



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 02:56 AM UTC

PDB ID : 7TEB / pdb_00007teb
EMDB ID : EMD-25844
Title : Cryo-EM structure of GluN1b-2B NMDAR complexed to Fab2 non-active1-like
Authors : Tajima, N.; Furukawa, H.
Deposited on : 2022-01-04
Resolution : 4.23 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

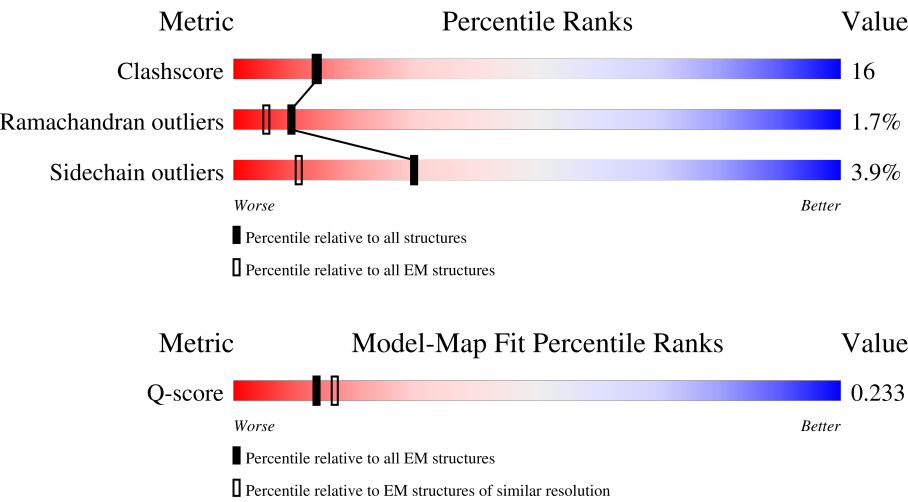
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.23 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4685 (3.74 - 4.73)

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

Mol	Chain	Length	Quality of chain
1	A	862	5% 63% 24% • 9%
1	C	862	5% 65% 22% • 9%
2	B	883	7% 62% 23% • 11%
2	D	883	7% 62% 23% • 11%

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Mol	Chain	Length	Quality of chain
3	H	223	42% 39% 13% 48%
3	M	223	43% 39% 13% 48%
4	L	213	44% 36% 13% 50%
4	N	213	45% 35% 14% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28161 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	783	Total	C	N	O	S	0	0
			6177	3928	1070	1142	37		
1	C	784	Total	C	N	O	S	0	0
			6186	3933	1071	1145	37		

There are 30 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	784	Total	C	N	O	S	0	0
			6177	3974	996	1165	42		
2	D	784	Total	C	N	O	S	0	0
			6177	3974	996	1165	42		

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		

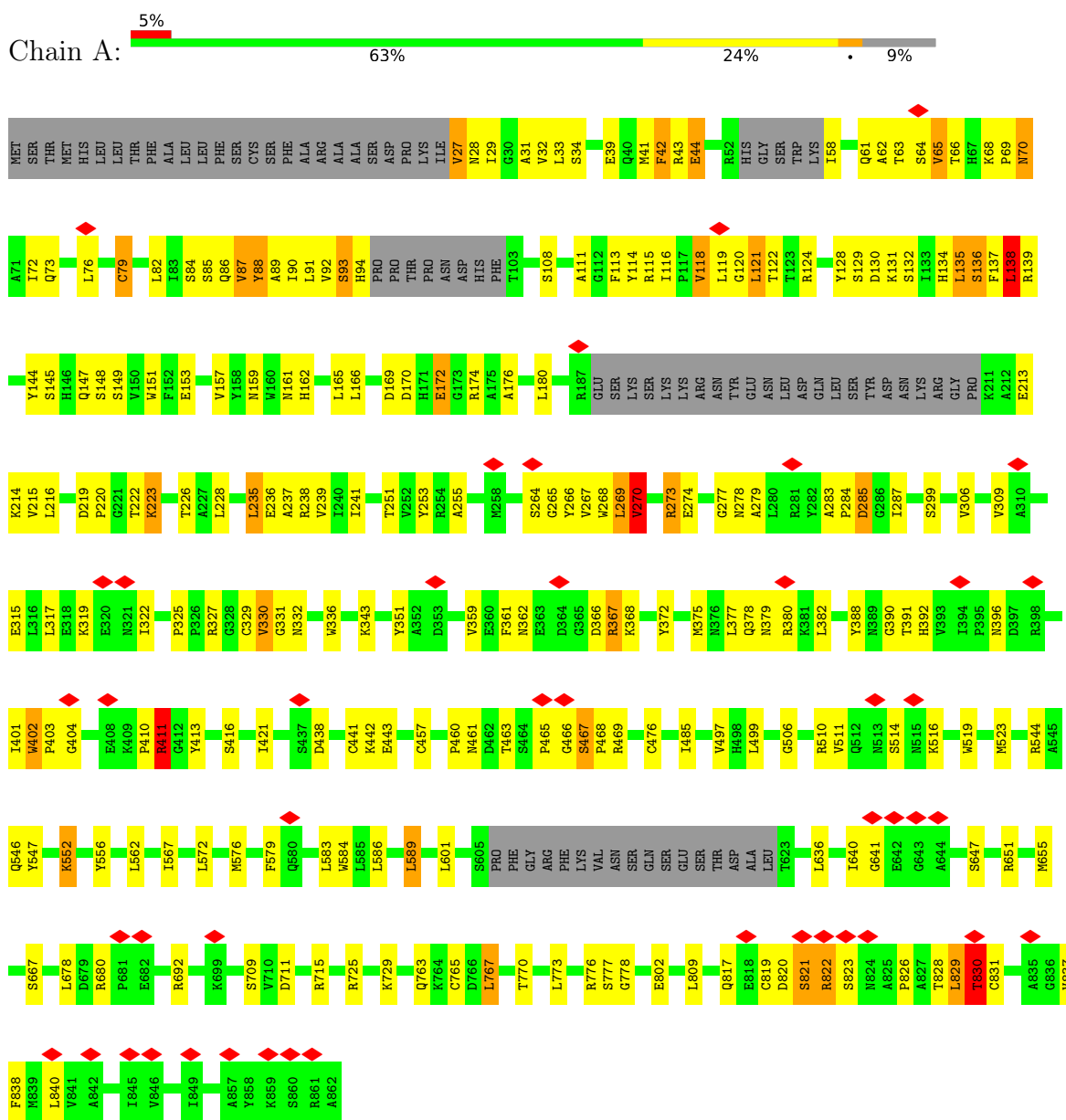
- Molecule 4 is a protein called Fab2 light chain.

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		

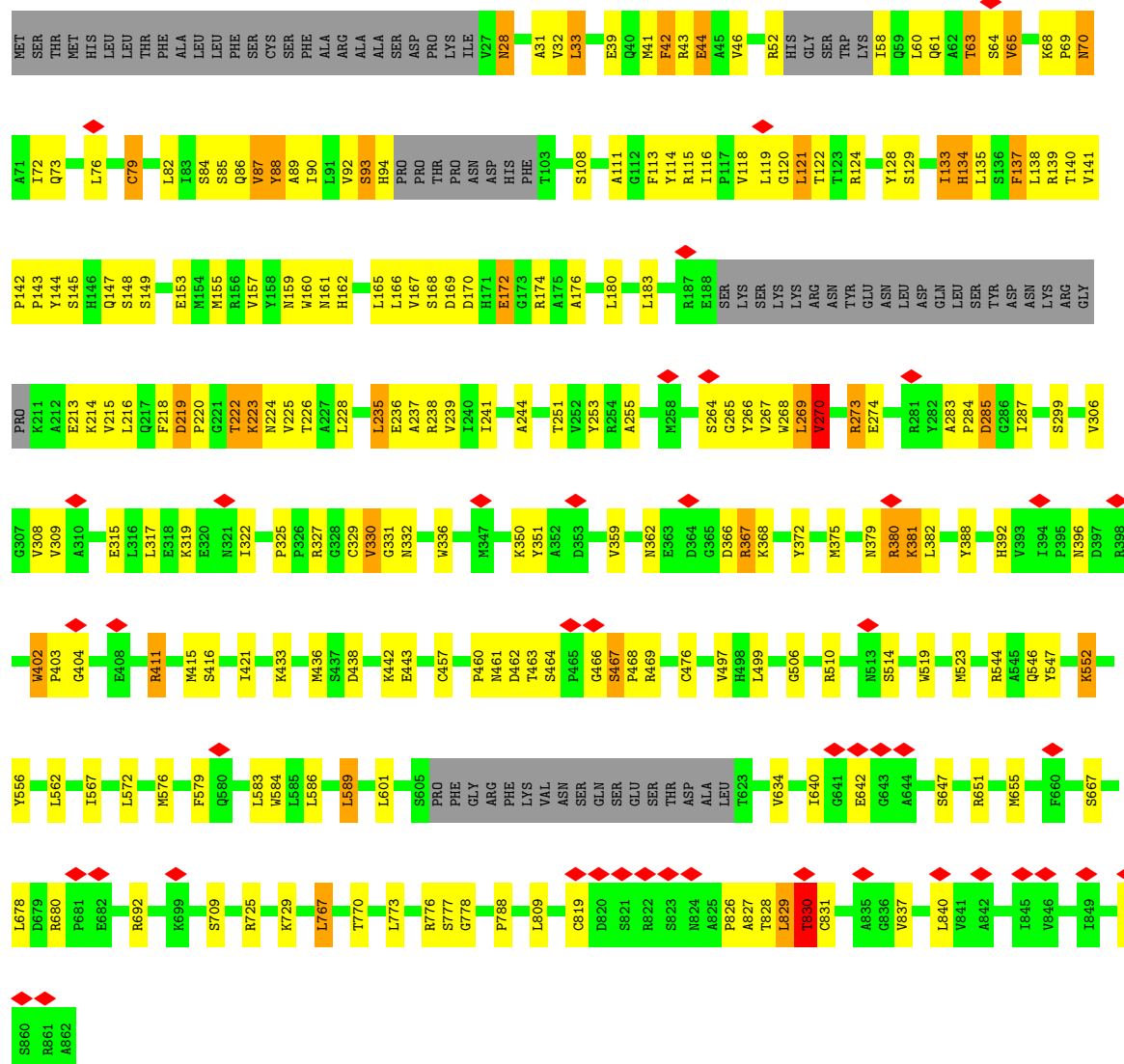
3 Residue-property plots

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

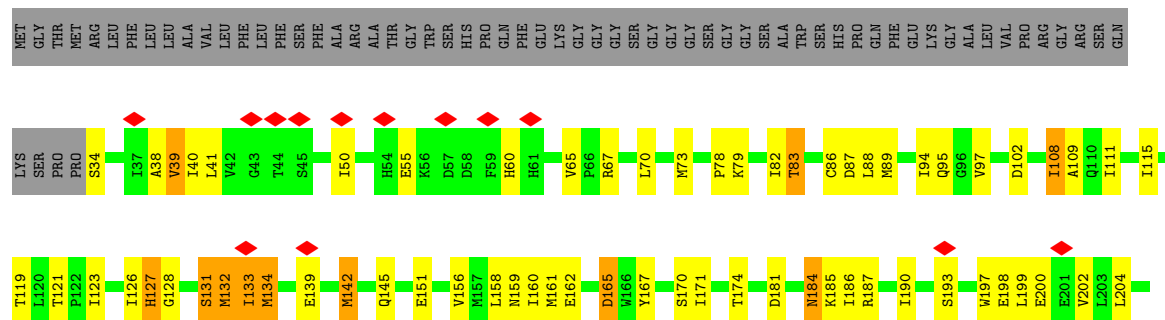
- Molecule 1: Glutamate receptor ionotropic, NMDA 1

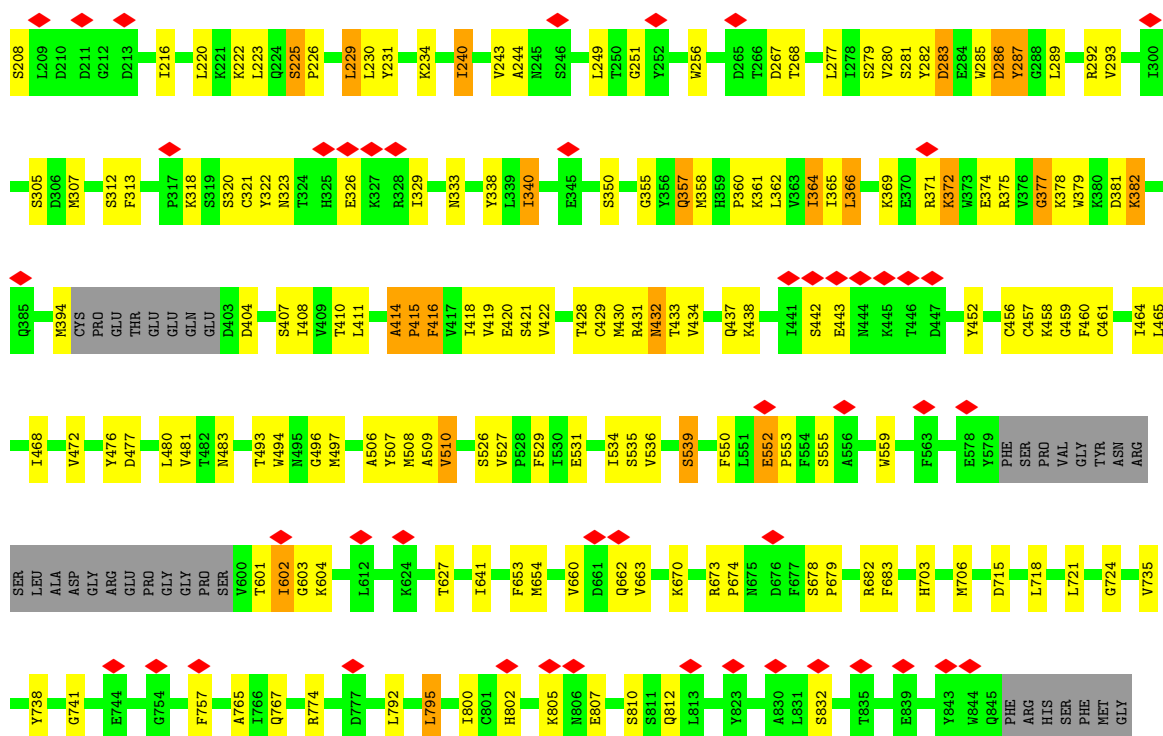


- Molecule 1: Glutamate receptor ionotropic, NMDA 1

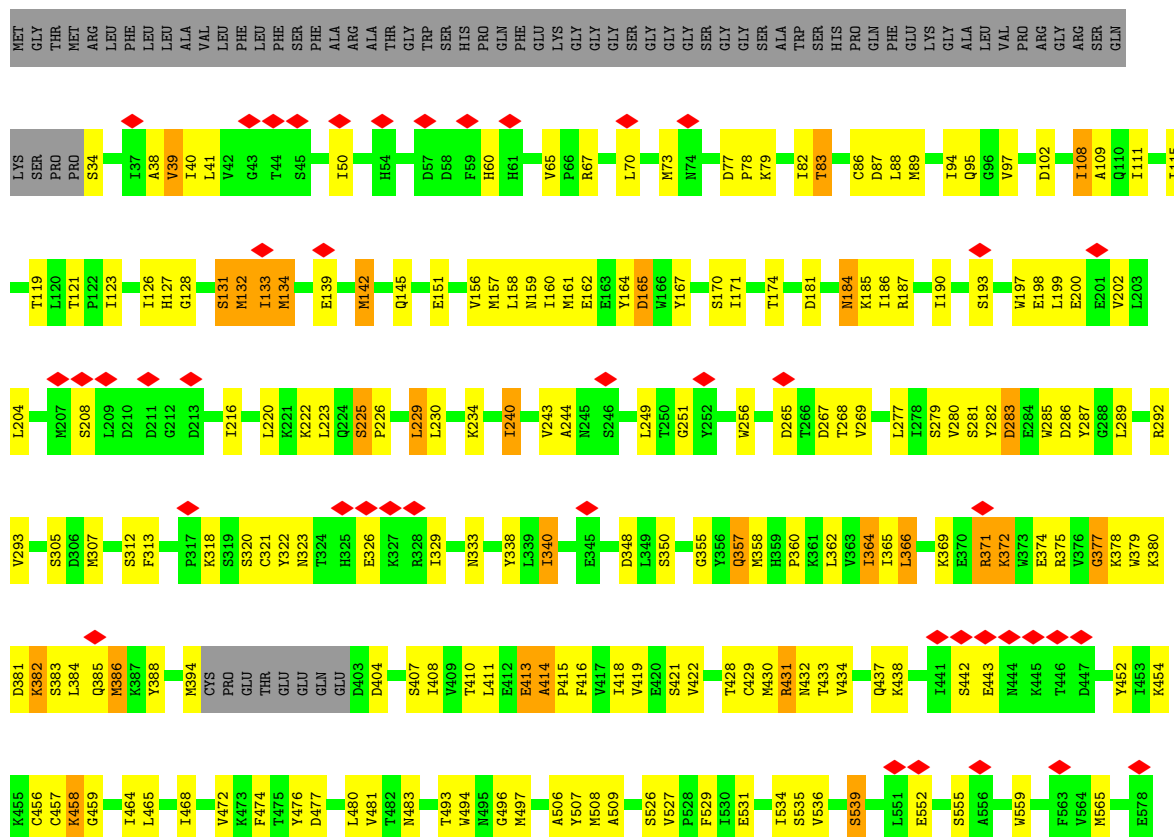


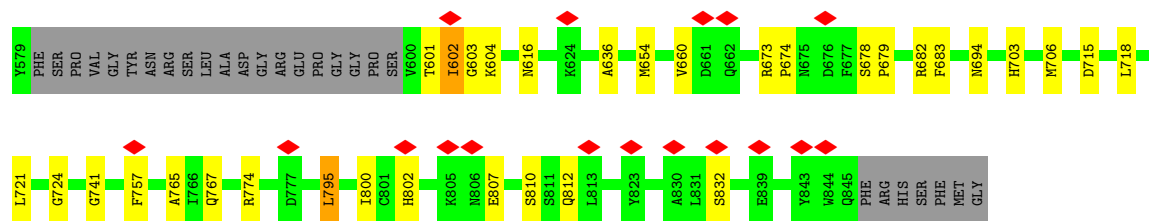
- Molecule 2: Glutamate receptor ionotropic, NMDA 2B



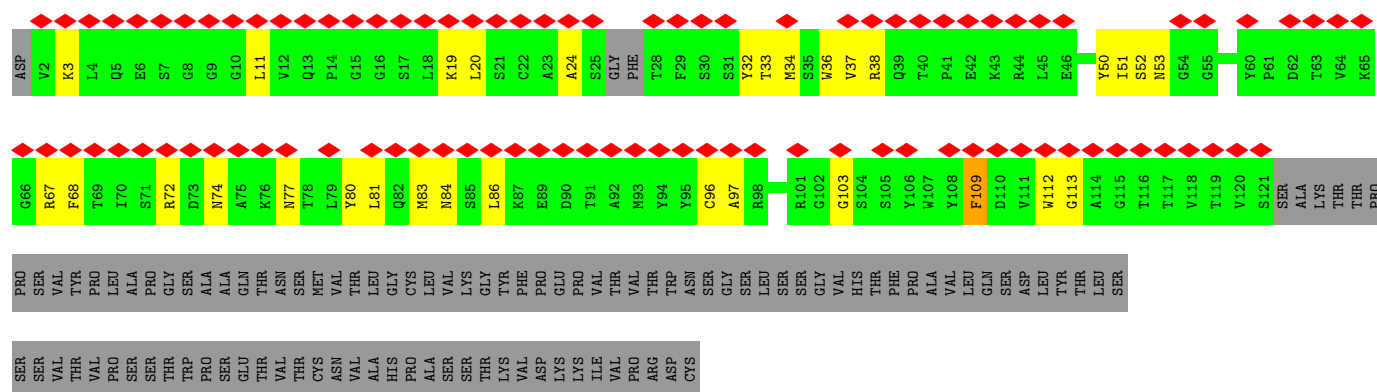
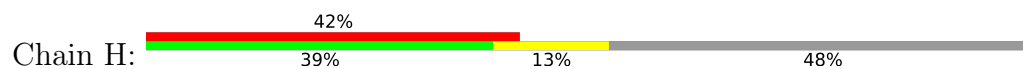


