



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:52 PM UTC

PDB ID : 9I7W / pdb_00009i7w
EMDB ID : EMD-52389
Title : Extended and wrapped protein P7 dimers of dimers, the P1 layer and the RNA-dependent RNA polymerase P2 in transcribing particles of bacteriophage phi6
Authors : Kumpula, E.-P.; Ilca, S.L.; Huiskonen, J.T.
Deposited on : 2025-02-03
Resolution : 4.80 Å (reported)
Based on initial models : 9HTW, 9I5C, 1HHT

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

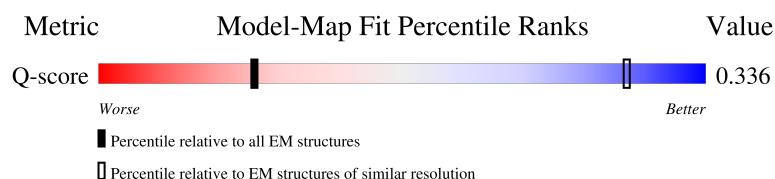
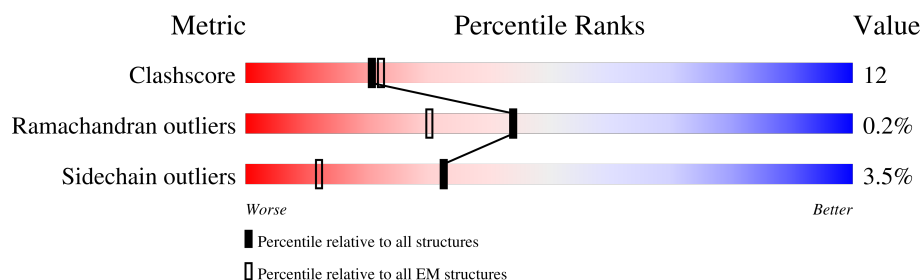
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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	1575 (4.30 - 5.30)

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	x	5	
2	U	664	
3	A	111	
3	B	111	

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Mol	Chain	Length	Quality of chain
3	E	111	<div> <div>47%</div> <div>83%</div> <div>17%</div> </div>
3	F	111	<div> <div>72%</div> <div>83%</div> <div>17%</div> </div>
3	M	111	<div> <div>49%</div> <div>73%</div> <div>27%</div> </div>
3	N	111	<div> <div>77%</div> <div>86%</div> <div>14%</div> </div>
3	S	111	<div> <div>68%</div> <div>86%</div> <div>14%</div> </div>
3	T	111	<div> <div>61%</div> <div>77%</div> <div>23%</div> </div>
4	V	766	<div> <div>26%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
4	W	766	<div> <div>17%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
4	X	766	<div> <div>28%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>
4	Z	766	<div> <div>25%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 35915 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 DNA chain called DNA (5'-D(*TP*TP*TP*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
1	x	5	Total	C	N	O	P	0	0
			95	48	12	31	4		

- Molecule 2 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	655	Total	C	N	O	S	0	0
			5204	3306	901	966	31		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	456	MET	ILE	conflict	UNP P11124

- Molecule 3 is a protein called Nucleocapsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	111	Total	C	N	O	S	0	0
			845	546	140	155	4		
3	B	111	Total	C	N	O	S	0	0
			845	546	140	155	4		
3	E	111	Total	C	N	O	S	0	0
			845	546	140	155	4		
3	F	111	Total	C	N	O	S	0	0
			845	546	140	155	4		
3	M	111	Total	C	N	O	S	0	0
			845	546	140	155	4		
3	N	111	Total	C	N	O	S	0	0
			845	546	140	155	4		
3	S	111	Total	C	N	O	S	0	0
			845	546	140	155	4		
3	T	111	Total	C	N	O	S	0	0
			841	544	140	153	4		

- Molecule 4 is a protein called Major inner protein P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	766	Total 5965	C 3767	N 1053	O 1122	S 23	0	0
4	W	766	Total 5965	C 3767	N 1053	O 1122	S 23	0	0
4	X	766	Total 5965	C 3767	N 1053	O 1122	S 23	0	0
4	Z	766	Total 5965	C 3767	N 1053	O 1122	S 23	0	0

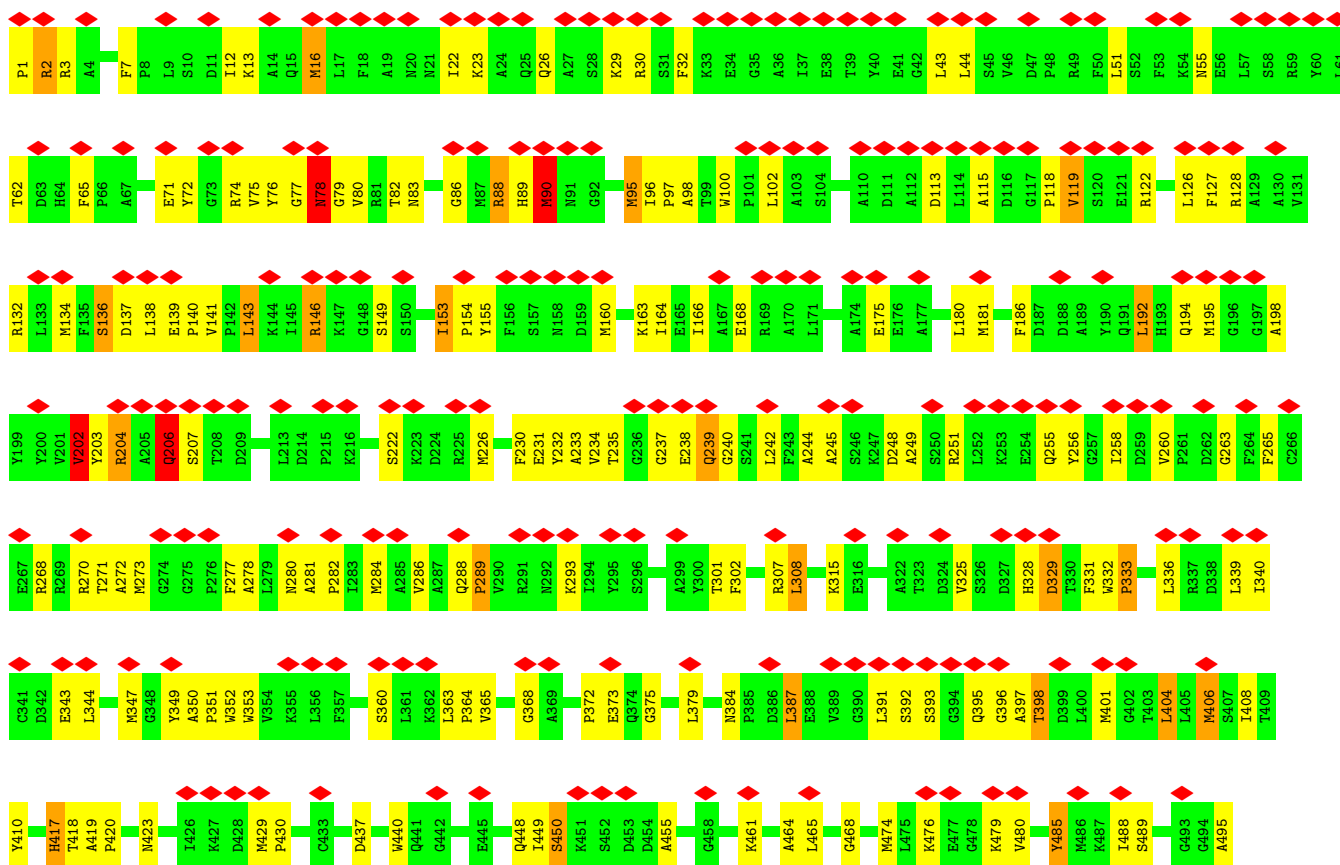
3 Residue-property plots

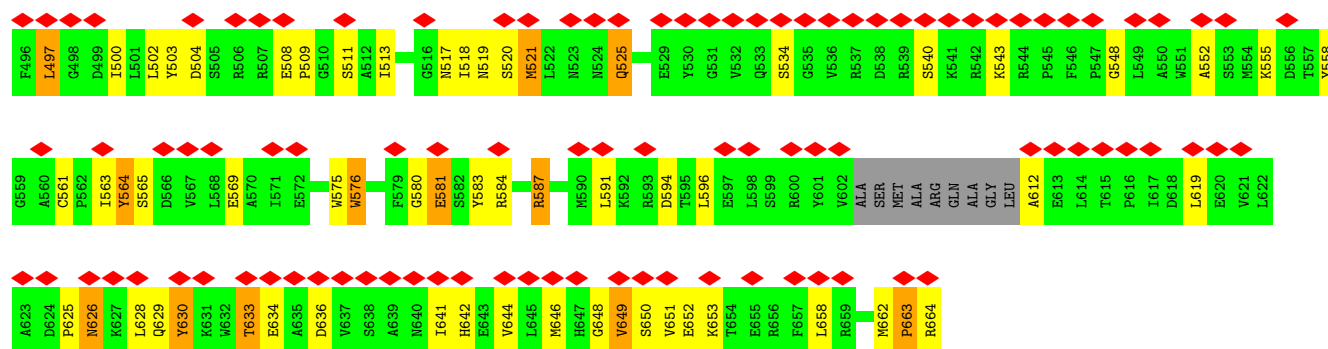
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DNA (5'-D(*TP*TP*TP*CP*C)-3')

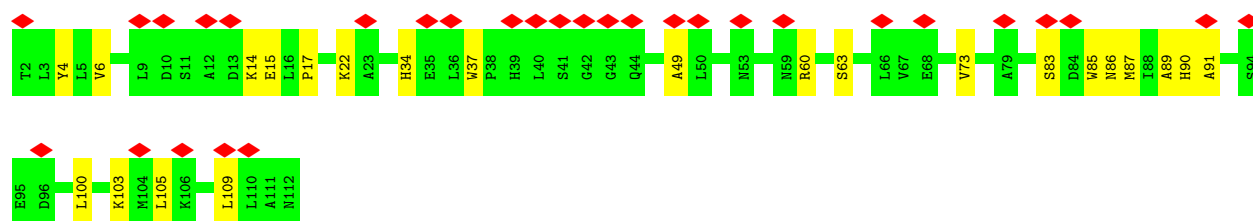


- Molecule 2: RNA-directed RNA polymerase

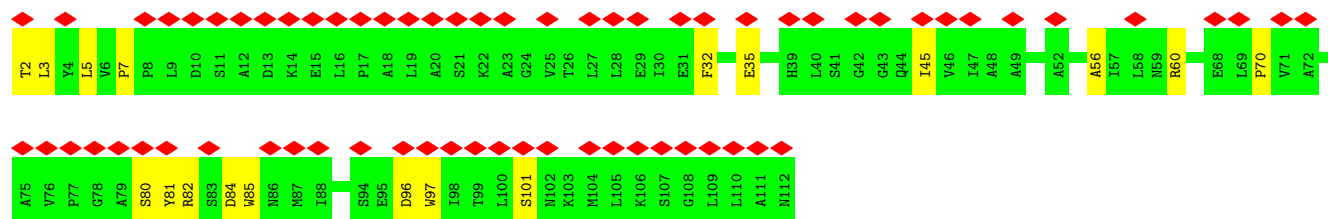
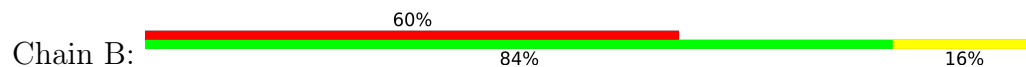




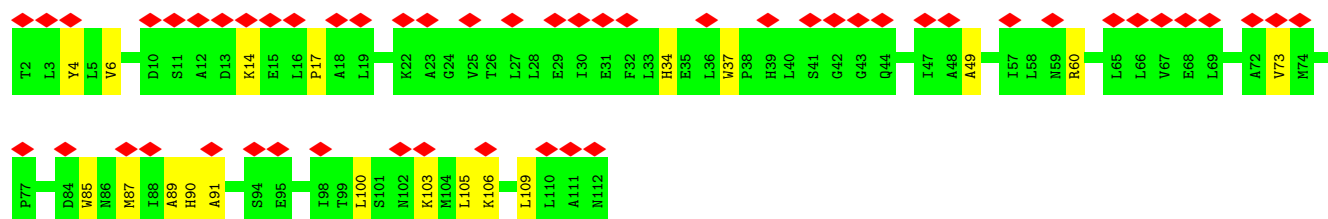
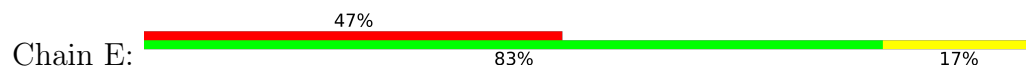
• Molecule 3: Nucleocapsid protein



