432:ASN:OD1	4:D:432:ASN:N	2.50	0.44
1:H:49:GLY:HA3	1:H:70:ILE:HD11	1.98	0.44
1:H:121:PRO:HG3	1:H:197:HIS:HB2	1.99	0.44
3:A:302:THR:H	3:A:317:THR:HG21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:262:SER:O	4:B:262:SER:OG	2.31	0.44
2:F:33:LEU:HD12	2:F:33:LEU:HA	1.73	0.44
3:A:283:ASP:OD2	3:A:338:VAL:HG21	2.18	0.44
4:B:138:LYS:HE2	4:B:353:GLU:O	2.18	0.44
5:C:151:TRP:CZ3	5:C:248:LEU:HB3	2.53	0.44
5:C:163:ILE:H	5:C:218:VAL:HG21	1.83	0.44
2:F:163:GLU:HG2	2:F:177:LEU:HD21	2.00	0.44
3:A:113:PHE:CE2	4:B:79:PRO:HD3	2.53	0.44
4:B:350:PHE:HD1	4:B:356:GLN:HA	1.83	0.44
4:B:379:GLU:HG2	4:B:380:ASN:H	1.82	0.44
4:D:273:PRO:HB2	4:D:395:SER:O	2.18	0.44
4:D:535:VAL:HG22	4:D:709:ILE:HG22	2.00	0.44
2:F:24:ARG:HD2	2:F:70:GLU:HB3	1.99	0.44
1:H:97:ALA:CB	1:H:102:PHE:HB3	2.47	0.44
1:H:97:ALA:HB3	1:H:102:PHE:CD2	2.52	0.44
3:A:272:ILE:HD12	3:A:350:ASN:O	2.18	0.44
5:C:32:VAL:HG22	5:C:65:VAL:HG13	2.00	0.44
3:A:91:LEU:HD22	3:A:119:LEU:HB2	1.99	0.43
3:A:356:LEU:HD12	3:A:357:GLN:N	2.32	0.43
3:A:410:TYR:HB3	3:A:456:TYR:CZ	2.53	0.43
3:A:538:LEU:HD12	3:A:538:LEU:HA	1.86	0.43
4:B:528:PHE:CD2	4:B:529:VAL:HG12	2.52	0.43
4:D:459:PHE:HB2	4:D:775:TRP:CD1	2.53	0.43
3:A:275:LYS:HE2	3:A:275:LYS:HB2	1.87	0.43
4:B:36:ILE:HD11	4:B:296:ILE:HD12	1.99	0.43
4:D:450:MET:H	4:D:450:MET:HG2	1.62	0.43
2:F:32:ASN:HB3	2:F:91:TYR:CZ	2.53	0.43
4:B:90:MET:HA	4:B:95:ILE:CG2	2.49	0.43
5:C:325:LEU:O	5:C:328:SER:OG	2.28	0.43
2:L:46:LEU:HD21	2:L:49:TYR:HD2	1.83	0.43
5:C:661:ILE:H	5:C:707:LEU:HD22	1.84	0.43
1:H:45:LEU:HB2	2:L:100:PHE:CD2	2.53	0.43
1:H:101:VAL:HG13	1:H:103:ASP:OD1	2.18	0.43
3:A:85:SER:O	3:A:85:SER:OG	2.29	0.43
3:A:128:TYR:HA	3:A:134:HIS:CD2	2.54	0.43
5:C:226:ASP:N	5:C:226:ASP:OD1	2.51	0.43
5:C:412:LYS:HG3	5:C:454:CYS:HB3	2.01	0.43
4:D:124:ILE:O	4:D:125:LEU:HD23	2.18	0.43
4:D:129:GLY:O	4:D:132:SER:HB2	2.19	0.43
1:H:2:VAL:HB	1:H:104:TYR:CD2	2.49	0.43
3:A:350:ASN:OD1	3:A:350:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:125:MET:H	5:C:139:ARG:NH2	2.07	0.43
5:C:266:ILE:H	5:C:266:ILE:HG13	1.69	0.43
4:D:54:LEU:O	4:D:293:ARG:NH1	2.45	0.43
4:D:493:TRP:CD1	4:D:501:VAL:HG21	2.54	0.43
3:A:118:VAL:O	3:A:119:LEU:HD23	2.19	0.43
4:B:659:PRO:HB2	4:B:684:TYR:OH	2.19	0.43
3:A:102:PHE:HB3	3:A:103:THR:H	1.63	0.43
4:D:213:ALA:HA	4:D:216:GLN:HG2	2.01	0.43
2:L:83:PHE:O	2:L:83:PHE:CG	2.71	0.42
4:B:772:GLU:O	4:B:776:LEU:N	2.52	0.42
2:F:7:SER:O	2:F:22:SER:OG	2.35	0.42
3:A:296:LEU:HD23	3:A:296:LEU:HA	1.77	0.42
3:A:521:ASN:HA	3:A:524:ALA:HB3	2.01	0.42
5:C:312:THR:HG21	4:D:76:ARG:HG3	2.01	0.42
2:F:34:ALA:HA	2:F:48:ILE:O	2.19	0.42
3:A:29:ILE:HD12	3:A:60:LEU:HD23	2.01	0.42
3:A:43:ARG:O	3:A:46:VAL:HG12	2.19	0.42
4:B:523:ASP:OD1	4:B:524:PHE:N	2.53	0.42
4:D:184:ILE:O	4:D:188:LYS:HG2	2.19	0.42
2:F:163:GLU:OE2	2:F:165:VAL:HG23	2.19	0.42
1:H:3:GLN:OE1	1:H:3:GLN:N	2.52	0.42
1:H:52:TYR:HD1	1:H:54:GLY:H	1.67	0.42
3:A:33:LEU:HB2	3:A:39:GLU:OE2	2.19	0.42
4:D:138:LYS:HD3	4:D:144:PHE:CE1	2.55	0.42
4:D:390:TRP:CD2	4:D:391:PRO:HD2	2.54	0.42
4:D:408:ILE:O	4:D:477:LEU:HA	2.20	0.42
3:A:157:VAL:HG13	3:A:158:TYR:CD1	2.55	0.42
4:B:34:LEU:HA	4:B:96:HIS:CD2	2.55	0.42
5:C:161:ASN:HD22	5:C:187:ARG:HH22	1.68	0.42
4:D:265:THR:OG1	4:D:266:GLU:N	2.52	0.42
2:F:200:HIS:CD2	2:F:201:GLN:N	2.87	0.42
1:H:178:VAL:HG11	2:L:137:LEU:HD22	2.02	0.42
2:L:14:SER:O	2:L:16:GLY:N	2.50	0.42
3:A:360:LYS:HE2	3:A:360:LYS:HB2	1.87	0.42
4:B:168:HIS:CD2	4:B:168:HIS:N	2.85	0.42
4:B:745:LEU:HD23	4:B:752:LYS:HG2	2.02	0.42
5:C:215:GLU:HA	5:C:393:GLN:HE22	1.85	0.42
4:D:36:ILE:HD12	4:D:299:LEU:HG	2.01	0.42
2:F:74:THR:O	2:F:74:THR:OG1	2.36	0.42
1:H:23:LYS:HB3	1:H:78:THR:HG22	2.01	0.42
4:B:414:ALA:HB3	4:B:415:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:144:TYR:N	5:C:144:TYR:CD1	2.88	0.42
3:A:540:ILE:HD11	3:A:709:ALA:HB1	2.01	0.42
4:D:265:THR:HG23	4:D:267:LEU:HB2	2.01	0.42
1:H:45:LEU:HD12	2:L:100:PHE:CE2	2.54	0.42
4:B:499:GLU:OE1	4:B:504:ARG:NH1	2.53	0.42
5:C:148:SER:O	5:C:151:TRP:HB2	2.20	0.42
5:C:217:ARG:O	5:C:246:VAL:N	2.53	0.42
4:D:251:TYR:CE1	4:D:394:LYS:HA	2.54	0.42
2:L:39:LYS:HG2	2:L:84:ALA:HB2	2.02	0.42
2:L:196:CYS:O	2:L:208:THR:HG23	2.20	0.42
4:B:523:ASP:OD2	4:B:752:LYS:NZ	2.42	0.42
5:C:115:ARG:HB2	5:C:318:GLY:HA3	2.02	0.42
4:D:414:ALA:HB1	4:D:415:PRO:HD2	2.02	0.42
4:D:485:HIS:CE1	4:D:512:LEU:HA	2.54	0.42
