Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 05:37 PM EST

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

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

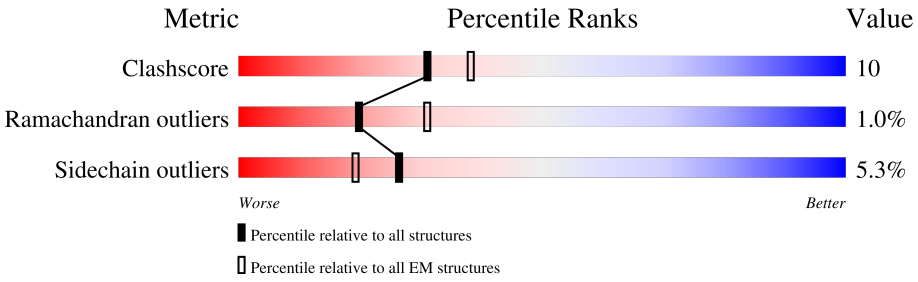
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 6.59 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	862	12% 67% 22% · 8%
1	C	862	12% 66% 22% · 8%
2	B	883	13% 61% 23% · 13%
2	D	883	13% 60% 23% · 13%
3	H	223	42% 37% 16% 48%
3	M	223	41% 36% 15% · 48%
4	L	213	46% 35% 13% · 50%
4	N	213	46% 35% 13% · 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 28054 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	790	Total	C	N	O	S	0	0
			6230	3961	1081	1151	37		
1	C	790	Total	C	N	O	S	0	0
			6230	3961	1081	1151	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	771	Total	C	N	O	S	0	0
			6075	3914	979	1141	41		
2	D	771	Total	C	N	O	S	0	0
			6075	3914	979	1141	41		

There are 126 discrepancies between the modelled and reference sequences:

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

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

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

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

- Molecule 3 is a protein called Fab2 heavy chain.

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

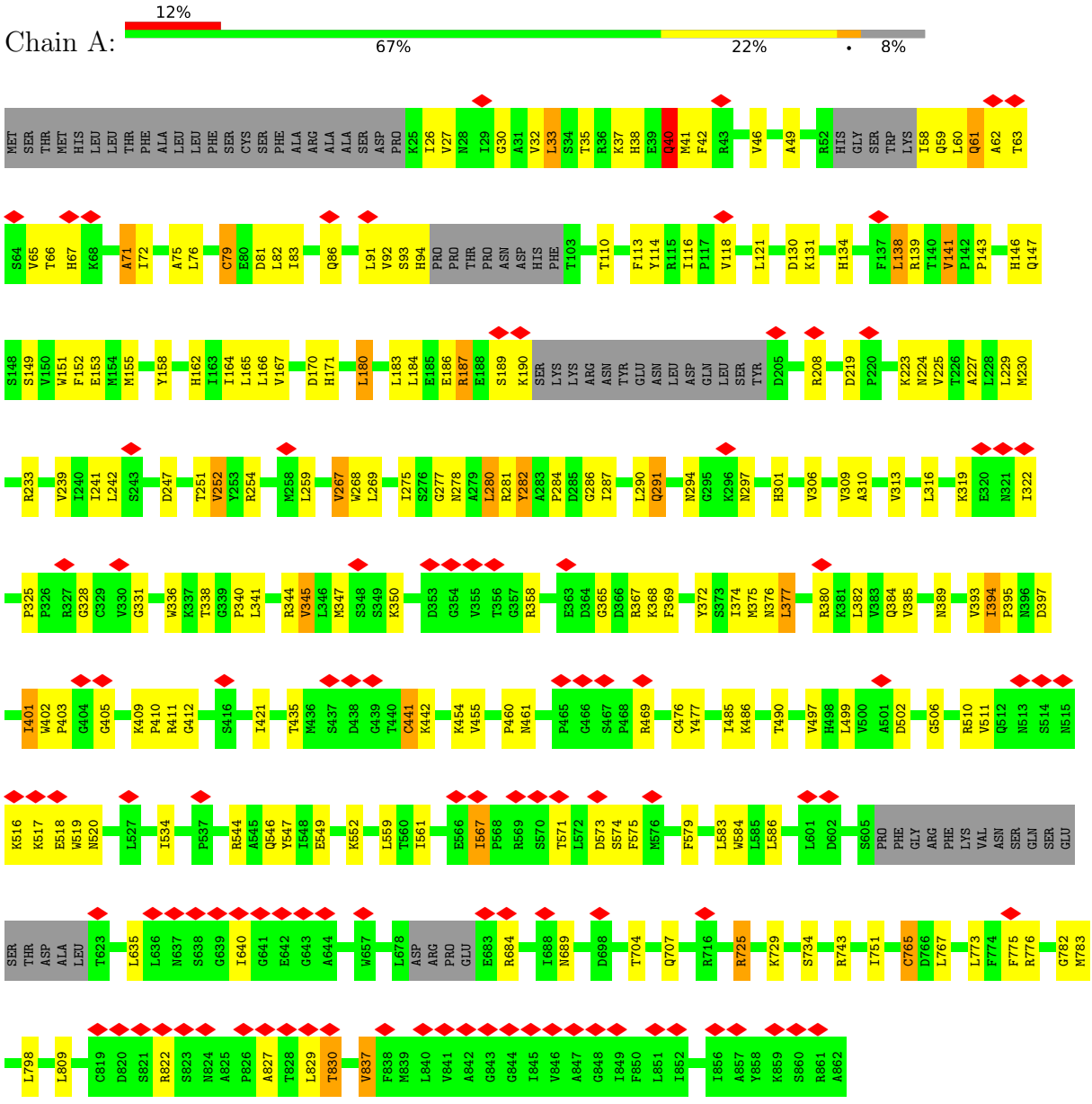
- Molecule 4 is a protein called Fab2 light chain.

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

3 Residue-property plots (i)

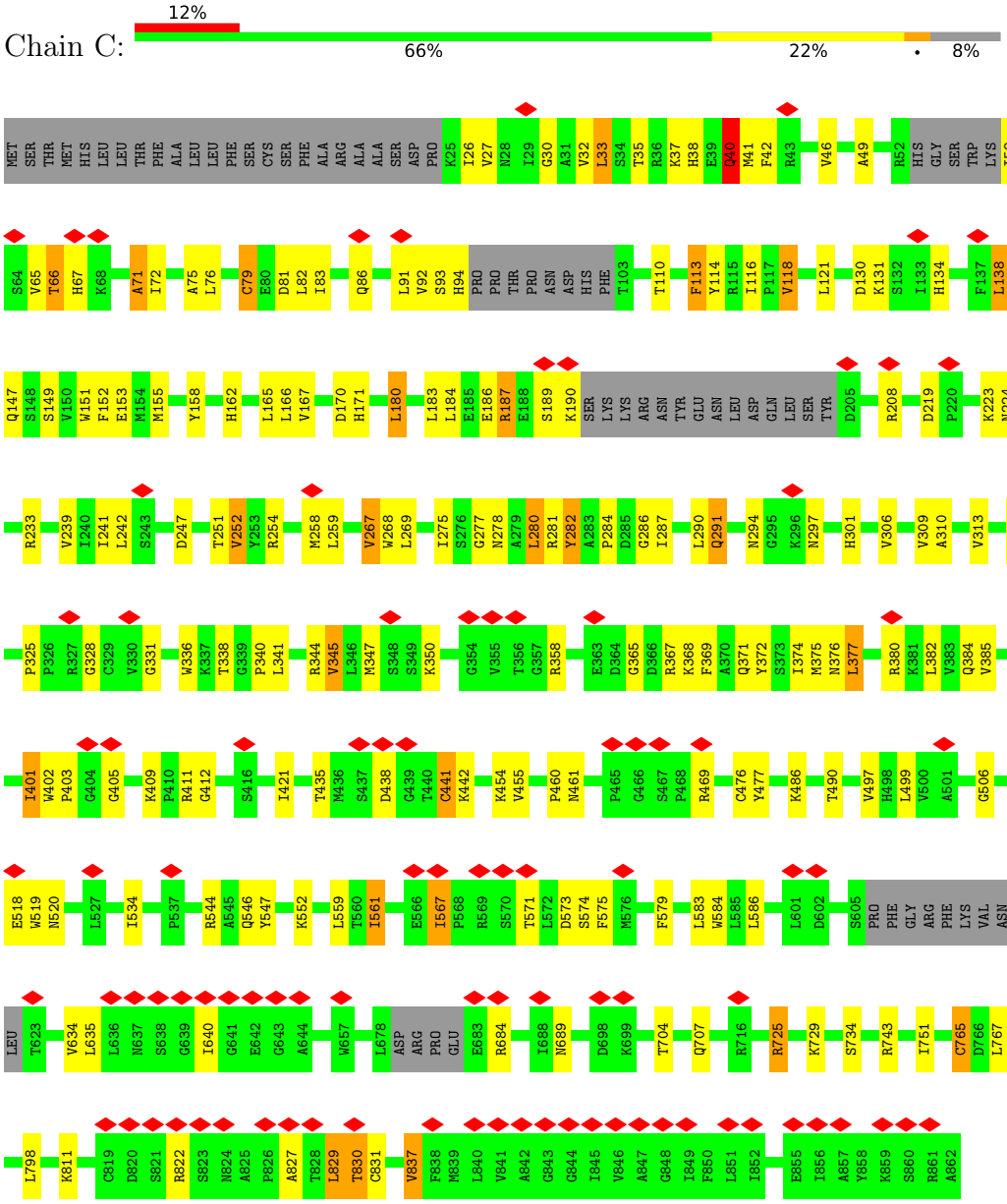
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



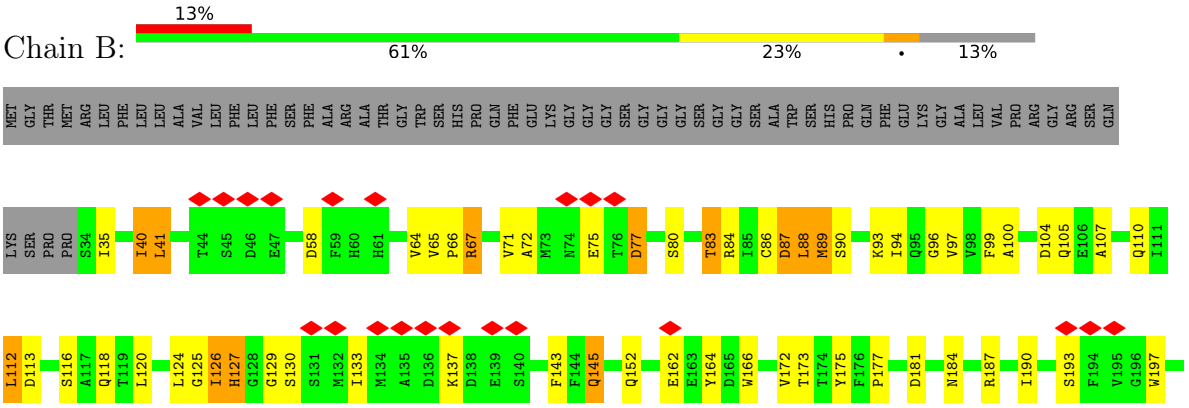
• Molecule 1: Glutamate receptor ionotropic, NMDA 1

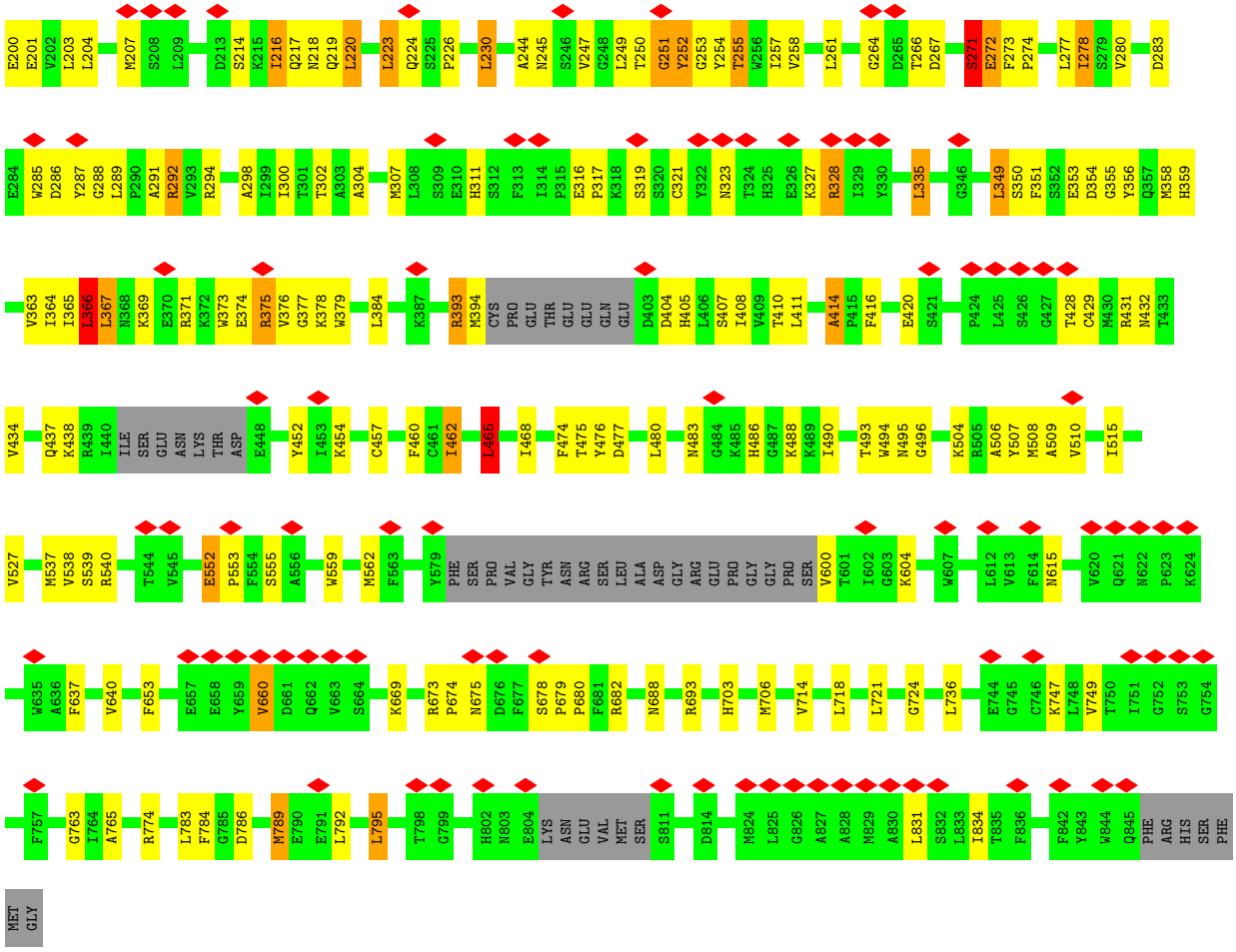
Chain C:



• Molecule 2: Glutamate receptor ionotropic, NMDA 2B

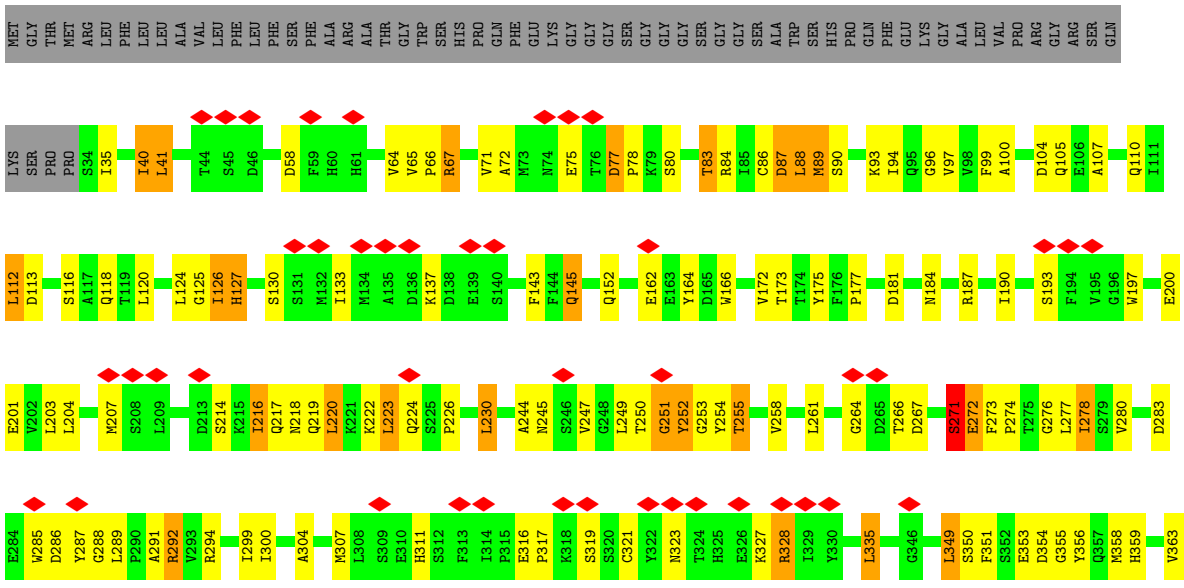
Chain B:

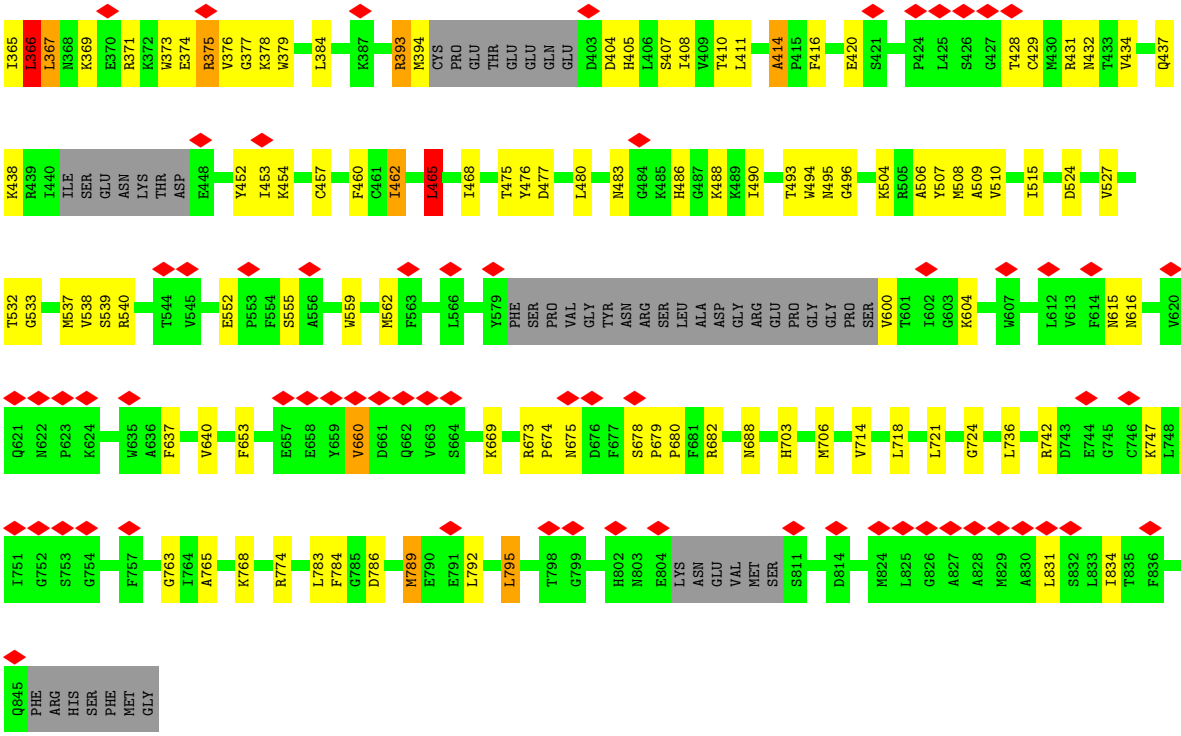




• Molecule 2: Glutamate receptor ionotropic, NMDA 2B

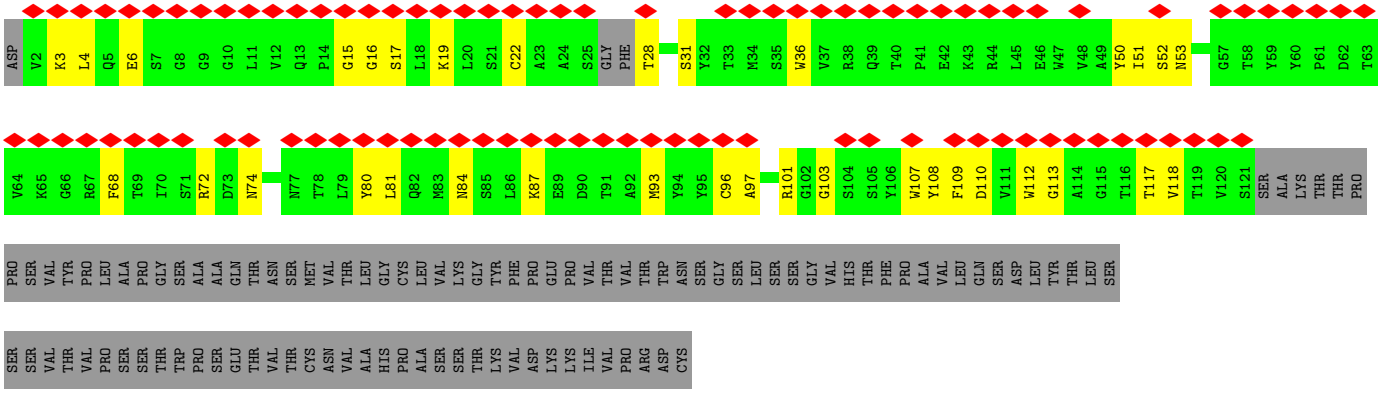
Chain D:





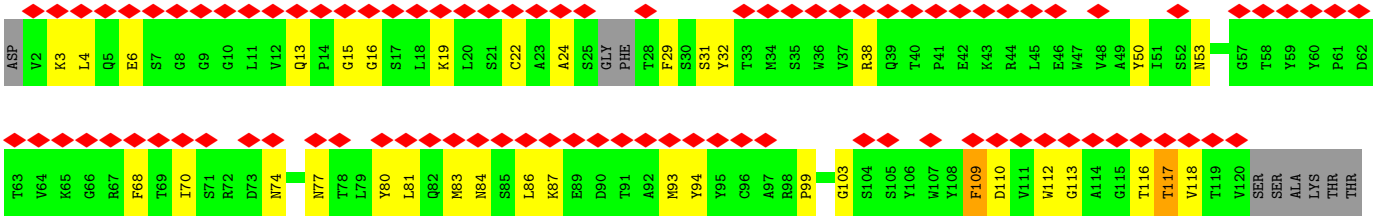
• Molecule 3: Fab2 heavy chain

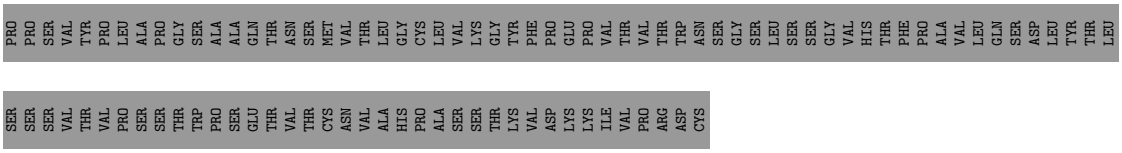
Chain H:



• Molecule 3: Fab2 heavy chain

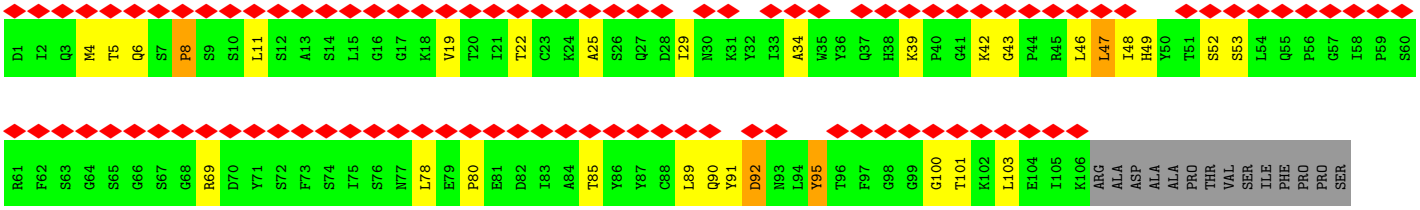
Chain M:





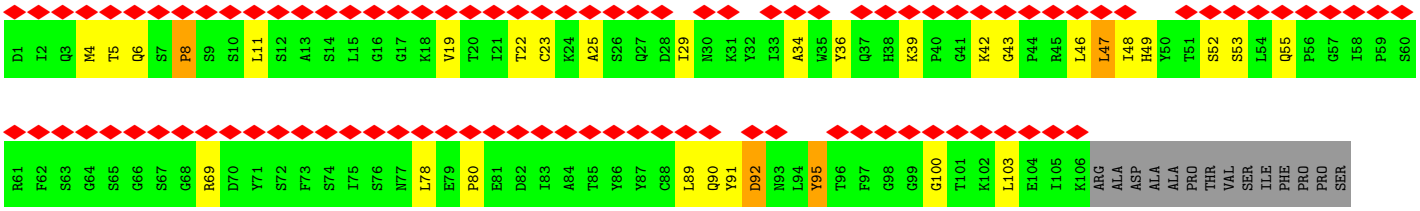
• Molecule 4: Fab2 light chain

Chain L:



• Molecule 4: Fab2 light chain

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18851	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	7.430	Depositor
Minimum map value	-1.126	Depositor
Average map value	0.054	Depositor
Map value standard deviation	0.431	Depositor
Recommended contour level	3.0	Depositor
Map size (Å)	350.72, 350.72, 350.72	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.34	0/6358	0.73	7/8599 (0.1%)
1	C	0.34	1/6358 (0.0%)	0.73	7/8599 (0.1%)
2	B	0.34	0/6209	0.75	9/8411 (0.1%)
2	D	0.34	0/6209	0.75	9/8411 (0.1%)
3	H	0.31	0/927	0.59	0/1255
3	M	0.32	0/921	0.61	0/1247
4	L	0.35	0/840	0.68	1/1136 (0.1%)
4	N	0.35	0/840	0.68	1/1136 (0.1%)
All	All	0.34	1/28662 (0.0%)	0.73	34/38794 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	18
1	C	0	18
2	B	0	24
2	D	0	24
3	H	0	2
3	M	0	1
4	L	0	3
4	N	0	3
All	All	0	93

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	118	VAL	CB-CG2	-5.03	1.42	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	367	LEU	CA-CB-CG	9.45	137.04	115.30
2	B	367	LEU	CA-CB-CG	9.44	137.02	115.30
1	A	138	LEU	CA-CB-CG	9.11	136.25	115.30
1	C	138	LEU	CA-CB-CG	9.10	136.22	115.30
2	D	465	LEU	CA-CB-CG	8.15	134.04	115.30
2	B	465	LEU	CA-CB-CG	8.13	134.00	115.30
1	C	377	LEU	CA-CB-CG	7.50	132.55	115.30
1	A	377	LEU	CA-CB-CG	7.49	132.54	115.30
2	D	224	GLN	C-N-CA	6.75	138.57	121.70
2	B	224	GLN	C-N-CA	6.71	138.48	121.70
2	B	335	LEU	CA-CB-CG	6.58	130.44	115.30
2	D	335	LEU	CA-CB-CG	6.58	130.42	115.30
2	B	58	ASP	CB-CG-OD1	6.48	124.14	118.30
2	D	58	ASP	CB-CG-OD1	6.44	124.10	118.30
1	C	180	LEU	CA-CB-CG	6.18	129.52	115.30
1	A	180	LEU	CA-CB-CG	6.17	129.50	115.30
1	A	282	TYR	C-N-CA	6.05	136.82	121.70
1	C	282	TYR	C-N-CA	6.04	136.79	121.70
2	D	718	LEU	CA-CB-CG	5.85	128.75	115.30
2	B	718	LEU	CA-CB-CG	5.84	128.73	115.30
2	B	562	MET	CA-CB-CG	5.74	123.06	113.30
2	D	562	MET	CA-CB-CG	5.73	123.03	113.30
1	A	401	ILE	C-N-CA	5.66	135.85	121.70
1	C	401	ILE	C-N-CA	5.61	135.73	121.70
2	B	795	LEU	CA-CB-CG	5.43	127.79	115.30
2	D	795	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	180	LEU	CB-CG-CD1	5.28	119.98	111.00
1	C	180	LEU	CB-CG-CD1	5.26	119.95	111.00
2	B	264	GLY	N-CA-C	5.19	126.08	113.10
2	D	264	GLY	N-CA-C	5.18	126.05	113.10
1	A	40	GLN	C-N-CA	5.15	134.57	121.70
1	C	40	GLN	C-N-CA	5.14	134.54	121.70
4	L	78	LEU	CA-CB-CG	5.04	126.89	115.30
4	N	78	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (93) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	252	VAL	Peptide
1	A	284	PRO	Peptide
1	A	33	LEU	Peptide
1	A	35	THR	Peptide

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

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Mol	Chain	Res	Type	Group
1	C	372	TYR	Peptide
1	C	394	ILE	Peptide
1	C	40	GLN	Peptide
1	C	405	GLY	Peptide
1	C	552	LYS	Peptide
1	C	567	ILE	Peptide
1	C	61	GLN	Peptide
1	C	62	ALA	Peptide
1	C	640	ILE	Peptide
1	C	66	THR	Peptide
1	C	71	ALA	Peptide
1	C	79	CYS	Peptide
1	C	829	LEU	Peptide
1	C	830	THR	Peptide
2	D	126	ILE	Peptide
2	D	145	GLN	Peptide
2	D	193	SER	Peptide
2	D	197	TRP	Peptide
2	D	216	ILE	Mainchain
2	D	251	GLY	Peptide
2	D	255	THR	Peptide
2	D	271	SER	Peptide
2	D	278	ILE	Peptide
2	D	283	ASP	Peptide
2	D	285	TRP	Peptide
2	D	311	HIS	Peptide
2	D	350	SER	Peptide
2	D	354	ASP	Peptide
2	D	366	LEU	Peptide
2	D	414	ALA	Peptide
2	D	476	TYR	Peptide
2	D	506	ALA	Peptide
2	D	552	GLU	Peptide
2	D	660	VAL	Peptide
2	D	678	SER	Peptide
2	D	72	ALA	Peptide
2	D	795	LEU	Peptide
2	D	83	THR	Mainchain
3	H	109	PHE	Peptide
3	H	36	TRP	Peptide
4	L	47	LEU	Peptide
4	L	8	PRO	Peptide