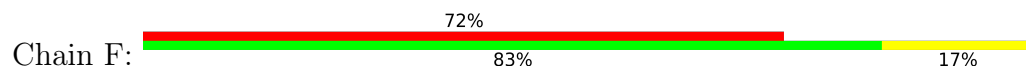
• Molecule 3: Nucleocapsid protein

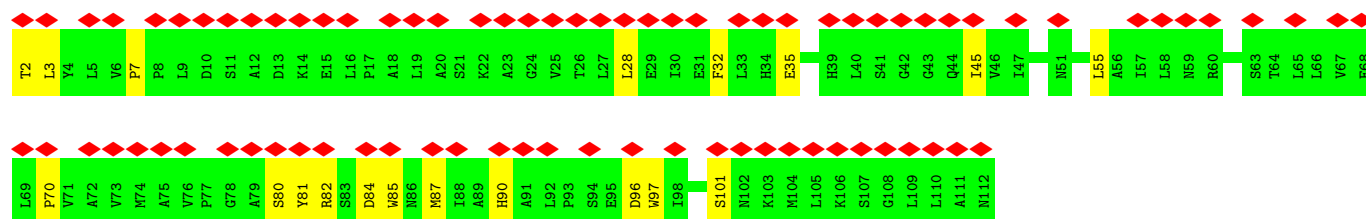


• Molecule 3: Nucleocapsid protein

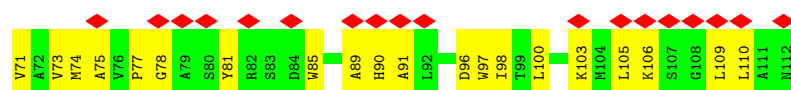
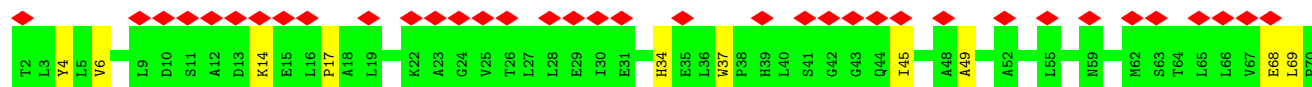
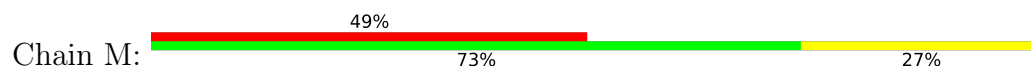


• Molecule 3: Nucleocapsid protein

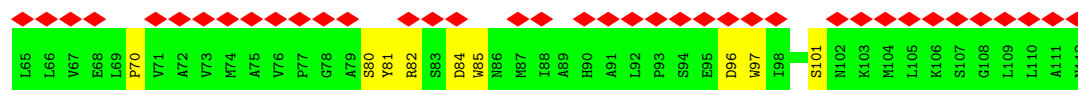
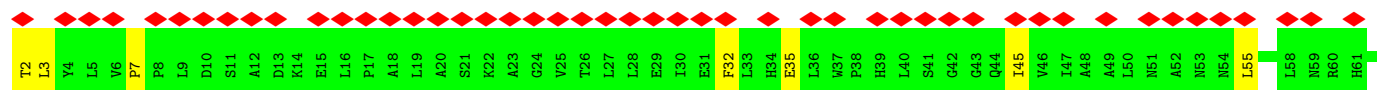
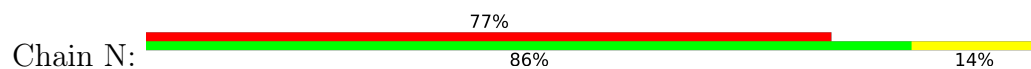




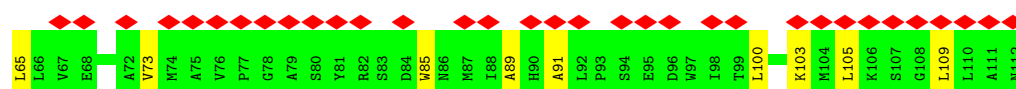
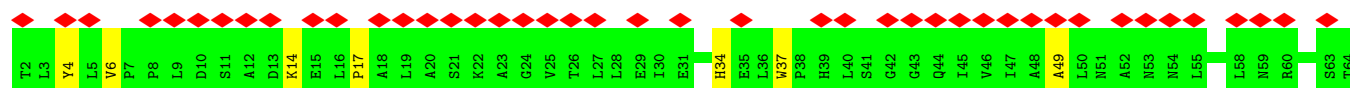
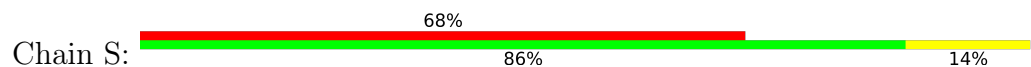
• Molecule 3: Nucleocapsid protein



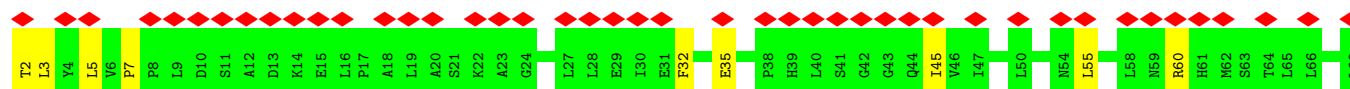
• Molecule 3: Nucleocapsid protein



• Molecule 3: Nucleocapsid protein

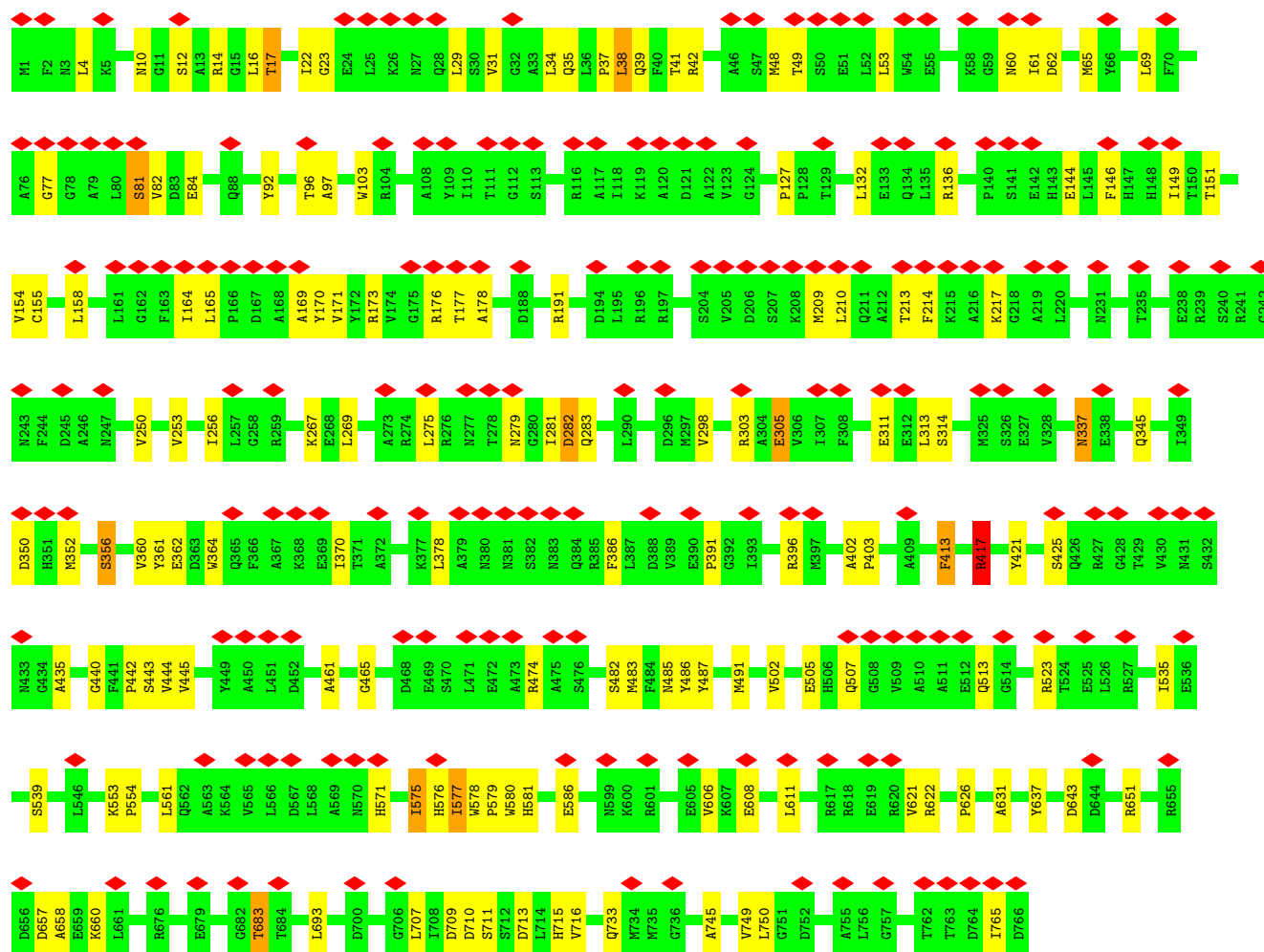
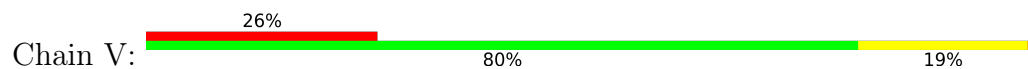


• Molecule 3: Nucleocapsid protein

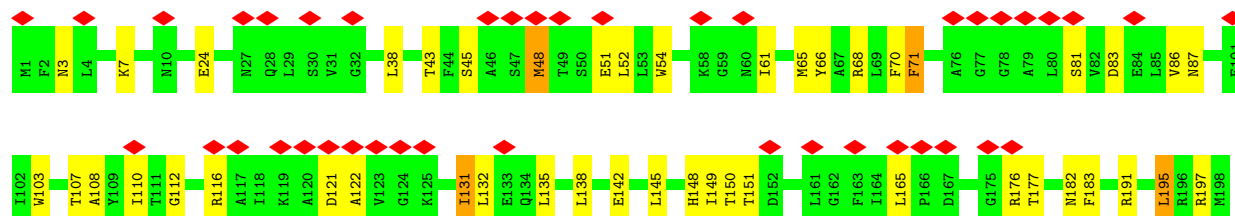
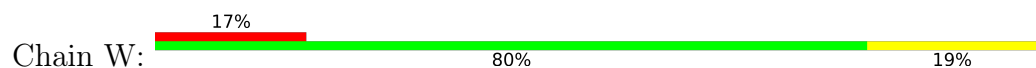