• Molecule 2: Glutamate receptor ionotropic, NMDA 2B

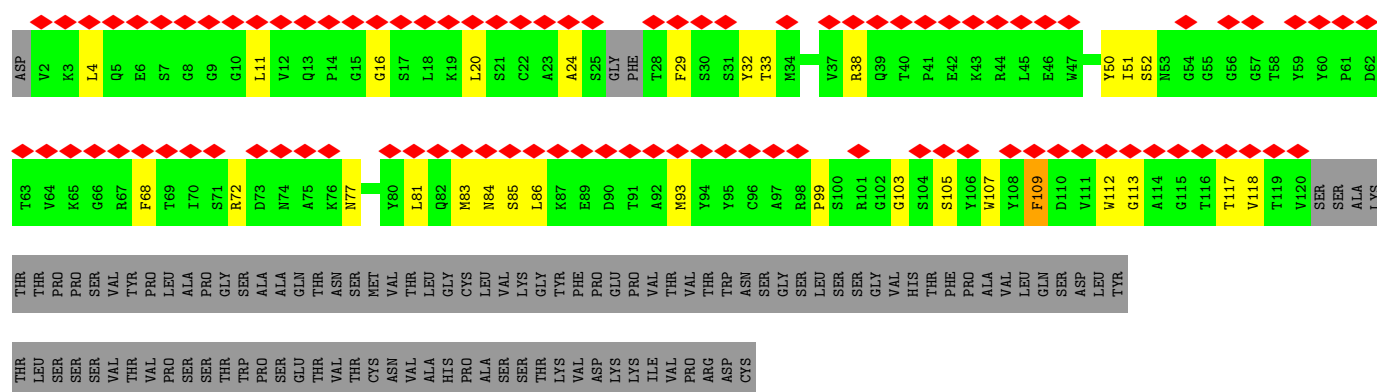
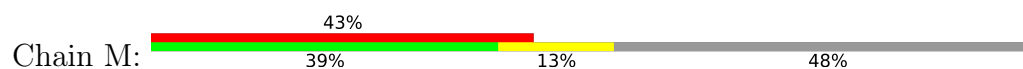




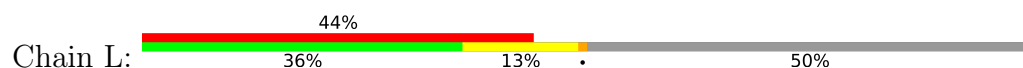
• Molecule 3: Fab2 heavy chain



• Molecule 3: Fab2 heavy chain



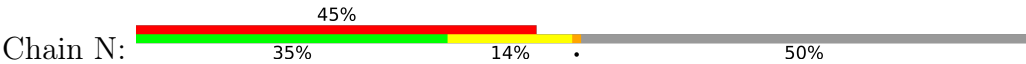
• Molecule 4: Fab2 light chain



LEU THR
GLU TYR
SER GLY
GLY ARG
HIS GLY
ASN ALA
SER SER
VAL VAL
THR CYS
GLU PHE
LEU LEU
ASN ASN
ASN ASN
PHE THR
LYS TYR
THR PRO
SER LYS
ASP ASP
ILE ILE
VAL VAL
LYS LYS
TRP TRP
LYS LYS
ILE ILE
ASP ASP
GLY GLY
SER SER
GLU GLU
ARG ARG
GLN GLN
ASN ASN
GLY GLY
VAL VAL
LEU LEU
ASN ASN
SER SER
TRP TRP
THR THR
ASP ASP
GLN GLN
ASP ASP
SER SER
LYS LYS
ASP ASP
SER SER
THR THR
TYR TYR
SER SER
MET MET
SER SER
THR THR
THR THR
LEU LEU
THR THR
LYS LYS
ASP ASP

GLU TYR
TYR ARG
GLU ARG
HIS HIS
ASN ASN
SER SER
TYR TYR
THR THR
CYS CYS
GLU GLU
ALA ALA
THR THR
HIS HIS
LYS LYS
THR THR
SER SER
PRO PRO
SER SER
PRO PRO
ILE ILE
VAL VAL
LYS LYS
SER SER
PHE PHE
ASN ASN
ARG ARG
ASN ASN
GLU GLU
SER SER

● Molecule 4: Fab2 light chain



D1 I2 Q3 M4 T5 Q6 S7 P8 S9 S10 L11 S12 A13 S14 L15 G16 G17 K18 V19 T20 T21 T22 C23 K24 A25 S26 Q27 D28 I29 A34 I35 Y36 Q37 H38 K39 P40 G41 K42 Q43 P44 R45 L46 L47 I48 H49 Y50 T51 S52 S53 L54 Q55 P56 G57 I58 P59 S60 R61 F62 S63

G64 S65 G66 S67 R69 D70 Y71 S72 F73 S74 I75 S76 N77 L78 E79 P80 E81 D82 I83 A84 T85 Y86 Y87 C88 L89 Q90 Y91 D92 Y95 T96 F97 Q98 G99 G100 T101 K102 L103 E104 I105 K106 ARG ALA ASP ALA ALA ALA PRO THR VAL SER ILE PHE PRO PRO SER SER GLN LEU

THR SER
GLU GLY
SER ALA
SER VAL
VAL VAL
CYS CYS
PHE PHE
LEU LEU
ASN ASN
ASN PHE
TYR TYR
PRO PRO
LYS LYS
ASP ASP
ILE ILE
ASN ASN
VAL VAL
LYS LYS
TRP TRP
LYS LYS
ILE ILE
ASP ASP
GLY GLY
SER SER
GLU GLU
ARG ARG
GLN GLN
ASN ASN
VAL VAL
GLY GLY
LEU LEU
ASN ASN
SER SER
TRP TRP
THR THR
ASP ASP
GLN GLN
ASP ASP
SER SER
LYS LYS
ASP ASP
SER SER
THR THR
TYR TYR
MET MET
SER SER
SER SER
THR THR
LEU LEU
THR THR
LEU LEU
THR THR
LYS LYS
ASP ASP
GLU GLU

TYR GLU
ARG ARG
HIS HIS
ASN ASN
SER SER
TYR TYR
THR THR
CYS CYS
GLU GLU
ALA ALA
THR THR
HIS HIS
LYS LYS
THR THR
SER SER
PRO PRO
ILE ILE
VAL VAL
LYS LYS
SER SER
PHE PHE
ASN ASN
ARG ARG
ASN ASN
GLU GLU
SER SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30424	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	9.079	Depositor
Minimum map value	-2.019	Depositor
Average map value	0.054	Depositor
Map value standard deviation	0.469	Depositor
Recommended contour level	3	Depositor
Map size ($\text{\AA}$)	350.72, 350.72, 350.72	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.37, 1.37, 1.37	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.28	0/6306	0.85	20/8534 (0.2%)
1	C	0.28	0/6315	0.84	18/8546 (0.2%)
2	B	0.32	0/6312	0.93	27/8550 (0.3%)
2	D	0.32	0/6312	0.92	25/8550 (0.3%)
3	H	0.28	0/927	0.68	1/1255 (0.1%)
3	M	0.24	0/921	0.63	0/1247
4	L	0.31	0/840	0.76	2/1136 (0.2%)
4	N	0.31	0/840	0.76	2/1136 (0.2%)
All	All	0.30	0/28773	0.87	95/38954 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	C	0	6
2	B	0	18
2	D	0	19
3	H	0	2
3	M	0	1
4	L	0	3
4	N	0	2
All	All	0	57

There are no bond length outliers.

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	476	CYS	CA-CB-SG	9.49	136.22	114.40
1	A	476	CYS	CA-CB-SG	9.49	136.22	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	GLY	N-CA-C	-9.24	98.40	110.69
2	B	377	GLY	N-CA-C	9.24	128.21	110.66
2	D	377	GLY	N-CA-C	9.23	128.21	110.66
1	C	265	GLY	N-CA-C	-9.22	98.42	110.69
2	B	414	ALA	CA-C-N	9.18	131.32	119.84
2	B	414	ALA	C-N-CA	9.18	131.32	119.84
1	C	402	TRP	CB-CA-C	7.56	120.20	109.92
1	A	402	TRP	CB-CA-C	7.53	120.17	109.92
2	D	127	HIS	N-CA-C	-7.39	99.05	109.69
2	B	127	HIS	N-CA-C	-7.36	99.09	109.69
1	C	148	SER	CA-C-N	7.11	131.98	120.60
1	C	148	SER	C-N-CA	7.11	131.98	120.60
1	A	148	SER	CA-C-N	7.09	131.95	120.60
1	A	148	SER	C-N-CA	7.09	131.95	120.60
1	C	367	ARG	CA-C-N	7.09	135.08	121.54
1	C	367	ARG	C-N-CA	7.09	135.08	121.54
1	A	367	ARG	CA-C-N	7.09	135.07	121.54
1	A	367	ARG	C-N-CA	7.09	135.07	121.54
1	C	264	SER	CA-C-N	6.99	130.56	120.91
1	C	264	SER	C-N-CA	6.99	130.56	120.91
1	A	264	SER	CA-C-N	6.97	130.53	120.91
1	A	264	SER	C-N-CA	6.97	130.53	120.91
1	A	402	TRP	N-CA-C	-6.86	99.26	108.11
1	C	402	TRP	N-CA-C	-6.83	99.30	108.11
1	A	476	CYS	N-CA-CB	-6.75	99.81	111.55
1	C	476	CYS	N-CA-CB	-6.72	99.86	111.55
2	D	372	LYS	N-CA-C	6.53	119.47	107.73
2	B	372	LYS	N-CA-C	6.52	119.47	107.73
2	D	108	ILE	CB-CG1-CD1	6.29	127.01	113.80
2	B	108	ILE	CB-CG1-CD1	6.28	126.99	113.80
2	D	229	LEU	CA-C-N	6.14	131.97	121.29
2	D	229	LEU	C-N-CA	6.14	131.97	121.29
1	C	44	GLU	CA-C-N	6.13	129.63	120.31
1	C	44	GLU	C-N-CA	6.13	129.63	120.31
2	B	229	LEU	CA-C-N	6.12	131.93	121.29
2	B	229	LEU	C-N-CA	6.12	131.93	121.29
1	A	44	GLU	CA-C-N	6.12	129.60	120.31
1	A	44	GLU	C-N-CA	6.12	129.60	120.31
2	D	355	GLY	CA-C-N	-6.02	112.27	123.05
2	D	355	GLY	C-N-CA	-6.02	112.27	123.05
2	B	355	GLY	CA-C-N	-6.00	112.30	123.05
2	B	355	GLY	C-N-CA	-6.00	112.30	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	103	GLY	N-CA-C	5.95	122.58	112.22
2	B	338	TYR	CA-CB-CG	-5.94	103.20	113.90
2	D	134	MET	N-CA-C	5.94	118.35	108.13
2	B	134	MET	N-CA-C	5.93	118.32	108.13
2	D	338	TYR	CA-CB-CG	-5.93	103.23	113.90
1	C	42	PHE	N-CA-CB	5.85	118.56	110.07
1	A	42	PHE	N-CA-CB	5.83	118.53	110.07
1	A	391	THR	N-CA-C	-5.81	99.93	109.40
2	D	131	SER	CA-C-N	5.78	132.57	121.54
2	D	131	SER	C-N-CA	5.78	132.57	121.54
2	B	131	SER	CA-C-N	5.77	132.56	121.54
2	B	131	SER	C-N-CA	5.77	132.56	121.54
2	B	340	ILE	N-CA-C	-5.70	100.39	109.17
2	D	340	ILE	N-CA-C	-5.69	100.41	109.17
2	B	204	LEU	N-CA-C	5.68	118.50	109.24
2	D	204	LEU	N-CA-C	5.66	118.47	109.24
1	A	149	SER	N-CA-C	5.63	119.25	112.38
1	C	149	SER	N-CA-C	5.59	119.19	112.38
1	A	336	TRP	CA-CB-CG	-5.50	103.15	113.60
1	C	336	TRP	CA-CB-CG	-5.50	103.15	113.60
1	A	42	PHE	CA-CB-CG	5.46	119.27	113.80
1	C	42	PHE	CA-CB-CG	5.37	119.17	113.80
2	B	108	ILE	CA-CB-CG1	5.33	119.45	110.40
2	D	108	ILE	CA-CB-CG1	5.33	119.45	110.40
2	B	109	ALA	CA-C-N	5.27	131.61	121.54
2	B	109	ALA	C-N-CA	5.27	131.61	121.54
2	D	109	ALA	CA-C-N	5.26	131.58	121.54
2	D	109	ALA	C-N-CA	5.26	131.58	121.54
2	B	240	ILE	N-CA-C	-5.25	105.20	112.50
2	D	348	ASP	N-CA-C	5.23	117.00	108.63
2	D	240	ILE	N-CA-C	-5.22	105.24	112.50
2	B	472	VAL	CA-C-N	5.16	131.40	121.54
2	B	472	VAL	C-N-CA	5.16	131.40	121.54
2	D	60	HIS	CA-C-N	5.16	135.21	125.66
2	D	60	HIS	C-N-CA	5.16	135.21	125.66
2	B	60	HIS	CA-C-N	5.16	135.21	125.66
2	B	60	HIS	C-N-CA	5.16	135.21	125.66
2	D	472	VAL	CA-C-N	5.14	131.37	121.54
2	D	472	VAL	C-N-CA	5.14	131.37	121.54
2	D	161	MET	CA-C-N	5.06	132.83	122.55
2	D	161	MET	C-N-CA	5.06	132.83	122.55
2	B	161	MET	CA-C-N	5.05	132.81	122.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	161	MET	C-N-CA	5.05	132.81	122.55
1	A	390	GLY	N-CA-C	-5.05	101.21	113.18
1	A	270	VAL	CA-CB-CG1	5.04	118.97	110.40
4	N	49	HIS	CA-C-N	5.04	128.38	120.82
4	N	49	HIS	C-N-CA	5.04	128.38	120.82
2	B	231	TYR	N-CA-CB	5.02	118.81	110.47
1	C	270	VAL	CA-CB-CG1	5.02	118.93	110.40
4	L	49	HIS	CA-C-N	5.01	128.34	120.82
4	L	49	HIS	C-N-CA	5.01	128.34	120.82

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	403	PRO	Peptide
1	A	552	LYS	Peptide
1	A	567	ILE	Peptide
1	A	79	CYS	Peptide
1	A	829	LEU	Peptide
1	A	830	THR	Peptide
2	B	128	GLY	Peptide
2	B	132	MET	Peptide
2	B	142	MET	Peptide
2	B	165	ASP	Peptide
2	B	184	ASN	Mainchain
2	B	222	LYS	Peptide
2	B	225	SER	Peptide
2	B	251	GLY	Peptide
2	B	283	ASP	Peptide
2	B	340	ILE	Peptide
2	B	357	GLN	Peptide
2	B	371	ARG	Peptide
2	B	476	TYR	Peptide
2	B	506	ALA	Peptide
2	B	552	GLU	Peptide
2	B	678	SER	Peptide
2	B	795	LEU	Peptide
2	B	83	THR	Mainchain
1	C	403	PRO	Peptide
1	C	552	LYS	Peptide
1	C	567	ILE	Peptide
1	C	79	CYS	Peptide

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Mol	Chain	Res	Type	Group
1	C	829	LEU	Peptide
1	C	830	THR	Peptide
2	D	128	GLY	Peptide
2	D	132	MET	Peptide
2	D	142	MET	Peptide
2	D	165	ASP	Peptide
2	D	184	ASN	Mainchain
2	D	222	LYS	Peptide
2	D	225	SER	Peptide
2	D	251	GLY	Peptide
2	D	283	ASP	Peptide
2	D	340	ILE	Peptide
2	D	357	GLN	Peptide
2	D	371	ARG	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	795	LEU	Peptide
2	D	83	THR	Mainchain
3	H	109	PHE	Peptide
3	H	36	TRP	Peptide
4	L	47	LEU	Peptide
4	L	8	PRO	Peptide
4	L	80	PRO	Peptide
3	M	109	PHE	Peptide
4	N	8	PRO	Peptide
4	N	80	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6177	0	6171	253	0
1	C	6186	0	6172	258	0
2	B	6177	0	6095	171	0
2	D	6177	0	6095	179	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	905	0	867	20	0
3	M	899	0	862	20	0
4	L	820	0	802	15	0
4	N	820	0	802	14	0
All	All	28161	0	27866	885	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 16.