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Mol	Chain	Res	Type	Group
4	L	80	PRO	Peptide
3	M	109	PHE	Peptide
4	N	47	LEU	Peptide
4	N	8	PRO	Peptide
4	N	80	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6230	0	6230	110	0
1	C	6230	0	6230	118	0
2	B	6075	0	5994	127	0
2	D	6075	0	5994	134	0
3	H	905	0	867	21	0
3	M	899	0	862	23	0
4	L	820	0	802	18	0
4	N	820	0	802	19	0
All	All	28054	0	27781	542	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 (542) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:THR:O	2:B:87:ASP:HB2	1.71	0.90
2:D:83:THR:O	2:D:87:ASP:HB2	1.71	0.88
2:B:615:ASN:HD21	2:D:615:ASN:HD21	1.33	0.75
3:M:15:GLY:H	3:M:87:LYS:HE3	1.54	0.72
4:L:29:ILE:HG12	4:L:69:ARG:HA	1.76	0.68
2:B:65:VAL:HG23	2:B:67:ARG:HH12	1.60	0.67
2:D:65:VAL:HG23	2:D:67:ARG:HH12	1.60	0.67
4:N:29:ILE:HG12	4:N:69:ARG:HA	1.76	0.67
1:A:79:CYS:HA	1:A:82:LEU:HB2	1.77	0.67
1:A:319:LYS:HB2	1:A:322:ILE:HD11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:LYS:HB2	1:C:322:ILE:HD11	1.78	0.66
1:C:79:CYS:HA	1:C:82:LEU:HB2	1.77	0.66
2:B:462:ILE:HA	2:B:465:LEU:HG	1.79	0.65
3:H:53:ASN:O	3:H:74:ASN:ND2	2.29	0.65
2:D:88:LEU:O	2:D:90:SER:N	2.29	0.65
1:A:546:GLN:O	2:D:774:ARG:NH2	2.30	0.65
2:D:462:ILE:HA	2:D:465:LEU:HG	1.79	0.65
2:B:88:LEU:O	2:B:90:SER:N	2.29	0.65
1:A:725:ARG:HH12	1:A:729:LYS:HE3	1.62	0.65
2:D:555:SER:HA	2:D:559:TRP:HB2	1.78	0.64
2:B:555:SER:HA	2:B:559:TRP:HB2	1.78	0.63
3:M:110:ASP:OD2	4:N:55:GLN:NE2	2.32	0.63
1:A:230:MET:SD	1:A:233:ARG:NH2	2.72	0.62
1:C:86:GLN:NE2	1:C:328:GLY:O	2.33	0.62
4:N:11:LEU:HB2	4:N:103:LEU:HA	1.81	0.62
1:C:331:GLY:H	2:D:77:ASP:HB2	1.64	0.62
1:C:230:MET:SD	1:C:233:ARG:NH2	2.72	0.62
1:C:725:ARG:HH12	1:C:729:LYS:HE3	1.62	0.62
4:L:11:LEU:HB2	4:L:103:LEU:HA	1.81	0.62
2:D:410:THR:OG1	2:D:411:LEU:N	2.33	0.62
1:A:86:GLN:NE2	1:A:328:GLY:O	2.33	0.61
2:B:410:THR:OG1	2:B:411:LEU:N	2.33	0.61
1:C:634:VAL:O	2:D:616:ASN:ND2	2.29	0.61
3:M:19:LYS:HE2	3:M:80:TYR:HB3	1.82	0.61
3:H:4:LEU:HB2	3:H:113:GLY:HA2	1.84	0.60
3:M:53:ASN:O	3:M:74:ASN:ND2	2.34	0.60
4:N:49:HIS:HB2	4:N:53:SER:HB3	1.83	0.60
2:D:271:SER:O	2:D:273:PHE:N	2.34	0.60
4:L:49:HIS:HB2	4:L:53:SER:HB3	1.83	0.60
2:B:653:PHE:HA	1:C:827:ALA:HB1	1.84	0.59
1:C:38:HIS:O	1:C:42:PHE:HB3	2.02	0.59
1:A:38:HIS:O	1:A:42:PHE:HB3	2.02	0.59
2:B:250:THR:OG1	2:B:251:GLY:N	2.35	0.59
2:D:250:THR:OG1	2:D:251:GLY:N	2.35	0.59
2:B:438:LYS:HB2	2:B:480:LEU:HD12	1.85	0.59
1:C:350:LYS:HE3	1:C:358:ARG:HH12	1.68	0.59
2:D:220:LEU:HD13	2:D:223:LEU:HD13	1.84	0.59
3:H:6:GLU:HA	3:H:22:CYS:HA	1.84	0.59
2:B:223:LEU:HD12	2:B:249:LEU:HD13	1.85	0.59
1:C:38:HIS:O	1:C:42:PHE:CB	2.51	0.59
2:D:145:GLN:H	2:D:355:GLY:HA3	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:HA	1:A:60:LEU:HD12	1.85	0.59
1:A:162:HIS:NE2	1:A:412:GLY:O	2.36	0.59
2:B:271:SER:O	2:B:273:PHE:N	2.34	0.59
2:B:539:SER:HA	2:B:721:LEU:HD21	1.85	0.59
2:D:438:LYS:HB2	2:D:480:LEU:HD12	1.85	0.59
1:A:38:HIS:O	1:A:42:PHE:CB	2.51	0.59
1:C:46:VAL:HA	1:C:60:LEU:HD12	1.85	0.58
2:B:145:GLN:H	2:B:355:GLY:HA3	1.68	0.58
3:H:19:LYS:HE2	3:H:80:TYR:HB3	1.85	0.58
3:M:93:MET:HA	3:M:117:THR:HA	1.85	0.58
1:A:58:ILE:HG13	1:A:59:GLN:HE21	1.68	0.58
1:C:58:ILE:HG13	1:C:59:GLN:HE21	1.68	0.58
2:B:682:ARG:NH2	2:B:724:GLY:O	2.37	0.58
1:C:162:HIS:NE2	1:C:412:GLY:O	2.36	0.58
2:B:220:LEU:HD13	2:B:223:LEU:HD13	1.85	0.58
1:A:350:LYS:HE3	1:A:358:ARG:HH12	1.68	0.58
2:D:539:SER:HA	2:D:721:LEU:HD21	1.85	0.57
1:A:519:TRP:NE1	1:A:547:TYR:OH	2.37	0.57
1:C:519:TRP:NE1	1:C:547:TYR:OH	2.37	0.57
2:D:223:LEU:HD12	2:D:249:LEU:HD13	1.85	0.57
1:A:579:PHE:O	1:A:583:LEU:N	2.36	0.57
1:A:72:ILE:HG23	1:A:75:ALA:HB3	1.87	0.57
2:D:245:ASN:ND2	2:D:272:GLU:O	2.37	0.57
2:B:245:ASN:ND2	2:B:272:GLU:O	2.37	0.57
1:C:114:TYR:HB2	1:C:116:ILE:HD11	1.87	0.57
1:C:579:PHE:O	1:C:583:LEU:N	2.36	0.56
2:D:682:ARG:NH2	2:D:724:GLY:O	2.37	0.56
3:M:16:GLY:O	3:M:84:ASN:ND2	2.38	0.56
3:H:51:ILE:HD12	3:H:72:ARG:HD2	1.87	0.56
1:C:72:ILE:HG23	1:C:75:ALA:HB3	1.87	0.56
1:C:316:LEU:HG	1:C:345:VAL:HG11	1.87	0.56
3:M:4:LEU:HB2	3:M:113:GLY:HA2	1.86	0.56
1:A:441:CYS:SG	1:A:442:LYS:N	2.79	0.56
1:C:82:LEU:HD22	1:C:86:GLN:HB3	1.87	0.56
1:C:441:CYS:SG	1:C:442:LYS:N	2.79	0.56
1:A:239:VAL:HA	1:A:267:VAL:HG23	1.88	0.56
1:A:316:LEU:HG	1:A:345:VAL:HG11	1.87	0.56
2:B:319:SER:H	2:B:327:LYS:HE2	1.71	0.56
2:D:319:SER:H	2:D:327:LYS:HE2	1.71	0.56
1:A:114:TYR:HB2	1:A:116:ILE:HD11	1.87	0.56
2:B:66:PRO:O	2:B:67:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:52:SER:O	3:H:72:ARG:NH1	2.38	0.56
1:A:82:LEU:HD22	1:A:86:GLN:HB3	1.87	0.56
1:C:743:ARG:HG2	1:C:767:LEU:HD21	1.88	0.55
2:B:789:MET:SD	2:B:789:MET:N	2.72	0.55
2:D:483:ASN:HD21	2:D:496:GLY:H	1.55	0.55
2:D:66:PRO:O	2:D:67:ARG:NH1	2.39	0.55
1:C:239:VAL:HA	1:C:267:VAL:HG23	1.88	0.55
2:B:253:GLY:HA2	2:B:394:MET:HB3	1.89	0.55
2:D:41:LEU:HA	2:D:100:ALA:HB2	1.89	0.55
4:N:4:MET:HA	4:N:25:ALA:HA	1.89	0.55
4:L:4:MET:HA	4:L:25:ALA:HA	1.89	0.55
3:M:50:TYR:HE1	4:N:95:TYR:HB2	1.72	0.55
2:D:366:LEU:HB3	2:D:376:VAL:HB	1.89	0.54
2:B:41:LEU:HA	2:B:100:ALA:HB2	1.89	0.54
2:B:86:CYS:HA	2:B:89:MET:HB2	1.90	0.54
2:B:288:GLY:O	2:B:292:ARG:N	2.37	0.54
1:A:37:LYS:NZ	1:A:40:GLN:OE1	2.40	0.54
2:B:252:TYR:O	2:B:393:ARG:NH2	2.41	0.54
2:D:252:TYR:O	2:D:393:ARG:NH2	2.41	0.54
1:C:83:ILE:HA	1:C:328:GLY:HA2	1.90	0.54
2:D:437:GLN:NE2	2:D:452:TYR:O	2.34	0.54
1:A:743:ARG:HG2	1:A:767:LEU:HD21	1.88	0.54
2:B:353:GLU:O	2:B:356:TYR:N	2.41	0.54
2:B:483:ASN:HD21	2:B:496:GLY:H	1.55	0.54
3:H:93:MET:HA	3:H:117:THR:HA	1.90	0.54
4:L:25:ALA:O	4:L:69:ARG:NH2	2.40	0.54
1:A:83:ILE:HA	1:A:328:GLY:HA2	1.90	0.54
2:B:366:LEU:HB3	2:B:376:VAL:HB	1.89	0.54
2:B:437:GLN:NE2	2:B:452:TYR:O	2.34	0.53
1:C:421:ILE:HB	1:C:497:VAL:HG22	1.89	0.53
2:D:488:LYS:NZ	2:D:688:ASN:OD1	2.42	0.53
4:N:25:ALA:O	4:N:69:ARG:NH2	2.40	0.53
2:D:253:GLY:HA2	2:D:394:MET:HB3	1.89	0.53
2:B:364:ILE:HB	2:B:377:GLY:HA3	1.91	0.53
2:D:669:LYS:NZ	2:D:673:ARG:O	2.41	0.53
2:B:316:GLU:OE1	2:B:328:ARG:NH2	2.42	0.53
2:B:488:LYS:NZ	2:B:688:ASN:OD1	2.42	0.53
2:D:86:CYS:HA	2:D:89:MET:HB2	1.90	0.53
3:H:107:TRP:O	4:L:95:TYR:OH	2.26	0.53
4:N:48:ILE:HG23	4:N:52:SER:HA	1.91	0.53
1:C:294:ASN:O	1:C:301:HIS:NE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ILE:HB	1:A:497:VAL:HG22	1.89	0.52
2:D:364:ILE:HB	2:D:377:GLY:HA3	1.91	0.52
1:C:37:LYS:NZ	1:C:40:GLN:OE1	2.40	0.52
3:H:50:TYR:HE1	4:L:95:TYR:HB2	1.74	0.52
1:A:306:VAL:HA	1:A:309:VAL:HG12	1.92	0.52
2:D:230:LEU:HD11	2:D:255:THR:HG22	1.92	0.52
2:D:316:GLU:OE1	2:D:328:ARG:NH2	2.42	0.52
1:C:306:VAL:HA	1:C:309:VAL:HG12	1.92	0.52
1:C:186:GLU:O	1:C:208:ARG:NH2	2.43	0.52
3:M:38:ARG:HD3	3:M:86:LEU:HD22	1.92	0.52
4:L:48:ILE:HG23	4:L:52:SER:HA	1.91	0.52
1:A:375:MET:HE3	1:A:382:LEU:HD13	1.92	0.52
2:D:291:ALA:HA	2:D:294:ARG:HG2	1.91	0.51
2:B:291:ALA:HA	2:B:294:ARG:HG2	1.91	0.51
2:D:353:GLU:O	2:D:356:TYR:N	2.41	0.51
1:A:331:GLY:H	2:B:77:ASP:HB2	1.75	0.51
2:B:230:LEU:HD11	2:B:255:THR:HG22	1.92	0.51
2:B:669:LYS:NZ	2:B:673:ARG:O	2.41	0.51
1:C:384:GLN:NE2	1:C:385:VAL:O	2.44	0.51
1:C:506:GLY:O	1:C:544:ARG:NH1	2.44	0.51
2:D:216:ILE:O	2:D:220:LEU:HG	2.11	0.51
1:A:294:ASN:O	1:A:301:HIS:NE2	2.41	0.51
2:D:410:THR:HG23	2:D:480:LEU:HD23	1.93	0.51
1:A:186:GLU:O	1:A:208:ARG:NH2	2.43	0.51
1:A:506:GLY:O	1:A:544:ARG:NH1	2.44	0.51
1:C:510:ARG:HD3	2:D:190:ILE:HG12	1.93	0.51
2:D:789:MET:SD	2:D:789:MET:N	2.72	0.51
2:B:216:ILE:O	2:B:220:LEU:HG	2.11	0.51
2:B:407:SER:HA	2:B:477:ASP:HB2	1.92	0.51
1:A:384:GLN:NE2	1:A:385:VAL:O	2.44	0.51
2:D:288:GLY:O	2:D:292:ARG:N	2.37	0.51
4:N:34:ALA:HB3	4:N:89:LEU:HB2	1.93	0.51
1:A:139:ARG:N	1:A:365:GLY:O	2.44	0.51
2:D:407:SER:HA	2:D:477:ASP:HB2	1.92	0.51
2:B:214:SER:O	2:B:218:ASN:ND2	2.44	0.50
2:B:468:ILE:HD11	2:B:783:LEU:HD11	1.93	0.50
3:H:68:PHE:HB3	3:H:81:LEU:HD11	1.94	0.50
3:M:68:PHE:HB3	3:M:81:LEU:HD11	1.92	0.50
2:D:214:SER:O	2:D:218:ASN:ND2	2.44	0.50
2:D:75:GLU:OE1	2:D:84:ARG:NH1	2.44	0.50
1:A:229:LEU:HG	1:A:259:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:ASP:OD1	2:B:104:ASP:N	2.45	0.50
2:B:107:ALA:O	2:B:110:GLN:NE2	2.37	0.50
2:B:271:SER:N	2:B:272:GLU:OE1	2.45	0.50
2:B:217:GLN:HE22	2:B:247:VAL:HB	1.77	0.50
1:C:152:PHE:HB2	1:C:183:LEU:HD13	1.93	0.50
1:C:229:LEU:HG	1:C:259:LEU:HD22	1.94	0.50
1:A:139:ARG:HH21	1:A:141:VAL:HG12	1.77	0.50
3:M:81:LEU:HD23	3:M:83:MET:HE1	1.93	0.50
2:D:468:ILE:HD11	2:D:783:LEU:HD11	1.93	0.50
3:M:29:PHE:HA	3:M:32:TYR:HB2	1.94	0.50
1:A:152:PHE:HB2	1:A:183:LEU:HD13	1.93	0.50
2:B:75:GLU:OE1	2:B:84:ARG:NH1	2.45	0.50
2:D:126:ILE:HD13	2:D:292:ARG:HG2	1.94	0.50
2:D:271:SER:N	2:D:272:GLU:OE1	2.45	0.50
2:B:675:ASN:OD1	2:B:675:ASN:N	2.44	0.49
1:C:139:ARG:HH21	1:C:141:VAL:HG12	1.77	0.49
2:B:410:THR:HG23	2:B:480:LEU:HD23	1.93	0.49
2:D:105:GLN:HB2	2:D:130:SER:H	1.77	0.49
2:D:137:LYS:HG3	2:D:143:PHE:HZ	1.77	0.49
2:D:104:ASP:N	2:D:104:ASP:OD1	2.45	0.49
1:A:92:VAL:HG23	1:A:121:LEU:HG	1.94	0.49
2:D:217:GLN:HE22	2:D:247:VAL:HB	1.77	0.49
2:D:253:GLY:HA3	2:D:393:ARG:HH21	1.78	0.49
2:D:277:LEU:HD13	2:D:369:LYS:HG2	1.94	0.49
2:D:393:ARG:HE	2:D:393:ARG:HA	1.78	0.49
4:L:34:ALA:HB3	4:L:89:LEU:HB2	1.93	0.49
3:M:6:GLU:HA	3:M:22:CYS:HA	1.93	0.49
2:D:244:ALA:HB1	2:D:249:LEU:HB3	1.95	0.49
4:N:92:ASP:OD1	4:N:92:ASP:N	2.41	0.49
2:B:105:GLN:HB2	2:B:130:SER:H	1.77	0.49
2:B:253:GLY:HA3	2:B:393:ARG:HH21	1.78	0.49
2:B:431:ARG:NH1	2:B:431:ARG:O	2.43	0.49
1:A:338:THR:HG23	1:A:341:LEU:HD23	1.95	0.49
2:B:77:ASP:OD2	2:B:80:SER:N	2.37	0.49
2:B:349:LEU:HD22	2:B:359:HIS:H	1.77	0.49
1:C:92:VAL:HG23	1:C:121:LEU:HG	1.94	0.49
2:D:414:ALA:O	2:D:416:PHE:N	2.45	0.49
1:A:71:ALA:HB1	2:B:118:GLN:HE21	1.78	0.49
2:B:323:ASN:OD1	2:B:323:ASN:N	2.46	0.49
2:B:414:ALA:O	2:B:416:PHE:N	2.45	0.49
1:C:139:ARG:N	1:C:365:GLY:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:349:LEU:HD22	2:D:359:HIS:H	1.77	0.49
2:B:126:ILE:HD13	2:B:292:ARG:HG2	1.93	0.49
2:D:431:ARG:O	2:D:431:ARG:NH1	2.43	0.49
2:B:393:ARG:HA	2:B:393:ARG:HE	1.78	0.48
3:H:101:ARG:HH22	3:H:108:TYR:HB2	1.76	0.48
1:A:166:LEU:N	1:A:241:ILE:O	2.44	0.48
2:B:137:LYS:HG3	2:B:143:PHE:HZ	1.77	0.48
2:B:465:LEU:HD23	2:B:510:VAL:HG21	1.96	0.48
2:D:465:LEU:HD23	2:D:510:VAL:HG21	1.96	0.48
1:A:340:PRO:HB3	1:A:344:ARG:HH21	1.78	0.48
2:B:273:PHE:CD2	2:B:274:PRO:HD2	2.49	0.48
2:B:437:GLN:OE1	2:B:454:LYS:NZ	2.39	0.48
1:C:573:ASP:OD1	1:C:573:ASP:N	2.45	0.48
1:A:189:SER:HA	1:A:190:LYS:HA	1.64	0.48
2:D:94:ILE:HG22	2:D:96:GLY:H	1.79	0.48
2:D:323:ASN:OD1	2:D:323:ASN:N	2.46	0.48
1:A:510:ARG:HD3	2:B:190:ILE:HG12	1.95	0.48
2:B:94:ILE:HG22	2:B:96:GLY:H	1.79	0.48
2:B:277:LEU:HD13	2:B:369:LYS:HG2	1.95	0.48
1:C:438:ASP:OD1	1:C:438:ASP:N	2.46	0.48
3:M:50:TYR:CE1	4:N:95:TYR:HB2	2.49	0.48
2:B:244:ALA:HB1	2:B:249:LEU:HB3	1.95	0.48
1:C:165:LEU:HA	1:C:241:ILE:HB	1.95	0.48
2:D:77:ASP:OD2	2:D:80:SER:N	2.37	0.48
1:A:367:ARG:HG3	1:A:369:PHE:H	1.78	0.48
2:B:379:TRP:HD1	2:B:384:LEU:HG	1.79	0.48
2:D:273:PHE:CD2	2:D:274:PRO:HD2	2.49	0.48
1:A:118:VAL:HG22	1:A:138:LEU:HB2	1.96	0.48
2:D:600:VAL:HA	2:D:604:LYS:HD2	1.96	0.48
2:B:280:VAL:HG22	2:B:364:ILE:HG13	1.96	0.47
2:B:286:ASP:HB3	2:B:289:LEU:HB2	1.96	0.47
1:C:189:SER:HA	1:C:190:LYS:HA	1.64	0.47
1:C:251:THR:HG23	1:C:254:ARG:HE	1.79	0.47
1:C:338:THR:HG23	1:C:341:LEU:HD23	1.95	0.47
2:D:379:TRP:HD1	2:D:384:LEU:HG	1.79	0.47
1:A:183:LEU:O	1:A:187:ARG:NH1	2.47	0.47
1:C:367:ARG:HG3	1:C:369:PHE:H	1.78	0.47
2:D:304:ALA:HA	2:D:307:MET:HE2	1.95	0.47
1:A:165:LEU:HA	1:A:241:ILE:HB	1.95	0.47
2:D:40:ILE:HG23	2:D:99:PHE:HA	1.96	0.47
1:C:520:ASN:ND2	1:C:707:GLN:OE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:304:ALA:HA	2:B:307:MET:HE2	1.96	0.47
1:A:573:ASP:N	1:A:573:ASP:OD1	2.45	0.47
1:C:118:VAL:HG22	1:C:138:LEU:HB2	1.96	0.47
1:C:138:LEU:HD12	1:C:365:GLY:HA2	1.96	0.47
1:C:344:ARG:HA	1:C:347:MET:HG2	1.97	0.47
2:D:437:GLN:OE1	2:D:454:LYS:NZ	2.39	0.47
1:A:143:PRO:HD2	1:A:146:HIS:HB2	1.97	0.47
1:A:520:ASN:ND2	1:A:707:GLN:OE1	2.48	0.47
2:B:86:CYS:HB2	2:B:321:CYS:HB3	1.66	0.47
2:B:105:GLN:HB2	2:B:130:SER:N	2.30	0.47
2:B:774:ARG:NH2	1:C:546:GLN:O	2.47	0.47
1:C:183:LEU:O	1:C:187:ARG:NH1	2.47	0.47
1:C:340:PRO:HB3	1:C:344:ARG:HH21	1.78	0.47
3:H:96:CYS:O	3:H:113:GLY:N	2.48	0.47
1:A:344:ARG:HA	1:A:347:MET:HG2	1.96	0.47
1:A:486:LYS:O	1:A:490:THR:OG1	2.29	0.47