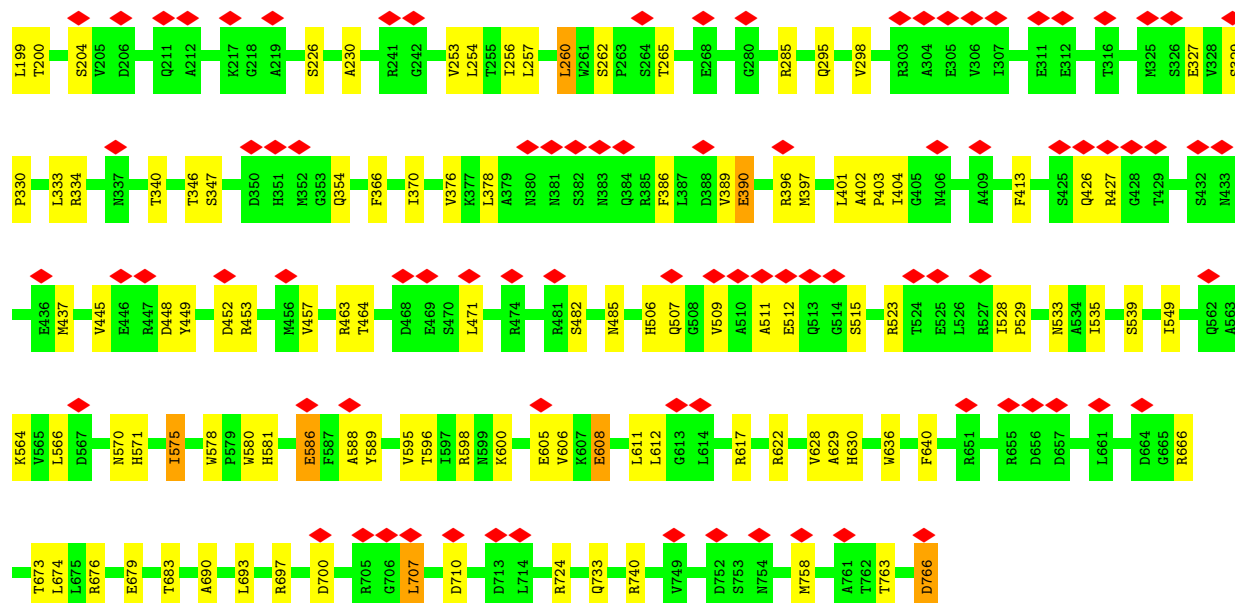


• Molecule 4: Major inner protein P1

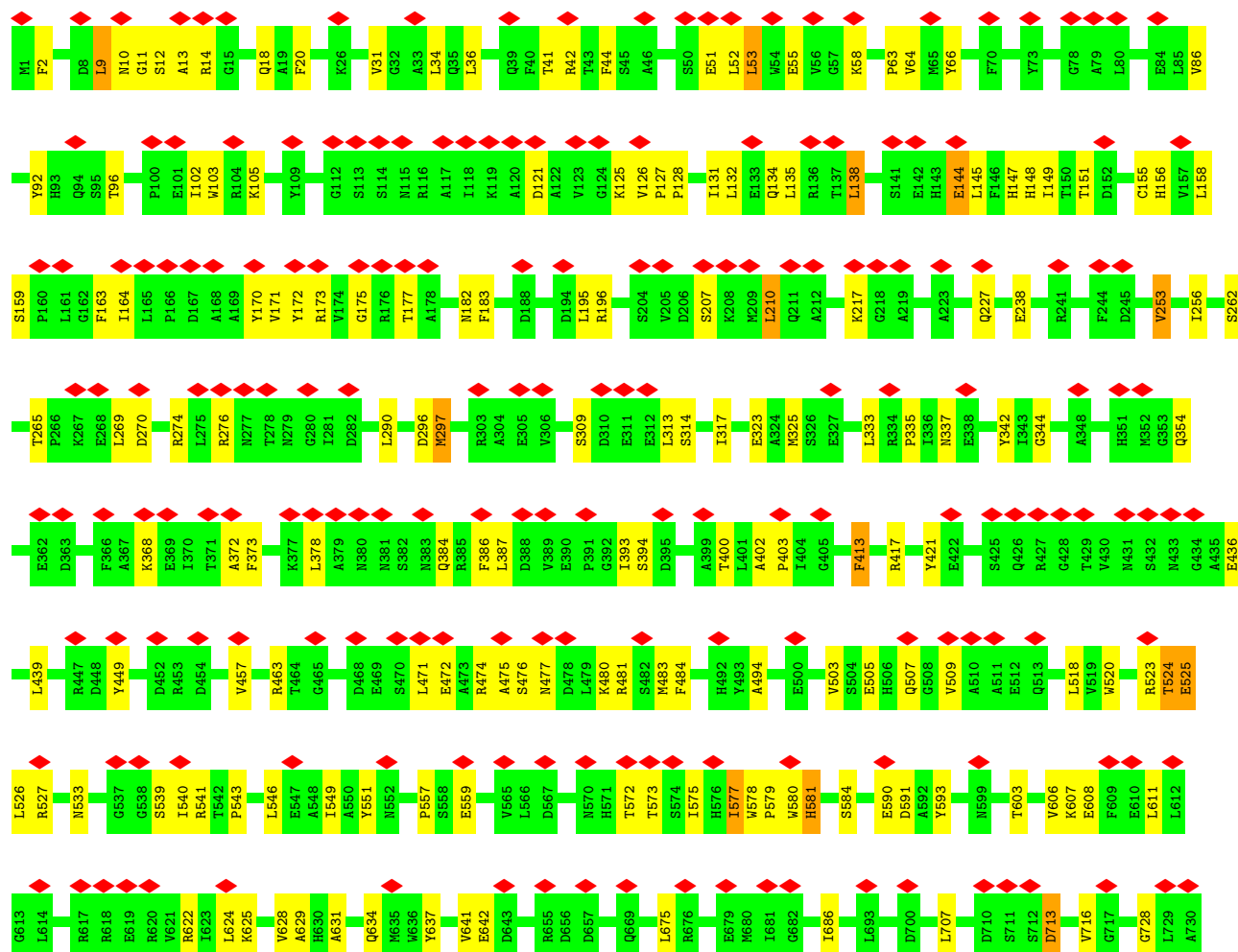
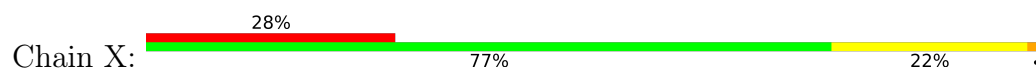


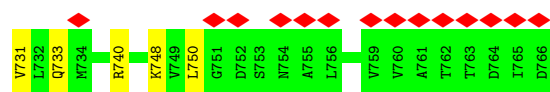
• Molecule 4: Major inner protein P1



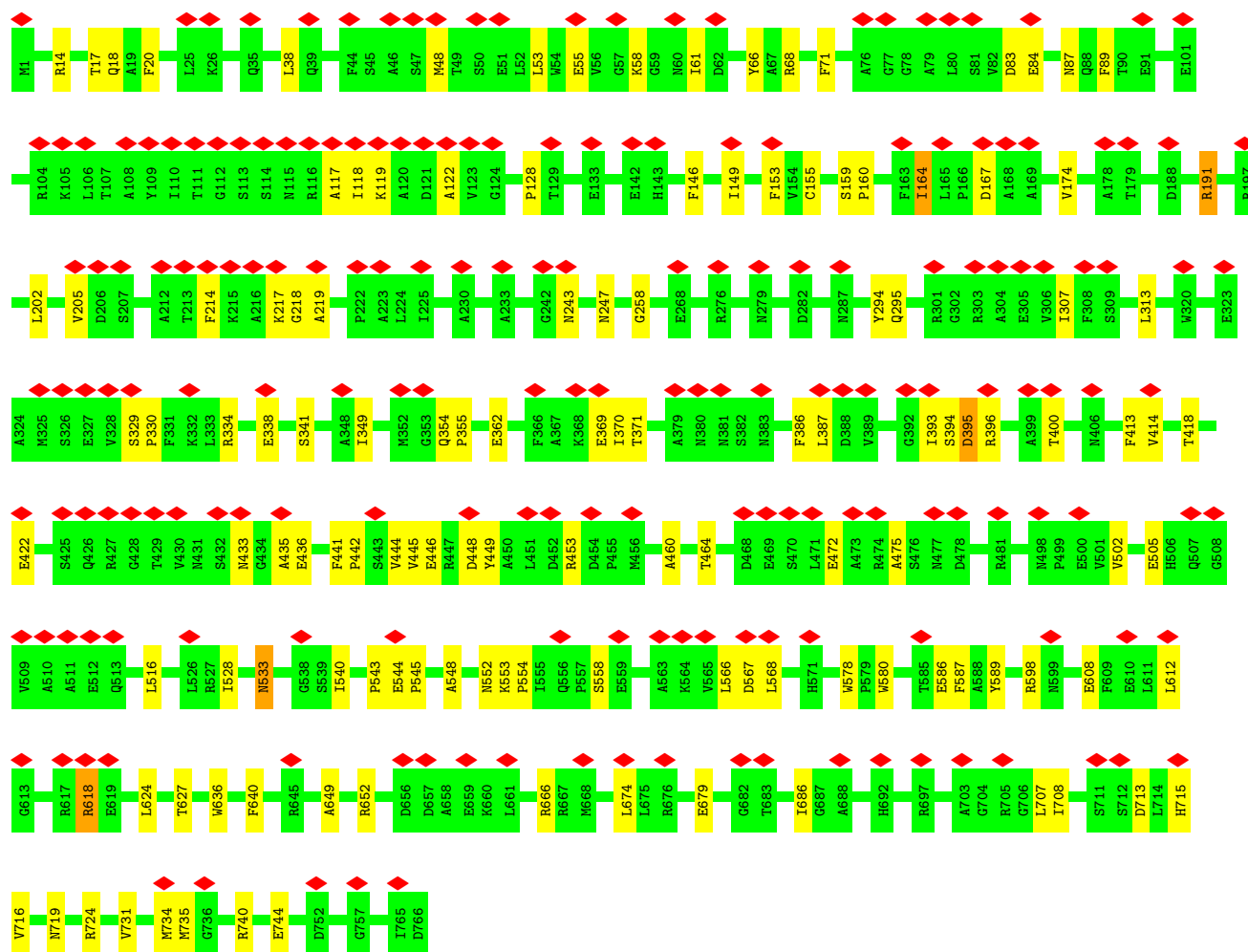
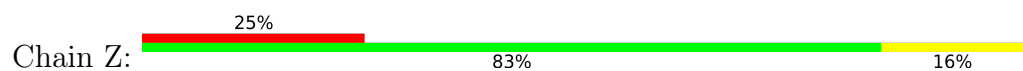


• Molecule 4: Major inner protein P1





• Molecule 4: Major inner protein P1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	18230	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	41000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.170	Depositor
Minimum map value	-0.105	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	268.8, 268.8, 268.8	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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	x	0.49	0/104	1.35	2/158 (1.3%)
2	U	0.73	2/5334 (0.0%)	1.12	35/7213 (0.5%)
3	A	0.38	0/864	0.56	0/1181
3	B	0.33	0/864	0.58	0/1181
3	E	0.38	0/864	0.56	0/1181
3	F	0.33	0/864	0.57	0/1181
3	M	0.38	0/864	0.56	0/1181
3	N	0.33	0/864	0.57	0/1181
3	S	0.38	0/864	0.56	0/1181
3	T	0.33	0/860	0.57	0/1176
4	V	0.29	0/6085	0.56	2/8267 (0.0%)
4	W	0.29	0/6085	0.53	0/8267
4	X	0.29	0/6085	0.55	0/8267
4	Z	0.28	0/6085	0.51	0/8267
All	All	0.40	2/36686 (0.0%)	0.66	39/49882 (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	x	0	2
4	V	0	4
4	W	0	2
4	X	0	1
4	Z	0	1
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	90	MET	SD-CE	-8.40	1.58	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	202	VAL	CA-CB	5.61	1.61	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	155	TYR	N-CA-C	9.31	123.14	111.69
2	U	525	GLN	N-CA-C	8.72	120.87	111.36
2	U	100	TRP	N-CA-C	-7.92	100.09	110.07
2	U	485	TYR	N-CA-C	7.24	122.17	113.12
2	U	141	VAL	CA-C-N	-7.15	112.56	120.14
2	U	141	VAL	C-N-CA	-7.15	112.56	120.14
2	U	206	GLN	N-CA-C	-7.05	96.85	108.49
2	U	521	MET	N-CA-C	-6.85	103.74	111.14
2	U	449	ILE	N-CA-C	-6.83	98.29	108.12
2	U	136	SER	N-CA-C	6.73	123.62	110.56
2	U	95	MET	N-CA-C	-6.67	100.61	110.48
2	U	384	ASN	CA-C-N	6.61	128.10	119.84
2	U	384	ASN	C-N-CA	6.61	128.10	119.84
2	U	450	SER	N-CA-C	6.46	118.68	108.79
2	U	153	ILE	N-CA-C	6.28	115.80	108.96
2	U	134	MET	N-CA-C	6.17	118.08	111.36
2	U	363	LEU	CA-C-N	6.00	125.97	120.21
2	U	363	LEU	C-N-CA	6.00	125.97	120.21
2	U	329	ASP	N-CA-C	5.95	117.76	111.28
2	U	302	PHE	N-CA-C	5.85	121.29	114.04
2	U	333	PRO	N-CA-C	5.82	119.75	110.21
1	x	5	DT	N1-C1'-C2'	-5.77	104.85	113.50
2	U	508	GLU	CA-C-N	5.73	126.12	119.47
2	U	508	GLU	C-N-CA	5.73	126.12	119.47
2	U	118	PRO	N-CA-C	-5.73	102.20	111.03
4	V	577	ILE	CA-C-N	5.65	135.59	121.80
4	V	577	ILE	C-N-CA	5.65	135.59	121.80
2	U	417	HIS	N-CA-C	5.65	120.17	113.28
2	U	95	MET	CA-C-N	-5.63	118.43	123.33
2	U	95	MET	C-N-CA	-5.63	118.43	123.33
2	U	479	LYS	N-CA-C	-5.52	106.91	113.97
2	U	98	ALA	N-CA-C	-5.47	101.88	110.36
2	U	393	SER	N-CA-C	5.41	120.29	111.37
2	U	115	ALA	N-CA-C	5.40	117.69	110.35
2	U	461	LYS	N-CA-C	-5.25	102.62	110.23
2	U	648	GLY	N-CA-C	5.17	120.57	111.57
2	U	78	ASN	N-CA-C	5.12	119.15	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	406	MET	N-CA-C	5.08	116.82	111.28
1	x	7	DC	C4'-C3'-O3'	5.08	117.61	110.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	V	191	ARG	Sidechain
4	V	269	LEU	Peptide
4	V	356	SER	Peptide
4	V	417	ARG	Sidechain
4	W	617	ARG	Sidechain
4	W	666	ARG	Sidechain
4	X	335	PRO	Peptide
4	Z	191	ARG	Sidechain
1	x	5	DT	Sidechain
1	x	6	DC	Sidechain