1:H:3:GLN:O	1:H:4:LEU:HD23	2.19	0.41
3:A:34:SER:OG	3:A:35:THR:N	2.53	0.41
3:A:93:SER:OG	3:A:277:GLU:OE2	2.21	0.41
3:A:460:ILE:O	3:A:464:ILE:HG12	2.20	0.41
3:A:518:THR:HG22	3:A:739:PHE:CZ	2.55	0.41
4:B:102:ASP:O	4:B:129:GLY:HA3	2.20	0.41
4:B:272:PHE:O	4:B:370:ARG:NH2	2.41	0.41
4:B:287:SER:O	4:B:291:ARG:HG3	2.20	0.41
5:C:735:PHE:HD1	5:C:735:PHE:O	2.03	0.41
2:F:89:GLN:HG3	2:F:100:PHE:CE1	2.55	0.41
1:H:29:PHE:CD1	1:H:77:SER:HB3	2.55	0.41
3:A:76:LEU:HD12	3:A:76:LEU:HA	1.76	0.41
1:H:97:ALA:HB3	1:H:102:PHE:HD2	1.85	0.41
4:B:530:GLU:CD	5:C:736:ARG:HH12	2.23	0.41
5:C:214:LEU:O	5:C:393:GLN:NE2	2.53	0.41
1:E:101:VAL:HG12	1:E:101:VAL:O	2.20	0.41
3:A:68:LYS:HB3	3:A:68:LYS:HE3	1.90	0.41
3:A:408:PHE:HB3	3:A:459:CYS:SG	2.61	0.41
4:B:307:LEU:HD12	4:B:311:SER:HA	2.03	0.41
3:A:82:LEU:HD12	3:A:87:VAL:HG11	2.02	0.41
3:A:335:THR:CG2	3:A:346:ARG:HH22	2.31	0.41
5:C:92:VAL:HG12	5:C:120:GLY:HA2	2.02	0.41
3:A:167:VAL:HG12	3:A:196:GLN:HB3	2.03	0.41
4:B:158:MET:O	4:B:161:ILE:HG22	2.21	0.41
4:B:286:TYR:CZ	4:B:291:ARG:HG2	2.56	0.41
4:B:531:THR:OG1	4:B:711:ASP:OD1	2.23	0.41
5:C:130:ASP:HB3	5:C:133:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:528:GLU:OE2	5:C:743:MET:HB3	2.21	0.41
4:D:508:ALA:O	4:D:512:LEU:HD11	2.20	0.41
2:L:121:PRO:HA	2:L:134:VAL:HG12	2.02	0.41
3:A:193:LYS:HG3	3:A:195:LEU:H	1.85	0.41
3:A:376:ASP:O	3:A:377:ARG:NE	2.49	0.41
3:A:698:ALA:O	3:A:702:VAL:HG13	2.20	0.41
4:B:191:VAL:HG23	4:B:198:TRP:CD1	2.56	0.41
4:B:298:ILE:HG12	4:B:348:LEU:HD11	2.03	0.41
5:C:147:GLN:O	5:C:150:VAL:HG12	2.20	0.41
2:L:35:TRP:CZ3	2:L:88:CYS:HB3	2.56	0.41
5:C:144:TYR:N	5:C:144:TYR:HD1	2.19	0.41
5:C:341:ASN:OD1	5:C:342:GLU:N	2.54	0.41
4:D:339:VAL:O	4:D:349:SER:HB2	2.21	0.41
1:E:60:TYR:HE2	1:E:68:VAL:HG23	1.86	0.41
1:E:72:ALA:HA	1:E:79:ALA:HA	2.03	0.41
2:L:39:LYS:HZ3	2:L:39:LYS:HG3	1.82	0.41
3:A:399:LYS:H	3:A:399:LYS:HG2	1.72	0.41
3:A:410:TYR:HB3	3:A:456:TYR:CE1	2.55	0.41
3:A:488:GLU:N	3:A:497:GLU:O	2.38	0.41
4:B:152:GLN:N	4:B:152:GLN:OE1	2.53	0.41
4:B:158:MET:HE1	4:B:258:PRO:HA	2.01	0.41
4:B:158:MET:HG2	4:B:256:ILE:HG21	2.02	0.41
4:B:485:HIS:O	4:B:495:GLY:HA3	2.21	0.41
4:B:493:TRP:CZ2	4:B:521:VAL:HG21	2.56	0.41
4:B:673:ASN:HA	4:B:676:ASN:HD21	1.86	0.41
4:B:749:SER:HA	4:B:750:PRO:HD3	1.88	0.41
5:C:131:LYS:HD3	5:C:131:LYS:HA	1.70	0.41
5:C:366:ILE:HD13	5:C:366:ILE:HA	1.92	0.41
5:C:538:LEU:HD13	5:C:735:PHE:HB3	2.01	0.41
4:D:158:MET:HA	4:D:161:ILE:HG22	2.03	0.41
4:D:234:ASP:O	4:D:237:VAL:HG22	2.21	0.41
2:F:189:GLU:OE1	2:F:213:ARG:NH1	2.53	0.41
1:H:140:LYS:HA	1:H:140:LYS:HD2	1.79	0.41
4:B:711:ASP:O	4:B:715:LEU:HG	2.21	0.41
5:C:466:LEU:HA	5:C:469:THR:HG22	2.01	0.41
4:D:162:MET:SD	4:D:226:VAL:HG11	2.60	0.41
4:D:463:ILE:HA	4:D:466:LYS:HE3	2.03	0.41
1:H:119:LYS:HE2	1:H:142:TYR:HA	2.03	0.40
3:A:124:ARG:H	3:A:124:ARG:HG2	1.72	0.40
3:A:356:LEU:HD11	3:A:359:ARG:HA	2.03	0.40
4:B:690:GLN:HG2	4:B:696:ALA:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:193:LYS:HB3	5:C:195:LEU:HG	2.03	0.40
3:A:129:SER:OG	3:A:139:ARG:NH1	2.54	0.40
3:A:162:HIS:NE2	3:A:392:TYR:HB3	2.36	0.40
3:A:254:ILE:HD13	3:A:268:GLY:HA3	2.02	0.40
5:C:170:ASP:O	5:C:174:ARG:HG3	2.21	0.40
5:C:353:ILE:HD11	5:C:365:GLY:HA3	2.03	0.40
1:E:12:LYS:O	1:E:113:VAL:HA	2.21	0.40
3:A:408:PHE:HZ	3:A:534:LYS:HE2	1.86	0.40
4:B:484:LYS:HA	4:B:484:LYS:HD3	1.83	0.40
5:C:58:ILE:HB	5:C:293:HIS:HE1	1.86	0.40
2:F:23:CYS:O	2:F:70:GLU:HA	2.21	0.40
3:A:260:ARG:HG3	3:A:261:TYR:CE1	2.56	0.40
4:B:771:LEU:HD12	4:B:771:LEU:O	2.21	0.40
5:C:145:SER:HB3	5:C:179:ARG:HD3	2.04	0.40
1:E:23:LYS:HE2	1:E:23:LYS:HB2	1.91	0.40
2:F:24:ARG:HD2	2:F:24:ARG:HA	1.91	0.40
2:L:168:GLN:HG2	2:L:175:TYR:CE1	2.57	0.40
4:D:55:TRP:HB3	4:D:56:GLY:H	1.51	0.40
4:D:147:PHE:HB2	4:D:356:GLN:OE1	2.21	0.40
4:D:672:ARG:HA	4:D:672:ARG:HD2	1.90	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	E	203/211 (96%)	180 (89%)	23 (11%)	0	100	100
1	H	209/211 (99%)	183 (88%)	26 (12%)	0	100	100
2	F	213/215 (99%)	190 (89%)	23 (11%)	0	100	100
2	L	213/215 (99%)	182 (85%)	31 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	656/776 (84%)	566 (86%)	85 (13%)	5 (1%)	16	53
4	B	650/771 (84%)	567 (87%)	80 (12%)	3 (0%)	25	61
4	D	642/771 (83%)	546 (85%)	91 (14%)	5 (1%)	16	53
5	C	659/776 (85%)	561 (85%)	96 (15%)	2 (0%)	37	71
All	All	3445/3946 (87%)	2975 (86%)	455 (13%)	15 (0%)	32	66