All (885) 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)
1:A:31:ALA:HB3	1:A:65:VAL:CG2	1.29	1.60
2:B:364:ILE:HG13	2:B:377:GLY:CA	1.29	1.58
2:D:364:ILE:HG13	2:D:377:GLY:CA	1.29	1.56
1:A:576:MET:HE1	1:A:840:LEU:CD1	1.27	1.56
1:C:576:MET:HE1	1:C:840:LEU:CD1	1.27	1.54
1:C:167:VAL:N	1:C:218:PHE:CE1	1.80	1.49
1:A:118:VAL:CG2	1:A:136:SER:O	1.65	1.42
1:C:576:MET:CE	1:C:840:LEU:CD1	1.97	1.41
1:A:31:ALA:CB	1:A:65:VAL:CG2	1.99	1.41
1:A:576:MET:CE	1:A:840:LEU:CD1	1.97	1.41
1:A:128:TYR:O	1:A:137:PHE:HZ	1.09	1.34
1:C:167:VAL:CA	1:C:218:PHE:CZ	2.15	1.30
1:A:128:TYR:O	1:A:137:PHE:CZ	1.84	1.28
2:D:364:ILE:CG1	2:D:377:GLY:HA3	1.64	1.27
2:B:364:ILE:CG1	2:B:377:GLY:HA3	1.63	1.26
1:A:214:LYS:HE2	1:A:235:LEU:CD1	1.63	1.26
1:A:86:GLN:O	1:A:325:PRO:HD2	1.33	1.24
1:C:467:SER:H	1:C:468:PRO:CD	1.50	1.24
1:A:467:SER:H	1:A:468:PRO:CD	1.52	1.21
1:A:33:LEU:HD12	1:A:39:GLU:OE2	1.36	1.19
1:C:86:GLN:O	1:C:325:PRO:HD2	1.36	1.19
2:D:364:ILE:CG1	2:D:377:GLY:CA	2.18	1.19
1:C:88:TYR:OH	1:C:90:ILE:HG22	1.43	1.19
1:C:167:VAL:N	1:C:218:PHE:CZ	2.10	1.19
1:A:214:LYS:CE	1:A:235:LEU:HD11	1.74	1.18
2:D:320:SER:OG	2:D:322:TYR:CD2	1.91	1.18
2:B:364:ILE:CG1	2:B:377:GLY:C	2.17	1.18
2:D:364:ILE:CG1	2:D:377:GLY:C	2.17	1.17
1:A:576:MET:CE	1:A:840:LEU:HD11	1.66	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:ILE:CG1	2:B:377:GLY:CA	2.18	1.17
1:A:115:ARG:CD	1:A:135:LEU:HD11	1.75	1.17
1:A:219:ASP:HB3	1:A:220:PRO:HD3	1.22	1.16
1:C:167:VAL:C	1:C:218:PHE:CZ	2.22	1.16
1:C:214:LYS:HE2	1:C:235:LEU:CD1	1.75	1.16
1:A:88:TYR:OH	1:A:90:ILE:HG22	1.43	1.15
1:C:576:MET:CE	1:C:840:LEU:HD11	1.66	1.15
2:D:414:ALA:CB	2:D:415:PRO:CD	2.25	1.14
1:C:159:ASN:HB3	1:C:411:ARG:HD2	1.30	1.14
1:C:467:SER:H	1:C:468:PRO:HD2	1.09	1.14
1:A:159:ASN:HB3	1:A:411:ARG:HD2	1.18	1.14
1:A:118:VAL:HG23	1:A:136:SER:O	0.97	1.13
1:C:213:GLU:OE2	1:C:235:LEU:CD2	1.97	1.12
2:D:320:SER:OG	2:D:322:TYR:CE2	1.93	1.12
2:D:414:ALA:HB3	2:D:415:PRO:HD2	1.22	1.11
1:A:214:LYS:NZ	1:A:235:LEU:HD11	1.64	1.11
1:A:31:ALA:HB3	1:A:65:VAL:HG22	1.23	1.11
1:A:213:GLU:OE2	1:A:235:LEU:CD2	1.98	1.11
1:A:214:LYS:HE2	1:A:235:LEU:HD13	1.32	1.10
1:C:214:LYS:NZ	1:C:235:LEU:HD11	1.64	1.10
1:C:219:ASP:HB3	1:C:220:PRO:CD	1.81	1.10
1:A:467:SER:H	1:A:468:PRO:HD2	1.04	1.09
1:A:88:TYR:OH	1:A:90:ILE:CG2	1.99	1.09
1:C:172:GLU:OE1	1:C:273:ARG:NH2	1.84	1.09
1:A:172:GLU:OE1	1:A:273:ARG:NH2	1.84	1.08
1:C:167:VAL:N	1:C:218:PHE:HE1	1.27	1.08
1:A:31:ALA:CB	1:A:65:VAL:HG22	1.72	1.08
1:A:31:ALA:HB3	1:A:65:VAL:HG23	1.11	1.07
1:A:159:ASN:HB3	1:A:411:ARG:CD	1.84	1.06
1:C:167:VAL:C	1:C:218:PHE:CE1	2.33	1.06
2:D:414:ALA:HB3	2:D:415:PRO:CD	1.85	1.06
1:C:93:SER:OG	1:C:122:THR:OG1	1.63	1.06
1:A:28:ASN:HA	1:A:61:GLN:O	1.55	1.04
1:C:128:TYR:O	1:C:137:PHE:CZ	2.11	1.04
1:A:93:SER:OG	1:A:122:THR:OG1	1.62	1.04
1:A:576:MET:HE1	1:A:840:LEU:CG	1.88	1.04
1:A:115:ARG:HD2	1:A:135:LEU:HD11	1.34	1.04
1:C:330:VAL:HG13	2:D:79:LYS:HE3	1.40	1.04
1:A:576:MET:HE3	1:A:840:LEU:HD11	1.39	1.03
1:C:88:TYR:OH	1:C:90:ILE:CG2	2.06	1.03
1:C:576:MET:HE1	1:C:840:LEU:CG	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:364:ILE:HG12	2:D:377:GLY:C	1.81	1.03
1:A:115:ARG:CD	1:A:135:LEU:CD1	2.36	1.03
2:B:364:ILE:HG12	2:B:377:GLY:C	1.80	1.03
1:C:219:ASP:HB3	1:C:220:PRO:HD3	1.07	1.03
1:C:214:LYS:HE2	1:C:235:LEU:HD13	1.33	1.03
1:C:214:LYS:CE	1:C:235:LEU:HD11	1.88	1.03
1:A:510:ARG:NH1	1:A:514:SER:O	1.92	1.02
2:D:432:ASN:ND2	2:D:456:CYS:HB3	1.74	1.02
1:A:93:SER:CB	1:A:122:THR:OG1	2.07	1.02
2:D:414:ALA:HB1	2:D:415:PRO:HD3	1.41	1.02
1:C:93:SER:CB	1:C:122:THR:OG1	2.08	1.02
1:C:576:MET:HE3	1:C:840:LEU:HD11	1.39	1.01
1:A:576:MET:CE	1:A:840:LEU:HD12	1.73	1.01
1:C:285:ASP:HB3	1:C:379:ASN:HB2	1.42	1.01
1:C:115:ARG:CD	1:C:135:LEU:HD11	1.91	1.00
1:C:576:MET:CE	1:C:840:LEU:HD12	1.73	1.00
1:C:330:VAL:CG1	2:D:79:LYS:HE3	1.90	0.99
1:A:88:TYR:HE1	1:A:90:ILE:HB	1.27	0.99
1:A:410:PRO:O	1:A:411:ARG:O	1.79	0.99
1:C:115:ARG:HD2	1:C:135:LEU:HD11	1.45	0.98
2:D:364:ILE:HG13	2:D:377:GLY:C	1.85	0.98
2:B:662:GLN:HG2	2:B:663:VAL:HG23	1.46	0.97
2:D:432:ASN:HD22	2:D:456:CYS:HB3	1.29	0.97
1:A:467:SER:N	1:A:468:PRO:HD2	1.79	0.97
1:A:214:LYS:CE	1:A:235:LEU:CD1	2.34	0.97
2:B:364:ILE:HG13	2:B:377:GLY:C	1.86	0.97
1:C:161:ASN:HB3	1:C:411:ARG:HH11	1.29	0.96
1:C:467:SER:N	1:C:468:PRO:HD2	1.81	0.96
1:C:214:LYS:CE	1:C:235:LEU:CD1	2.42	0.96
1:C:167:VAL:CA	1:C:218:PHE:CE1	2.44	0.95
1:C:219:ASP:CB	1:C:220:PRO:HD3	1.95	0.95
1:C:576:MET:HE1	1:C:840:LEU:HD12	0.96	0.95
2:B:416:PHE:HD1	2:B:461:CYS:HG	0.95	0.95
2:B:364:ILE:HD11	2:B:378:LYS:N	1.83	0.94
1:C:467:SER:N	1:C:468:PRO:CD	2.29	0.94
2:D:364:ILE:HD11	2:D:378:LYS:N	1.83	0.94
1:C:167:VAL:HA	1:C:218:PHE:CZ	2.03	0.93
1:A:576:MET:HE1	1:A:840:LEU:HD12	0.96	0.93
1:C:168:SER:N	1:C:218:PHE:CE2	2.35	0.93
1:A:115:ARG:HD3	1:A:135:LEU:CD1	1.99	0.91
1:A:31:ALA:CB	1:A:65:VAL:HG21	1.97	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ALA:HB1	1:A:65:VAL:CG2	2.01	0.90
1:C:88:TYR:HE1	1:C:90:ILE:HB	1.35	0.90
1:A:219:ASP:HB3	1:A:220:PRO:CD	2.01	0.89
2:B:320:SER:OG	2:B:322:TYR:HD2	1.54	0.89
1:A:68:LYS:HB2	1:A:69:PRO:HD2	1.53	0.89
1:C:68:LYS:HB2	1:C:69:PRO:HD2	1.53	0.89
1:A:115:ARG:HD3	1:A:135:LEU:HD12	1.56	0.87
1:C:128:TYR:HB3	1:C:137:PHE:HZ	1.39	0.87
1:C:166:LEU:C	1:C:218:PHE:CE1	2.53	0.87
1:C:88:TYR:CD1	1:C:89:ALA:N	2.43	0.87
1:A:115:ARG:HD2	1:A:135:LEU:CD1	2.03	0.86
1:C:167:VAL:CA	1:C:218:PHE:HZ	1.85	0.86
1:C:308:VAL:HB	1:C:351:TYR:CZ	2.11	0.86
1:C:167:VAL:H	1:C:218:PHE:HE1	0.87	0.86
2:B:465:LEU:HD13	2:B:510:VAL:HG11	1.58	0.85
2:B:414:ALA:HB1	2:B:415:PRO:HD2	1.58	0.85
1:A:31:ALA:HB1	1:A:65:VAL:HG21	1.59	0.85
1:C:108:SER:HB2	1:C:134:HIS:CE1	2.11	0.85
2:B:432:ASN:ND2	2:B:456:CYS:HB3	1.91	0.84
1:A:130:ASP:OD2	1:A:132:SER:OG	1.94	0.84
1:C:161:ASN:HB3	1:C:411:ARG:NH1	1.90	0.84
1:A:91:LEU:HD12	1:A:137:PHE:HB2	1.59	0.83
1:A:93:SER:HB2	1:A:122:THR:OG1	1.79	0.83
1:C:213:GLU:CD	1:C:235:LEU:HD22	2.04	0.83
1:C:88:TYR:CZ	1:C:90:ILE:HG22	2.14	0.83
1:A:88:TYR:CZ	1:A:90:ILE:HG22	2.14	0.82
1:C:214:LYS:HZ3	1:C:235:LEU:HD11	1.42	0.82
1:A:213:GLU:CD	1:A:235:LEU:HD22	2.04	0.82
2:D:414:ALA:CB	2:D:415:PRO:HD3	2.00	0.82
1:A:467:SER:N	1:A:468:PRO:CD	2.31	0.82
1:A:93:SER:CB	1:A:122:THR:HG1	1.89	0.81
1:C:93:SER:HB2	1:C:122:THR:OG1	1.80	0.81
1:C:120:GLY:HA2	1:C:138:LEU:O	1.80	0.81
2:B:414:ALA:CB	2:B:735:VAL:HG13	2.11	0.81
1:C:330:VAL:HG11	2:D:79:LYS:HZ1	1.45	0.81
1:A:213:GLU:CG	1:A:235:LEU:HD22	2.10	0.81
1:C:213:GLU:OE2	1:C:235:LEU:HD23	1.80	0.81
1:C:166:LEU:C	1:C:218:PHE:CZ	2.59	0.80
1:A:118:VAL:HG21	1:A:136:SER:O	1.79	0.79
1:C:93:SER:CB	1:C:122:THR:HG1	1.92	0.79
1:A:88:TYR:CD1	1:A:89:ALA:N	2.51	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:414:ALA:HB1	2:D:415:PRO:CD	2.03	0.79
1:A:236:GLU:OE2	1:A:416:SER:HB3	1.84	0.78
1:A:213:GLU:OE2	1:A:235:LEU:HD23	1.80	0.78
2:B:364:ILE:HD11	2:B:378:LYS:H	1.48	0.77
1:A:118:VAL:HG23	1:A:136:SER:C	2.05	0.77
1:A:159:ASN:CB	1:A:411:ARG:HD2	2.08	0.77
1:C:128:TYR:HB3	1:C:137:PHE:CZ	2.20	0.77
2:D:414:ALA:O	2:D:418:ILE:HG12	1.84	0.77
1:C:308:VAL:HB	1:C:351:TYR:OH	1.84	0.76
1:C:167:VAL:HA	1:C:218:PHE:HZ	1.43	0.76
1:C:115:ARG:HD3	1:C:135:LEU:HD11	1.66	0.76
1:A:213:GLU:CD	1:A:235:LEU:CD2	2.59	0.76
1:C:213:GLU:CG	1:C:235:LEU:HD22	2.16	0.76
1:C:168:SER:N	1:C:218:PHE:CZ	2.50	0.76
1:A:27:VAL:O	1:A:61:GLN:N	2.15	0.76
1:A:28:ASN:CA	1:A:61:GLN:O	2.33	0.75
1:A:821:SER:O	1:A:823:SER:N	2.19	0.75
1:C:214:LYS:NZ	1:C:235:LEU:CD1	2.48	0.75
1:A:88:TYR:HH	1:A:90:ILE:HG22	1.46	0.75
1:A:219:ASP:CB	1:A:220:PRO:HD3	2.08	0.75
1:A:31:ALA:C	1:A:65:VAL:HG22	2.12	0.75
2:D:364:ILE:HG13	2:D:377:GLY:HA3	0.75	0.75
2:D:364:ILE:HD11	2:D:378:LYS:H	1.48	0.75
1:A:88:TYR:HE1	1:A:90:ILE:CB	1.99	0.75
1:C:128:TYR:O	1:C:137:PHE:HZ	1.70	0.75
1:C:213:GLU:OE2	1:C:235:LEU:HD22	1.87	0.75
1:C:88:TYR:HE1	1:C:90:ILE:CB	2.00	0.74
1:A:118:VAL:O	1:A:137:PHE:HA	1.85	0.74
2:B:418:ILE:N	2:B:458:LYS:O	2.18	0.74
2:B:320:SER:OG	2:B:322:TYR:CD2	2.41	0.74
2:B:364:ILE:HG13	2:B:377:GLY:HA3	0.74	0.74
1:C:68:LYS:HB2	1:C:69:PRO:CD	2.18	0.73
2:B:320:SER:HG	2:B:322:TYR:HD2	1.34	0.73
1:A:121:LEU:HD23	1:A:121:LEU:N	2.04	0.73
1:C:330:VAL:HG11	2:D:79:LYS:NZ	2.03	0.73
1:C:88:TYR:HH	1:C:90:ILE:HG22	1.50	0.73
1:A:91:LEU:CD1	1:A:137:PHE:HB2	2.19	0.73
1:A:108:SER:HB2	1:A:134:HIS:CD2	2.23	0.73
1:A:222:THR:HG23	1:A:223:LYS:HD3	1.70	0.73
1:A:68:LYS:HB2	1:A:69:PRO:CD	2.18	0.72
1:A:88:TYR:OH	1:A:90:ILE:HG21	1.85	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:GLU:OE2	1:A:416:SER:CB	2.36	0.72
1:A:214:LYS:HZ3	1:A:235:LEU:HD11	1.53	0.71
1:C:330:VAL:CG1	2:D:79:LYS:CE	2.67	0.71
2:B:416:PHE:CD1	2:B:461:CYS:SG	2.83	0.71
1:A:93:SER:HB2	1:A:122:THR:H	1.55	0.71
2:B:414:ALA:HB1	2:B:735:VAL:HG13	1.73	0.71
1:A:169:ASP:HB3	1:A:219:ASP:HB2	1.71	0.71
1:C:121:LEU:N	1:C:121:LEU:HD23	2.05	0.71
1:C:159:ASN:HB3	1:C:411:ARG:CD	2.17	0.71
1:C:88:TYR:CE1	1:C:90:ILE:HB	2.24	0.70
1:C:93:SER:HB2	1:C:122:THR:H	1.55	0.70
1:C:167:VAL:O	1:C:218:PHE:CE1	2.44	0.70
1:A:33:LEU:HD12	1:A:39:GLU:CD	2.17	0.70
1:C:137:PHE:HD1	1:C:137:PHE:H	1.39	0.70
2:B:459:GLY:O	2:B:795:LEU:HD21	1.92	0.69
2:D:279:SER:C	2:D:365:ILE:HG23	2.17	0.69
1:A:213:GLU:HG2	1:A:235:LEU:HD22	1.75	0.69
1:A:576:MET:HE1	1:A:840:LEU:HG	1.75	0.69
1:C:330:VAL:HG21	2:D:79:LYS:NZ	2.08	0.69
2:B:460:PHE:HE1	2:B:792:LEU:HB3	1.59	0.68
1:C:46:VAL:HG13	1:C:60:LEU:HB3	1.75	0.68
2:D:364:ILE:CD1	2:D:378:LYS:N	2.56	0.68
2:B:279:SER:C	2:B:365:ILE:HG23	2.18	0.68
1:C:586:LEU:HA	1:C:589:LEU:HD22	1.76	0.68
1:C:467:SER:H	1:C:468:PRO:HD3	1.52	0.68
1:A:214:LYS:NZ	1:A:235:LEU:CD1	2.48	0.68
2:D:432:ASN:ND2	2:D:456:CYS:CB	2.56	0.68
1:C:330:VAL:HG11	2:D:79:LYS:CE	2.24	0.68
1:A:128:TYR:C	1:A:137:PHE:HZ	1.99	0.67
1:A:330:VAL:HG13	2:B:79:LYS:HE3	1.76	0.67
1:A:86:GLN:O	1:A:325:PRO:CD	2.28	0.67
1:C:213:GLU:CD	1:C:235:LEU:CD2	2.62	0.67
1:A:72:ILE:H	1:A:72:ILE:HD12	1.59	0.67
1:A:88:TYR:CE1	1:A:90:ILE:HB	2.18	0.66
1:A:236:GLU:OE1	1:A:413:TYR:OH	2.13	0.66
1:A:586:LEU:HA	1:A:589:LEU:HD22	1.75	0.66
2:B:364:ILE:CD1	2:B:378:LYS:N	2.56	0.66
1:C:119:LEU:HA	1:C:138:LEU:HB2	1.78	0.66
2:D:320:SER:CB	2:D:322:TYR:CE2	2.78	0.66
2:B:158:LEU:O	2:B:162:GLU:HB2	1.96	0.66
1:C:72:ILE:HD12	1:C:72:ILE:H	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:158:LEU:O	2:D:162:GLU:HB2	1.96	0.66
1:C:576:MET:SD	1:C:840:LEU:HD12	2.36	0.66
2:D:366:LEU:HG	2:D:375:ARG:HA	1.78	0.66
1:C:576:MET:HE1	1:C:840:LEU:HG	1.75	0.65
2:B:366:LEU:HG	2:B:375:ARG:HA	1.78	0.65
1:A:576:MET:SD	1:A:840:LEU:HD12	2.36	0.65
1:A:93:SER:HB2	1:A:122:THR:N	2.11	0.65
1:C:330:VAL:HG11	2:D:79:LYS:HE3	1.78	0.65
1:A:213:GLU:OE2	1:A:235:LEU:HD21	1.95	0.65
2:B:329:ILE:O	2:B:333:ASN:ND2	2.30	0.65
1:A:31:ALA:CA	1:A:65:VAL:HG22	2.27	0.65
1:C:93:SER:HB2	1:C:122:THR:N	2.11	0.65
1:A:330:VAL:CG1	2:B:79:LYS:HE3	2.28	0.64
2:D:329:ILE:O	2:D:333:ASN:ND2	2.30	0.64
1:A:330:VAL:HG11	2:B:79:LYS:HZ1	1.62	0.64
1:A:546:GLN:O	2:D:774:ARG:NH2	2.29	0.64
1:C:350:LYS:O	1:C:350:LYS:HD3	1.98	0.64
2:D:364:ILE:HG12	2:D:377:GLY:O	1.98	0.63
1:A:285:ASP:HB3	1:A:379:ASN:HB2	1.80	0.63
1:C:128:TYR:O	1:C:137:PHE:CE1	2.52	0.63
1:C:88:TYR:OH	1:C:90:ILE:HG21	1.97	0.63
2:B:364:ILE:HG12	2:B:377:GLY:O	1.98	0.63
2:D:459:GLY:O	2:D:795:LEU:HD21	1.98	0.62
1:C:226:THR:HG22	1:C:255:ALA:HB1	1.81	0.62
1:C:601:LEU:HD11	2:D:832:SER:HB2	1.81	0.62
1:A:467:SER:H	1:A:468:PRO:HD3	1.59	0.62
2:B:280:VAL:HB	2:B:365:ILE:HG12	1.81	0.62
1:A:128:TYR:O	1:A:137:PHE:CE1	2.49	0.62
3:H:68:PHE:HB3	3:H:81:LEU:HD11	1.82	0.62
1:C:167:VAL:N	1:C:218:PHE:HZ	1.89	0.62
2:D:416:PHE:O	2:D:459:GLY:HA3	1.99	0.62
3:H:19:LYS:HE2	3:H:80:TYR:HB3	1.80	0.62
1:A:161:ASN:HB3	1:A:411:ARG:NH1	2.14	0.61
2:D:280:VAL:HB	2:D:365:ILE:HG12	1.81	0.61
1:C:308:VAL:CB	1:C:351:TYR:CZ	2.82	0.61
1:C:153:GLU:O	1:C:157:VAL:HG23	2.00	0.61
1:A:773:LEU:HD12	1:A:776:ARG:HE	1.65	0.61
1:A:241:ILE:HG23	1:A:270:VAL:HG21	1.81	0.61
2:D:186:ILE:O	2:D:190:ILE:HB	2.01	0.61
2:B:186:ILE:O	2:B:190:ILE:HB	2.01	0.61
1:C:68:LYS:HD2	1:C:73:GLN:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:ILE:HG23	1:C:270:VAL:HG21	1.81	0.61
2:B:429:CYS:HB3	2:B:432:ASN:ND2	2.15	0.61
2:D:34:SER:N	2:D:65:VAL:O	2.34	0.60
3:M:99:PRO:HA	3:M:109:PHE:HB3	1.83	0.60
2:B:34:SER:N	2:B:65:VAL:O	2.34	0.60
2:D:438:LYS:HB2	2:D:480:LEU:HD12	1.83	0.60
1:C:225:VAL:O	1:C:225:VAL:HG23	2.01	0.60
2:B:534:ILE:HG23	2:B:757:PHE:HB3	1.82	0.60
1:C:128:TYR:CB	1:C:137:PHE:HZ	2.13	0.60
1:A:68:LYS:HD2	1:A:73:GLN:HB2	1.81	0.60
1:C:442:LYS:NZ	1:C:443:GLU:O	2.34	0.60
3:H:51:ILE:HD12	3:H:72:ARG:HD2	1.82	0.60
3:H:52:SER:O	3:H:72:ARG:NH1	2.34	0.60
2:D:534:ILE:HG23	2:D:757:PHE:HB3	1.82	0.60
1:C:576:MET:SD	1:C:840:LEU:CD1	2.90	0.60
1:C:579:PHE:O	1:C:583:LEU:N	2.35	0.60
1:C:87:VAL:HG22	1:C:87:VAL:O	2.02	0.59
1:C:380:ARG:HG3	1:C:381:LYS:HG2	1.82	0.59
2:D:429:CYS:HB3	2:D:432:ASN:ND2	2.17	0.59
1:C:88:TYR:CE1	1:C:90:ILE:HG22	2.37	0.59
1:C:773:LEU:HD12	1:C:776:ARG:HE	1.65	0.59
2:B:364:ILE:CG1	2:B:378:LYS:N	2.66	0.59
2:D:83:THR:O	2:D:87:ASP:HB2	2.02	0.59
1:A:576:MET:SD	1:A:840:LEU:CD1	2.89	0.59
1:C:213:GLU:HG2	1:C:235:LEU:HD22	1.84	0.59
2:D:184:ASN:OD1	2:D:187:ARG:NH2	2.36	0.59
1:A:222:THR:HA	1:A:251:THR:HG21	1.85	0.59
2:B:83:THR:O	2:B:87:ASP:HB2	2.02	0.59
2:B:281:SER:OG	2:B:283:ASP:OD1	2.20	0.59
1:A:93:SER:OG	1:A:94:HIS:N	2.35	0.59
2:B:184:ASN:OD1	2:B:187:ARG:NH2	2.36	0.59
2:B:438:LYS:HB2	2:B:480:LEU:HD12	1.83	0.59
2:B:555:SER:HA	2:B:559:TRP:HB2	1.84	0.59
1:C:285:ASP:N	1:C:285:ASP:OD1	2.36	0.59
1:A:765:CYS:SG	1:A:819:CYS:SG	3.01	0.59
2:D:384:LEU:HD21	2:D:386:MET:HG2	1.85	0.59
1:C:72:ILE:HG21	2:D:321:CYS:O	2.03	0.58
2:D:181:ASP:N	2:D:181:ASP:OD1	2.37	0.58
2:D:364:ILE:CD1	2:D:377:GLY:HA3	2.30	0.58
1:C:283:ALA:HB1	1:C:287:ILE:HG13	1.86	0.58
2:D:555:SER:HA	2:D:559:TRP:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:109:PHE:O	4:N:36:TYR:OH	2.16	0.58
2:B:414:ALA:CB	2:B:735:VAL:CG1	2.82	0.58
1:A:253:TYR:HE1	1:A:284:PRO:HD3	1.68	0.58
1:A:410:PRO:O	1:A:411:ARG:C	2.47	0.58
2:B:366:LEU:HG	2:B:374:GLU:O	2.04	0.58
2:B:410:THR:OG1	2:B:411:LEU:N	2.37	0.58
1:C:462:ASP:OD1	1:C:464:SER:O	2.22	0.58
1:A:442:LYS:NZ	1:A:443:GLU:O	2.34	0.58
1:A:579:PHE:O	1:A:583:LEU:N	2.35	0.57
1:A:28:ASN:HD21	1:A:84:SER:HB2	1.70	0.57
1:C:253:TYR:HE1	1:C:284:PRO:HD3	1.68	0.57
2:D:366:LEU:HG	2:D:374:GLU:O	2.04	0.57
2:D:385:GLN:O	2:D:385:GLN:HG2	2.03	0.57
2:D:102:ASP:OD1	2:D:102:ASP:N	2.38	0.57
2:D:429:CYS:HB3	2:D:432:ASN:HD22	1.69	0.57
4:L:49:HIS:HB2	4:L:53:SER:HB2	1.86	0.57
1:A:124:ARG:HH21	1:A:144:TYR:HA	1.69	0.57
1:C:124:ARG:HH21	1:C:144:TYR:HA	1.70	0.57
2:D:281:SER:OG	2:D:282:TYR:N	2.36	0.57
1:C:236:GLU:OE2	1:C:416:SER:CB	2.53	0.57
2:D:229:LEU:HG	2:D:256:TRP:HB3	1.86	0.57
1:A:87:VAL:HG22	1:A:87:VAL:O	2.02	0.57
1:A:283:ALA:HB1	1:A:287:ILE:HG13	1.86	0.57
1:C:166:LEU:C	1:C:218:PHE:HE1	1.99	0.57
1:C:168:SER:CA	1:C:218:PHE:CD2	2.87	0.57
2:B:364:ILE:CD1	2:B:377:GLY:HA3	2.30	0.57
1:C:93:SER:OG	1:C:94:HIS:N	2.35	0.57
1:C:372:TYR:H	1:C:388:TYR:HB3	1.69	0.57
1:A:372:TYR:H	1:A:388:TYR:HB3	1.69	0.57
4:N:11:LEU:HB2	4:N:103:LEU:HA	1.87	0.57
1:A:159:ASN:HB3	1:A:411:ARG:HD3	1.81	0.57
1:A:216:LEU:HD13	1:A:228:LEU:HD22	1.86	0.57
2:B:429:CYS:HB3	2:B:432:ASN:HD22	1.70	0.57
1:C:222:THR:HA	1:C:251:THR:HG21	1.86	0.57
1:A:58:ILE:HG23	1:A:317:LEU:HD12	1.87	0.56
1:C:213:GLU:OE2	1:C:235:LEU:HD21	1.98	0.56
1:C:461:ASN:HB3	1:C:469:ARG:HD2	1.87	0.56
1:A:153:GLU:O	1:A:157:VAL:HG23	2.04	0.56
1:A:28:ASN:HB2	1:A:63:THR:HG23	1.87	0.56
2:B:539:SER:HA	2:B:721:LEU:HD21	1.87	0.56
1:C:576:MET:CE	1:C:840:LEU:HG	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:364:ILE:CG1	2:D:378:LYS:N	2.65	0.56
3:H:38:ARG:HD3	3:H:86:LEU:HD22	1.87	0.56
1:C:58:ILE:HG23	1:C:317:LEU:HD12	1.88	0.56
3:M:16:GLY:O	3:M:84:ASN:ND2	2.38	0.56
3:M:52:SER:O	3:M:72:ARG:NH1	2.38	0.56
2:B:281:SER:OG	2:B:282:TYR:N	2.36	0.56
2:D:281:SER:OG	2:D:283:ASP:OD1	2.20	0.56
2:B:229:LEU:HG	2:B:256:TRP:HB3	1.85	0.56
2:D:539:SER:HA	2:D:721:LEU:HD21	1.87	0.56
2:D:364:ILE:HG13	2:D:377:GLY:N	2.11	0.56
2:D:432:ASN:HD22	2:D:456:CYS:CB	2.09	0.56
4:L:11:LEU:HB2	4:L:103:LEU:HA	1.87	0.56
2:B:627:THR:HB	1:C:852:ILE:HG12	1.88	0.56
2:B:774:ARG:NH2	1:C:546:GLN:O	2.38	0.56
1:C:330:VAL:HG21	2:D:79:LYS:HZ1	1.69	0.56
4:N:50:TYR:HH	4:N:91:TYR:HH	1.50	0.56
4:N:49:HIS:HB2	4:N:53:SER:HB2	1.86	0.56
1:C:88:TYR:CE1	1:C:89:ALA:C	2.84	0.55
2:D:459:GLY:C	2:D:795:LEU:HD21	2.30	0.55
1:C:88:TYR:CE1	1:C:90:ILE:CG2	2.90	0.55
1:C:139:ARG:HB2	1:C:366:ASP:HA	1.89	0.55
1:C:438:ASP:N	1:C:438:ASP:OD1	2.37	0.55
3:H:50:TYR:HE1	4:L:95:TYR:HB2	1.71	0.55
1:A:552:LYS:NZ	2:D:526:SER:O	2.40	0.55
1:C:86:GLN:O	1:C:325:PRO:CD	2.31	0.55
1:C:308:VAL:HA	1:C:351:TYR:CE1	2.42	0.55
1:C:576:MET:CE	1:C:840:LEU:CG	2.65	0.55
3:M:68:PHE:HB3	3:M:81:LEU:HD11	1.88	0.55
1:C:634:VAL:O	2:D:616:ASN:ND2	2.35	0.55
1:A:115:ARG:NE	1:A:135:LEU:HD11	2.21	0.55
1:A:576:MET:CE	1:A:840:LEU:HG	2.34	0.55
1:A:28:ASN:HA	1:A:61:GLN:C	2.29	0.55
1:A:88:TYR:CE1	1:A:90:ILE:HG22	2.42	0.55
2:B:102:ASP:OD1	2:B:102:ASP:N	2.38	0.55
1:C:168:SER:CB	1:C:218:PHE:O	2.55	0.55
1:C:219:ASP:CB	1:C:220:PRO:CD	2.59	0.55
1:A:506:GLY:O	1:A:544:ARG:NH1	2.39	0.55
1:C:519:TRP:NE1	1:C:547:TYR:OH	2.40	0.55
2:D:305:SER:OG	2:D:313:PHE:O	2.18	0.55
2:B:181:ASP:N	2:B:181:ASP:OD1	2.37	0.54
2:B:526:SER:OG	2:B:527:VAL:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:VAL:O	1:C:218:PHE:CD1	2.59	0.54
2:D:535:SER:OG	2:D:536:VAL:N	2.40	0.54
1:C:510:ARG:NH1	1:C:514:SER:O	2.39	0.54
2:D:119:THR:HA	2:D:318:LYS:HZ1	1.73	0.54
2:B:305:SER:OG	2:B:313:PHE:O	2.18	0.54
1:A:285:ASP:OD1	1:A:285:ASP:N	2.36	0.54
1:A:170:ASP:HB3	1:A:172:GLU:HG3	1.90	0.54
1:A:519:TRP:NE1	1:A:547:TYR:OH	2.40	0.54
2:D:38:ALA:HB3	2:D:97:VAL:HA	1.90	0.54
2:D:164:TYR:OH	2:D:386:MET:HG3	2.07	0.54
1:A:32:VAL:H	1:A:92:VAL:HG21	1.73	0.54
2:D:526:SER:OG	2:D:527:VAL:N	2.40	0.54
3:M:4:LEU:HB2	3:M:113:GLY:HA2	1.88	0.54
1:A:33:LEU:CD1	1:A:39:GLU:OE2	2.30	0.54
1:A:88:TYR:CE1	1:A:90:ILE:CG2	2.91	0.54
2:B:682:ARG:NH2	2:B:724:GLY:O	2.41	0.54
1:A:88:TYR:CE1	1:A:90:ILE:CB	2.86	0.54
2:B:437:GLN:NE2	2:B:452:TYR:O	2.35	0.54
1:C:157:VAL:HG22	1:C:392:HIS:CE1	2.43	0.54
2:D:133:ILE:HG22	2:D:134:MET:HG2	1.90	0.54
2:B:442:SER:OG	2:B:443:GLU:N	2.41	0.54
1:A:396:ASN:N	1:A:396:ASN:OD1	2.41	0.54
2:B:133:ILE:HG22	2:B:134:MET:HG2	1.90	0.53
2:B:160:ILE:HG21	2:B:365:ILE:HD11	1.88	0.53
2:B:364:ILE:HG13	2:B:377:GLY:N	2.11	0.53
1:C:168:SER:HB3	1:C:218:PHE:CD2	2.43	0.53
1:A:157:VAL:HG22	1:A:392:HIS:CE1	2.42	0.53
1:C:41:MET:SD	1:C:299:SER:OG	2.66	0.53
2:D:160:ILE:HG21	2:D:365:ILE:HD11	1.88	0.53
1:A:680:ARG:HH22	1:A:826:PRO:HB3	1.73	0.53
2:B:526:SER:O	1:C:552:LYS:NZ	2.42	0.53
1:C:680:ARG:HH22	1:C:826:PRO:HB3	1.73	0.53
2:D:682:ARG:NH2	2:D:724:GLY:O	2.41	0.53
1:A:128:TYR:HB3	1:A:137:PHE:CZ	2.43	0.53
1:C:111:ALA:HA	1:C:116:ILE:HD12	1.90	0.53
1:C:114:TYR:OH	2:D:77:ASP:OD1	2.24	0.53
2:D:39:VAL:HG21	2:D:70:LEU:HA	1.91	0.53
2:B:535:SER:OG	2:B:536:VAL:N	2.41	0.53
3:H:33:THR:OG1	3:H:34:MET:N	2.42	0.53
1:C:380:ARG:O	1:C:381:LYS:CB	2.55	0.53
2:D:442:SER:OG	2:D:443:GLU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ALA:HA	1:A:116:ILE:HD12	1.90	0.52
1:C:506:GLY:O	1:C:544:ARG:NH1	2.39	0.52
1:A:820:ASP:O	1:A:822:ARG:N	2.42	0.52
1:C:73:GLN:O	1:C:76:LEU:HB2	2.10	0.52
1:C:692:ARG:HH21	2:D:800:ILE:HG21	1.74	0.52
2:B:38:ALA:HB3	2:B:97:VAL:HA	1.90	0.52
2:B:430:MET:O	2:B:433:THR:CG2	2.57	0.52
1:A:41:MET:SD	1:A:299:SER:OG	2.66	0.52