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	x	95	0	60	8	0
2	U	5204	0	5096	216	0
3	A	845	0	865	60	0
3	B	845	0	867	15	0
3	E	845	0	867	55	0
3	F	845	0	865	47	0
3	M	845	0	867	78	0
3	N	845	0	867	12	0
3	S	845	0	867	11	0
3	T	841	0	863	55	0
4	V	5965	0	5953	152	0
4	W	5965	0	5953	143	0
4	X	5965	0	5951	156	0
4	Z	5965	0	5953	96	0
All	All	35915	0	35894	864	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (864) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:110:LEU:CD2	3:T:91:ALA:HA	1.26	1.65
3:A:22:LYS:NZ	3:E:109:LEU:CD2	1.71	1.54
3:A:22:LYS:CE	3:E:109:LEU:HD22	1.34	1.52
2:U:576:TRP:CZ2	4:X:156:HIS:HE1	1.28	1.52
3:M:110:LEU:CD2	3:T:91:ALA:CA	1.92	1.48
3:A:22:LYS:NZ	3:E:109:LEU:HA	1.28	1.47
3:F:87:MET:CE	4:Z:349:ILE:HG21	1.44	1.47
3:M:110:LEU:HD23	3:T:91:ALA:CA	1.44	1.47
3:T:98:ILE:CD1	4:V:337:ASN:HD21	1.28	1.47
3:T:98:ILE:HD12	4:V:337:ASN:ND2	1.25	1.46
3:F:82:ARG:CD	4:X:525:GLU:OE2	1.64	1.45
3:T:98:ILE:CD1	4:V:337:ASN:ND2	1.80	1.45
3:M:110:LEU:HD21	3:T:91:ALA:N	1.31	1.39
3:F:87:MET:HE2	4:Z:349:ILE:CG1	1.51	1.38
3:A:22:LYS:NZ	3:E:109:LEU:CA	1.83	1.38
2:U:504:ASP:OD2	4:X:337:ASN:ND2	1.56	1.37
3:F:87:MET:CE	4:Z:349:ILE:HG12	1.57	1.33
3:A:22:LYS:NZ	3:E:109:LEU:CB	1.91	1.32
3:A:90:HIS:ND1	4:W:564:LYS:NZ	1.74	1.31
3:F:82:ARG:HD2	4:X:525:GLU:OE2	1.15	1.30
2:U:576:TRP:CZ2	4:X:156:HIS:CE1	2.19	1.29
3:A:83:SER:OG	4:W:570:ASN:HB3	1.35	1.23
3:F:90:HIS:CE1	4:Z:554:PRO:HD2	1.72	1.22
3:F:87:MET:CE	4:Z:349:ILE:CG2	2.16	1.21
3:F:82:ARG:CZ	4:X:525:GLU:HB2	1.71	1.20
3:M:78:GLY:HA3	4:V:279:ASN:ND2	1.57	1.19
3:A:22:LYS:NZ	3:E:109:LEU:HD23	1.55	1.19
3:A:90:HIS:CE1	4:W:564:LYS:NZ	2.13	1.17
3:F:82:ARG:NH1	4:X:525:GLU:HB2	1.60	1.16
3:A:105:LEU:HD12	3:E:109:LEU:HD11	1.18	1.15
3:M:110:LEU:CD2	3:T:91:ALA:N	2.08	1.13
3:A:15:GLU:OE1	3:E:106:LYS:HE2	1.47	1.12
3:A:105:LEU:CD1	3:E:109:LEU:HD11	1.82	1.08
2:U:576:TRP:HZ2	4:X:156:HIS:CE1	1.62	1.07
2:U:192:LEU:HD11	3:S:91:ALA:HB2	1.37	1.06
3:A:105:LEU:HD11	3:E:105:LEU:HG	1.14	1.06
3:A:22:LYS:CE	3:E:109:LEU:CD2	2.19	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:584:ARG:NH2	4:X:63:PRO:CD	2.19	1.03
3:F:87:MET:HE2	4:Z:349:ILE:HG12	1.12	1.03
3:A:22:LYS:NZ	3:E:109:LEU:CG	2.20	1.03
2:U:555:LYS:HE2	4:X:323:GLU:HA	1.03	1.03
3:T:98:ILE:HD13	4:V:337:ASN:ND2	1.70	1.02
2:U:612:ALA:CB	4:V:396:ARG:HH21	1.72	1.02
3:M:110:LEU:HD11	3:T:90:HIS:CE1	1.94	1.01
3:M:96:ASP:HB2	4:V:41:THR:HB	1.43	1.00
2:U:584:ARG:HH22	4:X:63:PRO:HD2	1.21	1.00
3:F:87:MET:CE	4:Z:349:ILE:CG1	2.24	1.00
3:F:87:MET:HE3	4:Z:349:ILE:CG2	1.89	0.98
3:A:22:LYS:HE2	3:E:109:LEU:CD2	1.87	0.98
3:M:110:LEU:HD11	3:T:90:HIS:NE2	1.78	0.97
3:M:110:LEU:CD2	3:T:91:ALA:H	1.75	0.97
3:A:87:MET:O	4:W:54:TRP:HZ3	1.44	0.96
3:F:82:ARG:HD3	4:X:525:GLU:OE2	1.63	0.96
3:F:90:HIS:HE1	4:Z:554:PRO:HD2	1.16	0.96
3:M:98:ILE:HB	4:V:42:ARG:HH12	1.28	0.96
3:F:87:MET:HE3	4:Z:349:ILE:HG21	0.96	0.96
2:U:555:LYS:HE2	4:X:323:GLU:CA	1.94	0.95
3:T:98:ILE:HD13	4:V:337:ASN:CG	1.92	0.94
3:A:22:LYS:HE2	3:E:109:LEU:HD22	0.96	0.94
1:x:6:DC:H2''	1:x:7:DC:H5'	1.46	0.94
3:F:87:MET:CE	4:Z:349:ILE:CB	2.47	0.93
2:U:555:LYS:CE	4:X:323:GLU:HA	1.98	0.92
3:A:63:SER:CB	4:W:327:GLU:OE2	2.18	0.91
2:U:226:MET:HE1	2:U:244:ALA:HB2	1.49	0.91
3:M:97:TRP:HD1	4:V:42:ARG:NH2	1.69	0.90
3:T:98:ILE:CD1	4:V:337:ASN:CG	2.44	0.90
3:A:22:LYS:NZ	3:E:109:LEU:HD22	1.53	0.89
3:M:90:HIS:CE1	4:V:38:LEU:HA	2.07	0.89
2:U:584:ARG:NH2	4:X:63:PRO:HD2	1.83	0.89
2:U:612:ALA:HB2	4:V:396:ARG:HH21	1.34	0.88
3:M:110:LEU:CD1	3:T:90:HIS:NE2	2.36	0.88
3:A:87:MET:O	4:W:54:TRP:CZ3	2.27	0.88
3:A:83:SER:OG	4:W:570:ASN:CB	2.21	0.87
2:U:192:LEU:CD1	3:S:91:ALA:HB2	2.05	0.87
3:M:110:LEU:HD21	3:T:91:ALA:CA	1.78	0.87
3:E:60:ARG:HH22	4:W:763:THR:HA	1.37	0.87
2:U:612:ALA:CB	4:V:396:ARG:NH2	2.37	0.86
3:A:22:LYS:NZ	3:E:109:LEU:HB3	1.88	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:584:ARG:NH2	4:X:63:PRO:CG	2.38	0.86
3:F:87:MET:HE2	4:Z:349:ILE:CB	2.06	0.86
3:A:60:ARG:NH1	4:W:61:ILE:O	2.09	0.86
3:M:78:GLY:HA3	4:V:279:ASN:HD22	1.38	0.85
2:U:132:ARG:NH1	2:U:343:GLU:OE2	2.10	0.85
3:F:90:HIS:CE1	4:Z:553:LYS:HB2	2.13	0.84
2:U:504:ASP:OD2	4:X:337:ASN:CG	2.21	0.84
3:A:90:HIS:HB3	4:W:52:LEU:HD22	1.58	0.83
3:M:97:TRP:HD1	4:V:42:ARG:HH22	1.20	0.83
3:A:22:LYS:HZ2	3:E:109:LEU:HA	1.03	0.83
3:F:87:MET:HE2	4:Z:349:ILE:HG13	1.60	0.83
3:F:82:ARG:CZ	4:X:525:GLU:CB	2.56	0.83
3:F:90:HIS:HE1	4:Z:553:LYS:HB2	1.44	0.83
3:M:78:GLY:CA	4:V:279:ASN:ND2	2.41	0.82
3:A:83:SER:HG	4:W:570:ASN:HB3	1.42	0.82
3:E:60:ARG:NH2	4:W:763:THR:HA	1.93	0.82
3:F:82:ARG:CD	4:X:525:GLU:CD	2.52	0.82
3:M:71:VAL:CG2	3:T:103:LYS:HE2	2.09	0.82
2:U:204:ARG:HH12	2:U:626:ASN:HD21	1.28	0.82
3:A:90:HIS:CE1	4:W:564:LYS:HZ3	1.86	0.82
2:U:137:ASP:H	2:U:293:LYS:NZ	1.77	0.82
4:X:584:SER:O	4:X:622:ARG:NH2	2.13	0.80
3:M:106:LYS:HE2	3:T:90:HIS:NE2	1.95	0.80
3:A:22:LYS:HZ2	3:E:109:LEU:HD23	1.45	0.80
2:U:251:ARG:HB2	2:U:255:GLN:HE21	1.44	0.80
3:M:110:LEU:HD21	3:T:91:ALA:H	1.00	0.80
2:U:364:PRO:HA	2:U:387:LEU:HD22	1.61	0.80
3:A:105:LEU:HD11	3:E:105:LEU:CG	1.99	0.79
2:U:612:ALA:HB1	4:V:396:ARG:NH2	1.96	0.79
3:A:63:SER:HB3	4:W:327:GLU:OE2	1.84	0.78
3:F:87:MET:HE1	4:Z:349:ILE:HG12	1.61	0.78
3:M:97:TRP:CD1	4:V:42:ARG:HH22	2.01	0.78
3:A:91:ALA:HB1	4:W:65:MET:CE	2.14	0.77
3:M:110:LEU:HD23	3:T:91:ALA:CB	2.15	0.76
2:U:576:TRP:CH2	4:X:156:HIS:CE1	2.73	0.76
3:F:87:MET:HE2	4:Z:349:ILE:CG2	2.00	0.76
3:A:83:SER:OG	4:W:570:ASN:C	2.29	0.75
3:A:83:SER:CB	4:W:570:ASN:HB3	2.16	0.75
2:U:576:TRP:HZ2	4:X:156:HIS:HE1	0.76	0.75
2:U:95:MET:HE3	2:U:245:ALA:CB	2.17	0.74
3:A:15:GLU:OE1	3:E:106:LYS:CE	2.33	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:417:HIS:ND1	2:U:474:MET:HE1	2.02	0.74
2:U:203:TYR:HE1	2:U:271:THR:HG22	1.51	0.74
4:Z:18:GLN:NE2	4:Z:543:PRO:O	2.20	0.74
3:A:91:ALA:CB	4:W:65:MET:HE3	2.18	0.73
2:U:251:ARG:HH11	2:U:255:GLN:HE22	1.35	0.73
2:U:51:LEU:CD1	2:U:90:MET:HE1	2.19	0.73
3:M:78:GLY:HA3	4:V:279:ASN:HD21	1.52	0.73
1:x:3:DT:H4'	1:x:4:DT:OP2	1.88	0.72
2:U:612:ALA:HB1	4:V:396:ARG:HH21	1.53	0.72
2:U:273:MET:HE1	2:U:365:VAL:HG11	1.69	0.72
3:M:81:TYR:CD2	4:V:282:ASP:OD2	2.42	0.72
2:U:78:ASN:ND2	2:U:80:VAL:H	1.88	0.72
3:A:105:LEU:CD1	3:E:109:LEU:CD1	2.66	0.72
2:U:203:TYR:CE1	2:U:271:THR:HG22	2.25	0.71
4:V:77:GLY:O	4:V:474:ARG:NH2	2.22	0.71
3:M:90:HIS:CE1	4:V:38:LEU:CA	2.72	0.71
4:Z:14:ARG:O	4:Z:17:THR:HG22	1.89	0.71
3:E:60:ARG:HH12	4:W:763:THR:HG22	1.55	0.71
3:E:90:HIS:CB	4:W:676:ARG:HB3	2.21	0.71
3:M:78:GLY:CA	4:V:279:ASN:HD22	2.01	0.70
2:U:1:PRO:HG2	2:U:238:GLU:OE1	1.90	0.70
2:U:128:ARG:HG3	2:U:339:LEU:HD21	1.74	0.70
2:U:417:HIS:CE1	2:U:474:MET:HE1	2.26	0.69
3:E:60:ARG:HH12	4:W:763:THR:HA	1.56	0.69
3:M:74:MET:CE	4:V:41:THR:CG2	2.71	0.69
3:E:60:ARG:NH1	4:W:763:THR:HA	2.07	0.69
3:E:60:ARG:HH12	4:W:763:THR:CB	2.04	0.69
4:V:425:SER:O	4:W:116:ARG:NH2	2.25	0.68