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	58	ILE
3	A	71	ALA
3	A	389	PRO
4	D	36	ILE
4	D	260	LEU
4	D	657	SER
3	A	135	LEU
5	C	163	ILE
4	D	414	ALA
4	D	430	VAL
4	B	781	HIS
5	C	665	VAL
3	A	406	GLU
4	B	507	MET
4	B	657	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	104/178 (58%)	99 (95%)	5 (5%)	21	45
1	H	150/178 (84%)	147 (98%)	3 (2%)	50	68
2	F	156/186 (84%)	153 (98%)	3 (2%)	52	70
2	L	139/186 (75%)	136 (98%)	3 (2%)	47	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	498/674 (74%)	475 (95%)	23 (5%)	23	46
4	B	421/675 (62%)	405 (96%)	16 (4%)	28	51
4	D	399/675 (59%)	378 (95%)	21 (5%)	19	43
5	C	474/674 (70%)	452 (95%)	22 (5%)	23	46
All	All	2341/3426 (68%)	2245 (96%)	96 (4%)	28	49

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	64	PHE
1	E	67	HIS
1	E	83	TRP
1	E	98	ARG
1	E	99	SER
2	F	21	LEU
2	F	70	GLU
2	F	110	ARG
1	H	40	MET
1	H	83	TRP
1	H	189	GLN
2	L	82	ASP
2	L	188	TYR
2	L	203	LEU
3	A	37	LYS
3	A	43	ARG
3	A	56	TRP
3	A	67	HIS
3	A	101	HIS
3	A	113	PHE
3	A	132	SER
3	A	226	ASP
3	A	247	TRP
3	A	290	GLN
3	A	313	ASN
3	A	359	ARG
3	A	371	HIS
3	A	446	SER
3	A	453	GLN
3	A	454	CYS
3	A	512	MET
3	A	526	TYR

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Mol	Chain	Res	Type
3	A	660	PHE
3	A	692	TYR
3	A	725	CYS
3	A	736	ARG
3	A	766	MET
4	B	88	ASP
4	B	147	PHE
4	B	180	TYR
4	B	241	SER
4	B	251	TYR
4	B	287	SER
4	B	319	SER
4	B	320	CYS
4	B	334	LEU
4	B	344	ASP
4	B	386	ARG
4	B	393	TYR
4	B	423	ASP
4	B	472	LYS
4	B	496	MET
4	B	650	PHE
5	C	43	ARG
5	C	59	GLN
5	C	85	SER
5	C	113	PHE
5	C	132	SER
5	C	134	HIS
5	C	158	TYR
5	C	177	GLN
5	C	185	GLU
5	C	226	ASP
5	C	252	ARG
5	C	315	TRP
5	C	322	LYS
5	C	360	LYS
5	C	441	ASP
5	C	523	ARG
5	C	684	TYR
5	C	710	PHE
5	C	736	ARG
5	C	743	MET
5	C	756	SER

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Mol	Chain	Res	Type
5	C	769	LEU
4	D	55	TRP
4	D	133	MET
4	D	154	GLN
4	D	162	MET
4	D	200	MET
4	D	244	ARG
4	D	251	TYR
4	D	286	TYR
4	D	326	ARG
4	D	338	MET
4	D	348	LEU
4	D	381	HIS
4	D	462	ASP
4	D	507	MET
4	D	524	PHE
4	D	660	PHE
4	D	688	PHE
4	D	710	TYR
4	D	745	LEU
4	D	753	ARG
4	D	762	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	32	ASN
2	L	168	GLN
4	B	676	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

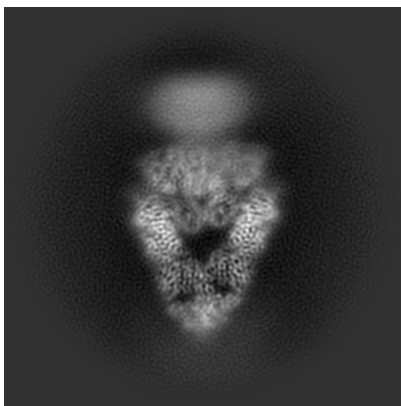
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43538. These allow visual inspection of the internal detail of the map and identification of artifacts.