2:B:432:ASN:HD22	2:B:456:CYS:HB3	1.72	0.52
1:C:84:SER:HA	1:C:327:ARG:NH1	2.24	0.52
1:C:170:ASP:HB3	1:C:172:GLU:HG3	1.90	0.52
1:C:380:ARG:O	1:C:381:LYS:HB3	2.09	0.52
1:A:33:LEU:N	1:A:65:VAL:HG13	2.25	0.52
1:A:315:GLU:O	1:A:319:LYS:NZ	2.43	0.52
1:C:236:GLU:OE2	1:C:416:SER:HB3	2.10	0.52
1:C:725:ARG:HH12	1:C:729:LYS:HE3	1.74	0.52
2:D:366:LEU:HG	2:D:374:GLU:C	2.34	0.52
1:A:576:MET:CE	1:A:840:LEU:CG	2.65	0.52
3:M:93:MET:HA	3:M:117:THR:HA	1.90	0.52
2:D:322:TYR:CD1	2:D:323:ASN:HB2	2.45	0.52
2:D:703:HIS:HA	2:D:706:MET:HB2	1.92	0.52
1:C:315:GLU:O	1:C:319:LYS:NZ	2.43	0.52
2:B:460:PHE:CE1	2:B:792:LEU:HB3	2.44	0.52
1:C:396:ASN:N	1:C:396:ASN:OD1	2.41	0.52
4:L:4:MET:HB2	4:L:96:THR:HG22	1.92	0.52
2:B:414:ALA:CB	2:B:415:PRO:HD2	2.26	0.51
1:C:169:ASP:OD1	1:C:174:ARG:NH1	2.43	0.51
4:N:4:MET:HB2	4:N:96:THR:HG22	1.92	0.51
1:A:115:ARG:CD	1:A:135:LEU:HD12	2.21	0.51
1:A:169:ASP:OD1	1:A:174:ARG:NH1	2.43	0.51
1:C:777:SER:OG	1:C:778:GLY:N	2.43	0.51
4:N:48:ILE:HG23	4:N:52:SER:HA	1.92	0.51
1:A:73:GLN:O	1:A:76:LEU:HB2	2.09	0.51
2:B:366:LEU:HG	2:B:374:GLU:C	2.35	0.51
1:C:166:LEU:C	1:C:218:PHE:HZ	2.12	0.51
2:B:653:PHE:HA	1:C:827:ALA:HB1	1.92	0.51
4:L:48:ILE:HG23	4:L:52:SER:HA	1.92	0.51
2:B:39:VAL:HG21	2:B:70:LEU:HA	1.91	0.51
2:B:350:SER:OG	2:B:358:MET:SD	2.66	0.51
2:B:703:HIS:HA	2:B:706:MET:HB2	1.92	0.51
1:C:168:SER:HA	1:C:218:PHE:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:279:SER:N	2:D:365:ILE:CG2	2.74	0.51
1:A:84:SER:HA	1:A:327:ARG:NH1	2.26	0.50
2:B:95:GLN:O	2:B:121:THR:OG1	2.29	0.50
2:D:437:GLN:NE2	2:D:452:TYR:O	2.35	0.50
1:A:725:ARG:HH12	1:A:729:LYS:HE3	1.75	0.50
1:C:85:SER:HA	1:C:88:TYR:HD2	1.76	0.50
1:C:169:ASP:HB3	1:C:219:ASP:HB2	1.94	0.50
1:A:88:TYR:CZ	1:A:90:ILE:CG2	2.82	0.50
1:A:214:LYS:HZ1	1:A:235:LEU:HD11	1.68	0.50
2:B:430:MET:O	2:B:433:THR:HG22	2.11	0.50
1:C:28:ASN:ND2	1:C:84:SER:HB2	2.27	0.50
1:C:584:TRP:HB3	1:C:586:LEU:H	1.77	0.50
2:D:95:GLN:O	2:D:121:THR:OG1	2.29	0.50
2:D:414:ALA:O	2:D:418:ILE:CG1	2.57	0.50
3:M:38:ARG:HD3	3:M:86:LEU:HD22	1.94	0.50
2:B:415:PRO:HG3	2:B:738:TYR:CD2	2.46	0.50
2:B:428:THR:OG1	2:B:429:CYS:N	2.45	0.50
2:B:432:ASN:ND2	2:B:456:CYS:CB	2.69	0.50
2:D:41:LEU:HB3	2:D:73:MET:H	1.77	0.50
4:N:29:ILE:HG12	4:N:69:ARG:HA	1.94	0.50
1:A:136:SER:HB3	1:A:343:LYS:HD2	1.93	0.50
1:A:284:PRO:HD2	1:A:287:ILE:HD11	1.94	0.50
2:D:419:VAL:HG22	2:D:457:CYS:SG	2.51	0.50
1:A:584:TRP:HB3	1:A:586:LEU:H	1.77	0.50
1:A:601:LEU:HD11	2:B:832:SER:HB2	1.94	0.50
2:B:65:VAL:HG11	3:M:105:SER:HA	1.94	0.50
1:C:88:TYR:CD1	1:C:88:TYR:C	2.90	0.50
2:D:497:MET:HE3	2:D:509:ALA:HB1	1.92	0.50
1:A:777:SER:OG	1:A:778:GLY:N	2.43	0.49
2:B:279:SER:N	2:B:365:ILE:CG2	2.75	0.49
2:B:509:ALA:HB3	2:B:765:ALA:HB3	1.95	0.49
2:B:810:SER:O	2:B:812:GLN:NE2	2.45	0.49
2:D:244:ALA:HB1	2:D:249:LEU:HB2	1.94	0.49
2:D:428:THR:OG1	2:D:429:CYS:N	2.45	0.49
2:D:810:SER:O	2:D:812:GLN:NE2	2.45	0.49
1:A:85:SER:HA	1:A:88:TYR:HD2	1.76	0.49
1:A:88:TYR:CE1	1:A:89:ALA:C	2.91	0.49
1:A:411:ARG:HA	1:A:411:ARG:NE	2.27	0.49
1:A:236:GLU:OE2	1:A:416:SER:HB2	2.12	0.49
2:B:97:VAL:HB	2:B:123:ILE:HG12	1.94	0.49
1:C:284:PRO:HD2	1:C:287:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:29:ILE:HG12	4:L:69:ARG:HA	1.94	0.49
2:B:289:LEU:HB2	2:B:292:ARG:HG2	1.93	0.49
1:C:120:GLY:C	1:C:121:LEU:HD23	2.38	0.49
2:D:357:GLN:HB2	2:D:360:PRO:HB3	1.94	0.49
2:D:366:LEU:CG	2:D:375:ARG:HA	2.42	0.49
2:B:357:GLN:HB2	2:B:360:PRO:HB3	1.94	0.49
2:D:277:LEU:O	2:D:372:LYS:NZ	2.45	0.49
2:B:41:LEU:HB3	2:B:73:MET:H	1.77	0.49
2:B:366:LEU:CG	2:B:375:ARG:HA	2.42	0.49
1:C:544:ARG:NH2	1:C:709:SER:OG	2.45	0.49
2:B:244:ALA:HB1	2:B:249:LEU:HB2	1.94	0.49
1:C:114:TYR:CZ	1:C:332:ASN:HB3	2.48	0.49
1:C:133:ILE:HD13	1:C:133:ILE:N	2.26	0.49
1:C:226:THR:HG22	1:C:255:ALA:CB	2.43	0.49
2:B:408:ILE:HG23	2:B:510:VAL:HG22	1.95	0.49
2:D:97:VAL:HB	2:D:123:ILE:HG12	1.94	0.49
2:D:126:ILE:H	2:D:131:SER:HB2	1.77	0.49
2:D:174:THR:H	2:D:230:LEU:HD13	1.77	0.49
2:D:289:LEU:HB2	2:D:292:ARG:HG2	1.93	0.49
1:A:70:ASN:HB3	1:A:73:GLN:HG2	1.95	0.48
1:A:572:LEU:HD11	1:A:830:THR:HG22	1.95	0.48
2:D:86:CYS:HA	2:D:89:MET:HB2	1.95	0.48
2:D:156:VAL:HG21	2:D:362:LEU:HD21	1.95	0.48
2:D:464:ILE:HG13	2:D:529:PHE:HZ	1.79	0.48
3:M:11:LEU:HG	3:M:118:VAL:HB	1.95	0.48
3:M:32:TYR:O	3:M:72:ARG:NH2	2.47	0.48
1:A:378:GLN:OE1	1:A:380:ARG:NH2	2.46	0.48
1:A:544:ARG:NH2	1:A:709:SER:OG	2.45	0.48
1:C:32:VAL:O	1:C:32:VAL:HG12	2.13	0.48
3:M:29:PHE:HA	3:M:32:TYR:HB2	1.94	0.48
1:A:120:GLY:C	1:A:121:LEU:HD23	2.37	0.48
2:B:86:CYS:HA	2:B:89:MET:HB2	1.96	0.48
2:B:464:ILE:HG13	2:B:529:PHE:HZ	1.79	0.48
2:D:350:SER:OG	2:D:358:MET:SD	2.66	0.48
2:B:174:THR:H	2:B:230:LEU:HD13	1.77	0.48
1:C:88:TYR:HD1	1:C:89:ALA:H	1.62	0.48
1:C:129:SER:O	1:C:129:SER:OG	2.28	0.48
1:C:375:MET:HB3	1:C:382:LEU:HG	1.96	0.48
1:C:572:LEU:HD11	1:C:830:THR:HG22	1.95	0.48
3:H:24:ALA:HB3	3:H:77:ASN:HB3	1.96	0.48
4:N:6:GLN:HB2	4:N:100:GLY:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:ILE:HG23	2:B:243:VAL:HG11	1.95	0.48
1:C:350:LYS:HD3	1:C:350:LYS:C	2.39	0.48
1:C:362:ASN:OD1	1:C:366:ASP:N	2.42	0.48
1:A:93:SER:HB2	1:A:122:THR:CB	2.43	0.48
1:A:114:TYR:CZ	1:A:332:ASN:HB3	2.48	0.48
2:B:277:LEU:O	2:B:372:LYS:NZ	2.45	0.48
2:D:216:ILE:HG23	2:D:243:VAL:HG11	1.95	0.48
3:H:67:ARG:HH21	3:H:84:ASN:HD21	1.61	0.48
1:A:31:ALA:CB	1:A:65:VAL:HG23	2.02	0.48
1:A:377:LEU:HG	1:A:379:ASN:H	1.76	0.48
1:A:441:CYS:SG	1:A:442:LYS:N	2.87	0.48
3:M:50:TYR:CE1	4:N:95:TYR:HB2	2.49	0.48
1:A:457:CYS:HA	1:A:497:VAL:HG23	1.96	0.47
1:A:692:ARG:HH21	2:B:800:ILE:HG21	1.78	0.47
2:B:415:PRO:CG	2:B:738:TYR:CD2	2.97	0.47
2:D:159:ASN:HA	2:D:162:GLU:HB3	1.96	0.47
2:D:362:LEU:HB3	2:D:379:TRP:HB3	1.96	0.47
1:C:457:CYS:HA	1:C:497:VAL:HG23	1.96	0.47
4:L:90:GLN:HB2	4:L:96:THR:HB	1.96	0.47
1:A:28:ASN:C	1:A:61:GLN:O	2.58	0.47
1:C:70:ASN:HB3	1:C:73:GLN:HG2	1.95	0.47
1:C:93:SER:HB2	1:C:122:THR:CB	2.43	0.47
1:A:91:LEU:HD23	1:A:91:LEU:HA	1.82	0.47
1:A:119:LEU:HA	1:A:138:LEU:HD12	1.97	0.47
1:A:362:ASN:OD1	1:A:366:ASP:N	2.42	0.47
1:C:88:TYR:CD1	1:C:89:ALA:C	2.92	0.47
3:M:24:ALA:HB3	3:M:77:ASN:HB3	1.96	0.47
1:A:226:THR:HG22	1:A:255:ALA:HB1	1.96	0.47
2:B:126:ILE:H	2:B:131:SER:HB2	1.77	0.47
2:B:216:ILE:HD11	2:B:240:ILE:HG23	1.97	0.47
2:D:459:GLY:O	2:D:795:LEU:CD2	2.60	0.47
1:A:378:GLN:HA	1:A:401:ILE:HD11	1.96	0.47
2:D:430:MET:O	2:D:433:THR:CG2	2.63	0.47
1:A:68:LYS:CB	1:A:69:PRO:CD	2.86	0.47
1:A:461:ASN:HB3	1:A:469:ARG:HD2	1.97	0.47
1:C:39:GLU:HA	1:C:42:PHE:CD2	2.50	0.47
2:D:170:SER:OG	2:D:171:ILE:N	2.48	0.47
2:D:171:ILE:HG22	2:D:202:VAL:HG22	1.96	0.47
2:D:382:LYS:HA	2:D:382:LYS:HD2	1.57	0.47
2:D:507:TYR:O	2:D:767:GLN:NE2	2.48	0.47
1:A:139:ARG:HB2	1:A:366:ASP:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:LEU:N	1:C:241:ILE:O	2.48	0.47
2:D:509:ALA:HB3	2:D:765:ALA:HB3	1.96	0.47
1:A:39:GLU:HA	1:A:42:PHE:CD2	2.50	0.47
1:A:266:TYR:HE1	1:A:268:TRP:HB2	1.80	0.47
1:A:375:MET:HB3	1:A:382:LEU:HG	1.96	0.47
2:B:170:SER:OG	2:B:171:ILE:N	2.48	0.47
2:B:408:ILE:CG2	2:B:510:VAL:HG22	2.44	0.47
2:B:497:MET:HE3	2:B:509:ALA:HB1	1.97	0.47
4:N:90:GLN:HB2	4:N:96:THR:HB	1.96	0.47
2:B:119:THR:HA	2:B:318:LYS:HZ1	1.80	0.46
1:C:121:LEU:N	1:C:121:LEU:CD2	2.75	0.46
2:B:156:VAL:HG21	2:B:362:LEU:HD21	1.95	0.46
1:C:222:THR:HG23	1:C:223:LYS:HD3	1.97	0.46
3:H:109:PHE:O	4:L:36:TYR:OH	2.26	0.46
1:A:238:ARG:HE	1:A:266:TYR:HB2	1.81	0.46
2:B:362:LEU:HB3	2:B:379:TRP:HB3	1.96	0.46
2:B:419:VAL:HG22	2:B:457:CYS:SG	2.55	0.46
1:A:576:MET:HE2	1:A:837:VAL:HA	1.98	0.46
2:B:507:TYR:O	2:B:767:GLN:NE2	2.48	0.46
2:D:216:ILE:HD11	2:D:240:ILE:HG23	1.97	0.46
2:D:410:THR:OG1	2:D:411:LEU:N	2.37	0.46
1:A:87:VAL:O	1:A:87:VAL:HG13	2.16	0.46
1:A:236:GLU:CD	1:A:413:TYR:HH	2.23	0.46
2:B:420:GLU:HG2	2:B:456:CYS:HB2	1.96	0.46
2:B:641:ILE:HG12	1:C:576:MET:HB3	1.98	0.46
1:C:266:TYR:HE1	1:C:268:TRP:HB2	1.80	0.46
2:B:171:ILE:HG22	2:B:202:VAL:HG22	1.96	0.46
2:B:465:LEU:HA	2:B:468:ILE:HG22	1.98	0.46
1:C:32:VAL:H	1:C:92:VAL:HG21	1.80	0.46
1:C:88:TYR:CE1	1:C:90:ILE:CB	2.88	0.46
4:L:6:GLN:HB2	4:L:100:GLY:H	1.79	0.46
2:B:159:ASN:HA	2:B:162:GLU:HB3	1.96	0.46
2:B:167:TYR:CE2	2:B:198:GLU:HB3	2.51	0.46
2:B:408:ILE:CG2	2:B:510:VAL:CG2	2.94	0.46
1:C:145:SER:HB2	1:C:176:ALA:HB2	1.98	0.46
2:D:279:SER:H	2:D:365:ILE:CG2	2.28	0.46
1:A:166:LEU:N	1:A:241:ILE:O	2.48	0.46
1:C:238:ARG:HE	1:C:266:TYR:HB2	1.81	0.46
1:C:576:MET:HE2	1:C:837:VAL:HA	1.98	0.46
1:C:31:ALA:HB3	1:C:65:VAL:HG22	1.98	0.45
1:A:124:ARG:HH22	1:A:147:GLN:HE21	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:LYS:HB2	2:B:369:LYS:HE3	1.70	0.45
1:C:39:GLU:H	1:C:39:GLU:HG3	1.65	0.45
1:C:68:LYS:CB	1:C:69:PRO:CD	2.86	0.45
2:D:683:PHE:HB2	2:D:706:MET:HG2	1.98	0.45
3:H:32:TYR:O	3:H:72:ARG:NH2	2.49	0.45
2:B:230:LEU:HD23	2:B:230:LEU:H	1.82	0.45
2:D:386:MET:HB3	2:D:388:TYR:O	2.15	0.45
1:A:421:ILE:HB	1:A:497:VAL:HG12	1.97	0.45
1:C:421:ILE:HB	1:C:497:VAL:HG12	1.97	0.45
2:D:230:LEU:HD23	2:D:230:LEU:H	1.82	0.45
1:A:711:ASP:O	1:A:715:ARG:HB2	2.17	0.45
1:A:802:GLU:OE1	2:D:694:ASN:ND2	2.47	0.45
2:B:216:ILE:O	2:B:220:LEU:HG	2.17	0.45
2:D:167:TYR:CE2	2:D:198:GLU:HB3	2.51	0.45
2:D:413:GLU:HB3	2:D:414:ALA:H	1.49	0.45
1:A:145:SER:HB2	1:A:176:ALA:HB2	1.98	0.45
2:B:279:SER:H	2:B:365:ILE:CG2	2.29	0.45
2:D:432:ASN:OD1	2:D:458:LYS:HG2	2.17	0.45
2:B:382:LYS:HA	2:B:382:LYS:HD2	1.49	0.45
1:C:43:ARG:HH21	1:C:44:GLU:HG3	1.82	0.45
1:C:88:TYR:CZ	1:C:90:ILE:CG2	2.86	0.45
2:D:465:LEU:HA	2:D:468:ILE:HG22	1.98	0.45
2:D:142:MET:HE2	2:D:142:MET:HB2	1.88	0.45
2:B:286:ASP:HB3	2:B:287:TYR:H	1.68	0.44
1:C:87:VAL:O	1:C:87:VAL:HG13	2.18	0.44
1:C:124:ARG:HH22	1:C:147:GLN:HE21	1.64	0.44
1:C:359:VAL:HG22	1:C:367:ARG:HD3	1.99	0.44
3:M:33:THR:OG1	3:M:51:ILE:O	2.35	0.44
1:C:155:MET:HG2	1:C:160:TRP:HA	1.99	0.44
1:A:129:SER:O	1:A:129:SER:OG	2.28	0.44
1:A:277:GLY:C	1:A:279:ALA:N	2.74	0.44
1:A:516:LYS:HA	1:A:516:LYS:HD3	1.73	0.44
2:B:279:SER:H	2:B:365:ILE:HG22	1.83	0.44
1:C:134:HIS:HB2	1:C:135:LEU:H	1.51	0.44
1:C:433:LYS:HA	1:C:433:LYS:HD3	1.83	0.44
2:D:279:SER:H	2:D:365:ILE:HG22	1.82	0.44
1:A:161:ASN:HB2	1:A:239:VAL:HG21	2.00	0.44
1:A:838:PHE:HD2	2:D:565:MET:HE3	1.83	0.44
1:C:33:LEU:HB2	1:C:65:VAL:HG12	2.00	0.44
1:A:43:ARG:HH21	1:A:44:GLU:HG3	1.82	0.44
1:C:63:THR:HB	1:C:64:SER:H	1.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ARG:HE	1:A:411:ARG:CA	2.30	0.44
2:B:459:GLY:O	2:B:795:LEU:CD2	2.63	0.44
2:B:683:PHE:HB2	2:B:706:MET:HG2	1.99	0.44
1:C:218:PHE:HE2	1:C:244:ALA:HB2	1.83	0.44
1:C:770:THR:O	1:C:770:THR:OG1	2.35	0.44
2:D:673:ARG:HA	2:D:674:PRO:HD3	1.90	0.44
1:A:770:THR:O	1:A:770:THR:OG1	2.35	0.44
2:D:216:ILE:O	2:D:220:LEU:HG	2.17	0.44
1:A:277:GLY:O	1:A:279:ALA:N	2.50	0.44
2:B:158:LEU:O	2:B:162:GLU:CB	2.65	0.44
2:D:86:CYS:HB2	2:D:321:CYS:HB3	1.62	0.44
2:D:407:SER:HA	2:D:477:ASP:HB2	2.00	0.44
2:B:88:LEU:HD23	2:B:94:ILE:HG13	2.00	0.44
1:A:118:VAL:C	1:A:137:PHE:HA	2.43	0.43
1:A:128:TYR:HB3	1:A:137:PHE:HZ	1.83	0.43
1:A:306:VAL:HA	1:A:309:VAL:HG12	2.00	0.43
1:C:167:VAL:C	1:C:218:PHE:CE2	2.75	0.43
1:C:216:LEU:HD13	1:C:228:LEU:HD22	2.00	0.43
2:D:654:MET:HE2	2:D:654:MET:HB3	1.67	0.43
2:B:151:GLU:HG2	2:B:185:LYS:HG2	2.01	0.43
2:B:805:LYS:HB2	2:B:805:LYS:HE3	1.79	0.43
1:C:161:ASN:HB2	1:C:239:VAL:HG21	2.00	0.43
1:C:306:VAL:HA	1:C:309:VAL:HG12	2.01	0.43
1:C:317:LEU:HD23	1:C:317:LEU:HA	1.89	0.43
1:C:392:HIS:O	1:C:392:HIS:CG	2.70	0.43
1:A:121:LEU:N	1:A:121:LEU:CD2	2.74	0.43
1:A:359:VAL:HG22	1:A:367:ARG:HD3	1.99	0.43
1:A:678:LEU:HD23	1:A:678:LEU:HA	1.90	0.43
2:B:234:LYS:NZ	2:B:268:THR:O	2.46	0.43
2:D:430:MET:O	2:D:433:THR:HG22	2.18	0.43
3:H:20:LEU:HD21	3:H:83:MET:HE3	1.99	0.43
1:A:829:LEU:HD13	1:A:831:CYS:SG	2.58	0.43
2:B:322:TYR:CE1	2:B:323:ASN:HB2	2.53	0.43
2:B:481:VAL:HG21	2:B:497:MET:HG3	2.00	0.43
3:H:11:LEU:HD12	3:H:11:LEU:HA	1.90	0.43
3:H:53:ASN:O	3:H:74:ASN:ND2	2.52	0.43
3:H:97:ALA:HA	3:H:112:TRP:HA	1.99	0.43
2:B:86:CYS:HB2	2:B:321:CYS:HB3	1.61	0.43
2:B:404:ASP:OD1	2:B:404:ASP:N	2.50	0.43
2:D:431:ARG:HD2	2:D:431:ARG:HA	1.54	0.43
2:B:55:GLU:O	3:M:103:GLY:HA2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ARG:HA	1:C:52:ARG:HD3	1.78	0.43
1:C:124:ARG:HE	1:C:124:ARG:HB3	1.60	0.43
2:D:267:ASP:OD1	2:D:267:ASP:N	2.52	0.43
1:A:236:GLU:HB3	1:A:413:TYR:HE1	1.82	0.43
2:B:394:MET:HE3	2:B:394:MET:HB2	1.93	0.43
2:D:234:LYS:NZ	2:D:268:THR:O	2.46	0.43
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.84	0.43
2:B:493:THR:OG1	2:B:494:TRP:N	2.52	0.43
1:C:33:LEU:HD12	1:C:39:GLU:OE2	2.19	0.43
1:C:809:LEU:HD12	1:C:809:LEU:HA	1.92	0.43
1:A:351:TYR:HE2	1:A:361:PHE:HE2	1.67	0.43
1:A:763:GLN:HB2	1:A:817:GLN:NE2	2.34	0.43
2:B:190:ILE:HD12	2:B:190:ILE:HA	1.86	0.43
1:C:140:THR:O	1:C:367:ARG:NE	2.46	0.43
1:C:168:SER:CA	1:C:218:PHE:CE2	3.02	0.43
1:C:829:LEU:HD13	1:C:831:CYS:SG	2.58	0.43
2:D:157:MET:HE3	2:D:157:MET:HB3	1.97	0.43
2:D:404:ASP:OD1	2:D:404:ASP:N	2.50	0.43
1:C:46:VAL:HG13	1:C:60:LEU:CB	2.47	0.42
2:D:67:ARG:NH1	4:L:32:TYR:OH	2.50	0.42
2:D:88:LEU:HD23	2:D:94:ILE:HG13	2.00	0.42
2:D:158:LEU:O	2:D:162:GLU:CB	2.65	0.42
2:D:493:THR:OG1	2:D:494:TRP:N	2.52	0.42
3:H:33:THR:OG1	3:H:51:ILE:O	2.35	0.42
1:C:415:MET:HE1	1:C:788:PRO:HG3	2.02	0.42
2:D:362:LEU:HD23	2:D:379:TRP:CG	2.54	0.42
4:L:38:HIS:HB3	4:L:44:PRO:HA	2.01	0.42
1:A:159:ASN:O	1:A:411:ARG:NH1	2.52	0.42
1:A:411:ARG:NE	1:A:411:ARG:CA	2.82	0.42
1:A:556:TYR:HB3	2:D:531:GLU:HG2	2.00	0.42
1:A:809:LEU:HD12	1:A:809:LEU:HA	1.93	0.42
2:B:362:LEU:HD23	2:B:379:TRP:CG	2.55	0.42
2:B:483:ASN:HD21	2:B:496:GLY:H	1.67	0.42
2:B:715:ASP:HA	2:B:718:LEU:HD12	2.02	0.42
1:C:269:LEU:HD23	1:C:274:GLU:HG2	2.01	0.42
2:D:151:GLU:HG2	2:D:185:LYS:HG2	2.01	0.42
2:D:408:ILE:HG12	2:D:508:MET:HB2	2.01	0.42
1:A:266:TYR:HA	1:A:402:TRP:HZ2	1.83	0.42
1:C:137:PHE:CD1	1:C:137:PHE:N	2.73	0.42
1:C:523:MET:HE1	1:C:544:ARG:HA	2.02	0.42
4:L:46:LEU:HD21	4:L:49:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:38:HIS:HB3	4:N:44:PRO:HA	2.01	0.42
2:B:361:LYS:HA	2:B:361:LYS:HD3	1.88	0.42
2:B:407:SER:HA	2:B:477:ASP:HB2	2.00	0.42
2:B:601:THR:O	2:B:601:THR:HG22	2.20	0.42
1:C:266:TYR:HA	1:C:402:TRP:HZ2	1.83	0.42
1:C:651:ARG:O	1:C:655:MET:HG2	2.20	0.42
2:D:481:VAL:HG21	2:D:497:MET:HG3	2.00	0.42
3:H:3:LYS:HD3	3:H:3:LYS:HA	1.87	0.42
1:C:79:CYS:HA	1:C:82:LEU:HB2	2.02	0.42
1:C:168:SER:HB3	1:C:218:PHE:O	2.19	0.42
1:C:330:VAL:CG1	2:D:79:LYS:HZ1	2.22	0.42
3:M:20:LEU:HD21	3:M:83:MET:HE3	2.02	0.42
1:A:277:GLY:C	1:A:279:ALA:H	2.28	0.42
1:A:651:ARG:O	1:A:655:MET:HG2	2.20	0.42
1:C:224:ASN:ND2	1:C:224:ASN:O	2.53	0.42
1:C:330:VAL:HG13	2:D:79:LYS:HB3	2.00	0.42
1:A:438:ASP:OD1	1:A:438:ASP:N	2.45	0.42
1:A:523:MET:HE1	1:A:544:ARG:HA	2.02	0.42
2:B:307:MET:HE2	2:B:307:MET:HB3	1.88	0.42
1:C:108:SER:O	1:C:134:HIS:ND1	2.53	0.42
4:L:47:LEU:HB3	4:L:48:ILE:HG12	2.02	0.42
1:A:108:SER:OG	1:A:134:HIS:NE2	2.40	0.42
1:A:238:ARG:NH1	1:A:411:ARG:O	2.53	0.42
1:C:267:VAL:HG12	1:C:269:LEU:HD11	2.02	0.42
1:A:180:LEU:HD12	1:A:180:LEU:HA	1.89	0.42
1:A:236:GLU:HB3	1:A:413:TYR:CE1	2.55	0.42
2:B:285:TRP:HB3	2:B:289:LEU:HD11	2.02	0.42
1:C:141:VAL:O	1:C:141:VAL:HG23	2.19	0.42
1:C:162:HIS:CE1	1:C:237:ALA:HA	2.55	0.42
4:N:47:LEU:HB3	4:N:48:ILE:HG12	2.02	0.42
1:A:82:LEU:HA	1:A:85:SER:HB3	2.02	0.41
1:A:382:LEU:HD12	1:A:382:LEU:HA	1.94	0.41
2:B:421:SER:OG	2:B:422:VAL:N	2.53	0.41
2:B:662:GLN:O	2:B:670:LYS:HE2	2.20	0.41
2:D:421:SER:OG	2:D:422:VAL:N	2.53	0.41
2:D:602:ILE:O	2:D:602:ILE:HG13	2.18	0.41
4:N:46:LEU:HD21	4:N:49:HIS:CE1	2.54	0.41
1:A:33:LEU:N	1:A:65:VAL:CG1	2.84	0.41
1:A:65:VAL:CG1	1:A:66:THR:N	2.82	0.41
2:D:50:ILE:HD12	2:D:293:VAL:HG21	2.03	0.41
2:D:225:SER:HA	2:D:226:PRO:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:269:VAL:O	2:D:371:ARG:NE	2.44	0.41
1:A:88:TYR:CD1	1:A:89:ALA:C	2.98	0.41
1:A:269:LEU:HD23	1:A:274:GLU:HG2	2.02	0.41
1:C:165:LEU:HB3	1:C:215:VAL:HG12	2.03	0.41
2:D:394:MET:HE3	2:D:394:MET:HB2	1.93	0.41
2:D:715:ASP:HA	2:D:718:LEU:HD12	2.02	0.41
3:H:96:CYS:O	3:H:113:GLY:N	2.52	0.41
3:M:85:SER:O	3:M:85:SER:OG	2.32	0.41
3:M:112:TRP:CH2	4:N:43:GLY:HA3	2.55	0.41
1:A:79:CYS:HA	1:A:82:LEU:HB2	2.02	0.41
1:A:222:THR:O	1:A:222:THR:OG1	2.36	0.41
1:A:267:VAL:HG12	1:A:269:LEU:HD11	2.02	0.41
1:A:636:LEU:O	2:D:636:ALA:HB1	2.21	0.41
2:B:50:ILE:HD12	2:B:293:VAL:HG21	2.03	0.41
2:B:78:PRO:O	2:B:82:ILE:HG12	2.21	0.41
1:A:460:PRO:HD3	1:A:499:LEU:HD12	2.02	0.41
1:A:821:SER:O	1:A:822:ARG:C	2.64	0.41
2:B:408:ILE:HG12	2:B:508:MET:HB2	2.01	0.41
2:B:432:ASN:ND2	2:B:456:CYS:SG	2.94	0.41
2:B:531:GLU:HG2	1:C:556:TYR:HB3	2.02	0.41
2:B:673:ARG:HA	2:B:674:PRO:HD3	1.90	0.41
2:D:483:ASN:HD21	2:D:496:GLY:H	1.67	0.41
3:H:50:TYR:CE1	4:L:95:TYR:HB2	2.53	0.41
2:B:318:LYS:HD3	2:B:320:SER:O	2.21	0.41
2:B:654:MET:HE2	2:B:654:MET:HB3	1.67	0.41
1:A:162:HIS:CE1	1:A:237:ALA:HA	2.55	0.41
2:B:67:ARG:HG3	3:M:107:TRP:CZ2	2.56	0.41
2:B:267:ASP:N	2:B:267:ASP:OD1	2.52	0.41
2:B:741:GLY:HA3	2:B:802:HIS:HE1	1.86	0.41
1:C:142:PRO:HA	1:C:143:PRO:HD3	1.91	0.41
2:D:369:LYS:HB2	2:D:369:LYS:HE3	1.70	0.41
1:A:29:ILE:H	1:A:62:ALA:HA	1.84	0.41
1:A:485:ILE:HD13	1:A:485:ILE:HA	1.95	0.41
2:B:550:PHE:CZ	1:C:829:LEU:HG	2.56	0.41
1:C:562:LEU:HD11	1:C:767:LEU:HB2	2.02	0.41
1:A:39:GLU:H	1:A:39:GLU:HG3	1.65	0.41
1:A:165:LEU:HB3	1:A:215:VAL:HG12	2.03	0.41
1:A:411:ARG:HA	1:A:411:ARG:HE	1.85	0.41
1:A:562:LEU:HD11	1:A:767:LEU:HB2	2.02	0.41
1:C:180:LEU:HD12	1:C:183:LEU:HD12	2.03	0.41
1:C:460:PRO:HD3	1:C:499:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:678:LEU:HD23	1:C:678:LEU:HA	1.90	0.41
2:D:39:VAL:HG11	2:D:70:LEU:HA	2.02	0.41
2:D:78:PRO:O	2:D:82:ILE:HG12	2.21	0.41
2:D:159:ASN:ND2	2:D:382:LYS:HE3	2.35	0.41
2:D:601:THR:HG22	2:D:601:THR:O	2.20	0.41
2:D:741:GLY:HA3	2:D:802:HIS:HE1	1.86	0.41
1:A:108:SER:CB	1:A:134:HIS:NE2	2.83	0.41
2:B:111:ILE:O	2:B:115:ILE:HG13	2.21	0.41
2:B:142:MET:HE2	2:B:142:MET:HB2	1.88	0.41
1:C:253:TYR:CE1	1:C:284:PRO:HD3	2.53	0.41
2:D:111:ILE:O	2:D:115:ILE:HG13	2.21	0.41
2:D:321:CYS:O	2:D:321:CYS:SG	2.79	0.41
2:B:552:GLU:HB3	2:B:553:PRO:HD3	2.03	0.40
2:D:265:ASP:OD1	2:D:265:ASP:N	2.49	0.40
2:D:285:TRP:HB3	2:D:289:LEU:HD11	2.02	0.40
2:B:127:HIS:CD2	2:B:287:TYR:HB3	2.57	0.40
2:B:225:SER:HA	2:B:226:PRO:HA	1.80	0.40
2:B:321:CYS:O	2:B:321:CYS:SG	2.79	0.40
2:D:133:ILE:H	2:D:133:ILE:HD12	1.86	0.40
2:D:307:MET:HB3	2:D:307:MET:HE2	1.88	0.40
2:D:318:LYS:HD3	2:D:320:SER:O	2.21	0.40
2:D:366:LEU:CD1	2:D:375:ARG:HA	2.51	0.40
1:A:151:TRP:CE2	1:A:270:VAL:HG22	2.56	0.40
2:B:366:LEU:CD1	2:B:375:ARG:HA	2.51	0.40
2:D:139:GLU:HG3	2:D:142:MET:HE2	2.03	0.40
2:D:160:ILE:HG21	2:D:365:ILE:CD1	2.52	0.40
2:B:432:ASN:HD22	2:B:456:CYS:CB	2.33	0.40
1:C:124:ARG:HH22	1:C:147:GLN:NE2	2.20	0.40
1:C:157:VAL:HG22	1:C:392:HIS:NE2	2.36	0.40
2:D:374:GLU:OE1	2:D:375:ARG:N	2.53	0.40
2:B:139:GLU:HG3	2:B:142:MET:HE2	2.03	0.40
2:B:415:PRO:HG3	2:B:738:TYR:CE2	2.57	0.40
2:B:602:ILE:O	2:B:602:ILE:HG13	2.18	0.40
2:D:437:GLN:OE1	2:D:454:LYS:NZ	2.45	0.40
2:D:474:PHE:HD1	2:D:474:PHE:HA	1.77	0.40
3:H:112:TRP:CH2	4:L:43:GLY:HA3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	773/862 (90%)	675 (87%)	80 (10%)	18 (2%)	5	28
1	C	774/862 (90%)	676 (87%)	83 (11%)	15 (2%)	6	32
2	B	774/883 (88%)	653 (84%)	108 (14%)	13 (2%)	7	35
2	D	774/883 (88%)	651 (84%)	111 (14%)	12 (2%)	7	36
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%)	92 (88%)	11 (11%)	1 (1%)	12	47
4	N	104/213 (49%)	92 (88%)	11 (11%)	1 (1%)	12	47
All	All	3528/4362 (81%)	3055 (87%)	413 (12%)	60 (2%)	9	35