3:F:87:MET:HE1	4:Z:349:ILE:CB	2.23	0.68
2:U:315:LYS:HZ2	4:X:41:THR:HG22	1.59	0.68
2:U:143:LEU:HD21	2:U:284:MET:HE2	1.75	0.68
3:M:74:MET:CE	4:V:41:THR:HG23	2.25	0.67
2:U:315:LYS:HZ2	4:X:41:THR:CG2	2.08	0.67
3:M:110:LEU:CD1	3:T:90:HIS:CE1	2.74	0.67
3:A:90:HIS:CE1	4:W:564:LYS:HZ1	2.00	0.67
3:M:96:ASP:OD2	4:V:41:THR:C	2.38	0.67
1:x:3:DT:H5'	2:U:26:GLN:HE21	1.60	0.67
3:M:71:VAL:CG2	3:T:103:LYS:CE	2.73	0.67
2:U:249:ALA:O	2:U:260:VAL:HG21	1.95	0.66
4:X:155:CYS:O	4:X:159:SER:N	2.29	0.66
4:X:483:MET:SD	4:X:484:PHE:N	2.69	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:69:LEU:CD1	3:T:107:SER:HB2	2.26	0.65
2:U:596:LEU:HD21	4:V:391:PRO:HG3	1.78	0.65
3:M:45:ILE:HD11	3:T:93:PRO:HB3	1.78	0.65
4:X:121:ASP:OD2	4:X:217:LYS:NZ	2.29	0.65
2:U:663:PRO:O	2:U:664:ARG:CZ	2.43	0.65
3:E:60:ARG:HH12	4:W:763:THR:CA	2.08	0.65
4:X:135:LEU:HD12	4:X:151:THR:HG22	1.78	0.65
4:X:9:LEU:HD22	4:X:13:ALA:HB2	1.78	0.65
3:M:74:MET:HE1	4:V:39:GLN:O	1.97	0.65
2:U:95:MET:HE3	2:U:245:ALA:HB3	1.79	0.64
4:X:342:TYR:N	4:X:559:GLU:OE2	2.30	0.64
2:U:518:ILE:HB	2:U:561:CYS:SG	2.37	0.64
3:F:82:ARG:NE	4:X:525:GLU:CD	2.56	0.64
3:M:97:TRP:CD1	4:V:42:ARG:NH2	2.60	0.64
2:U:552:ALA:HB3	2:U:619:LEU:HD13	1.79	0.63
2:U:663:PRO:HG2	2:U:664:ARG:H	1.64	0.63
3:A:83:SER:HA	4:W:570:ASN:OD1	1.97	0.63
4:Z:354:GLN:NE2	4:Z:528:ILE:O	2.31	0.63
3:A:105:LEU:CD1	3:E:105:LEU:HG	2.06	0.63
3:E:60:ARG:CZ	4:W:763:THR:HA	2.28	0.63
4:X:477:ASN:OD1	4:X:481:ARG:NH1	2.31	0.63
2:U:175:GLU:HA	2:U:352:TRP:CE3	2.34	0.63
3:A:91:ALA:HB2	4:W:65:MET:HE3	1.80	0.63
1:x:6:DC:H2''	1:x:7:DC:C5'	2.24	0.63
3:A:86:ASN:HB2	4:W:570:ASN:OD1	1.99	0.63
3:M:96:ASP:CB	4:V:41:THR:HB	2.25	0.63
3:F:90:HIS:CE1	4:Z:554:PRO:CD	2.66	0.62
4:V:578:TRP:HB2	4:V:579:PRO:HD2	1.81	0.62
2:U:650:SER:OG	2:U:653:LYS:HG3	1.99	0.62
4:W:707:LEU:HD12	4:W:707:LEU:O	1.98	0.62
3:M:74:MET:HE2	4:V:41:THR:HG21	1.81	0.62
4:V:345:GLN:NE2	4:V:553:LYS:O	2.31	0.62
2:U:251:ARG:HB2	2:U:255:GLN:NE2	2.14	0.62
3:E:60:ARG:HH12	4:W:763:THR:CG2	2.11	0.62
2:U:364:PRO:HA	2:U:387:LEU:CD2	2.29	0.62
2:U:401:MET:HE2	2:U:401:MET:HA	1.80	0.62
3:A:109:LEU:HD21	3:E:105:LEU:HD11	1.80	0.62
2:U:658:LEU:HG	2:U:662:MET:HE2	1.81	0.62
4:W:87:ASN:OD1	4:W:191:ARG:NH2	2.32	0.62
2:U:137:ASP:H	2:U:293:LYS:HZ2	1.47	0.62
3:S:34:HIS:HA	3:S:37:TRP:NE1	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:34:HIS:HA	3:A:37:TRP:NE1	2.15	0.62
2:U:465:LEU:O	2:U:465:LEU:HD12	2.00	0.62
3:E:34:HIS:HA	3:E:37:TRP:NE1	2.15	0.62
4:Z:740:ARG:NH2	4:Z:744:GLU:OE2	2.33	0.62
2:U:2:ARG:HD2	2:U:2:ARG:O	1.99	0.61
2:U:315:LYS:NZ	4:X:41:THR:CG2	2.63	0.61
2:U:78:ASN:HD22	2:U:79:GLY:N	1.98	0.61
2:U:584:ARG:NH2	4:X:63:PRO:HG3	2.14	0.61
2:U:652:GLU:CD	2:U:652:GLU:H	2.08	0.61
3:A:34:HIS:HA	3:A:37:TRP:HE1	1.66	0.61
3:M:34:HIS:HA	3:M:37:TRP:HE1	1.66	0.61
3:M:34:HIS:HA	3:M:37:TRP:NE1	2.15	0.61
4:V:586:GLU:OE2	4:V:622:ARG:NH1	2.34	0.61
2:U:391:LEU:HD22	2:U:398:THR:HG22	1.82	0.60
3:E:34:HIS:HA	3:E:37:TRP:HE1	1.66	0.60
3:M:68:GLU:HG2	3:T:45:ILE:HD12	1.83	0.60
2:U:137:ASP:H	2:U:293:LYS:HZ3	1.47	0.60
3:A:91:ALA:CB	4:W:65:MET:CE	2.77	0.60
2:U:251:ARG:HH11	2:U:255:GLN:NE2	2.00	0.60
2:U:86:GLY:O	2:U:89:HIS:HD2	1.85	0.60
3:S:34:HIS:HA	3:S:37:TRP:HE1	1.66	0.60
4:W:674:LEU:HD23	4:W:674:LEU:C	2.26	0.60
3:E:90:HIS:HB3	4:W:676:ARG:HB3	1.81	0.60
3:M:96:ASP:OD2	4:V:41:THR:O	2.20	0.60
4:W:700:ASP:OD2	4:X:31:VAL:N	2.35	0.60
3:E:60:ARG:NH1	4:W:763:THR:CB	2.65	0.60
3:M:91:ALA:O	3:T:106:LYS:HE2	2.02	0.60
4:V:48:MET:O	4:V:49:THR:HG22	2.01	0.59
4:W:24:GLU:OE1	4:W:506:HIS:NE2	2.28	0.59
4:V:657:ASP:OD1	4:V:658:ALA:N	2.36	0.59
4:X:713:ASP:O	4:X:716:VAL:HG22	2.02	0.59
2:U:90:MET:HA	2:U:90:MET:HE2	1.84	0.59
4:Z:396:ARG:NH2	4:Z:612:LEU:O	2.35	0.59
3:M:77:PRO:O	4:V:279:ASN:HB3	2.02	0.59
3:M:69:LEU:HD12	3:T:107:SER:HB2	1.85	0.59
3:M:74:MET:CE	4:V:39:GLN:O	2.51	0.59
2:U:301:THR:HG22	2:U:448:GLN:O	2.03	0.59
4:W:512:GLU:HB3	4:W:515:SER:HB2	1.85	0.58
3:M:73:VAL:HG11	3:M:100:LEU:HD11	1.84	0.58
3:S:73:VAL:HG11	3:S:100:LEU:HD11	1.84	0.58
3:M:98:ILE:HB	4:V:42:ARG:NH1	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:51:LEU:HD13	2:U:90:MET:HE1	1.85	0.58
2:U:76:TYR:HA	2:U:502:LEU:HD12	1.85	0.58
3:E:73:VAL:HG11	3:E:100:LEU:HD11	1.84	0.58
3:F:87:MET:HE1	4:Z:349:ILE:HG21	1.69	0.58
4:W:51:GLU:OE1	4:W:176:ARG:N	2.35	0.58
4:X:269:LEU:O	4:X:274:ARG:NH1	2.37	0.58
2:U:584:ARG:HH21	4:X:63:PRO:CD	2.10	0.58
2:U:206:GLN:HE21	2:U:268:ARG:HH11	1.51	0.58
3:A:73:VAL:HG11	3:A:100:LEU:HD11	1.84	0.58
3:M:81:TYR:CG	4:V:282:ASP:OD2	2.57	0.58
3:M:74:MET:CE	4:V:41:THR:HG21	2.34	0.58
4:W:598:ARG:NH1	4:W:710:ASP:OD1	2.36	0.58
2:U:181:MET:HG2	2:U:186:PHE:CD2	2.39	0.57
2:U:132:ARG:HA	2:U:347:MET:HE3	1.86	0.57
2:U:336:LEU:O	2:U:340:ILE:HG13	2.04	0.57
4:Z:17:THR:HG23	4:Z:20:PHE:H	1.69	0.57
2:U:88:ARG:HD3	2:U:263:GLY:O	2.04	0.57
3:F:82:ARG:NE	4:X:525:GLU:OE2	2.34	0.57
4:Z:448:ASP:OD1	4:Z:453:ARG:NH2	2.38	0.57
2:U:51:LEU:HD11	2:U:90:MET:HE1	1.85	0.57
4:X:314:SER:HA	4:X:317:ILE:HG12	1.87	0.57
3:M:110:LEU:HD13	3:T:90:HIS:NE2	2.18	0.57
4:Z:55:GLU:OE2	4:Z:58:LYS:NZ	2.35	0.57
1:x:3:DT:H5'	2:U:26:GLN:NE2	2.19	0.56
4:Z:83:ASP:OD1	4:Z:84:GLU:N	2.38	0.56
4:Z:395:ASP:OD1	4:Z:395:ASP:N	2.38	0.56
4:X:147:HIS:O	4:X:151:THR:HG23	2.05	0.56
3:E:90:HIS:HB2	4:W:676:ARG:HB3	1.87	0.56
4:V:710:ASP:O	4:V:713:ASP:N	2.39	0.56
4:X:210:LEU:HD23	4:X:210:LEU:H	1.69	0.56
2:U:71:GLU:H	2:U:71:GLU:CD	2.14	0.56
3:A:90:HIS:CE1	4:W:564:LYS:HZ2	2.19	0.56
3:F:82:ARG:NH1	4:X:525:GLU:CB	2.52	0.56
4:W:766:ASP:OD2	4:Z:666:ARG:NH2	2.39	0.56
2:U:32:PHE:CD2	2:U:372:PRO:HG3	2.41	0.56
3:N:82:ARG:NH1	3:N:84:ASP:OD2	2.39	0.56
4:V:22:ILE:HG22	4:V:23:GLY:N	2.21	0.56
3:M:71:VAL:HG23	3:T:103:LYS:HE2	1.88	0.56
2:U:72:TYR:CE1	2:U:476:LYS:HD3	2.41	0.55
3:B:82:ARG:NH1	3:B:84:ASP:OD2	2.39	0.55
3:M:75:ALA:HB1	4:V:283:GLN:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:110:LEU:HD23	3:T:91:ALA:HA	0.59	0.55
2:U:315:LYS:NZ	4:X:41:THR:HG22	2.20	0.55
2:U:55:ASN:OD1	2:U:88:ARG:NH2	2.37	0.55
2:U:280:ASN:HD21	2:U:395:GLN:HA	1.71	0.55
4:X:637:TYR:CZ	4:X:641:VAL:HG11	2.41	0.55
4:X:92:TYR:CZ	4:X:96:THR:HG21	2.42	0.55
2:U:420:PRO:HA	2:U:423:ASN:ND2	2.22	0.55
2:U:650:SER:OG	2:U:653:LYS:CG	2.54	0.55
4:W:389:VAL:HG22	4:W:390:GLU:N	2.22	0.55
4:X:417:ARG:NH1	4:X:642:GLU:OE1	2.40	0.55
4:X:675:LEU:HD21	4:X:750:LEU:HD22	1.89	0.54
2:U:584:ARG:HH21	4:X:63:PRO:CG	2.18	0.54
4:V:81:SER:N	4:V:84:GLU:OE2	2.34	0.54
4:Z:370:ILE:HD12	4:Z:371:THR:H	1.72	0.54
2:U:288:GLN:HB3	2:U:289:PRO:HD3	1.88	0.54
3:T:82:ARG:NH1	3:T:84:ASP:OD2	2.39	0.54
4:X:196:ARG:HG2	4:X:196:ARG:HH11	1.73	0.54
2:U:401:MET:HE2	2:U:401:MET:CA	2.37	0.54
3:E:90:HIS:CB	4:W:676:ARG:CB	2.85	0.54
2:U:74:ARG:HB3	2:U:503:TYR:CD2	2.42	0.54
3:M:106:LYS:HE2	3:T:90:HIS:CD2	2.42	0.54
3:M:90:HIS:CE1	4:V:38:LEU:C	2.86	0.54
2:U:584:ARG:HH21	4:X:63:PRO:HG3	1.72	0.54
3:M:110:LEU:CD2	3:T:91:ALA:CB	2.78	0.54