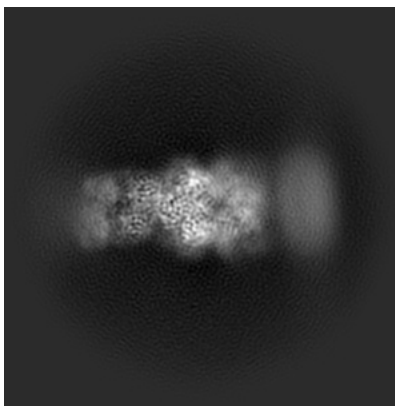
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

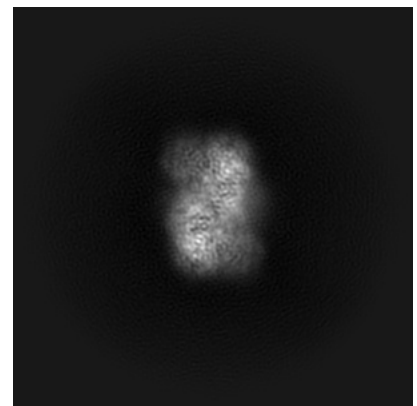
6.1.1 Primary map



X

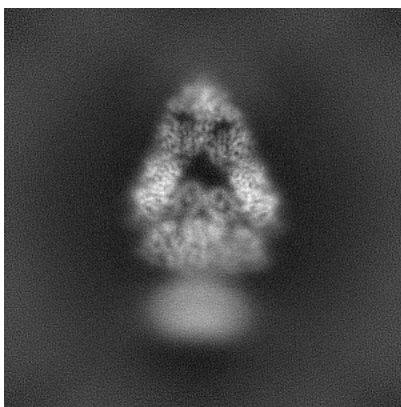


Y

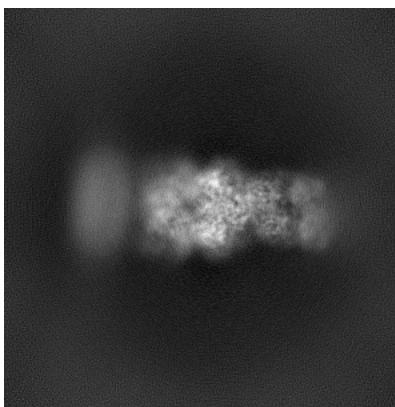


Z

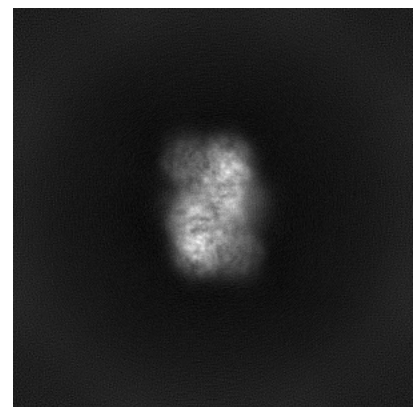
6.1.2 Raw map



X



Y

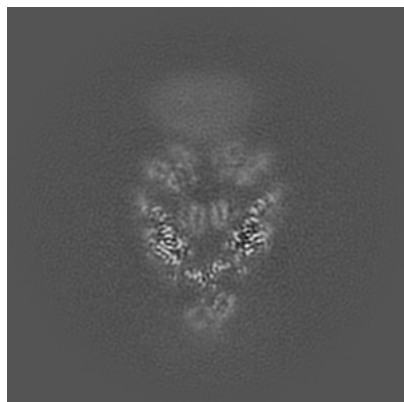


Z

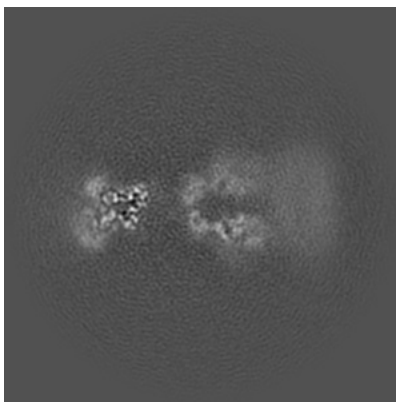
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

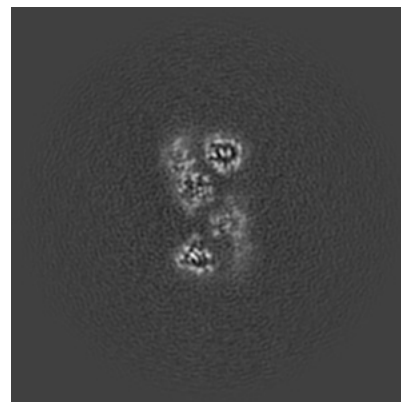
6.2.1 Primary map



X Index: 220

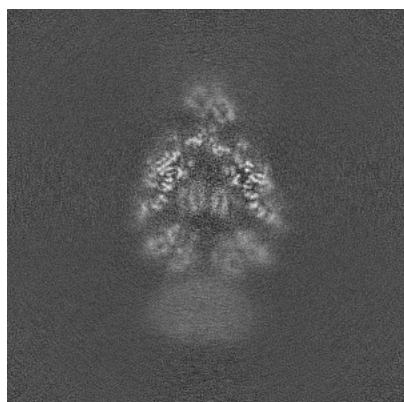


Y Index: 220

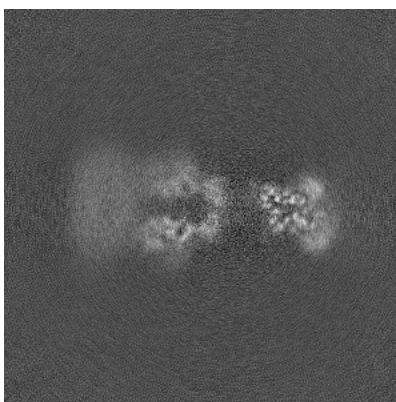


Z Index: 220

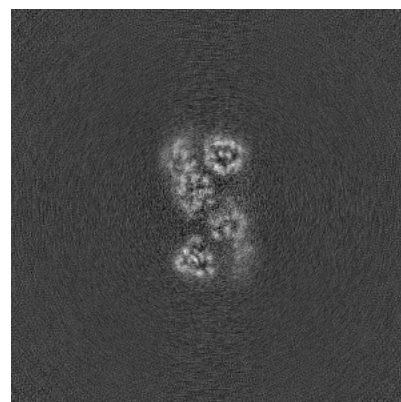
6.2.2 Raw map



X Index: 220



Y Index: 220

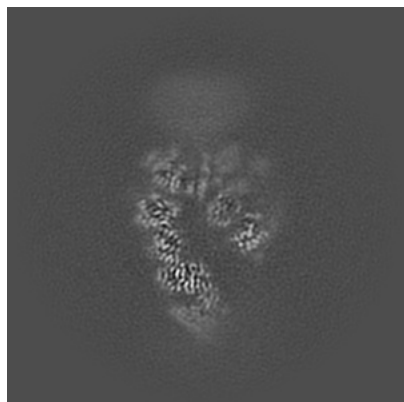


Z Index: 220

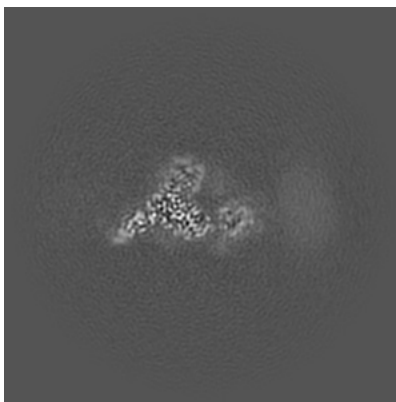
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