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	LEU
1	A	411	ARG
1	A	467	SER
1	A	821	SER
1	A	822	ARG
2	B	132	MET
2	B	133	ILE
2	B	223	LEU
2	B	415	PRO
1	C	381	LYS
1	C	467	SER
2	D	132	MET
2	D	133	ILE
2	D	223	LEU
2	D	414	ALA
1	A	87	VAL
1	A	368	LYS

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Mol	Chain	Res	Type
1	A	404	GLY
1	A	641	GLY
1	A	830	THR
1	C	87	VAL
1	C	368	LYS
1	C	404	GLY
1	C	436	MET
1	C	830	THR
1	A	172	GLU
1	A	278	ASN
1	C	172	GLU
1	C	331	GLY
1	A	34	SER
1	A	331	GLY
1	A	465	PRO
2	B	193	SER
2	B	287	TYR
1	C	380	ARG
2	D	193	SER
2	D	287	TYR
1	A	113	PHE
2	B	145	GLN
2	B	312	SER
2	B	416	PHE
1	C	113	PHE
1	C	219	ASP
2	D	145	GLN
2	D	312	SER
1	A	466	GLY
2	B	165	ASP
2	D	165	ASP
1	A	322	ILE
1	C	322	ILE
1	C	65	VAL
2	B	603	GLY
1	C	466	GLY
2	D	603	GLY
2	B	39	VAL
2	B	679	PRO
2	D	39	VAL
2	D	679	PRO
4	L	8	PRO