4:V:38:LEU:HD12	4:V:38:LEU:O	2.08	0.53
4:Z:334:ARG:NH1	4:Z:338:GLU:OE2	2.37	0.53
4:W:448:ASP:OD1	4:W:453:ARG:NH1	2.40	0.53
4:X:125:LYS:HB3	4:X:163:PHE:HA	1.90	0.53
4:Z:341:SER:HG	4:Z:558:SER:HG	1.54	0.53
2:U:3:ARG:O	2:U:3:ARG:HG3	2.09	0.53
2:U:194:GLN:O	2:U:278:ALA:HB3	2.09	0.53
2:U:525:GLN:NE2	2:U:583:TYR:OH	2.41	0.53
4:X:413:PHE:N	4:X:413:PHE:CD1	2.75	0.53
2:U:160:MET:O	2:U:164:ILE:HG12	2.09	0.53
3:F:82:ARG:NH1	3:F:84:ASP:OD2	2.39	0.53
3:M:81:TYR:HB2	4:V:282:ASP:OD2	2.09	0.53
4:W:354:GLN:OE1	4:W:528:ILE:HB	2.08	0.53
4:X:417:ARG:NH2	4:X:642:GLU:OE1	2.39	0.53
2:U:132:ARG:HD2	2:U:429:MET:HE2	1.91	0.53
2:U:138:LEU:HB2	2:U:662:MET:SD	2.48	0.53
4:X:387:LEU:CB	4:X:577:ILE:HD11	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:29:LYS:O	2:U:30:ARG:C	2.52	0.53
3:E:90:HIS:HB2	4:W:676:ARG:CB	2.39	0.53
4:V:413:PHE:CD1	4:V:413:PHE:N	2.76	0.53
4:X:584:SER:OG	4:X:624:LEU:HA	2.09	0.53
3:T:98:ILE:HD12	4:V:337:ASN:HD21	0.43	0.52
4:X:386:PHE:CZ	4:X:573:THR:HA	2.45	0.52
4:Z:400:THR:OG1	4:Z:735:MET:HE1	2.09	0.52
2:U:132:ARG:HA	2:U:347:MET:CE	2.38	0.52
4:Z:460:ALA:O	4:Z:464:THR:HG22	2.10	0.52
2:U:7:PHE:CD1	2:U:7:PHE:N	2.77	0.52
2:U:230:PHE:O	2:U:234:VAL:HG22	2.10	0.52
4:V:362:GLU:OE2	4:V:364:TRP:NE1	2.36	0.52
4:X:675:LEU:CD2	4:X:750:LEU:HD22	2.39	0.52
2:U:495:ALA:HB2	2:U:500:ILE:HG12	1.91	0.52
3:F:84:ASP:OD2	4:X:527:ARG:NH1	2.43	0.52
4:W:386:PHE:HB3	4:W:575:ILE:HA	1.92	0.52
2:U:280:ASN:ND2	2:U:396:GLY:H	2.07	0.52
2:U:596:LEU:HD21	4:V:391:PRO:HB3	1.91	0.52
4:W:566:LEU:HD22	4:W:566:LEU:H	1.74	0.52
4:X:18:GLN:NE2	4:X:543:PRO:O	2.42	0.52
4:V:417:ARG:CZ	4:V:421:TYR:CE2	2.93	0.52
2:U:146:ARG:NH2	2:U:540:SER:O	2.42	0.52
2:U:368:GLY:O	2:U:375:GLY:HA3	2.10	0.52
2:U:281:ALA:HB3	2:U:282:PRO:CD	2.40	0.51
3:E:60:ARG:NH1	4:W:763:THR:HG22	2.24	0.51
3:A:83:SER:CB	4:W:570:ASN:CB	2.85	0.51
4:V:158:LEU:HD11	4:V:164:ILE:HA	1.93	0.51
4:X:10:ASN:HA	4:X:13:ALA:HB3	1.92	0.51
4:V:402:ALA:HB3	4:V:403:PRO:HD3	1.93	0.51
4:W:3:ASN:O	4:W:463:ARG:NH2	2.24	0.51
2:U:328:HIS:HD2	2:U:329:ASP:OD1	1.94	0.51
2:U:140:PRO:HG3	2:U:658:LEU:HD23	1.91	0.51
3:A:63:SER:HB2	4:W:327:GLU:OE2	2.09	0.51
3:E:60:ARG:NH1	4:W:763:THR:CA	2.70	0.51
3:M:81:TYR:CB	4:V:282:ASP:OD2	2.58	0.51
4:V:362:GLU:OE2	4:V:443:SER:N	2.38	0.51
3:A:91:ALA:HB1	4:W:65:MET:HE3	1.83	0.51
4:W:586:GLU:OE1	4:W:622:ARG:NH2	2.42	0.51
4:X:572:THR:HG23	4:X:575:ILE:HD11	1.92	0.51
2:U:268:ARG:HH22	2:U:270:ARG:HH21	1.59	0.51
2:U:280:ASN:O	2:U:284:MET:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:91:ALA:HB2	4:W:676:ARG:CZ	2.41	0.51
3:F:82:ARG:NH2	4:X:525:GLU:HB2	2.21	0.51
4:V:209:MET:SD	4:V:209:MET:C	2.93	0.51
3:T:3:LEU:HD23	3:T:70:PRO:HB3	1.93	0.51
4:W:413:PHE:CE2	4:W:636:TRP:HB2	2.46	0.51
4:Z:55:GLU:CD	4:Z:55:GLU:H	2.19	0.51
3:M:110:LEU:HD11	3:T:90:HIS:CD2	2.44	0.51
4:Z:118:ILE:HD12	4:Z:119:LYS:N	2.26	0.51
4:V:417:ARG:NH1	4:V:643:ASP:OD1	2.44	0.50
3:N:3:LEU:HD23	3:N:70:PRO:HB3	1.93	0.50
4:X:578:TRP:HB2	4:X:579:PRO:HD2	1.92	0.50
3:E:60:ARG:NH1	4:W:763:THR:HB	2.25	0.50
4:W:598:ARG:NH2	4:W:710:ASP:OD1	2.42	0.50
2:U:584:ARG:HH22	4:X:63:PRO:CD	1.88	0.50
4:V:176:ARG:CZ	4:V:176:ARG:HA	2.41	0.50
4:Z:258:GLY:HA3	4:Z:294:TYR:CE2	2.47	0.50
2:U:332:TRP:CZ2	2:U:401:MET:HB3	2.47	0.50
4:V:214:PHE:CE1	4:V:217:LYS:HE2	2.47	0.50
4:V:523:ARG:HA	4:V:539:SER:HA	1.93	0.50
4:W:71:PHE:CD1	4:W:71:PHE:N	2.78	0.50
4:V:96:THR:HG23	4:V:97:ALA:N	2.26	0.50
3:E:87:MET:SD	4:W:758:MET:SD	3.10	0.50
3:E:90:HIS:CD2	4:W:673:THR:HG22	2.47	0.50
4:V:31:VAL:HG12	4:V:31:VAL:O	2.12	0.50
4:Z:413:PHE:CE2	4:Z:636:TRP:HB2	2.47	0.50
2:U:78:ASN:HD22	2:U:78:ASN:C	2.19	0.50
2:U:364:PRO:HB3	2:U:379:LEU:O	2.12	0.50
3:B:3:LEU:HD23	3:B:70:PRO:HB3	1.93	0.50
3:E:90:HIS:HB3	4:W:676:ARG:CB	2.42	0.50
3:M:90:HIS:NE2	4:V:38:LEU:HA	2.27	0.50
4:V:4:LEU:HA	4:V:12:SER:HB3	1.94	0.50
4:W:605:GLU:O	4:W:697:ARG:NH1	2.40	0.50
2:U:429:MET:HB2	2:U:430:PRO:HD3	1.93	0.49
4:V:209:MET:SD	4:V:210:LEU:N	2.85	0.49
4:X:269:LEU:O	4:X:270:ASP:C	2.55	0.49
2:U:175:GLU:HA	2:U:352:TRP:CD2	2.46	0.49
4:Z:329:SER:OG	4:Z:330:PRO:HD2	2.11	0.49
4:Z:567:ASP:OD1	4:Z:568:LEU:N	2.45	0.49
2:U:119:VAL:HG12	2:U:485:TYR:CZ	2.48	0.49
4:W:427:ARG:HD2	4:Z:708:ILE:HG23	1.95	0.49
4:Z:679:GLU:OE2	4:Z:724:ARG:NH1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:121:ASP:OD1	4:W:122:ALA:N	2.45	0.49
2:U:95:MET:HE3	2:U:245:ALA:HB2	1.94	0.49
3:F:3:LEU:HD23	3:F:70:PRO:HB3	1.93	0.49
3:M:68:GLU:OE2	3:T:2:THR:HG21	2.11	0.49
4:X:51:GLU:OE1	4:X:173:ARG:NH2	2.42	0.49
4:Z:472:GLU:HG2	4:Z:475:ALA:H	1.77	0.49
2:U:268:ARG:NH2	2:U:270:ARG:HH21	2.10	0.49
2:U:596:LEU:HD21	4:V:391:PRO:CG	2.41	0.49
3:A:83:SER:OG	4:W:571:HIS:N	2.46	0.49
4:X:472:GLU:OE2	4:X:475:ALA:N	2.43	0.49
2:U:273:MET:HE1	2:U:365:VAL:CG1	2.42	0.49
3:B:56:ALA:HB1	4:W:204:SER:HB2	1.94	0.49
4:X:417:ARG:NE	4:X:421:TYR:OH	2.46	0.49
4:X:584:SER:OG	4:X:625:LYS:N	2.45	0.49
2:U:662:MET:HB3	2:U:663:PRO:HD2	1.95	0.48
4:V:350:ASP:C	4:V:350:ASP:OD1	2.55	0.48
4:V:360:VAL:O	4:V:440:GLY:N	2.36	0.48
4:X:126:VAL:O	4:X:164:ILE:HA	2.12	0.48
2:U:286:VAL:HG21	2:U:353:TRP:CZ2	2.48	0.48
4:W:606:VAL:HG11	4:W:611:LEU:HD21	1.95	0.48
4:Z:155:CYS:O	4:Z:159:SER:N	2.45	0.48
4:X:387:LEU:HB3	4:X:577:ILE:HD11	1.95	0.48
4:Z:544:GLU:CD	4:Z:545:PRO:HD2	2.38	0.48
2:U:642:HIS:CE1	2:U:646:MET:HG3	2.48	0.48
2:U:119:VAL:HG12	2:U:485:TYR:OH	2.14	0.48
3:M:71:VAL:HG21	3:T:103:LYS:CE	2.43	0.48
4:W:589:TYR:N	4:W:608:GLU:OE2	2.47	0.48
4:X:172:TYR:HA	4:X:578:TRP:HB3	1.96	0.48
4:Z:53:LEU:HG	4:Z:566:LEU:HD11	1.94	0.48
2:U:232:TYR:CE1	2:U:242:LEU:HB2	2.49	0.48
2:U:62:THR:HG23	2:U:83:ASN:HB2	1.95	0.48
4:X:402:ALA:HB3	4:X:403:PRO:HD3	1.96	0.48
4:Z:295:GLN:NE2	4:Z:516:LEU:O	2.39	0.48
4:Z:548:ALA:O	4:Z:552:ASN:ND2	2.44	0.48
2:U:232:TYR:CE2	2:U:237:GLY:HA2	2.49	0.48
3:M:74:MET:HE3	4:V:41:THR:HG23	1.96	0.48
4:V:136:ARG:NH1	4:V:144:GLU:OE1	2.46	0.48
4:X:631:ALA:HA	4:X:634:GLN:HE21	1.79	0.48
3:B:56:ALA:CB	4:W:204:SER:HB2	2.43	0.48
4:W:262:SER:OG	4:W:265:THR:HG23	2.14	0.48
4:X:183:PHE:CD1	4:X:297:MET:HB3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:373:PHE:CE1	4:X:622:ARG:HB2	2.49	0.48
2:U:136:SER:OG	2:U:293:LYS:NZ	2.46	0.48
4:W:676:ARG:NH1	4:W:679:GLU:OE1	2.34	0.48
3:E:91:ALA:HB2	4:W:676:ARG:NH1	2.28	0.47
4:X:105:LYS:HD2	4:X:138:LEU:HD21	1.96	0.47
4:V:158:LEU:HD11	4:V:164:ILE:CA	2.44	0.47
4:X:207:SER:HA	4:X:210:LEU:HD21	1.95	0.47
2:U:102:LEU:HD12	2:U:233:ALA:HA	1.96	0.47
4:X:507:GLN:HB2	4:X:509:VAL:HG23	1.96	0.47
4:W:262:SER:CB	4:W:265:THR:HG23	2.43	0.47
4:W:595:VAL:HG22	4:W:596:THR:N	2.30	0.47
4:X:66:TYR:CD1	4:X:149:ILE:HD13	2.48	0.47
4:X:707:LEU:HD23	4:X:707:LEU:N	2.29	0.47
4:Z:649:ALA:O	4:Z:652:ARG:HG2	2.15	0.47
3:F:87:MET:SD	4:Z:349:ILE:HG12	2.51	0.47
4:Z:341:SER:OG	4:Z:558:SER:OG	2.27	0.47
2:U:7:PHE:CE2	2:U:13:LYS:HD2	2.49	0.47
2:U:12:ILE:O	2:U:16:MET:HG3	2.15	0.47