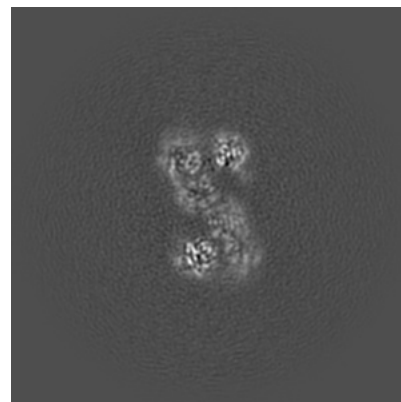
6.3.1 Primary map



X Index: 206

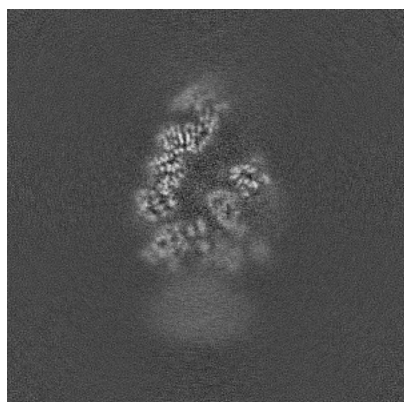


Y Index: 175



Z Index: 209

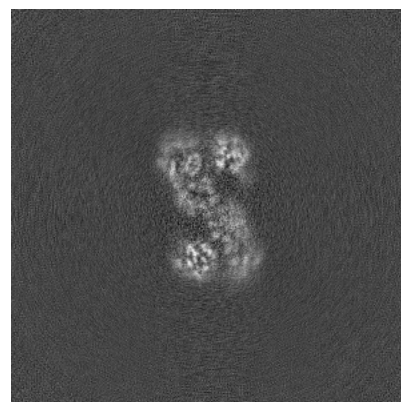
6.3.2 Raw map



X Index: 209



Y Index: 182

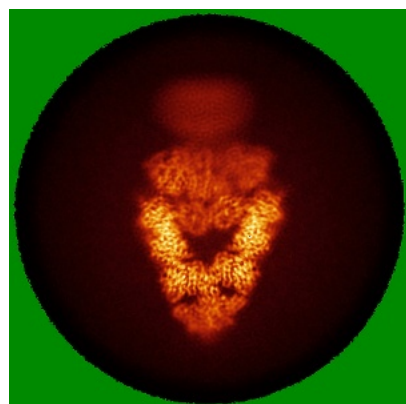


Z Index: 230

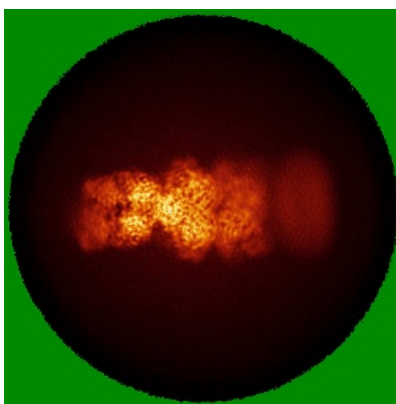
The images above show the largest variance slices of the map in three orthogonal directions.

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

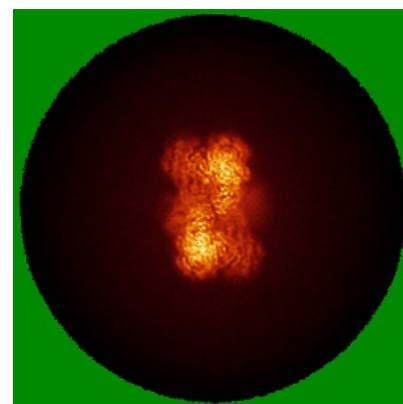
6.4.1 Primary map



X

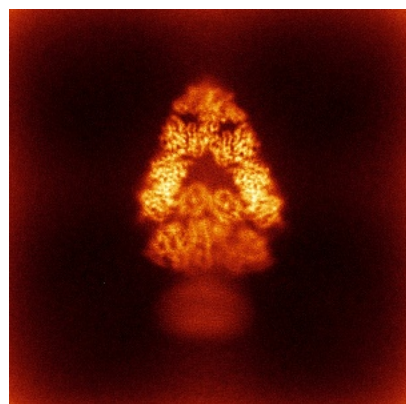


Y

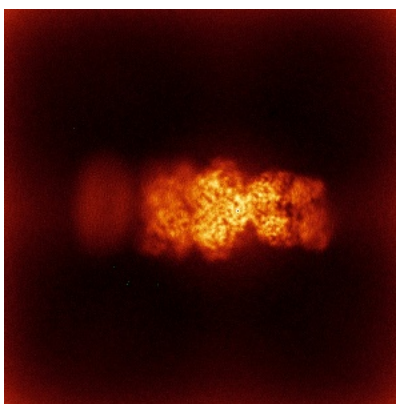


Z

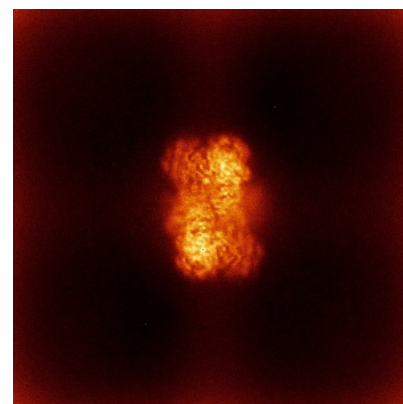
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



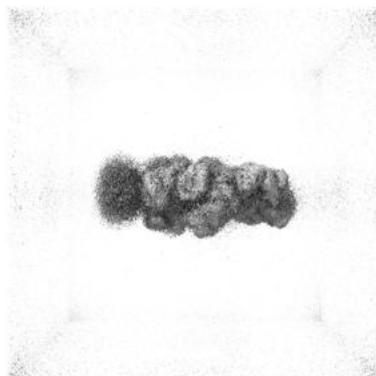
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0508. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

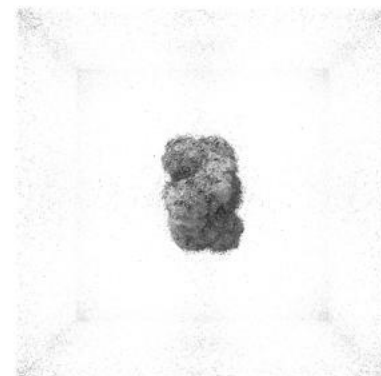
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