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Mol	Chain	Res	Type
4	N	8	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	673/744 (90%)	644 (96%)	29 (4%)	26	48
1	C	674/744 (91%)	643 (95%)	31 (5%)	24	46
2	B	681/762 (89%)	660 (97%)	21 (3%)	35	56
2	D	681/762 (89%)	658 (97%)	23 (3%)	32	54
3	H	96/189 (51%)	95 (99%)	1 (1%)	68	75
3	M	95/189 (50%)	95 (100%)	0	100	100
4	L	91/189 (48%)	84 (92%)	7 (8%)	12	33
4	N	91/189 (48%)	84 (92%)	7 (8%)	12	33
All	All	3082/3768 (82%)	2963 (96%)	119 (4%)	30	50

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	64	SER
1	A	65	VAL
1	A	70	ASN
1	A	88	TYR
1	A	93	SER
1	A	118	VAL
1	A	121	LEU
1	A	131	LYS
1	A	135	LEU
1	A	136	SER
1	A	138	LEU
1	A	223	LYS
1	A	235	LEU

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Mol	Chain	Res	Type
1	A	269	LEU
1	A	270	VAL
1	A	273	ARG
1	A	285	ASP
1	A	329	CYS
1	A	330	VAL
1	A	411	ARG
1	A	463	THR
1	A	511	VAL
1	A	589	LEU
1	A	640	ILE
1	A	647	SER
1	A	667	SER
1	A	767	LEU
1	A	828	THR
2	B	40	ILE
2	B	108	ILE
2	B	197	TRP
2	B	199	LEU
2	B	200	GLU
2	B	208	SER
2	B	286	ASP
2	B	326	GLU
2	B	364	ILE
2	B	366	LEU
2	B	381	ASP
2	B	382	LYS
2	B	431	ARG
2	B	432	ASN
2	B	434	VAL
2	B	510	VAL
2	B	539	SER
2	B	602	ILE
2	B	604	LYS
2	B	660	VAL
2	B	807	GLU
1	C	28	ASN
1	C	33	LEU
1	C	61	GLN
1	C	63	THR
1	C	70	ASN
1	C	88	TYR

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Mol	Chain	Res	Type
1	C	93	SER
1	C	118	VAL
1	C	121	LEU
1	C	133	ILE
1	C	134	HIS
1	C	137	PHE
1	C	222	THR
1	C	223	LYS
1	C	235	LEU
1	C	269	LEU
1	C	270	VAL
1	C	273	ARG
1	C	285	ASP
1	C	329	CYS
1	C	330	VAL
1	C	411	ARG
1	C	463	THR
1	C	589	LEU
1	C	640	ILE
1	C	642	GLU
1	C	647	SER
1	C	667	SER
1	C	767	LEU
1	C	819	CYS
1	C	828	THR
2	D	40	ILE
2	D	108	ILE
2	D	197	TRP
2	D	199	LEU
2	D	200	GLU
2	D	208	SER
2	D	286	ASP
2	D	326	GLU
2	D	364	ILE
2	D	366	LEU
2	D	380	LYS
2	D	381	ASP
2	D	382	LYS
2	D	383	SER
2	D	386	MET
2	D	413	GLU
2	D	431	ARG

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Mol	Chain	Res	Type
2	D	434	VAL
2	D	458	LYS
2	D	539	SER
2	D	602	ILE
2	D	604	LYS
2	D	807	GLU
3	H	37	VAL
4	L	5	THR
4	L	22	THR
4	L	26	SER
4	L	67	SER
4	L	72	SER
4	L	83	ILE
4	L	105	ILE
4	N	5	THR
4	N	22	THR
4	N	26	SER
4	N	67	SER
4	N	72	SER
4	N	83	ILE
4	N	105	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	40	GLN
1	A	61	GLN
1	A	146	HIS
1	A	426	GLN
1	A	515	ASN
1	A	726	HIS
2	B	118	GLN
2	B	192	ASN
2	B	432	ASN
2	B	486	HIS
2	B	491	ASN
2	B	495	ASN
2	B	656	GLN
2	B	697	ASN
2	B	698	ASN
2	B	767	GLN

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Mol	Chain	Res	Type
2	B	782	GLN
2	B	812	GLN
1	C	40	GLN
1	C	146	HIS
1	C	224	ASN
1	C	426	GLN
1	C	726	HIS
2	D	118	GLN
2	D	192	ASN
2	D	432	ASN
2	D	486	HIS
2	D	491	ASN
2	D	495	ASN
2	D	656	GLN
2	D	697	ASN
2	D	698	ASN
2	D	767	GLN
2	D	812	GLN
3	H	5	GLN
3	H	84	ASN
4	L	38	HIS
4	L	49	HIS
4	L	55	GLN
4	N	38	HIS
4	N	49	HIS
4	N	55	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2
2	D	2

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	5.22
1	D	44:THR	C	45:SER	N	5.22
1	B	63:SER	C	64:VAL	N	3.24
1	D	63:SER	C	64:VAL	N	3.24

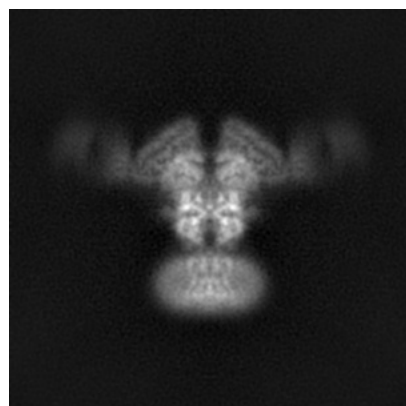
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25844. These allow visual inspection of the internal detail of the map and identification of artifacts.