2:U:331:PHE:O	2:U:332:TRP:C	2.58	0.47
3:M:90:HIS:HE1	4:V:39:GLN:N	2.13	0.47
4:V:370:ILE:CD1	4:V:626:PRO:HB3	2.45	0.47
4:X:314:SER:HA	4:X:317:ILE:CG1	2.45	0.47
4:X:675:LEU:HG	4:X:750:LEU:HD22	1.95	0.47
4:Z:307:ILE:HD12	4:Z:307:ILE:N	2.30	0.47
2:U:202:VAL:HG22	2:U:272:ALA:HB3	1.96	0.47
2:U:222:SER:HB3	2:U:265:PHE:CD2	2.49	0.47
3:M:4:TYR:OH	3:M:103:LYS:NZ	2.32	0.47
4:V:177:THR:HG22	4:V:178:ALA:N	2.29	0.47
2:U:488:ILE:HG22	2:U:489:SER:N	2.30	0.47
4:X:175:GLY:O	4:X:177:THR:HG23	2.15	0.47
4:X:400:THR:OG1	4:X:686:ILE:HG12	2.14	0.47
4:X:483:MET:SD	4:X:483:MET:C	2.98	0.47
3:B:96:ASP:OD1	3:B:97:TRP:N	2.48	0.47
4:Z:362:GLU:CG	4:Z:442:PRO:HD2	2.46	0.47
4:Z:589:TYR:CD1	4:Z:734:MET:HA	2.49	0.47
4:Z:618:ARG:HH11	4:Z:618:ARG:HG2	1.80	0.47
4:Z:707:LEU:HD12	4:Z:707:LEU:C	2.40	0.47
3:F:96:ASP:OD1	3:F:97:TRP:N	2.48	0.46
4:X:53:LEU:HA	4:X:173:ARG:HA	1.98	0.46
2:U:308:LEU:HD11	4:X:42:ARG:NH2	2.30	0.46
2:U:543:LYS:O	2:U:625:PRO:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:65:MET:SD	4:V:65:MET:C	2.99	0.46
4:W:145:LEU:HA	4:W:148:HIS:ND1	2.31	0.46
4:W:449:TYR:CE1	4:W:630:HIS:CE1	3.03	0.46
4:Z:68:ARG:CZ	4:Z:174:VAL:HG11	2.45	0.46
4:V:483:MET:SD	4:V:483:MET:C	2.98	0.46
4:Z:449:TYR:HB2	4:Z:627:THR:HG23	1.96	0.46
2:U:143:LEU:HB3	2:U:649:VAL:HG23	1.98	0.46
3:A:4:TYR:OH	3:A:103:LYS:NZ	2.32	0.46
3:A:22:LYS:CD	3:E:109:LEU:HB3	2.45	0.46
3:A:105:LEU:O	3:A:109:LEU:HG	2.15	0.46
3:E:105:LEU:O	3:E:109:LEU:HG	2.15	0.46
3:N:96:ASP:OD1	3:N:97:TRP:N	2.48	0.46
4:V:709:ASP:OD1	4:V:709:ASP:N	2.49	0.46
4:X:145:LEU:O	4:X:149:ILE:HG22	2.15	0.46
4:X:387:LEU:HD22	4:X:572:THR:HG21	1.98	0.46
4:W:108:ALA:O	4:W:112:GLY:N	2.43	0.46
4:W:260:LEU:HD13	4:W:285:ARG:HE	1.80	0.46
4:Z:442:PRO:O	4:Z:445:VAL:HG22	2.16	0.46
4:Z:448:ASP:OD1	4:Z:453:ARG:NH1	2.48	0.46
2:U:231:GLU:O	2:U:235:THR:HG23	2.15	0.46
4:V:716:VAL:HG13	4:W:386:PHE:CE2	2.51	0.46
2:U:504:ASP:OD2	4:X:337:ASN:OD1	2.33	0.46
3:F:84:ASP:OD1	3:F:84:ASP:N	2.48	0.46
3:S:105:LEU:O	3:S:109:LEU:HG	2.15	0.46
3:T:96:ASP:OD1	3:T:97:TRP:N	2.48	0.46
4:V:214:PHE:CD1	4:V:217:LYS:HE2	2.50	0.46
4:V:482:SER:HA	4:V:485:ASN:ND2	2.31	0.46
3:M:69:LEU:HD11	3:T:107:SER:HB2	1.96	0.46
4:X:265:THR:HG23	4:X:265:THR:O	2.16	0.46
2:U:301:THR:HG23	2:U:440:TRP:O	2.16	0.46
4:Z:191:ARG:NH1	4:Z:243:ASN:OD1	2.49	0.46
2:U:630:TYR:CD1	2:U:630:TYR:C	2.94	0.45
4:V:127:PRO:HD3	4:V:165:LEU:HD23	1.98	0.45
4:W:132:LEU:HG	4:W:151:THR:HG21	1.96	0.45
4:X:344:GLY:CA	4:X:557:PRO:HG3	2.45	0.45
4:Z:400:THR:HG21	4:Z:686:ILE:CG1	2.46	0.45
4:Z:713:ASP:O	4:Z:716:VAL:HG12	2.16	0.45
4:X:9:LEU:HD23	4:X:12:SER:OG	2.17	0.45
4:X:55:GLU:HA	4:X:170:TYR:O	2.16	0.45
2:U:280:ASN:ND2	2:U:396:GLY:N	2.64	0.45
4:W:329:SER:HB2	4:W:330:PRO:CD	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:149:SER:OG	2:U:163:LYS:HE3	2.16	0.45
2:U:418:THR:HG21	2:U:468:GLY:HA2	1.98	0.45
2:U:596:LEU:HD21	4:V:391:PRO:CB	2.46	0.45
4:W:45:SER:O	4:W:334:ARG:NH2	2.40	0.45
4:W:70:PHE:CD1	4:W:145:LEU:HD21	2.51	0.45
4:X:471:LEU:HD11	4:X:476:SER:HB3	1.99	0.45
4:X:524:THR:CG2	4:X:526:LEU:H	2.29	0.45
4:X:675:LEU:CG	4:X:750:LEU:HD22	2.47	0.45
3:M:105:LEU:O	3:M:109:LEU:HG	2.15	0.45
4:X:577:ILE:HG22	4:X:578:TRP:N	2.32	0.45
4:Z:87:ASN:OD1	4:Z:191:ARG:NH2	2.48	0.45
2:U:86:GLY:O	2:U:89:HIS:CD2	2.69	0.45
3:A:83:SER:OG	4:W:570:ASN:CA	2.64	0.45
3:T:7:PRO:HB2	3:T:80:SER:H	1.82	0.45
4:V:606:VAL:HG21	4:V:611:LEU:HD21	1.99	0.45
4:W:595:VAL:HG22	4:W:596:THR:H	1.81	0.45
4:X:144:GLU:OE1	4:X:148:HIS:ND1	2.49	0.45
4:X:523:ARG:HA	4:X:539:SER:HA	1.97	0.45
4:W:43:THR:O	4:W:333:LEU:HA	2.17	0.45
4:W:107:THR:OG1	4:W:226:SER:OG	2.33	0.45
4:W:378:LEU:HD13	4:W:378:LEU:C	2.41	0.45
4:W:426:GLN:OE1	4:Z:598:ARG:NH2	2.50	0.45
2:U:286:VAL:HG21	2:U:353:TRP:CE2	2.51	0.45
4:W:182:ASN:OD1	4:W:183:PHE:N	2.48	0.45
4:W:437:MET:HE1	4:W:549:ILE:HG21	1.97	0.45
4:W:683:THR:CG2	4:W:724:ARG:HE	2.29	0.45
4:Z:386:PHE:C	4:Z:387:LEU:HD22	2.41	0.45
4:W:48:MET:HE2	4:W:48:MET:HA	1.98	0.45
4:W:195:LEU:HD13	4:W:195:LEU:O	2.17	0.45
4:W:578:TRP:CZ3	4:W:580:TRP:HA	2.52	0.45
4:X:591:ASP:O	4:X:606:VAL:HG12	2.17	0.45
4:Z:370:ILE:HD11	4:Z:624:LEU:O	2.17	0.45
3:B:7:PRO:HG2	3:B:81:TYR:H	1.83	0.44
4:V:92:TYR:CE2	4:V:96:THR:HG21	2.52	0.44
4:V:745:ALA:O	4:V:749:VAL:HG23	2.17	0.44
4:X:105:LYS:CD	4:X:138:LEU:HD21	2.47	0.44
4:X:590:GLU:OE1	4:X:607:LYS:NZ	2.47	0.44
2:U:16:MET:HB3	2:U:16:MET:HE2	1.75	0.44
2:U:564:TYR:O	2:U:565:SER:C	2.59	0.44
3:B:84:ASP:OD1	3:B:85:TRP:N	2.47	0.44
3:M:74:MET:HE3	4:V:41:THR:CG2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:84:ASP:OD1	3:N:84:ASP:N	2.48	0.44
4:V:96:THR:CG2	4:V:97:ALA:N	2.80	0.44
4:V:303:ARG:HH11	4:V:513:GLN:HB3	1.83	0.44
4:W:66:TYR:O	4:W:70:PHE:CD1	2.71	0.44
4:X:128:PRO:O	4:X:131:ILE:HG22	2.18	0.44
2:U:239:GLN:HB3	2:U:240:GLY:H	1.69	0.44
2:U:584:ARG:NH2	4:X:63:PRO:HD3	2.25	0.44
3:F:87:MET:HE1	4:Z:349:ILE:CG1	2.24	0.44
3:M:90:HIS:CE1	4:V:39:GLN:N	2.86	0.44
4:W:588:ALA:HA	4:W:608:GLU:OE2	2.17	0.44
1:x:3:DT:C4'	1:x:4:DT:OP2	2.60	0.44
2:U:521:MET:HB2	2:U:558:TYR:CD2	2.51	0.44
3:B:84:ASP:OD1	3:B:84:ASP:N	2.48	0.44
4:V:155:CYS:HA	4:V:158:LEU:HB3	1.98	0.44
4:Z:117:ALA:HB1	4:Z:122:ALA:HB3	1.99	0.44
2:U:83:ASN:C	2:U:83:ASN:OD1	2.61	0.44
3:B:7:PRO:HB2	3:B:80:SER:H	1.82	0.44
4:V:275:LEU:HA	4:V:311:GLU:HG2	1.99	0.44
4:X:276:ARG:HG2	4:X:276:ARG:HH11	1.83	0.44
4:Z:128:PRO:HD2	4:Z:167:ASP:HB2	1.99	0.44
2:U:168:GLU:HG2	2:U:649:VAL:CG1	2.47	0.44
4:V:14:ARG:HA	4:V:17:THR:CG2	2.48	0.44
4:X:102:ILE:CG2	4:X:103:TRP:N	2.80	0.44
4:Z:71:PHE:O	4:Z:71:PHE:CD1	2.71	0.44
2:U:126:LEU:HA	2:U:126:LEU:HD23	1.75	0.44
3:F:7:PRO:HB2	3:F:80:SER:H	1.82	0.44
4:V:505:GLU:OE2	4:V:507:GLN:HA	2.17	0.44
4:W:197:ARG:O	4:W:200:THR:HG22	2.18	0.44
4:X:9:LEU:HD21	4:X:546:LEU:HD12	2.00	0.44
2:U:583:TYR:CE2	2:U:587:ARG:HD3	2.53	0.44
4:W:346:THR:HG22	4:W:347:SER:N	2.32	0.44
4:X:503:VAL:HG12	4:X:518:LEU:CD2	2.48	0.44
2:U:122:ARG:NH1	2:U:423:ASN:OD1	2.45	0.44
2:U:166:ILE:HG21	2:U:277:PHE:HD2	1.83	0.44
2:U:195:MET:HE2	2:U:278:ALA:O	2.18	0.44
2:U:256:TYR:HB2	2:U:258:ILE:HG13	1.99	0.44
3:T:7:PRO:HG2	3:T:81:TYR:H	1.82	0.44
4:X:393:ILE:HG23	4:X:394:SER:N	2.33	0.44
4:Z:118:ILE:HD12	4:Z:118:ILE:C	2.42	0.44
3:E:14:LYS:O	3:E:17:PRO:HD2	2.18	0.43
4:V:35:GLN:HB3	4:V:502:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:61:ILE:O	4:V:62:ASP:C	2.60	0.43
4:W:401:LEU:HD12	4:W:404:ILE:HD12	2.00	0.43
4:X:628:VAL:HG13	4:X:629:ALA:N	2.33	0.43
2:U:325:VAL:HG21	2:U:406:MET:HE2	2.01	0.43
2:U:401:MET:HE2	2:U:401:MET:N	2.33	0.43
3:N:7:PRO:HB2	3:N:80:SER:H	1.82	0.43
4:V:461:ALA:O	4:V:465:GLY:N	2.51	0.43
4:W:366:PHE:CZ	4:W:629:ALA:HB1	2.53	0.43
4:X:86:VAL:HG22	4:X:195:LEU:HD13	1.99	0.43
4:Z:61:ILE:CD1	4:Z:149:ILE:CD1	2.96	0.43
2:U:450:SER:HB3	2:U:455:ALA:CB	2.49	0.43
3:B:5:LEU:HD23	3:B:5:LEU:HA	1.79	0.43
3:N:7:PRO:HG2	3:N:81:TYR:H	1.83	0.43