2:B:600:VAL:HA	2:B:604:LYS:HD2	1.96	0.47
1:C:143:PRO:HD2	1:C:146:HIS:HB2	1.97	0.47
3:H:16:GLY:O	3:H:84:ASN:ND2	2.48	0.47
3:H:31:SER:O	3:H:103:GLY:N	2.48	0.47
4:L:92:ASP:OD1	4:L:92:ASP:N	2.41	0.47
1:A:275:ILE:O	1:A:278:ASN:ND2	2.48	0.47
2:D:286:ASP:HB3	2:D:289:LEU:HB2	1.96	0.47
2:D:428:THR:OG1	2:D:429:CYS:N	2.48	0.47
2:D:538:VAL:N	2:D:749:VAL:O	2.47	0.47
2:D:280:VAL:HG22	2:D:364:ILE:HG13	1.96	0.47
2:B:353:GLU:HB3	2:B:356:TYR:HB2	1.97	0.46
1:C:275:ILE:O	1:C:278:ASN:ND2	2.48	0.46
1:C:282:TYR:O	1:C:380:ARG:NH1	2.42	0.46
2:D:172:VAL:HG12	2:D:203:LEU:HB2	1.97	0.46
2:D:637:PHE:HA	2:D:640:VAL:HG22	1.96	0.46
1:A:251:THR:HG23	1:A:254:ARG:HE	1.79	0.46
1:A:389:ASN:OD1	1:A:389:ASN:N	2.49	0.46
1:C:375:MET:HE3	1:C:382:LEU:HD13	1.96	0.46
1:C:460:PRO:HD3	1:C:499:LEU:HD12	1.98	0.46
1:C:225:VAL:HG11	1:C:252:VAL:HG12	1.97	0.46
2:B:226:PRO:HA	2:B:252:TYR:HE1	1.80	0.46
2:B:637:PHE:HA	2:B:640:VAL:HG22	1.96	0.46
2:D:353:GLU:HB3	2:D:356:TYR:HB2	1.98	0.46
1:A:184:LEU:O	1:A:187:ARG:NH2	2.48	0.46
2:B:40:ILE:HG23	2:B:99:PHE:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ASP:OD1	1:C:171:HIS:ND1	2.49	0.46
2:D:105:GLN:HB2	2:D:130:SER:N	2.30	0.46
1:A:138:LEU:HD12	1:A:365:GLY:HA2	1.96	0.46
1:C:131:LYS:HB2	2:D:177:PRO:HG3	1.96	0.46
1:A:460:PRO:HD3	1:A:499:LEU:HD12	1.98	0.46
2:B:172:VAL:HG12	2:B:203:LEU:HB2	1.98	0.46
1:C:584:TRP:HB3	1:C:586:LEU:H	1.80	0.46
1:A:225:VAL:HG11	1:A:252:VAL:HG12	1.97	0.46
1:A:584:TRP:HB3	1:A:586:LEU:H	1.80	0.46
1:A:773:LEU:HD12	1:A:776:ARG:HE	1.80	0.46
1:A:827:ALA:HB1	2:D:653:PHE:HA	1.97	0.46
2:B:175:TYR:CZ	2:B:204:LEU:HB3	2.51	0.46
2:B:540:ARG:HD3	2:B:747:LYS:HE3	1.98	0.46
2:D:226:PRO:HA	2:D:252:TYR:HE1	1.80	0.46
4:N:39:LYS:HD2	4:N:42:LYS:HD3	1.98	0.46
1:A:170:ASP:OD1	1:A:171:HIS:ND1	2.49	0.46
2:B:349:LEU:HD22	2:B:358:MET:HG3	1.98	0.46
2:B:428:THR:OG1	2:B:429:CYS:N	2.48	0.46
1:C:773:LEU:HD12	1:C:776:ARG:HE	1.80	0.46
2:D:540:ARG:HD3	2:D:747:LYS:HE3	1.98	0.46
3:M:109:PHE:O	4:N:36:TYR:OH	2.20	0.46
2:B:374:GLU:HG3	2:B:375:ARG:HE	1.81	0.45
2:D:107:ALA:O	2:D:110:GLN:NE2	2.37	0.45
4:L:39:LYS:HD2	4:L:42:LYS:HD3	1.98	0.45
2:D:349:LEU:HD22	2:D:358:MET:HG3	1.98	0.45
3:M:31:SER:O	3:M:103:GLY:N	2.49	0.45
3:M:99:PRO:HA	3:M:109:PHE:HB3	1.98	0.45
1:C:184:LEU:O	1:C:187:ARG:NH2	2.48	0.45
2:D:133:ILE:O	2:D:356:TYR:OH	2.34	0.45
2:D:374:GLU:HG3	2:D:375:ARG:HE	1.81	0.45
2:D:175:TYR:CZ	2:D:204:LEU:HB3	2.51	0.45
3:M:94:TYR:N	3:M:116:THR:O	2.45	0.45
2:B:434:VAL:HG21	2:B:457:CYS:HB2	1.98	0.45
2:B:460:PHE:HE1	2:B:792:LEU:HB3	1.82	0.45
1:C:389:ASN:OD1	1:C:389:ASN:N	2.49	0.45
2:B:493:THR:OG1	2:B:494:TRP:N	2.50	0.45
2:D:408:ILE:HG12	2:D:508:MET:HB2	1.98	0.45
2:D:493:THR:OG1	2:D:494:TRP:N	2.50	0.45
1:A:151:TRP:CG	1:A:269:LEU:HD21	2.52	0.45
2:B:420:GLU:OE2	2:B:432:ASN:ND2	2.50	0.45
2:D:222:LYS:HD2	2:D:222:LYS:HA	1.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:SER:OG	1:C:94:HIS:N	2.47	0.45
1:C:704:THR:HB	1:C:751:ILE:HG23	1.99	0.45
2:D:152:GLN:NE2	2:D:358:MET:HA	2.32	0.45
2:D:420:GLU:OE2	2:D:432:ASN:ND2	2.50	0.45
1:C:71:ALA:HB1	2:D:118:GLN:HE21	1.81	0.45
1:A:310:ALA:HA	1:A:313:VAL:HG22	1.98	0.45
1:C:397:ASP:OD1	1:C:397:ASP:N	2.49	0.45
2:D:125:GLY:HA3	2:D:127:HIS:NE2	2.31	0.44
1:A:93:SER:OG	1:A:94:HIS:N	2.47	0.44
2:B:133:ILE:O	2:B:356:TYR:OH	2.34	0.44
2:B:152:GLN:NE2	2:B:358:MET:HA	2.32	0.44
2:B:408:ILE:HG12	2:B:508:MET:HB2	1.98	0.44
1:C:310:ALA:HA	1:C:313:VAL:HG22	1.98	0.44
3:H:50:TYR:CE1	4:L:95:TYR:HB2	2.52	0.44
3:H:112:TRP:CH2	4:L:43:GLY:HA3	2.53	0.44
1:A:49:ALA:HB3	1:A:60:LEU:HD11	1.99	0.44
1:A:571:THR:HG22	1:A:574:SER:HB3	2.00	0.44
2:B:125:GLY:HA3	2:B:127:HIS:NE2	2.31	0.44
1:C:38:HIS:O	1:C:42:PHE:HB2	2.18	0.44
2:D:434:VAL:HG21	2:D:457:CYS:HB2	1.98	0.44
1:A:454:LYS:HG2	1:A:477:TYR:HB3	1.98	0.44
2:B:93:LYS:HD2	2:B:317:PRO:HG2	2.00	0.44
2:B:124:LEU:HD22	2:B:300:ILE:HD11	2.00	0.44
1:C:454:LYS:HG2	1:C:477:TYR:HB3	1.98	0.44
2:D:431:ARG:HA	2:D:431:ARG:HD2	1.66	0.44
2:D:509:ALA:HB3	2:D:765:ALA:HB3	1.99	0.44
3:H:110:ASP:OD1	3:H:110:ASP:N	2.41	0.44
2:D:130:SER:O	2:D:130:SER:OG	2.33	0.44
2:D:460:PHE:HE1	2:D:792:LEU:HB3	1.82	0.44
2:D:537:MET:HB2	2:D:736:LEU:HD22	1.99	0.44
1:A:223:LYS:HE2	1:A:223:LYS:HB2	1.83	0.44
2:B:99:PHE:HZ	2:B:112:LEU:HD22	1.82	0.44
2:B:509:ALA:HB3	2:B:765:ALA:HB3	1.99	0.44
1:C:151:TRP:CG	1:C:269:LEU:HD21	2.52	0.44
1:C:811:LYS:HA	1:C:811:LYS:HD2	1.73	0.44
2:D:99:PHE:HZ	2:D:112:LEU:HD22	1.82	0.44
1:C:149:SER:HA	1:C:152:PHE:HB3	2.00	0.44
1:C:33:LEU:O	1:C:38:HIS:NE2	2.51	0.44
2:D:675:ASN:OD1	2:D:675:ASN:N	2.44	0.44
1:A:149:SER:HA	1:A:152:PHE:HB3	2.00	0.44
1:A:290:LEU:HD23	1:A:374:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ASP:OD1	1:A:397:ASP:N	2.49	0.44
2:B:831:LEU:HD23	2:B:834:ILE:HD12	2.00	0.44
1:C:290:LEU:HD23	1:C:374:ILE:HG12	2.00	0.44
1:C:765:CYS:O	1:C:822:ARG:NH2	2.51	0.44
1:A:33:LEU:O	1:A:38:HIS:NE2	2.51	0.43
1:A:224:ASN:HD21	1:A:227:ALA:HB3	1.83	0.43
1:A:516:LYS:HA	1:A:516:LYS:HD3	1.79	0.43
2:D:365:ILE:HA	2:D:375:ARG:HA	2.00	0.43
1:A:502:ASP:OD1	1:A:502:ASP:N	2.50	0.43
1:C:166:LEU:N	1:C:241:ILE:O	2.44	0.43
1:C:571:THR:HG22	1:C:574:SER:HB3	2.00	0.43
1:A:38:HIS:O	1:A:42:PHE:HB2	2.18	0.43
2:B:537:MET:HB2	2:B:736:LEU:HD22	1.99	0.43
2:D:366:LEU:HG	2:D:373:TRP:HB3	2.00	0.43
1:A:286:GLY:HA3	1:A:403:PRO:HA	1.99	0.43
1:A:294:ASN:HD22	1:A:297:ASN:HB3	1.84	0.43
1:C:49:ALA:HB3	1:C:60:LEU:HD11	2.00	0.43
2:D:405:HIS:HA	2:D:475:THR:HB	2.00	0.43
3:M:112:TRP:CH2	4:N:43:GLY:HA3	2.53	0.43
1:A:704:THR:HB	1:A:751:ILE:HG23	1.99	0.43
1:C:435:THR:HG22	1:C:441:CYS:HB2	2.01	0.43
4:N:47:LEU:HB3	4:N:48:ILE:HG12	2.00	0.43
1:A:75:ALA:HB1	1:A:110:THR:HG21	2.01	0.43
2:B:405:HIS:HA	2:B:475:THR:HB	1.99	0.43
2:D:201:GLU:HG3	2:D:203:LEU:HG	2.01	0.43
2:B:693:ARG:HD2	2:B:693:ARG:HA	1.92	0.43
1:C:75:ALA:HB1	1:C:110:THR:HG21	2.01	0.43
1:C:534:ILE:N	1:C:782:GLY:O	2.47	0.43
1:A:765:CYS:O	1:A:822:ARG:NH2	2.51	0.43
2:B:784:PHE:HA	2:B:789:MET:HE1	2.01	0.43
1:A:131:LYS:HB2	2:B:177:PRO:HG3	1.99	0.43
2:B:184:ASN:OD1	2:B:187:ARG:NH1	2.52	0.43
1:C:72:ILE:HG13	2:D:118:GLN:NE2	2.34	0.43
1:C:268:TRP:HB2	1:C:287:ILE:HG23	2.01	0.43
1:C:499:LEU:HD23	1:C:499:LEU:HA	1.91	0.43
3:H:3:LYS:HD3	3:H:3:LYS:HA	1.84	0.43
1:C:72:ILE:HG13	2:D:118:GLN:HE22	1.84	0.43
2:D:86:CYS:HB2	2:D:321:CYS:HB3	1.66	0.43
1:A:158:TYR:HD1	1:A:409:LYS:HE3	1.84	0.42
1:C:286:GLY:HA3	1:C:403:PRO:HA	1.99	0.42
2:D:35:ILE:HG23	2:D:64:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:124:LEU:HD22	2:D:300:ILE:HD11	2.00	0.42
2:D:831:LEU:HD23	2:D:834:ILE:HD12	2.00	0.42
1:A:574:SER:O	1:A:574:SER:OG	2.26	0.42
2:B:365:ILE:HA	2:B:375:ARG:HA	2.00	0.42
2:D:93:LYS:HD2	2:D:317:PRO:HG2	2.00	0.42
2:D:453:ILE:HD12	2:D:453:ILE:HA	1.90	0.42
2:B:267:ASP:N	2:B:267:ASP:OD1	2.52	0.42
1:C:277:GLY:HA2	1:C:280:LEU:HB2	2.02	0.42
1:C:294:ASN:HD22	1:C:297:ASN:HB3	1.84	0.42
1:A:534:ILE:N	1:A:782:GLY:O	2.46	0.42
2:B:164:TYR:HB2	2:B:166:TRP:CD1	2.55	0.42
2:B:181:ASP:N	2:B:181:ASP:OD1	2.52	0.42
1:C:224:ASN:HD21	1:C:227:ALA:HB3	1.83	0.42
3:H:15:GLY:H	3:H:87:LYS:HE2	1.84	0.42
3:H:97:ALA:HA	3:H:112:TRP:HA	2.01	0.42
2:D:181:ASP:N	2:D:181:ASP:OD1	2.52	0.42
2:D:184:ASN:OD1	2:D:187:ARG:NH1	2.52	0.42
4:L:47:LEU:HB3	4:L:48:ILE:HG12	2.00	0.42
1:A:282:TYR:O	1:A:380:ARG:NH1	2.43	0.42
1:A:376:ASN:HD21	1:A:385:VAL:HG11	1.85	0.42
2:B:366:LEU:HG	2:B:373:TRP:HB3	2.00	0.42
2:D:404:ASP:N	2:D:404:ASP:OD1	2.53	0.42
2:D:703:HIS:HA	2:D:706:MET:HB2	2.01	0.42
2:B:404:ASP:N	2:B:404:ASP:OD1	2.53	0.42
1:C:113:PHE:CE2	2:D:78:PRO:HG3	2.55	0.42
2:D:299:ILE:HD13	2:D:299:ILE:HA	1.91	0.42
2:B:201:GLU:HG3	2:B:203:LEU:HG	2.01	0.42
1:A:58:ILE:HG13	1:A:59:GLN:NE2	2.35	0.42
1:A:325:PRO:HG3	1:A:336:TRP:CD2	2.55	0.42
1:A:435:THR:HG22	1:A:441:CYS:HB2	2.01	0.42
2:B:116:SER:O	2:B:120:LEU:N	2.51	0.42
2:B:703:HIS:HA	2:B:706:MET:HB2	2.01	0.42
1:C:275:ILE:HG21	1:C:291:GLN:HE21	1.85	0.42
2:D:254:TYR:CZ	2:D:278:ILE:HG23	2.55	0.42
2:D:669:LYS:HA	2:D:669:LYS:HD2	1.90	0.42
3:M:24:ALA:HB3	3:M:77:ASN:HB3	2.01	0.42
4:N:6:GLN:HB2	4:N:100:GLY:H	1.85	0.42
1:A:130:ASP:H	1:A:134:HIS:CE1	2.37	0.42
2:B:674:PRO:HB2	2:B:680:PRO:HB2	2.02	0.42
1:C:30:GLY:HA3	1:C:91:LEU:HA	2.02	0.42
1:C:321:ASN:OD1	1:C:321:ASN:N	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:559:LEU:HG	1:C:775:PHE:HB3	2.02	0.42
2:D:742:ARG:HD2	2:D:742:ARG:HA	1.91	0.42
3:M:3:LYS:HD3	3:M:3:LYS:HA	1.84	0.42
1:A:268:TRP:HB2	1:A:287:ILE:HG23	2.01	0.41
2:B:538:VAL:N	2:B:749:VAL:O	2.47	0.41
1:C:32:VAL:HG22	1:C:91:LEU:HB3	2.02	0.41
1:C:517:LYS:HE2	2:D:190:ILE:HD13	2.01	0.41
1:C:561:ILE:HD11	1:C:774:PHE:HZ	1.85	0.41
4:L:46:LEU:HD21	4:L:49:HIS:CE1	2.55	0.41
1:A:147:GLN:HE21	1:A:290:LEU:HB2	1.84	0.41
1:A:219:ASP:OD1	1:A:219:ASP:N	2.52	0.41
1:A:517:LYS:HE2	2:B:190:ILE:HD13	2.02	0.41
2:D:164:TYR:HB2	2:D:166:TRP:CD1	2.55	0.41
4:N:23:CYS:HB3	4:N:90:GLN:HE22	1.86	0.41
1:C:130:ASP:H	1:C:134:HIS:CE1	2.37	0.41
1:C:376:ASN:HD21	1:C:385:VAL:HG11	1.85	0.41
2:D:504:LYS:HA	2:D:507:TYR:HE2	1.85	0.41
4:N:46:LEU:HD21	4:N:49:HIS:CE1	2.55	0.41
2:B:35:ILE:HG23	2:B:64:VAL:HG21	2.01	0.41
2:B:298:ALA:O	2:B:302:THR:OG1	2.26	0.41
2:B:429:CYS:HB3	2:B:432:ASN:HD22	1.85	0.41
1:C:147:GLN:HE21	1:C:290:LEU:HB2	1.84	0.41
1:C:158:TYR:HD1	1:C:409:LYS:HE3	1.84	0.41
1:C:325:PRO:HG3	1:C:336:TRP:CD2	2.55	0.41
1:C:369:PHE:HD2	1:C:371:GLN:HE22	1.68	0.41
1:C:770:THR:O	1:C:770:THR:OG1	2.38	0.41
2:D:116:SER:O	2:D:120:LEU:N	2.51	0.41
1:A:559:LEU:HG	1:A:775:PHE:HB3	2.02	0.41
2:B:515:ILE:HD11	2:B:763:GLY:HA3	2.03	0.41
1:C:223:LYS:HB2	1:C:223:LYS:HE2	1.84	0.41
2:D:515:ILE:HD11	2:D:763:GLY:HA3	2.03	0.41
3:M:70:ILE:HD13	3:M:81:LEU:HD13	2.03	0.41
1:A:277:GLY:HA2	1:A:280:LEU:HB2	2.01	0.41
1:A:409:LYS:HA	1:A:410:PRO:HD3	1.85	0.41
2:B:474:PHE:HD1	2:B:474:PHE:HA	1.78	0.41
4:L:29:ILE:HG21	4:L:90:GLN:HG2	2.02	0.41
2:B:366:LEU:HD12	2:B:367:LEU:H	1.86	0.41
2:B:490:ILE:HD13	2:B:495:ASN:HD21	1.86	0.41
1:C:461:ASN:HB3	1:C:469:ARG:HD2	2.03	0.41
1:C:486:LYS:O	1:C:490:THR:OG1	2.29	0.41
1:C:511:VAL:HG21	1:C:518:GLU:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:267:ASP:OD1	2:D:267:ASP:N	2.52	0.41
2:D:524:ASP:HB2	2:D:768:LYS:HA	2.03	0.41
1:A:485:ILE:HD13	1:A:485:ILE:HA	1.96	0.41
1:A:809:LEU:HD12	1:A:809:LEU:HA	1.94	0.41
2:B:230:LEU:H	2:B:257:ILE:HG22	1.86	0.41
2:B:254:TYR:CZ	2:B:278:ILE:HG23	2.55	0.41
1:C:33:LEU:HA	1:C:66:THR:HG23	2.02	0.41
1:C:393:VAL:O	1:C:395:PRO:HD3	2.21	0.41
1:A:164:ILE:HD13	1:A:164:ILE:HA	1.89	0.41
1:C:516:LYS:HD3	1:C:516:LYS:HA	1.79	0.41
2:D:490:ILE:HD13	2:D:495:ASN:HD21	1.85	0.41
2:D:674:PRO:HB2	2:D:680:PRO:HB2	2.02	0.41
1:A:30:GLY:HA3	1:A:91:LEU:HA	2.02	0.40
1:A:32:VAL:HG22	1:A:91:LEU:HB3	2.02	0.40
1:A:461:ASN:HB3	1:A:469:ARG:HD2	2.03	0.40
1:C:219:ASP:OD1	1:C:219:ASP:N	2.52	0.40
4:N:29:ILE:HG21	4:N:90:GLN:HG2	2.02	0.40
2:B:673:ARG:HA	2:B:674:PRO:HD3	1.93	0.40
1:C:258:MET:HB2	1:C:258:MET:HE3	1.94	0.40
2:D:532:THR:OG1	2:D:533:GLY:N	2.55	0.40
3:M:13:GLN:HB3	3:M:16:GLY:HA3	2.02	0.40
1:A:511:VAL:HG21	1:A:518:GLU:HG2	2.03	0.40
2:B:504:LYS:HA	2:B:507:TYR:HE2	1.86	0.40
1:C:350:LYS:HA	1:C:350:LYS:HD2	1.90	0.40
2:D:366:LEU:HD12	2:D:367:LEU:H	1.86	0.40
4:L:85:THR:OG1	4:L:101:THR:O	2.29	0.40
1:A:393:VAL:O	1:A:395:PRO:HD3	2.21	0.40
1:A:575:PHE:HB3	1:A:837:VAL:HG13	2.03	0.40
2:B:105:GLN:HG3	2:B:129:GLY:H	1.86	0.40
2:D:254:TYR:CZ	2:D:276:GLY:HA2	2.57	0.40
2:D:429:CYS:HB3	2:D:432:ASN:HD22	1.85	0.40
1:A:275:ILE:HG21	1:A:291:GLN:HE21	1.85	0.40
1:A:549:GLU:HG3	1:A:783:MET:HB2	2.03	0.40
2:B:552:GLU:HB3	2:B:553:PRO:HD3	2.04	0.40
1:C:58:ILE:HG13	1:C:59:GLN:NE2	2.35	0.40
1:C:575:PHE:HB3	1:C:837:VAL:HG13	2.03	0.40
1:C:829:LEU:HD13	1:C:831:CYS:SG	2.62	0.40
2:D:784:PHE:HA	2:D:789:MET:HE1	2.03	0.40
3:H:17:SER:OG	3:H:84:ASN:ND2	2.46	0.40
4:L:6:GLN:HB2	4:L:100:GLY:H	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	778/862 (90%)	688 (88%)	81 (10%)	9 (1%)	13	50
1	C	778/862 (90%)	688 (88%)	81 (10%)	9 (1%)	13	50
2	B	759/883 (86%)	647 (85%)	104 (14%)	8 (1%)	14	52
2	D	759/883 (86%)	647 (85%)	104 (14%)	8 (1%)	14	52
3	H	113/223 (51%)	107 (95%)	6 (5%)	0	100	100
3	M	112/223 (50%)	109 (97%)	3 (3%)	0	100	100
4	L	104/213 (49%)	90 (86%)	13 (12%)	1 (1%)	15	54
4	N	104/213 (49%)	90 (86%)	13 (12%)	1 (1%)	15	54
All	All	3507/4362 (80%)	3066 (87%)	405 (12%)	36 (1%)	20	54