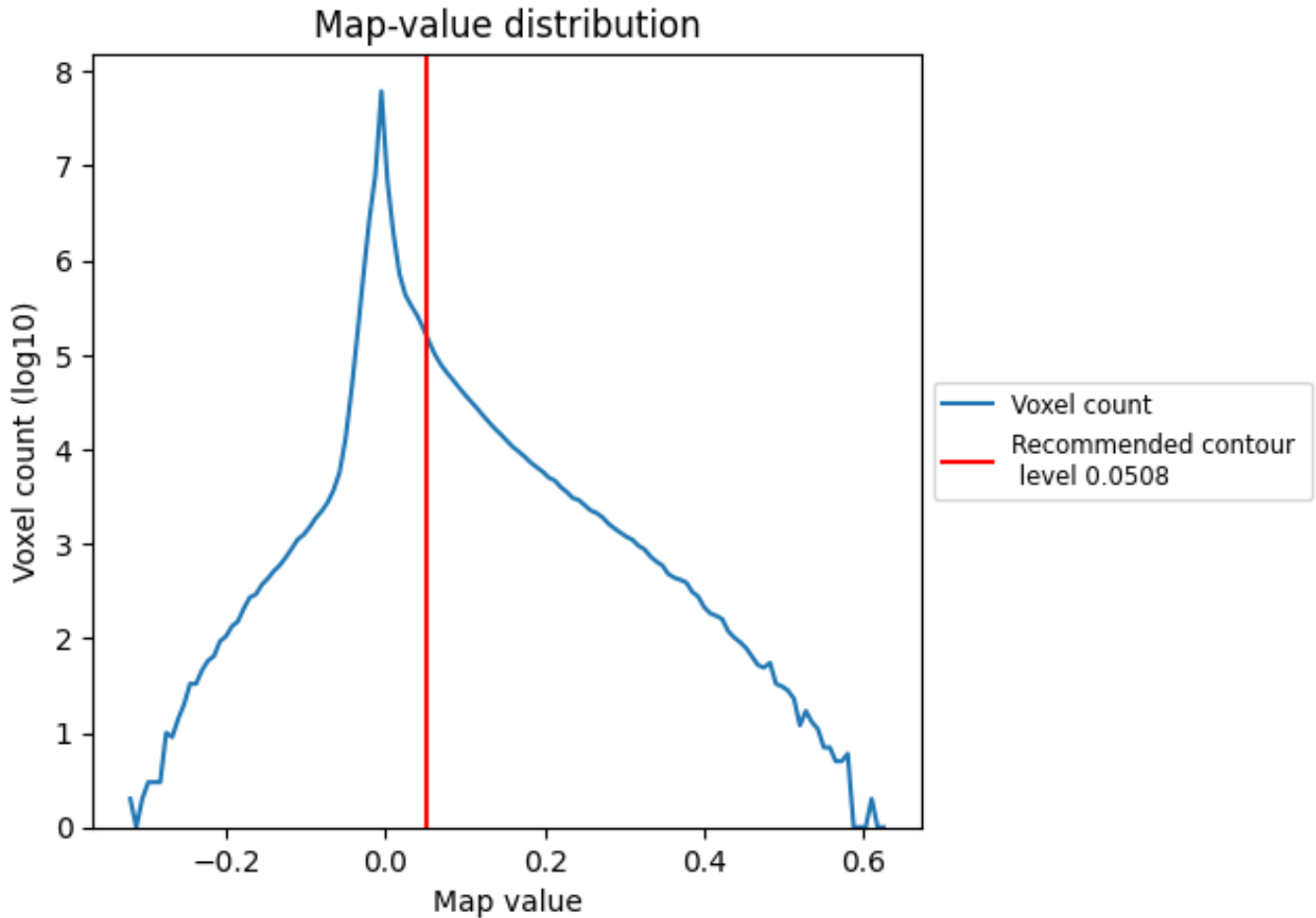
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

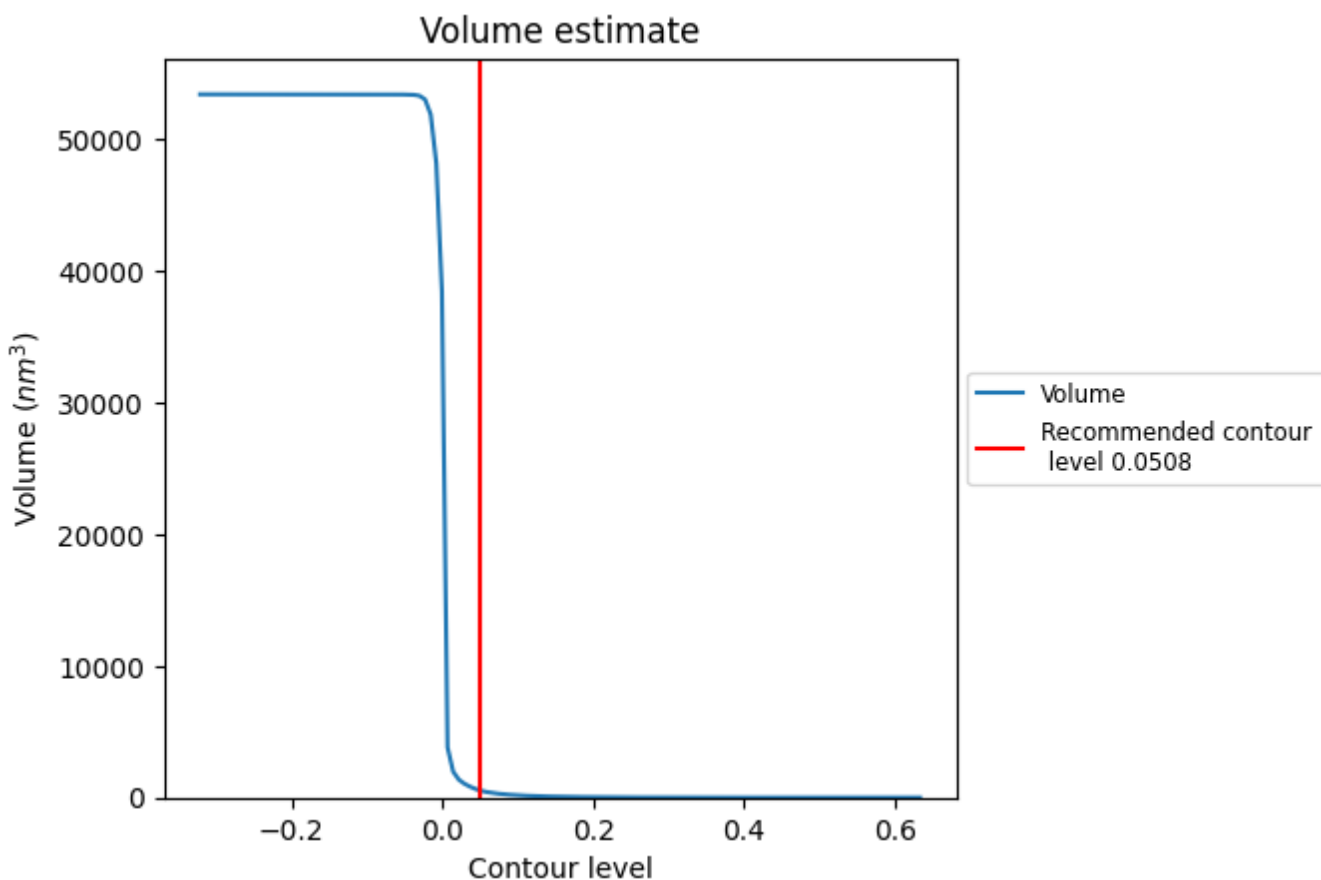
This section contains the results of statistical analysis of the map.

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.