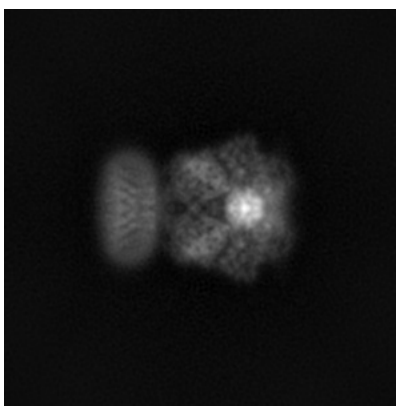
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

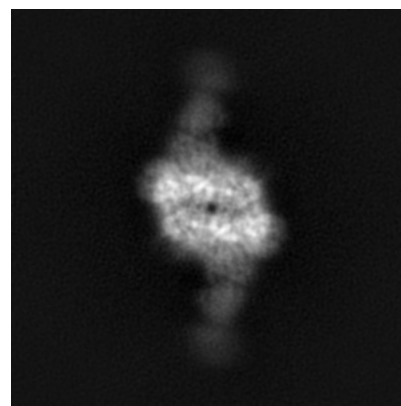
6.1.1 Primary map



X

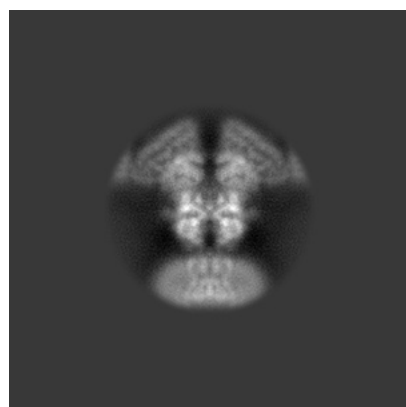


Y

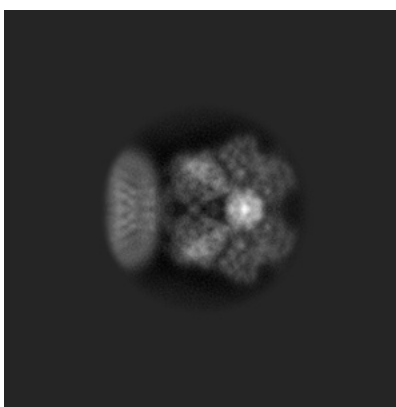


Z

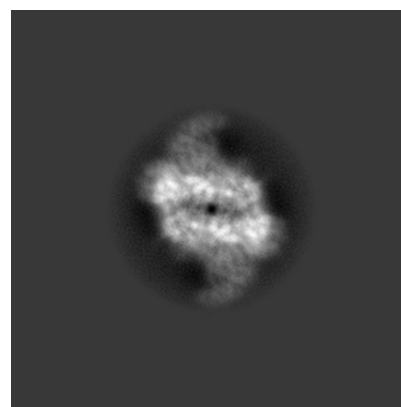
6.1.2 Raw map



X



Y

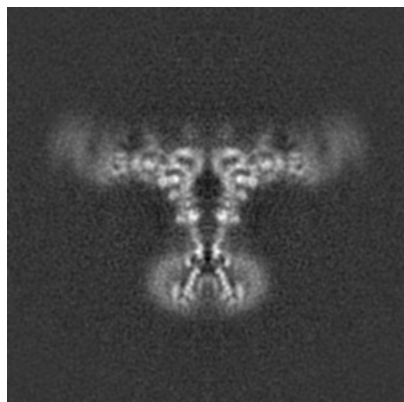


Z

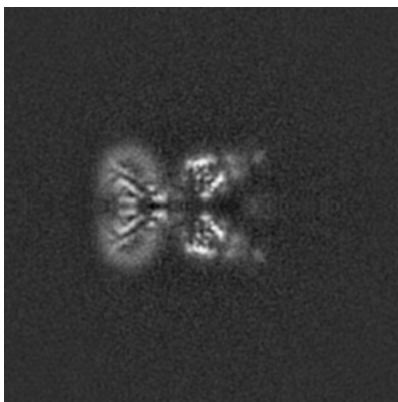
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

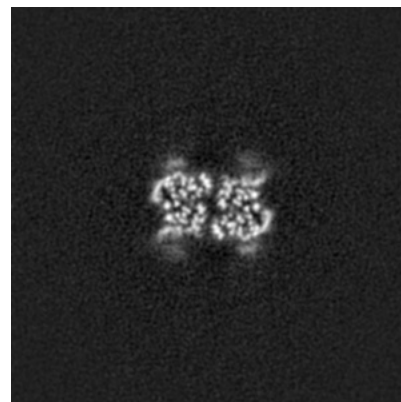
6.2.1 Primary map



X Index: 128

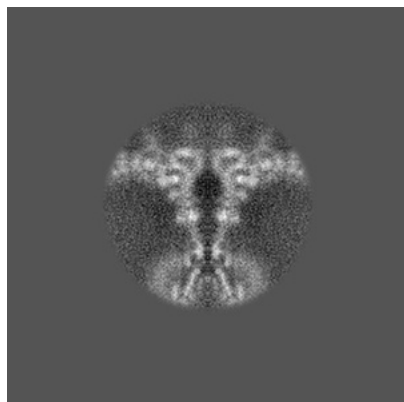


Y Index: 128

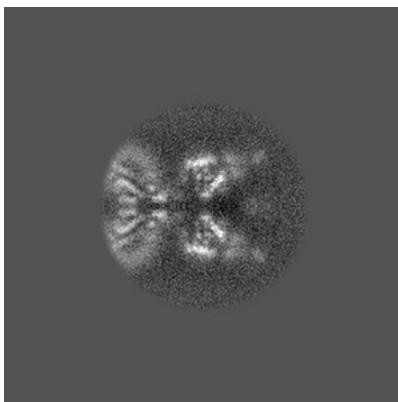


Z Index: 128

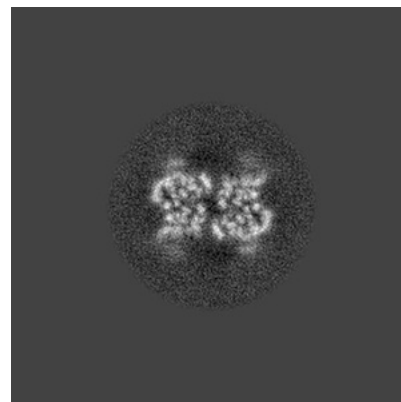
6.2.2 Raw map



X Index: 128



Y Index: 128

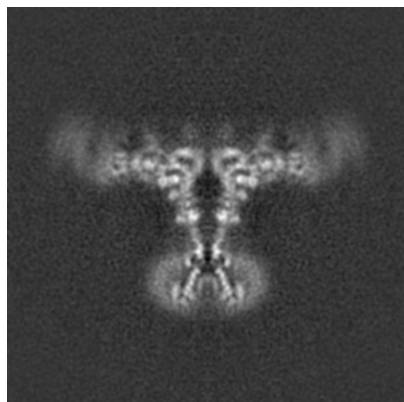


Z Index: 128

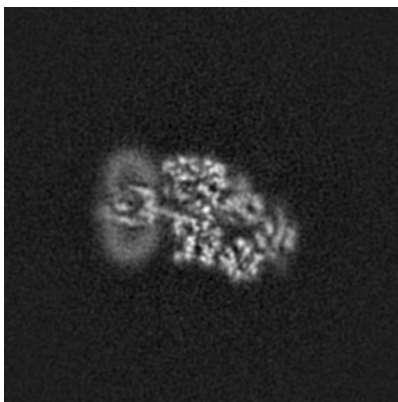
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

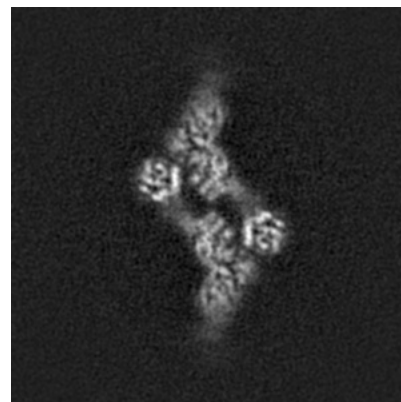
6.3.1 Primary map



X Index: 128

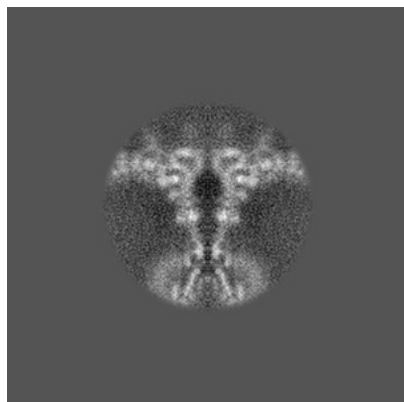


Y Index: 141

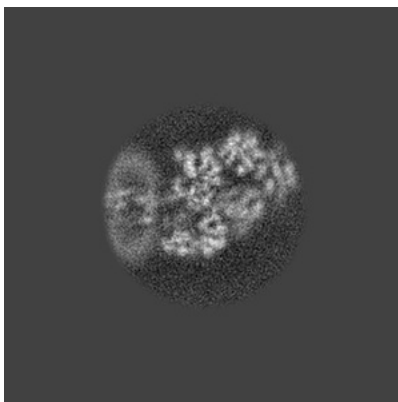


Z Index: 152

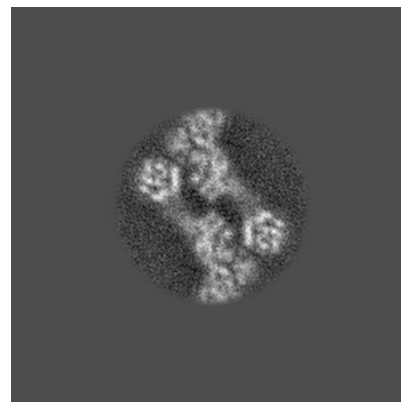
6.3.2 Raw map



X Index: 128



Y Index: 114

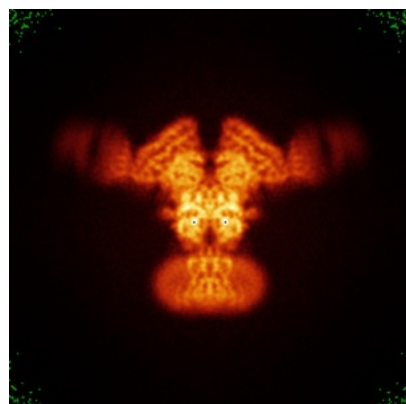


Z Index: 152

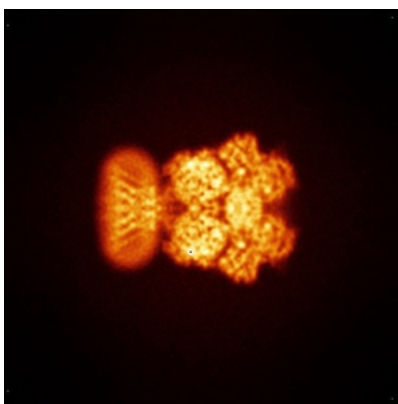
The images above show the largest variance slices of the map in three orthogonal directions.

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

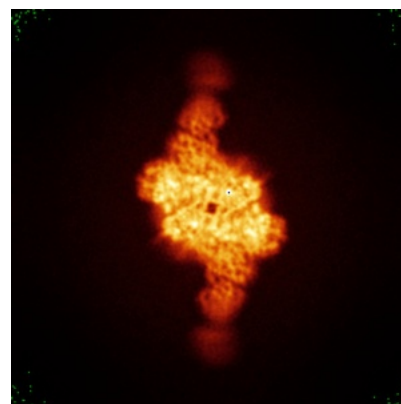
6.4.1 Primary map



X

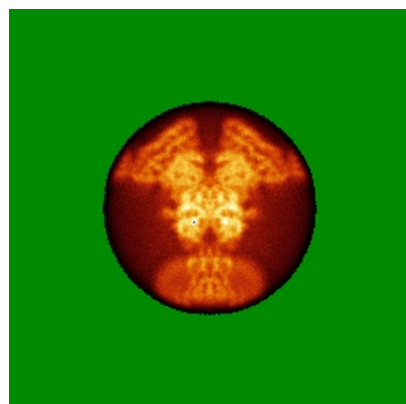


Y

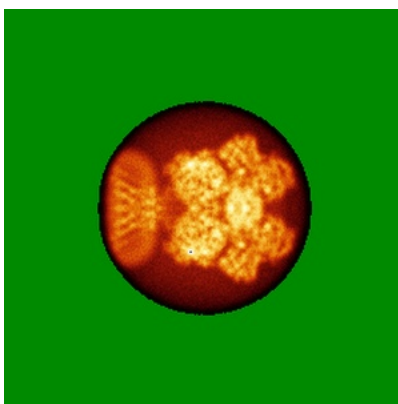


Z

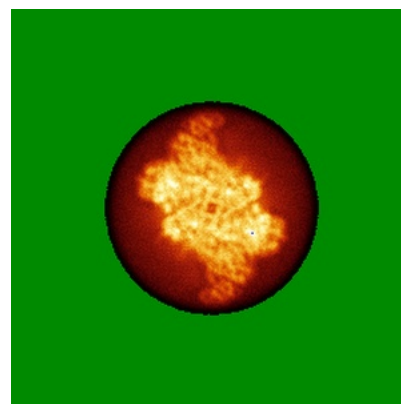
6.4.2 Raw map



X



Y

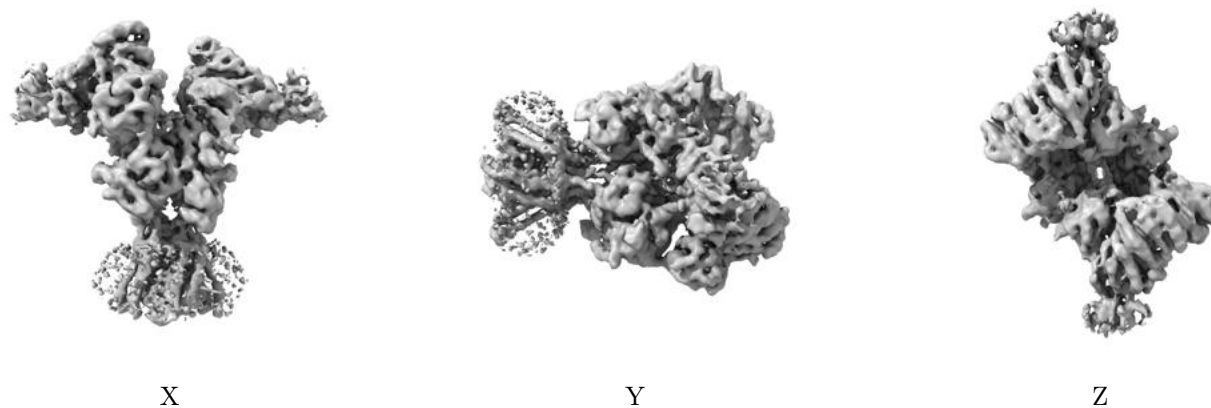


Z

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

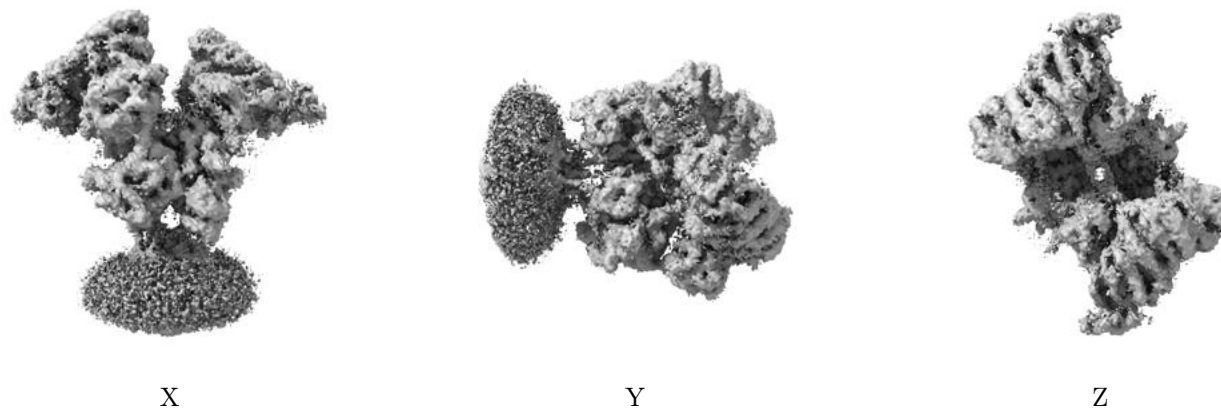
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

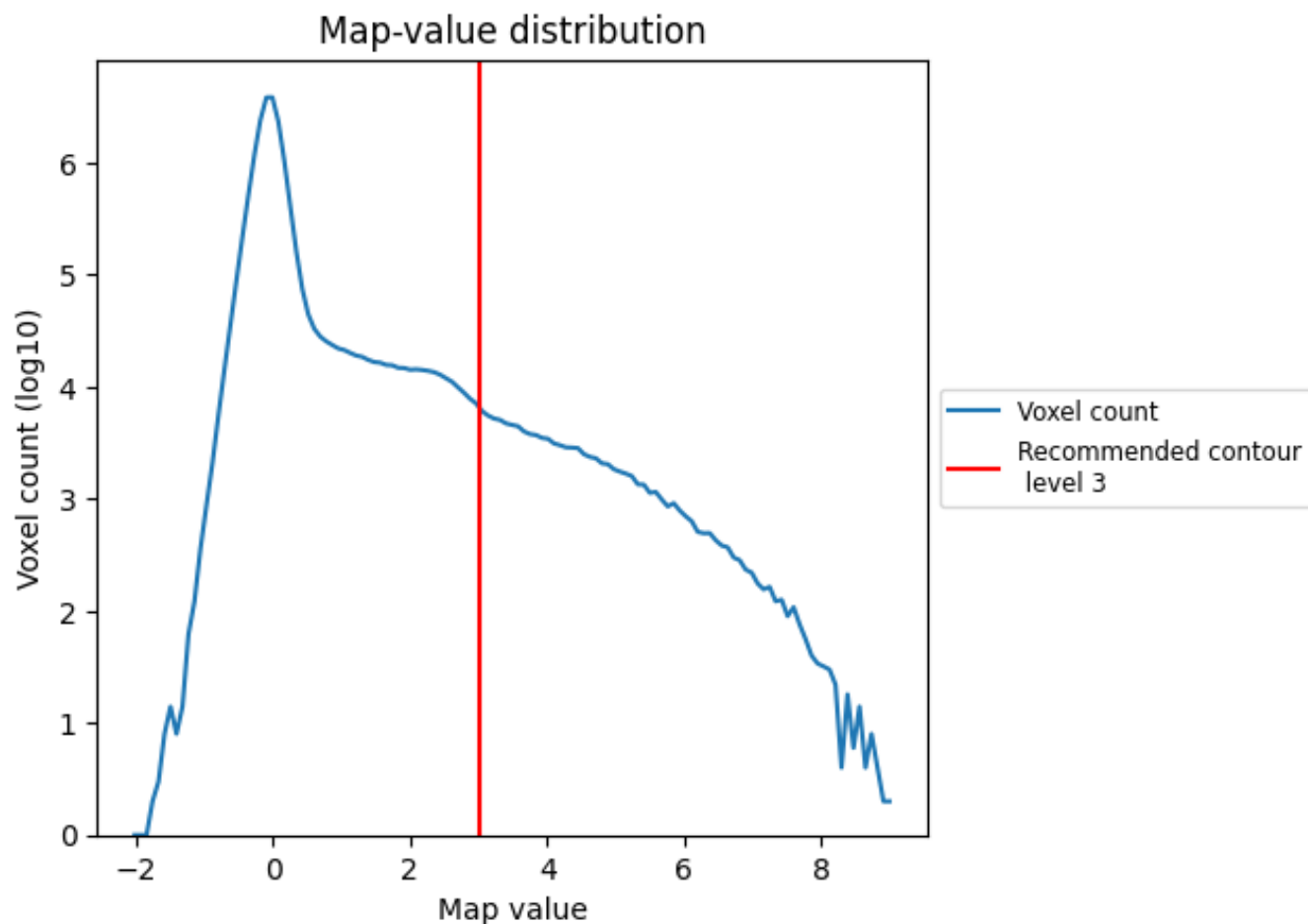
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