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	41	MET
1	A	402	TRP
2	B	89	MET
2	B	272	GLU
1	C	40	GLN
1	C	41	MET
1	C	402	TRP
2	D	89	MET
2	D	272	GLU
1	A	394	ILE
1	A	830	THR
2	B	351	PHE
1	C	394	ILE
1	C	830	THR
2	D	351	PHE
1	A	281	ARG

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Mol	Chain	Res	Type
1	A	401	ILE
2	B	88	LEU
2	B	220	LEU
2	B	252	TYR
1	C	281	ARG
1	C	401	ILE
2	D	88	LEU
2	D	220	LEU
2	D	252	TYR
1	A	67	HIS
1	A	368	LYS
1	C	67	HIS
1	C	368	LYS
2	B	200	GLU
2	D	200	GLU
2	B	679	PRO
2	D	679	PRO
4	L	8	PRO
4	N	8	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	679/744 (91%)	644 (95%)	35 (5%)	23	48
1	C	679/744 (91%)	644 (95%)	35 (5%)	23	48
2	B	668/762 (88%)	629 (94%)	39 (6%)	20	45
2	D	668/762 (88%)	629 (94%)	39 (6%)	20	45
3	H	96/189 (51%)	94 (98%)	2 (2%)	53	72
3	M	95/189 (50%)	93 (98%)	2 (2%)	53	72
4	L	91/189 (48%)	85 (93%)	6 (7%)	16	41
4	N	91/189 (48%)	85 (93%)	6 (7%)	16	41
All	All	3067/3768 (81%)	2903 (95%)	164 (5%)	26	47