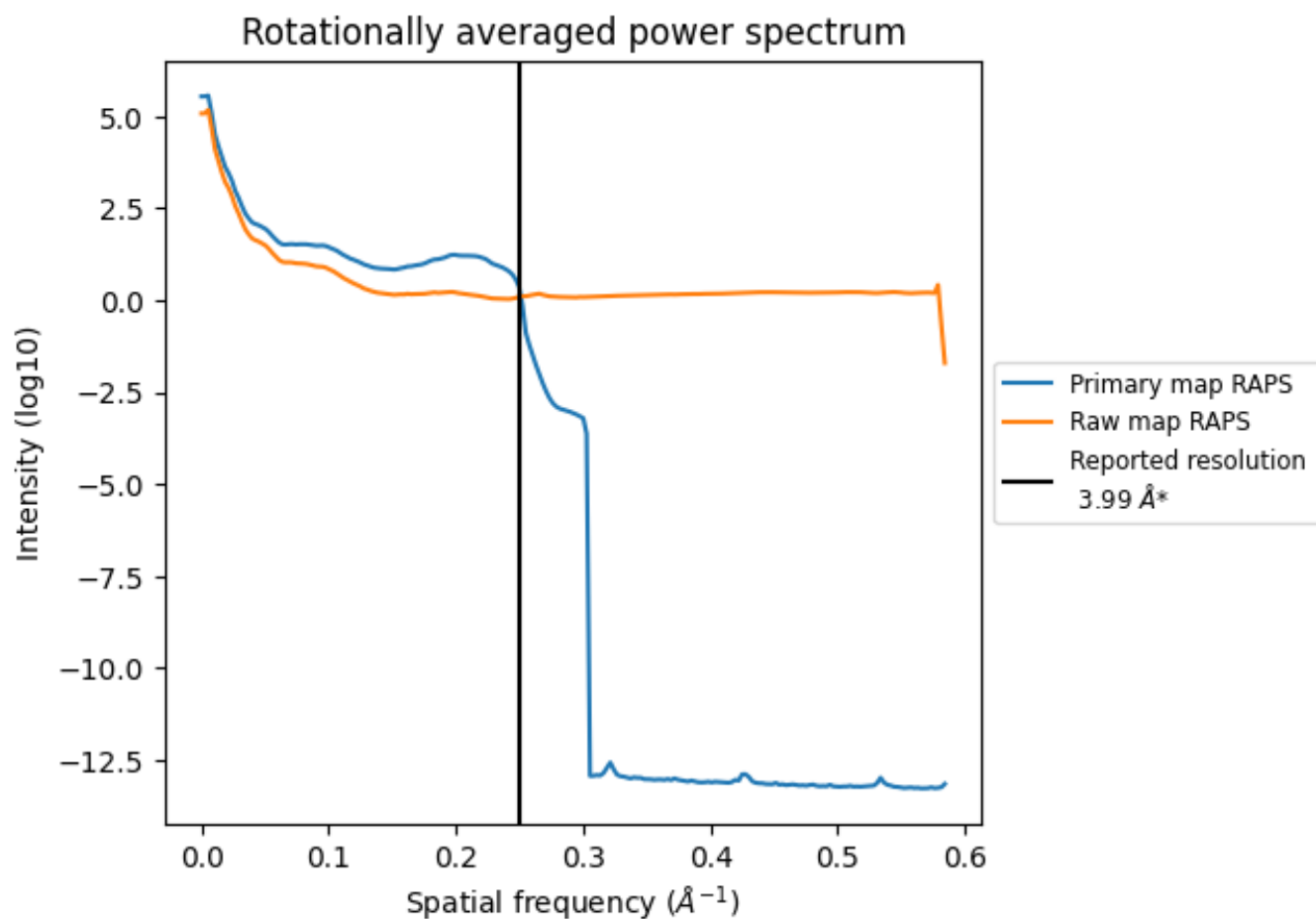
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 536 nm^3 ; this corresponds to an approximate mass of 484 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

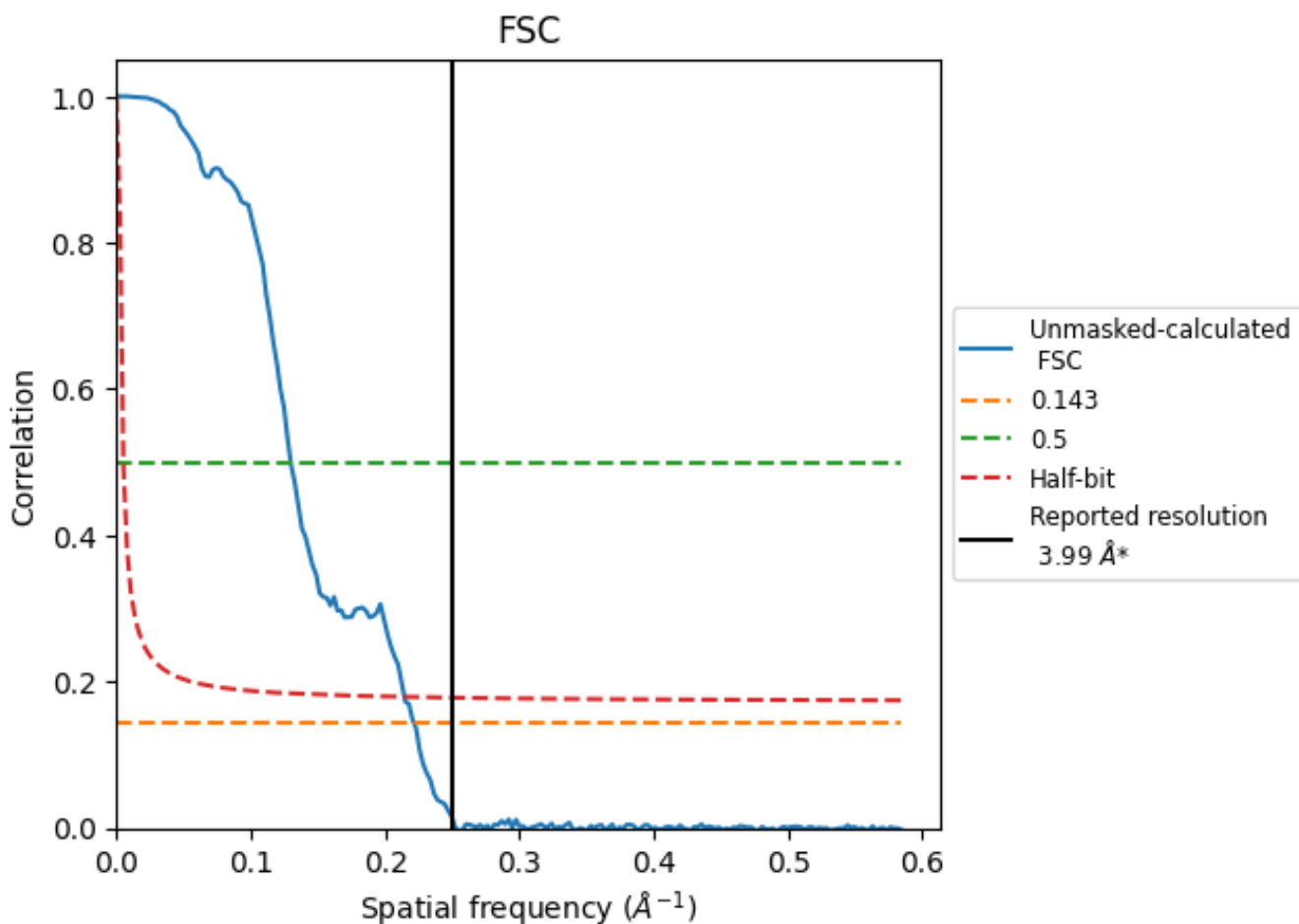


*Reported resolution corresponds to spatial frequency of 0.251 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.251 Å⁻¹