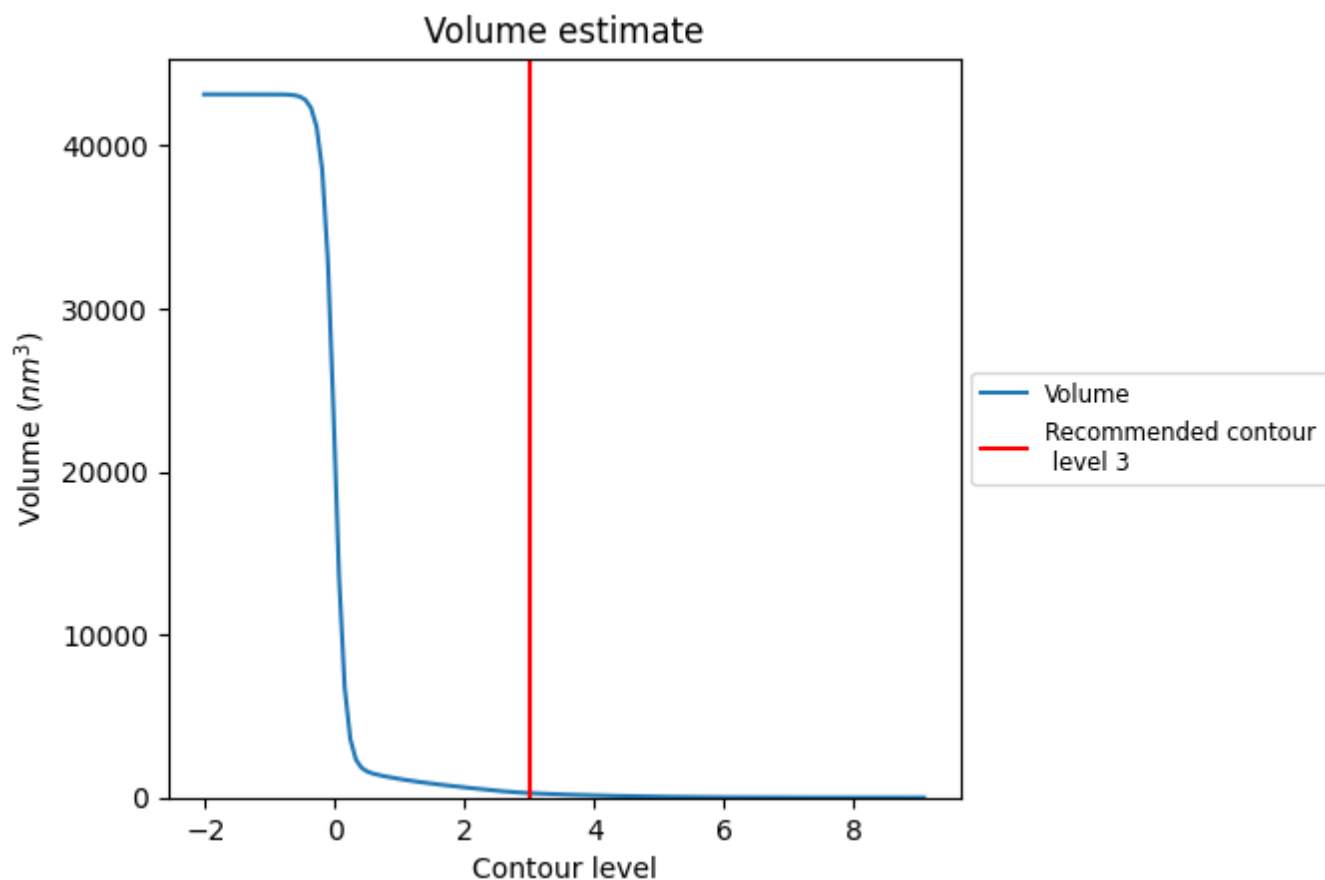
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

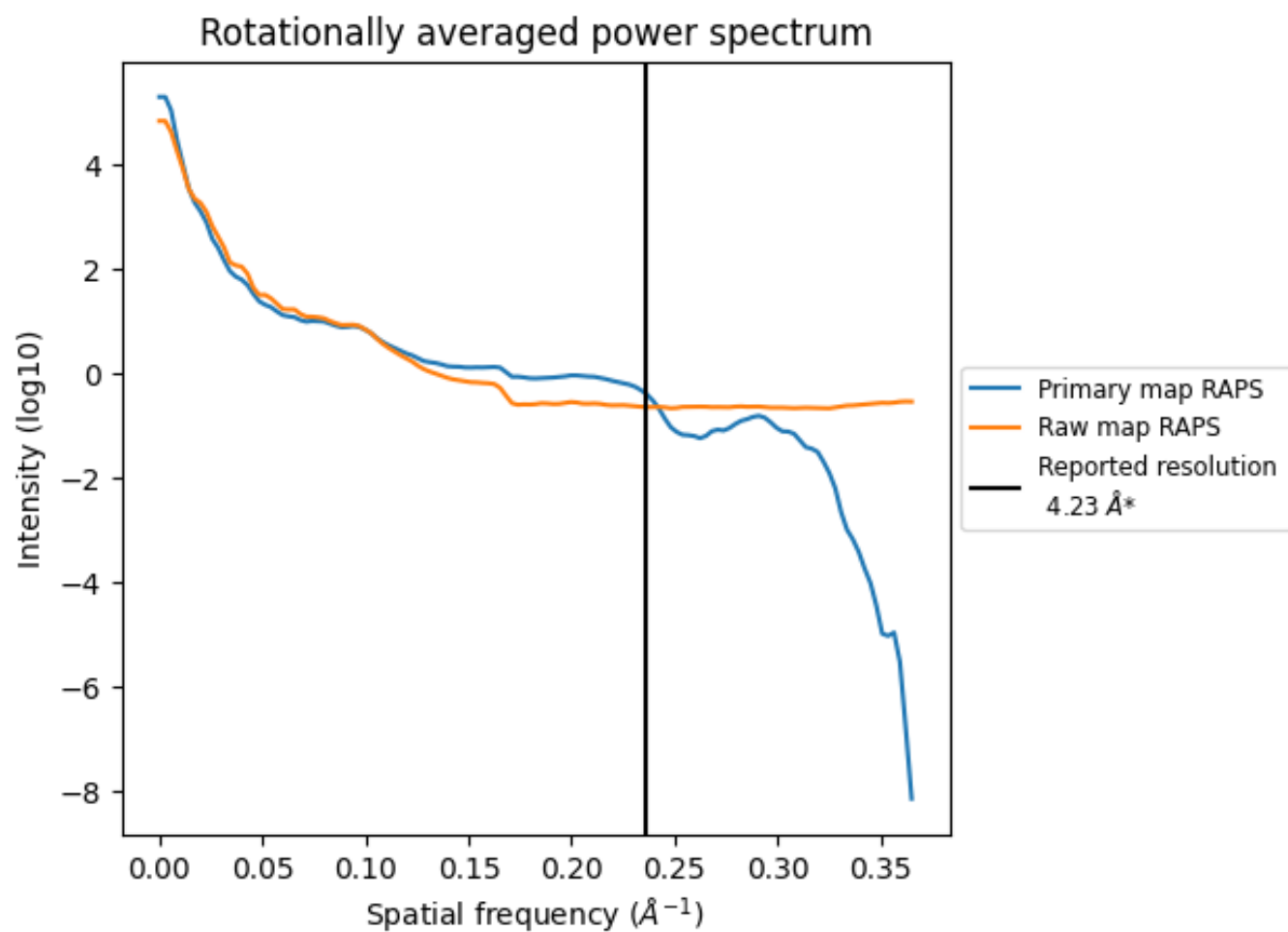
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 272 nm³; this corresponds to an approximate mass of 246 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

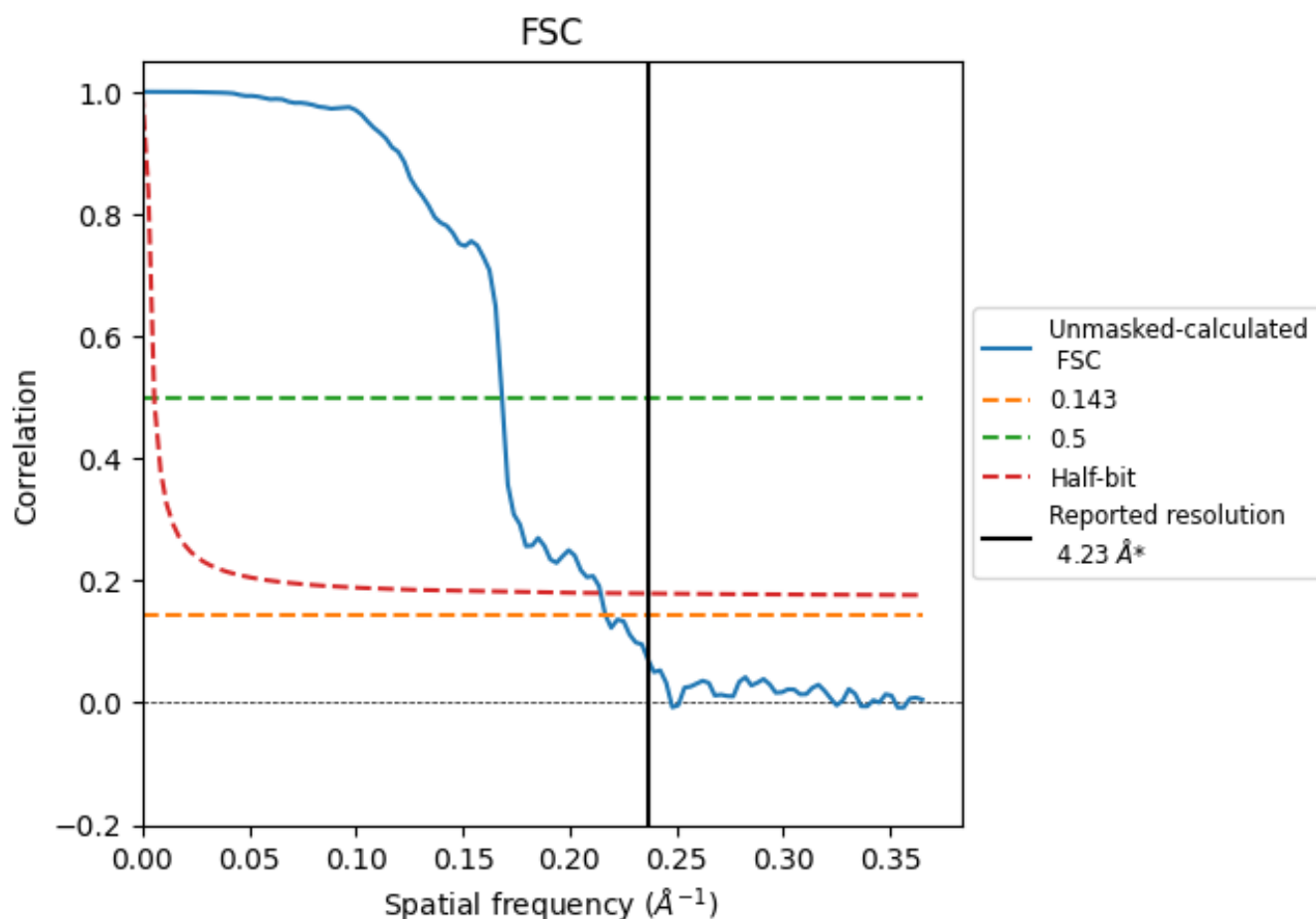


*Reported resolution corresponds to spatial frequency of 0.236 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.236 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

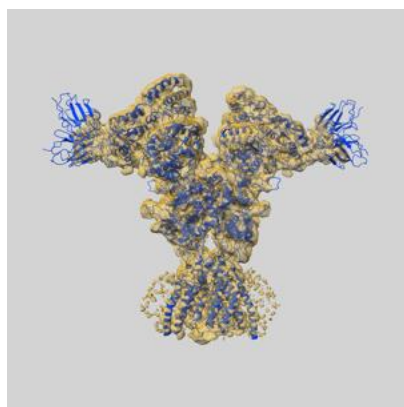
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.23	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.61	5.94	4.66

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

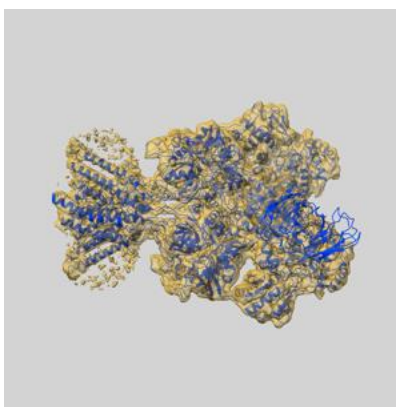
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25844 and PDB model 7TEB. Per-residue inclusion information can be found in section [3](#) on page [9](#).

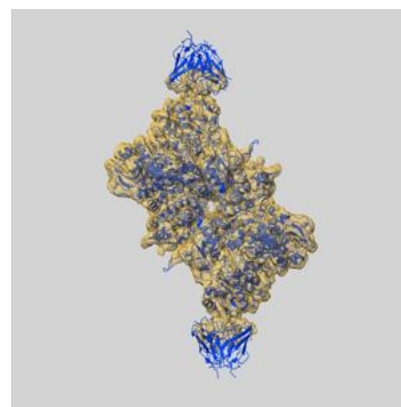
9.1 Map-model overlay [i](#)



X



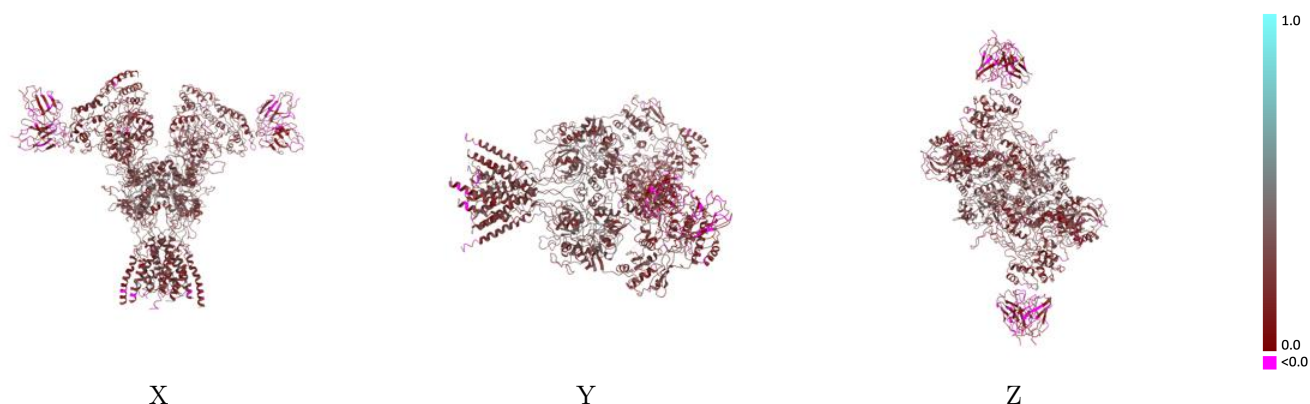
Y



Z

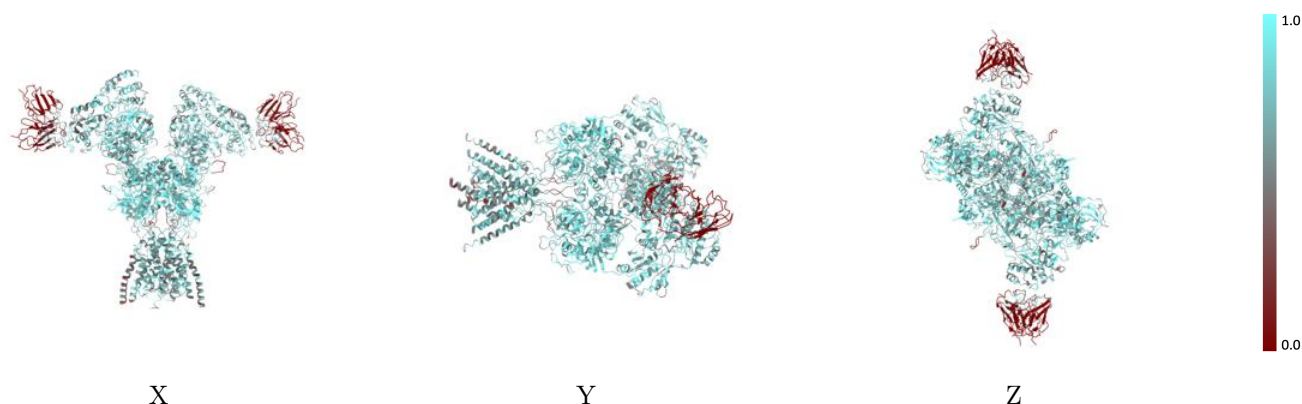
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



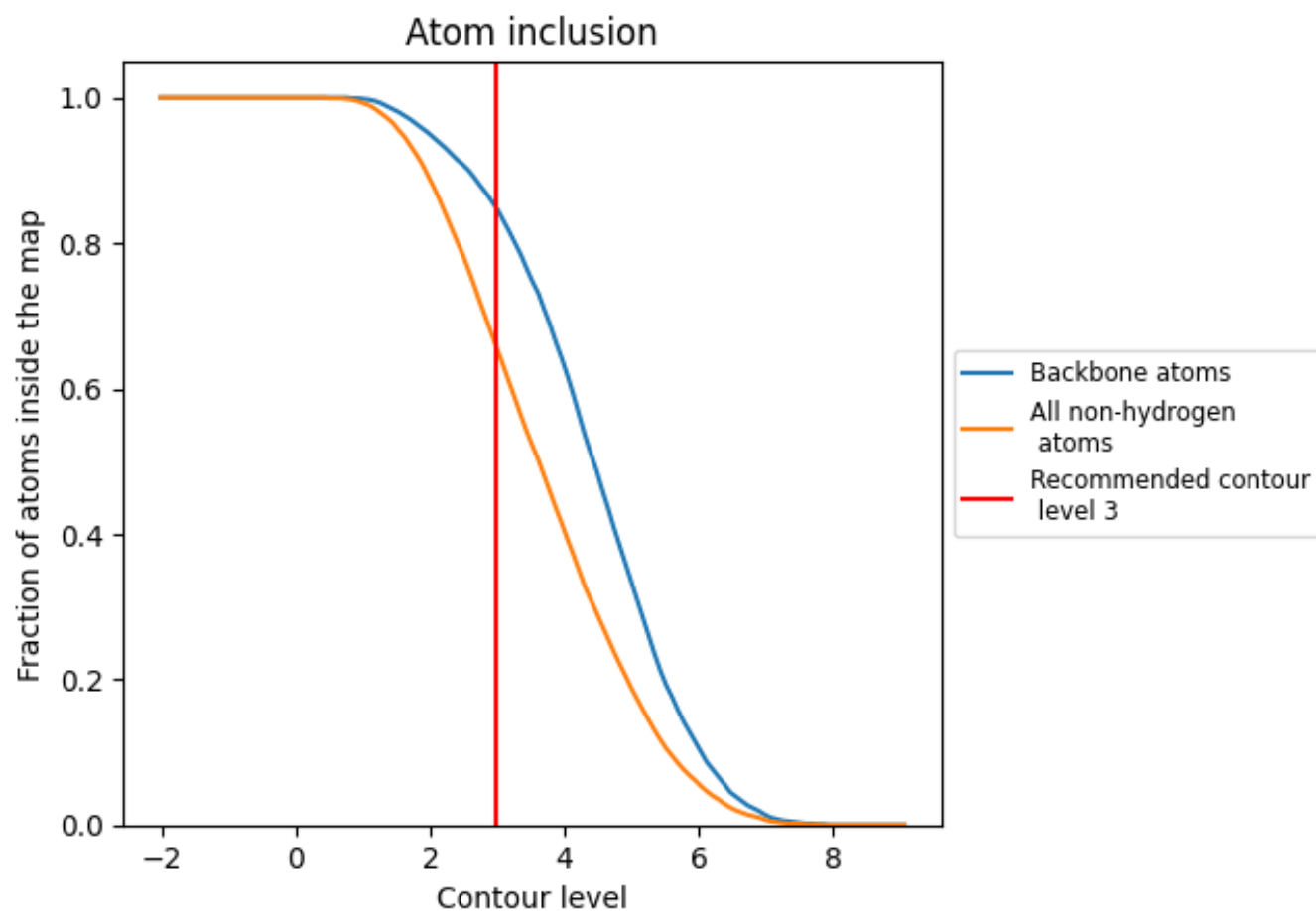
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6550	0.2330
A	0.7420	0.2600
B	0.7120	0.2450
C	0.7410	0.2620
D	0.7060	0.2450
H	0.1720	0.1040
L	0.1270	0.0860
M	0.1910	0.1130
N	0.1180	0.0620

1.0

0.0

<0.0