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ILE
1	A	27	VAL
1	A	61	GLN
1	A	63	THR
1	A	65	VAL
1	A	76	LEU
1	A	81	ASP
1	A	113	PHE
1	A	141	VAL
1	A	153	GLU
1	A	155	MET
1	A	167	VAL
1	A	180	LEU
1	A	187	ARG
1	A	242	LEU
1	A	247	ASP
1	A	267	VAL
1	A	280	LEU
1	A	291	GLN
1	A	345	VAL
1	A	377	LEU
1	A	411	ARG
1	A	441	CYS
1	A	455	VAL
1	A	476	CYS
1	A	561	ILE
1	A	567	ILE
1	A	635	LEU
1	A	684	ARG
1	A	689	ASN
1	A	725	ARG
1	A	734	SER
1	A	765	CYS
1	A	798	LEU
1	A	837	VAL
2	B	40	ILE
2	B	41	LEU
2	B	67	ARG
2	B	71	VAL
2	B	77	ASP
2	B	87	ASP
2	B	97	VAL

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Mol	Chain	Res	Type
2	B	112	LEU
2	B	113	ASP
2	B	127	HIS
2	B	162	GLU
2	B	173	THR
2	B	207	MET
2	B	219	GLN
2	B	223	LEU
2	B	230	LEU
2	B	258	VAL
2	B	261	LEU
2	B	266	THR
2	B	271	SER
2	B	287	TYR
2	B	292	ARG
2	B	328	ARG
2	B	335	LEU
2	B	349	LEU
2	B	363	VAL
2	B	366	LEU
2	B	371	ARG
2	B	375	ARG
2	B	378	LYS
2	B	393	ARG
2	B	462	ILE
2	B	465	LEU
2	B	486	HIS
2	B	527	VAL
2	B	660	VAL
2	B	714	VAL
2	B	786	ASP
2	B	789	MET
1	C	26	ILE
1	C	27	VAL
1	C	61	GLN
1	C	63	THR
1	C	65	VAL
1	C	76	LEU
1	C	81	ASP
1	C	113	PHE
1	C	141	VAL
1	C	153	GLU

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Mol	Chain	Res	Type
1	C	155	MET
1	C	167	VAL
1	C	180	LEU
1	C	187	ARG
1	C	242	LEU
1	C	247	ASP
1	C	267	VAL
1	C	280	LEU
1	C	291	GLN
1	C	345	VAL
1	C	377	LEU
1	C	411	ARG
1	C	441	CYS
1	C	455	VAL
1	C	476	CYS
1	C	561	ILE
1	C	567	ILE
1	C	635	LEU
1	C	684	ARG
1	C	689	ASN
1	C	725	ARG
1	C	734	SER
1	C	765	CYS
1	C	798	LEU
1	C	837	VAL
2	D	40	ILE
2	D	41	LEU
2	D	67	ARG
2	D	71	VAL
2	D	77	ASP
2	D	87	ASP
2	D	97	VAL
2	D	112	LEU
2	D	113	ASP
2	D	127	HIS
2	D	162	GLU
2	D	173	THR
2	D	207	MET
2	D	219	GLN
2	D	223	LEU
2	D	230	LEU
2	D	258	VAL

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Mol	Chain	Res	Type
2	D	261	LEU
2	D	266	THR
2	D	271	SER
2	D	287	TYR
2	D	292	ARG
2	D	328	ARG
2	D	335	LEU
2	D	349	LEU
2	D	363	VAL
2	D	366	LEU
2	D	371	ARG
2	D	375	ARG
2	D	378	LYS
2	D	393	ARG
2	D	462	ILE
2	D	465	LEU
2	D	486	HIS
2	D	527	VAL
2	D	660	VAL
2	D	714	VAL
2	D	786	ASP
2	D	789	MET
3	H	28	THR
3	H	118	VAL
4	L	5	THR
4	L	19	VAL
4	L	22	THR
4	L	91	TYR
4	L	92	ASP
4	L	95	TYR
3	M	117	THR
3	M	118	VAL
4	N	5	THR
4	N	19	VAL
4	N	22	THR
4	N	91	TYR
4	N	92	ASP
4	N	95	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	291	GLN
1	A	817	GLN
2	B	95	GLN
2	B	152	GLN
2	B	218	ASN
2	B	357	GLN
2	B	432	ASN
2	B	495	ASN
2	B	615	ASN
2	B	656	GLN
2	B	698	ASN
2	B	711	GLN
1	C	59	GLN
1	C	291	GLN
1	C	817	GLN
2	D	95	GLN
2	D	152	GLN
2	D	218	ASN
2	D	357	GLN
2	D	432	ASN
2	D	495	ASN
2	D	656	GLN
2	D	698	ASN
2	D	711	GLN
3	H	84	ASN
4	L	3	GLN
4	L	38	HIS
4	L	77	ASN
3	M	84	ASN
4	N	3	GLN
4	N	38	HIS
4	N	77	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
2	D	1

All chain breaks are listed below:

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

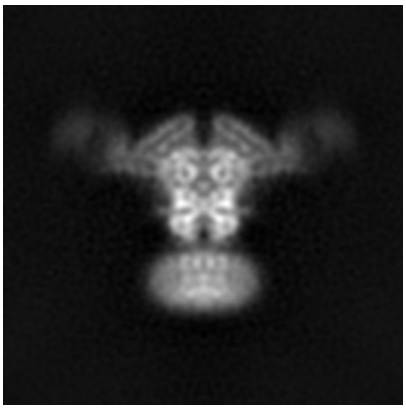
6 Map visualisation

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

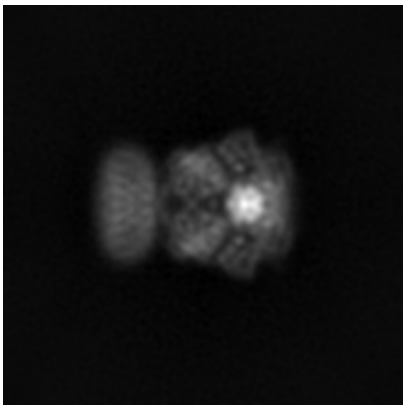
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

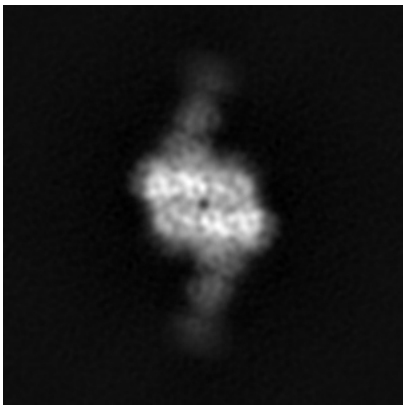
6.1.1 Primary map



X

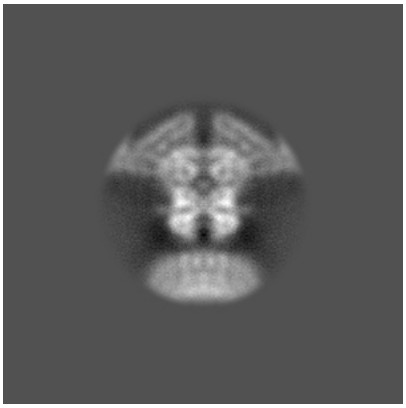


Y

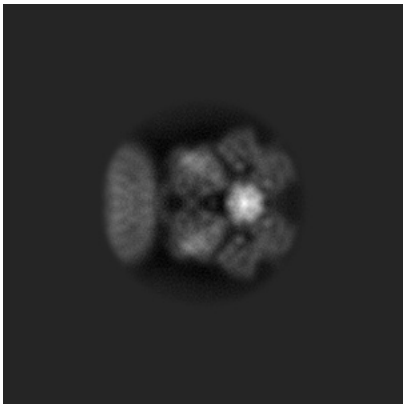


Z

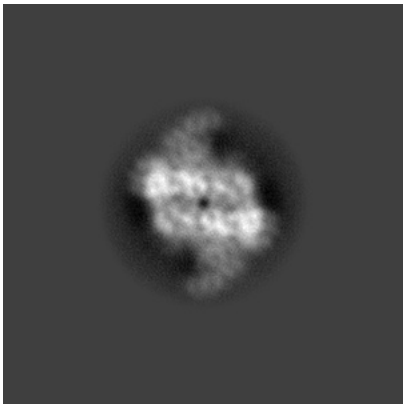
6.1.2 Raw map



X



Y

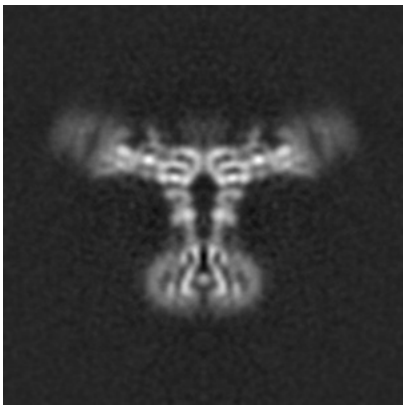


Z

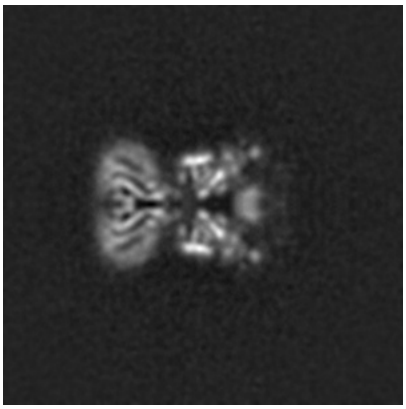
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

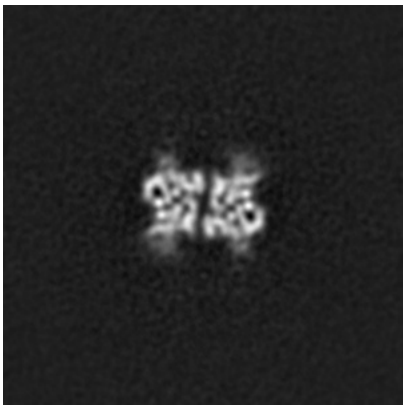
6.2.1 Primary map



X Index: 128

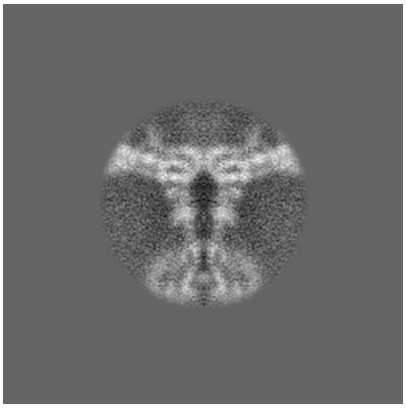


Y Index: 128

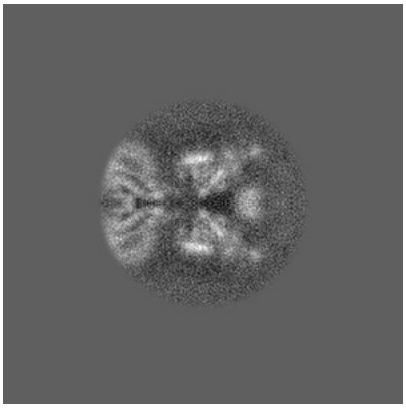


Z Index: 128

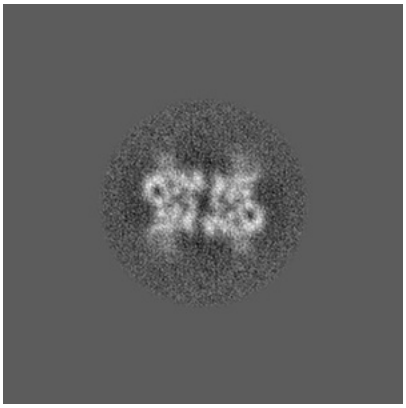
6.2.2 Raw map



X Index: 128



Y Index: 128

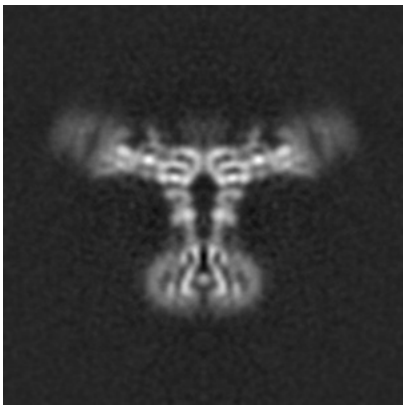


Z Index: 128

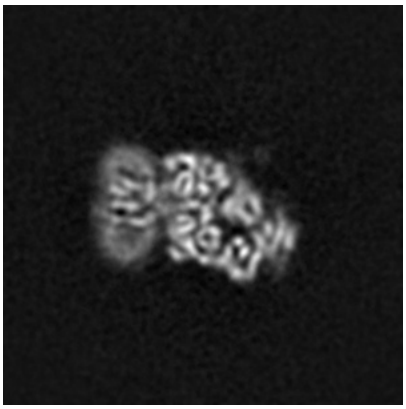
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