8.2 Resolution estimates [i](#)

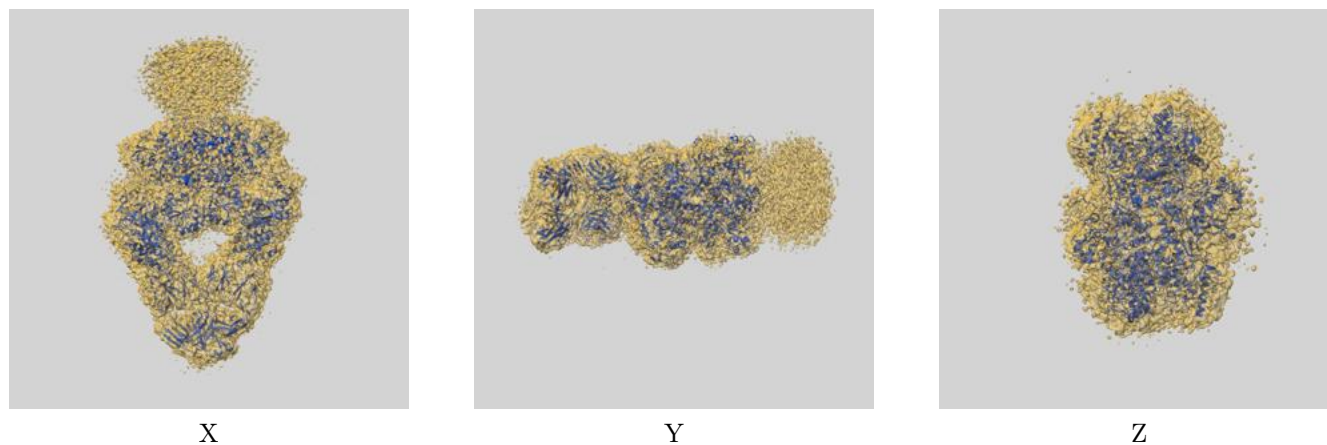
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.99	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.51	7.70	4.67

*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 4.51 differs from the reported value 3.99 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43538 and PDB model 8VUS. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



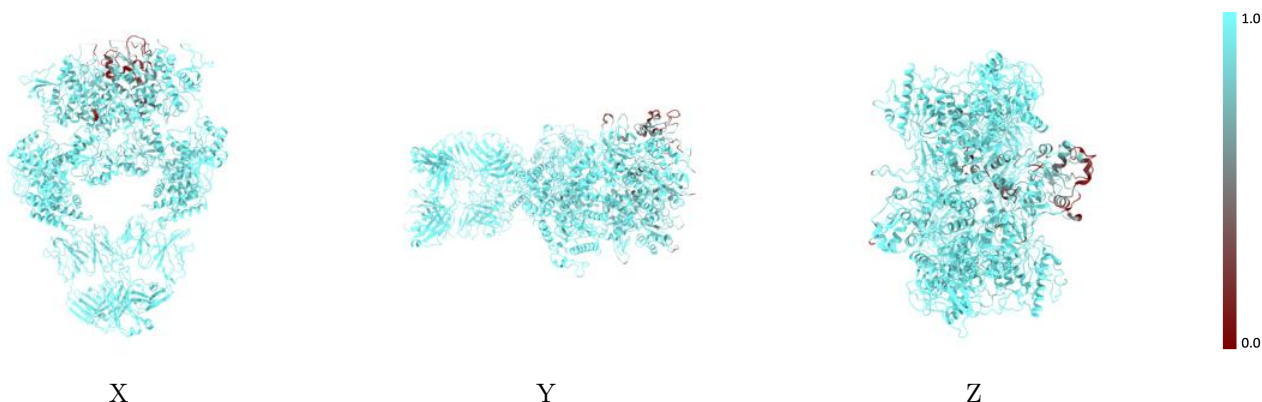
The images above show the 3D surface view of the map at the recommended contour level 0.0508 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



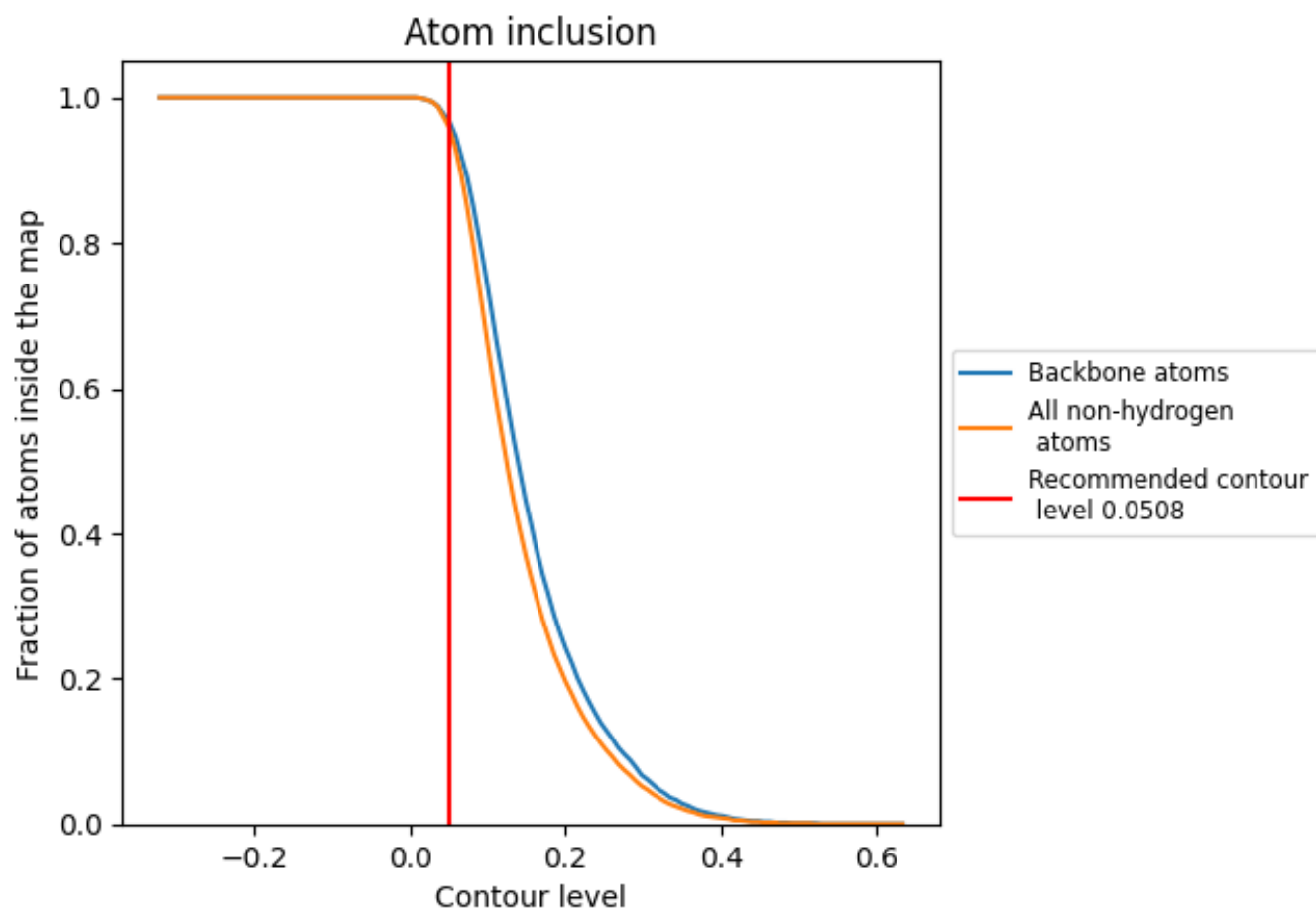
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0508).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0508) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9600	 0.3810
A	 0.9640	 0.3510
B	 0.9730	 0.3820
C	 0.9820	 0.4140
D	 0.8710	 0.2900
E	 0.9980	 0.4500
F	 0.9900	 0.4190
H	 0.9970	 0.4630
L	 0.9970	 0.4620