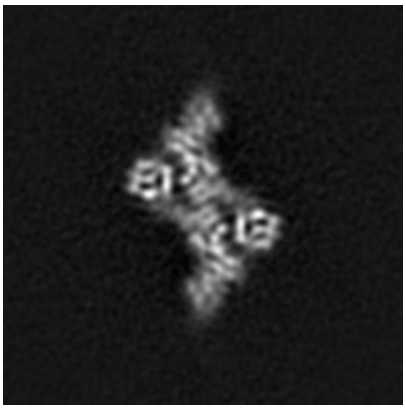
6.3.1 Primary map



X Index: 128

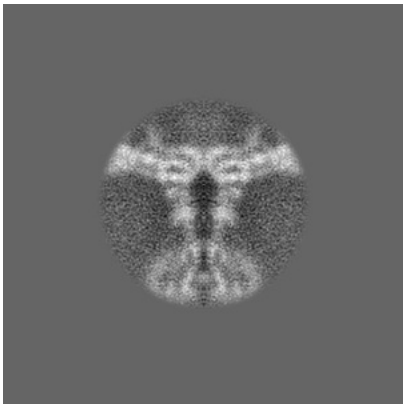


Y Index: 138

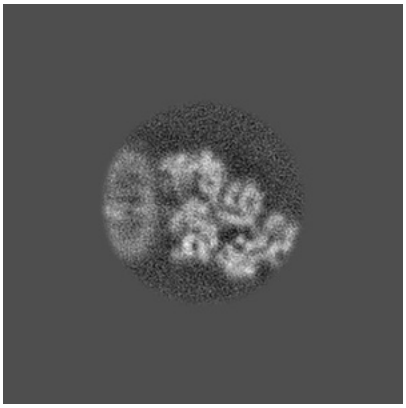


Z Index: 151

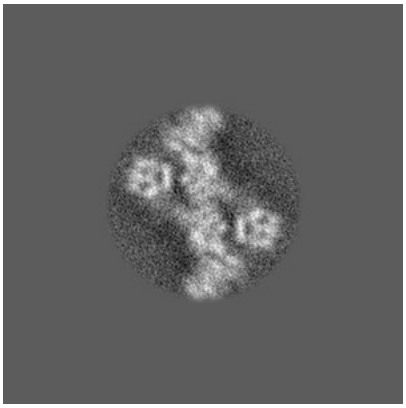
6.3.2 Raw map



X Index: 128



Y Index: 143

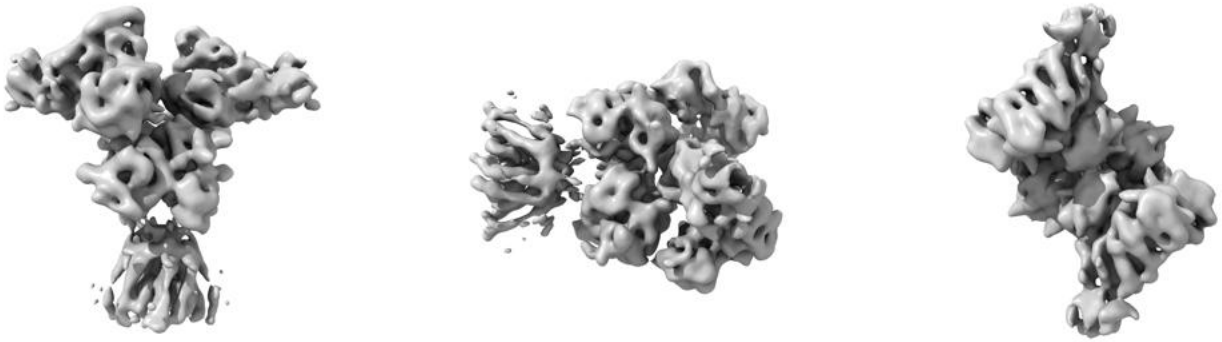


Z Index: 152

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

6.4 Orthogonal surface views (i)

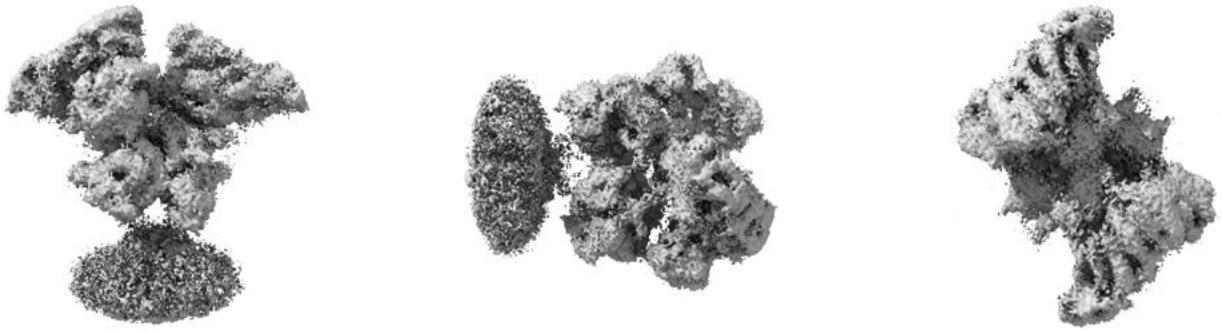
6.4.1 Primary map



X Y Z

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.

6.4.2 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.

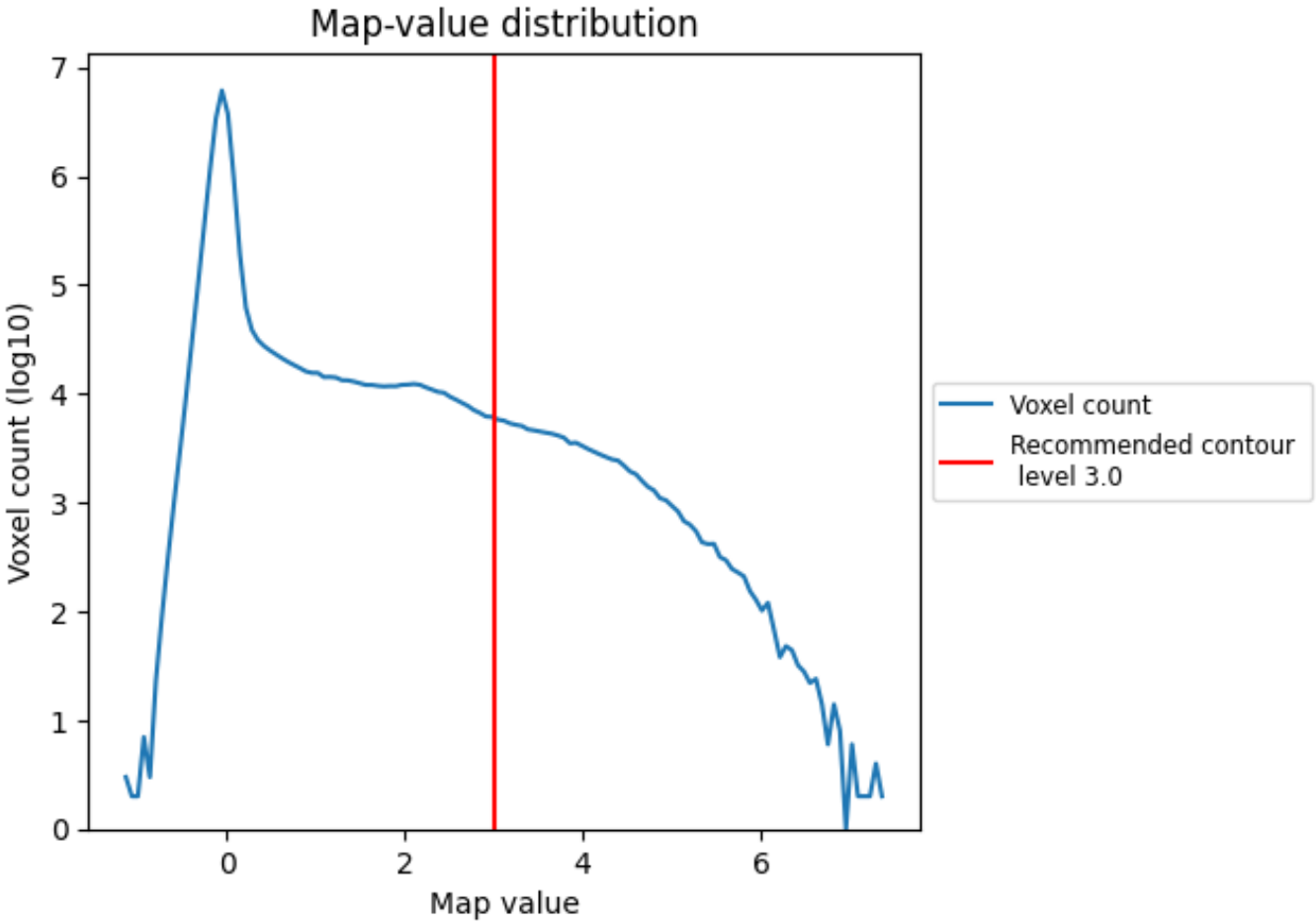
6.5 Mask visualisation (i)

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

7 Map analysis

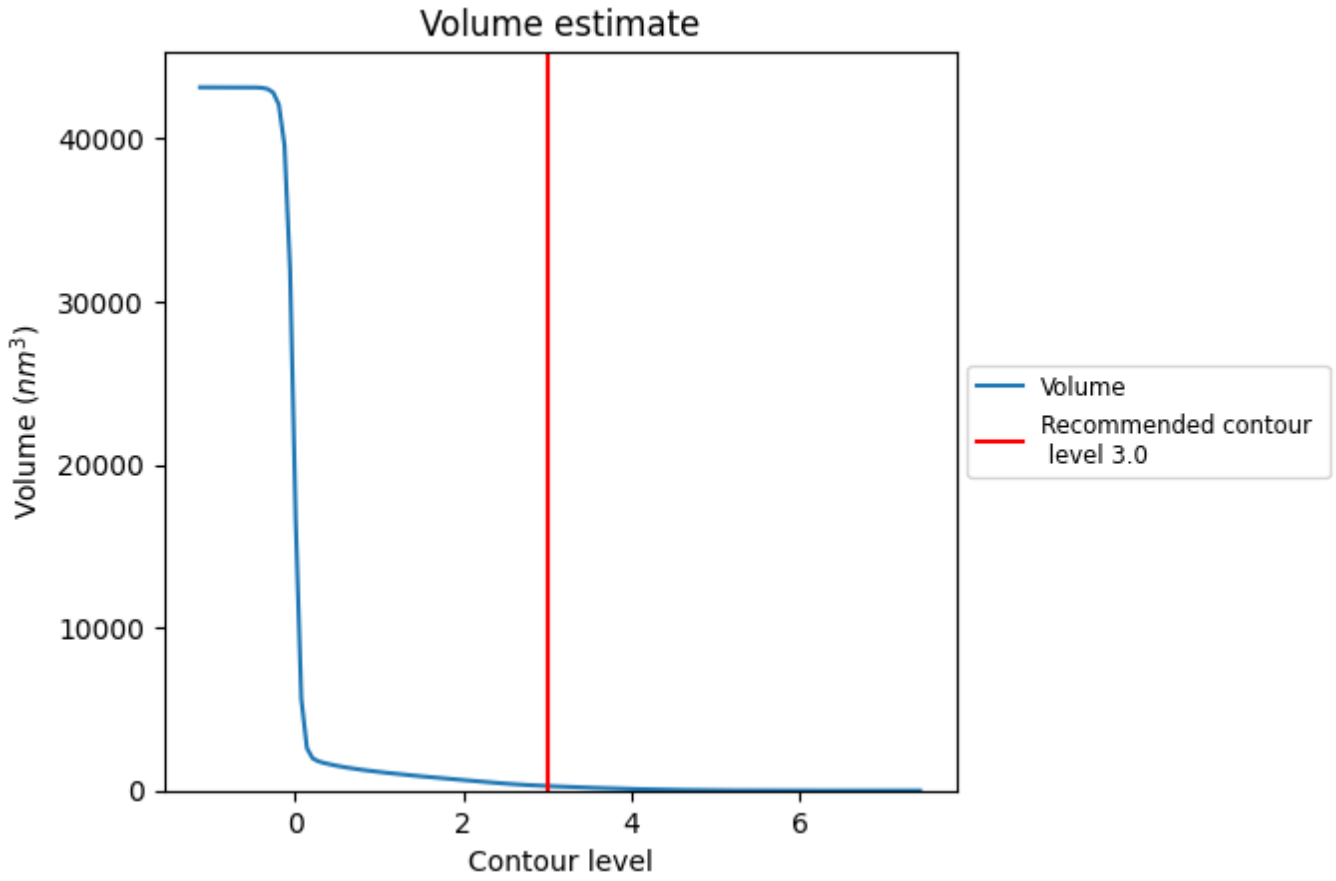
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

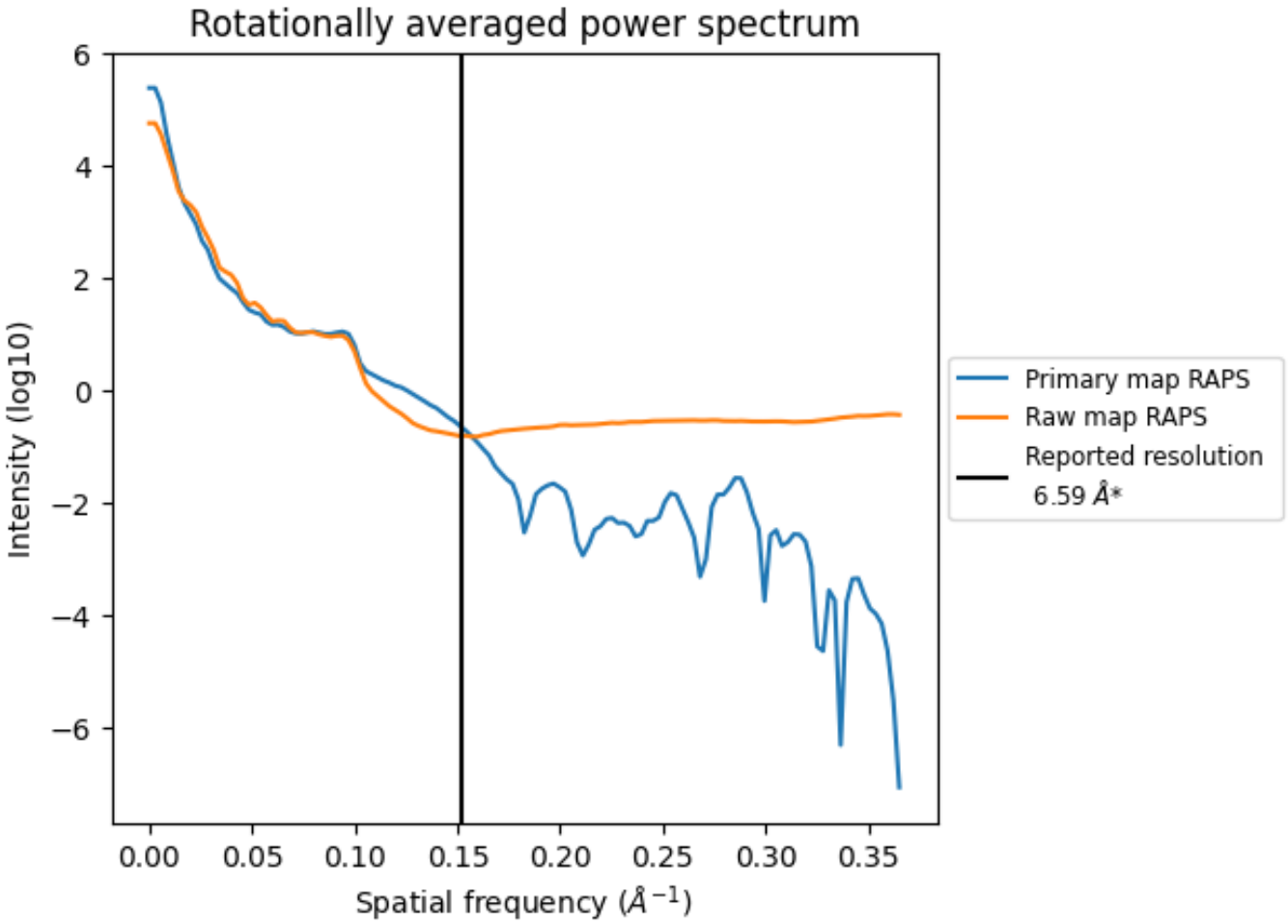
7.2 Volume estimate



The volume at the recommended contour level is 279 nm^3; this corresponds to an approximate mass of 252 kDa.

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

7.3 Rotationally averaged power spectrum (i)

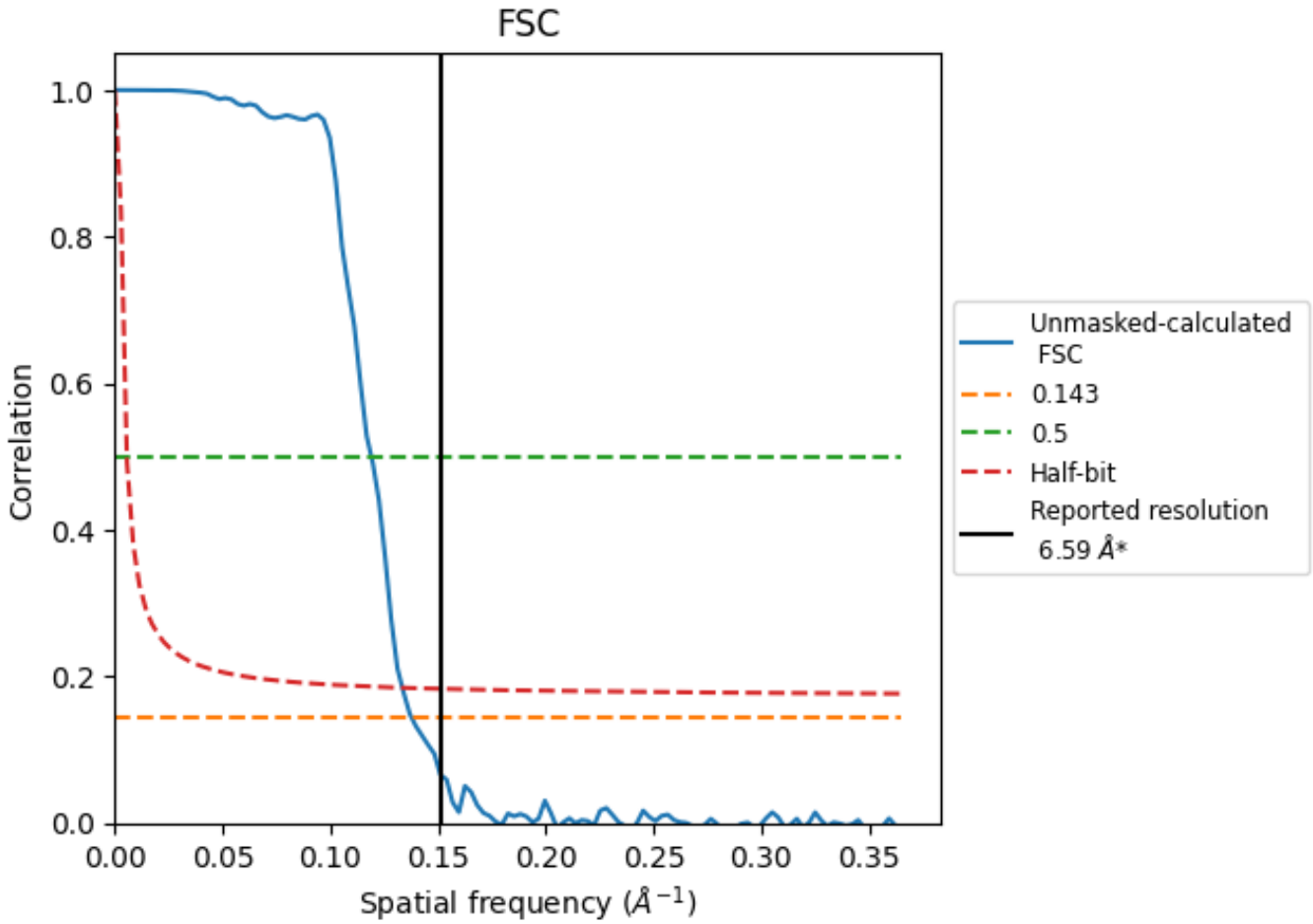


*Reported resolution corresponds to spatial frequency of 0.152 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.152 Å^{-1}

8.2 Resolution estimates (i)

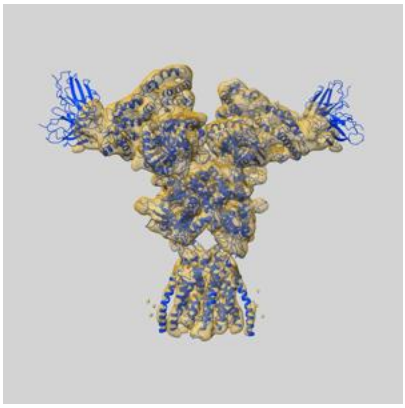
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.59	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.26	8.40	7.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.26 differs from the reported value 6.59 by more than 10 %

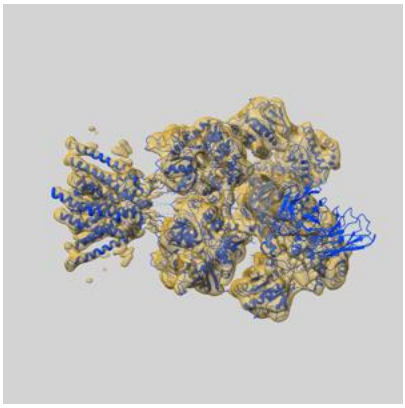
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25845 and PDB model 7TEE. Per-residue inclusion information can be found in section 3 on page 8.

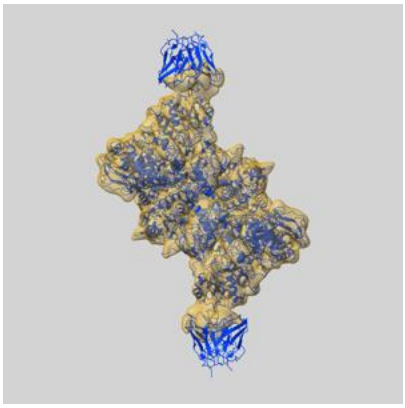
9.1 Map-model overlay



X



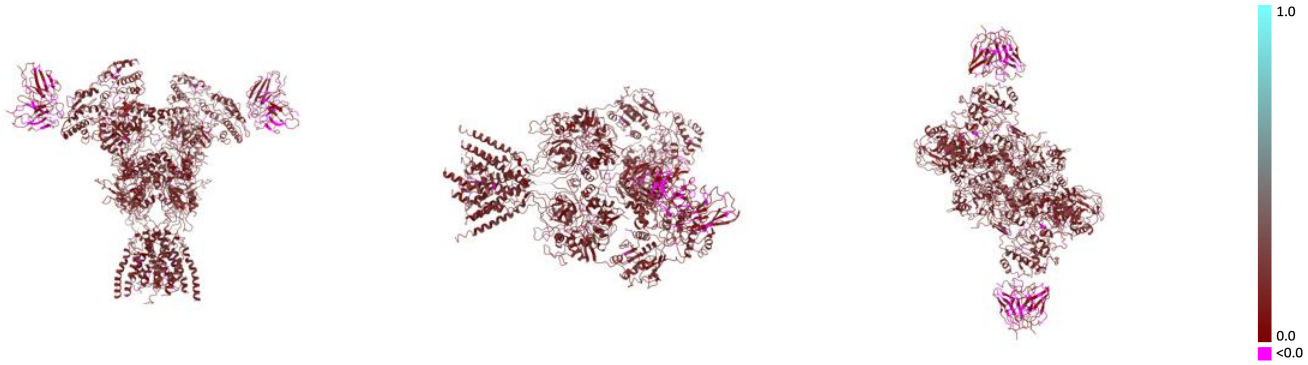
Y



Z

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

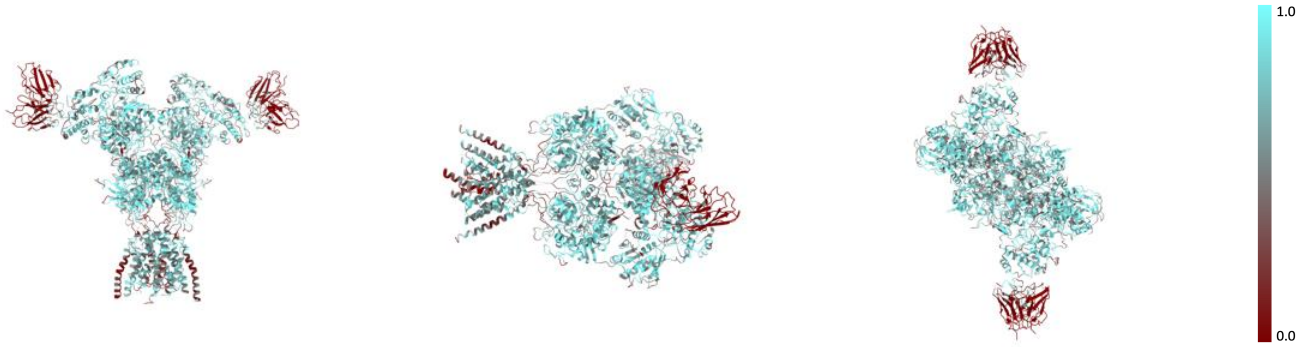
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

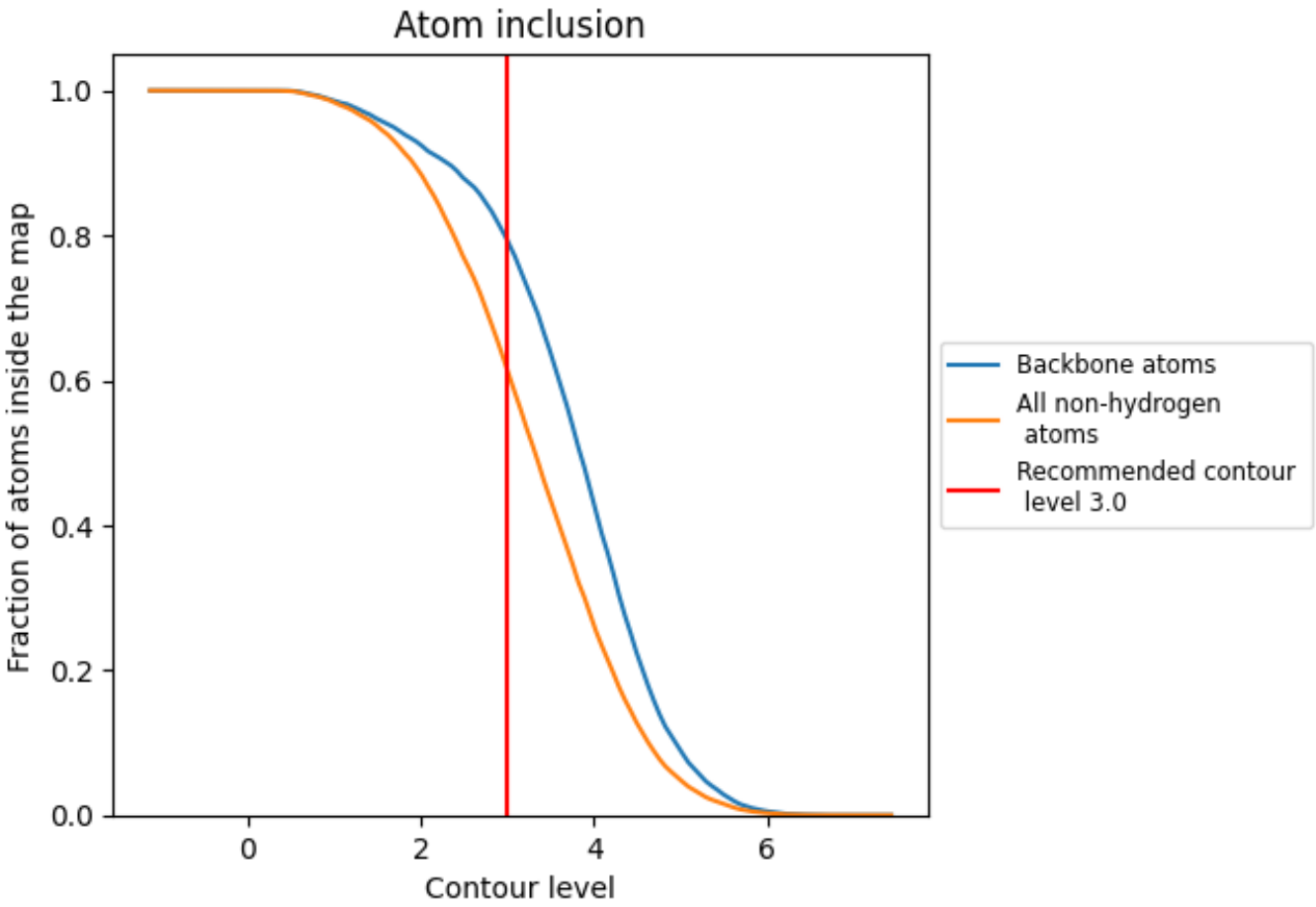
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (3.0).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6131	0.1570
A	0.6825	0.1740
B	0.6739	0.1680
C	0.6841	0.1740
D	0.6749	0.1700
H	0.1852	0.0260
L	0.0907	0.0730
M	0.1842	0.0280
N	0.0944	0.0950