3:T:84:ASP:OD1	3:T:84:ASP:N	2.48	0.43
4:V:356:SER:OG	4:V:435:ALA:HA	2.19	0.43
2:U:65:PHE:CD1	2:U:563:ILE:HG21	2.54	0.43
2:U:168:GLU:HG2	2:U:649:VAL:HG11	2.00	0.43
3:A:6:VAL:HG23	3:A:49:ALA:HA	2.00	0.43
3:M:90:HIS:NE2	4:V:37:PRO:O	2.51	0.43
3:T:2:THR:HB	3:T:45:ILE:HA	2.01	0.43
4:V:444:VAL:HG22	4:V:486:TYR:CE1	2.53	0.43
4:W:103:TRP:CD1	4:W:230:ALA:HB2	2.53	0.43
4:W:396:ARG:CZ	4:W:612:LEU:O	2.67	0.43
2:U:2:ARG:HD2	2:U:2:ARG:C	2.43	0.43
2:U:575:TRP:CG	2:U:583:TYR:HB2	2.53	0.43
3:S:14:LYS:O	3:S:17:PRO:HD2	2.18	0.43
4:V:158:LEU:O	4:V:158:LEU:HG	2.19	0.43
4:V:378:LEU:HD22	4:V:576:HIS:CE1	2.54	0.43
4:W:528:ILE:HG23	4:W:529:PRO:HD2	1.99	0.43
4:X:55:GLU:HA	4:X:171:VAL:HA	2.01	0.43
2:U:349:TYR:O	2:U:350:ALA:C	2.58	0.43
3:B:7:PRO:CG	3:B:81:TYR:H	2.32	0.43
2:U:76:TYR:CD1	2:U:77:GLY:N	2.87	0.43
2:U:82:THR:OG1	2:U:83:ASN:N	2.52	0.43
2:U:450:SER:HB3	2:U:455:ALA:HB2	2.00	0.43
2:U:569:GLU:HG2	4:X:64:VAL:HG11	2.01	0.43
2:U:580:GLY:C	2:U:581:GLU:HG2	2.43	0.43
2:U:663:PRO:CG	2:U:664:ARG:H	2.29	0.43
4:W:523:ARG:HA	4:W:539:SER:HA	2.00	0.43
4:X:372:ALA:N	4:X:394:SER:OG	2.52	0.43
4:X:471:LEU:C	4:X:471:LEU:HD12	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:95:MET:SD	2:U:268:ARG:HA	2.59	0.43
2:U:511:SER:HB2	4:X:337:ASN:ND2	2.34	0.43
3:E:6:VAL:HG23	3:E:49:ALA:HA	2.00	0.43
3:F:7:PRO:HG2	3:F:81:TYR:H	1.82	0.43
3:A:14:LYS:O	3:A:17:PRO:HD2	2.18	0.43
3:B:2:THR:HB	3:B:45:ILE:HA	2.01	0.43
3:M:74:MET:HE1	4:V:39:GLN:C	2.42	0.43
4:V:92:TYR:CD2	4:V:146:PHE:HB3	2.54	0.43
4:V:313:LEU:N	4:V:313:LEU:HD12	2.33	0.43
4:Z:159:SER:OG	4:Z:160:PRO:HD3	2.19	0.43
2:U:628:LEU:HD12	2:U:628:LEU:HA	1.81	0.43
3:B:97:TRP:CE2	3:B:101:SER:HB3	2.54	0.43
4:V:97:ALA:O	4:V:103:TRP:CZ3	2.71	0.43
4:W:142:GLU:OE1	4:W:142:GLU:N	2.50	0.43
4:W:256:ILE:HG13	4:W:257:LEU:N	2.33	0.43
4:W:448:ASP:O	4:W:452:ASP:N	2.51	0.43
4:X:44:PHE:CE1	4:X:333:LEU:HD13	2.54	0.43
4:X:44:PHE:CE2	4:X:290:LEU:HD13	2.54	0.43
3:F:97:TRP:CE2	3:F:101:SER:HB3	2.54	0.42
3:M:14:LYS:O	3:M:17:PRO:HD2	2.18	0.42
4:X:126:VAL:HG13	4:X:127:PRO:HD2	2.00	0.42
4:X:480:LYS:HA	4:X:483:MET:HG3	2.01	0.42
4:X:524:THR:HG22	4:X:526:LEU:H	1.84	0.42
4:Z:578:TRP:CZ3	4:Z:580:TRP:HA	2.54	0.42
2:U:315:LYS:HA	2:U:509:PRO:O	2.19	0.42
2:U:404:LEU:CD1	2:U:404:LEU:C	2.92	0.42
2:U:418:THR:O	2:U:464:ALA:HA	2.19	0.42
3:F:7:PRO:CG	3:F:81:TYR:H	2.32	0.42
4:V:716:VAL:HG21	4:W:376:VAL:HG11	2.00	0.42
4:W:596:THR:HA	4:W:600:LYS:O	2.19	0.42
4:Z:640:PHE:CZ	4:Z:674:LEU:HD13	2.54	0.42
2:U:226:MET:CE	2:U:244:ALA:HB2	2.36	0.42
3:N:2:THR:HB	3:N:45:ILE:HA	2.01	0.42
3:N:97:TRP:CE2	3:N:101:SER:HB3	2.54	0.42
3:S:4:TYR:OH	3:S:103:LYS:NZ	2.32	0.42
4:V:146:PHE:O	4:V:149:ILE:HG22	2.19	0.42
4:V:362:GLU:CG	4:V:442:PRO:HD2	2.49	0.42
4:V:710:ASP:OD1	4:V:711:SER:N	2.52	0.42
4:W:295:GLN:O	4:W:298:VAL:HG12	2.19	0.42
4:W:449:TYR:CZ	4:W:630:HIS:CE1	3.08	0.42
4:X:520:TRP:O	4:X:541:ARG:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:76:TYR:HA	2:U:502:LEU:CD1	2.50	0.42
2:U:164:ILE:O	2:U:168:GLU:HG3	2.18	0.42
2:U:663:PRO:HG2	2:U:664:ARG:N	2.34	0.42
3:N:7:PRO:CG	3:N:81:TYR:H	2.32	0.42
4:V:651:ARG:NH2	4:V:660:LYS:HE2	2.34	0.42
4:X:439:LEU:HD23	4:X:439:LEU:N	2.35	0.42
4:Z:533:ASN:HB3	4:Z:540:ILE:HD11	2.00	0.42
2:U:139:GLU:HA	2:U:140:PRO:HD3	1.89	0.42
2:U:497:LEU:HD12	2:U:497:LEU:HA	1.75	0.42
3:F:2:THR:HB	3:F:45:ILE:HA	2.01	0.42
3:M:90:HIS:O	3:T:106:LYS:NZ	2.52	0.42
3:T:7:PRO:CG	3:T:81:TYR:H	2.32	0.42
3:T:97:TRP:CE2	3:T:101:SER:HB3	2.54	0.42
4:V:171:VAL:HG21	4:V:575:ILE:HG21	2.01	0.42
4:W:640:PHE:CZ	4:W:674:LEU:HD13	2.54	0.42
4:X:9:LEU:HB3	4:X:13:ALA:HB2	2.02	0.42
4:X:138:LEU:HD13	4:X:138:LEU:O	2.19	0.42
4:X:182:ASN:ND2	4:X:296:ASP:OD2	2.52	0.42
4:X:728:GLY:O	4:X:731:VAL:HG12	2.19	0.42
2:U:596:LEU:CD2	4:V:391:PRO:HB3	2.49	0.42
3:M:85:TRP:CZ3	3:M:89:ALA:HB2	2.55	0.42
4:V:34:LEU:H	4:V:34:LEU:HD22	1.85	0.42
4:V:60:ASN:ND2	4:V:62:ASP:OD1	2.52	0.42
4:V:305:GLU:H	4:V:305:GLU:CD	2.28	0.42
4:W:110:ILE:CD1	4:W:131:ILE:HG22	2.50	0.42
4:Z:355:PRO:O	4:Z:435:ALA:HB2	2.20	0.42
2:U:563:ILE:O	2:U:564:TYR:C	2.63	0.42
3:N:32:PHE:O	3:N:35:GLU:HB3	2.20	0.42
3:S:6:VAL:HG23	3:S:49:ALA:HA	2.00	0.42
3:T:84:ASP:OD1	3:T:85:TRP:N	2.47	0.42
4:V:298:VAL:HG13	4:V:303:ARG:NE	2.35	0.42
4:V:578:TRP:HB2	4:V:579:PRO:CD	2.48	0.42
4:X:572:THR:O	4:X:572:THR:HG22	2.20	0.42
4:Z:38:LEU:C	4:Z:38:LEU:HD12	2.44	0.42
2:U:502:LEU:HB3	2:U:513:ILE:HG13	2.01	0.42
4:V:364:TRP:CH2	4:V:561:LEU:HD23	2.55	0.42
4:W:333:LEU:C	4:W:333:LEU:HD12	2.45	0.42
4:W:580:TRP:CE3	4:W:581:HIS:HA	2.55	0.42
4:X:44:PHE:CZ	4:X:325:MET:HG2	2.55	0.42
4:Z:393:ILE:HG13	4:Z:394:SER:N	2.35	0.42
2:U:22:ILE:O	2:U:23:LYS:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:28:LEU:HA	3:F:28:LEU:HD12	1.82	0.42
3:M:6:VAL:HG23	3:M:49:ALA:HA	2.00	0.42
3:T:60:ARG:O	3:T:60:ARG:NH1	2.50	0.42
4:V:151:THR:O	4:V:154:VAL:HG22	2.20	0.42
4:V:253:VAL:O	4:V:256:ILE:HG22	2.19	0.42
4:X:9:LEU:HD22	4:X:13:ALA:CB	2.47	0.42
4:X:449:TYR:CZ	4:X:634:GLN:OE1	2.72	0.42
2:U:344:LEU:HD23	2:U:344:LEU:HA	1.94	0.42
2:U:641:ILE:O	2:U:644:VAL:HB	2.20	0.42
3:B:32:PHE:O	3:B:35:GLU:HB3	2.20	0.42
3:E:85:TRP:CZ3	3:E:89:ALA:HB2	2.55	0.42
4:W:48:MET:SD	4:W:68:ARG:NH2	2.88	0.42
4:W:396:ARG:NH2	4:W:611:LEU:O	2.53	0.42
4:X:309:SER:HB3	4:X:313:LEU:HD23	2.02	0.42
4:Z:164:ILE:HD12	4:Z:164:ILE:O	2.20	0.42
2:U:265:PHE:CD1	2:U:265:PHE:N	2.88	0.41
2:U:633:THR:O	2:U:636:ASP:N	2.50	0.41
3:S:65:LEU:HD23	3:S:65:LEU:HA	1.86	0.41
4:V:445:VAL:HG23	4:V:631:ALA:HB1	2.01	0.41
4:V:553:LYS:HB3	4:V:554:PRO:HD2	2.02	0.41
4:W:611:LEU:HD22	4:W:690:ALA:HB2	2.02	0.41
4:X:262:SER:OG	4:X:505:GLU:OE1	2.37	0.41
4:X:494:ALA:HB2	4:X:549:ILE:HD11	2.02	0.41
4:X:593:TYR:O	4:X:603:THR:HG23	2.20	0.41
2:U:180:LEU:HD23	2:U:180:LEU:HA	1.86	0.41
3:F:32:PHE:O	3:F:35:GLU:HB3	2.20	0.41
3:M:71:VAL:HG22	3:T:103:LYS:HE2	1.96	0.41
4:V:173:ARG:HB2	4:V:578:TRP:CD1	2.55	0.41
1:x:7:DC:O2	2:U:633:THR:HA	2.20	0.41
2:U:397:ALA:O	2:U:398:THR:C	2.60	0.41
2:U:406:MET:HB3	2:U:410:TYR:CE2	2.55	0.41
3:B:60:ARG:O	3:B:60:ARG:NH1	2.50	0.41
3:M:106:LYS:HE2	3:T:90:HIS:CE1	2.52	0.41
3:T:32:PHE:O	3:T:35:GLU:HB3	2.20	0.41
4:V:535:ILE:O	4:V:535:ILE:CG2	2.68	0.41
4:W:48:MET:HG3	4:W:177:THR:OG1	2.19	0.41
4:X:439:LEU:HD23	4:X:439:LEU:H	1.84	0.41
4:Z:89:PHE:HA	4:Z:146:PHE:CE2	2.54	0.41
4:Z:413:PHE:N	4:Z:413:PHE:CD1	2.87	0.41
2:U:325:VAL:CG2	2:U:406:MET:HE2	2.51	0.41
4:V:378:LEU:HD11	4:V:386:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:149:ILE:HD11	4:W:199:LEU:HD22	2.03	0.41
4:W:566:LEU:HD22	4:W:566:LEU:N	2.36	0.41
4:X:128:PRO:O	4:X:131:ILE:CG2	2.69	0.41
4:X:134:GLN:HE22	4:X:138:LEU:HD23	1.85	0.41
4:X:472:GLU:HG2	4:X:474:ARG:H	1.85	0.41
2:U:450:SER:CB	2:U:455:ALA:HB2	2.51	0.41
3:A:85:TRP:CZ3	3:A:89:ALA:HB2	2.55	0.41
3:S:85:TRP:CZ3	3:S:89:ALA:HB2	2.55	0.41
4:V:154:VAL:O	4:V:158:LEU:N	2.48	0.41
4:X:14:ARG:O	4:X:20:PHE:CG	2.73	0.41
4:W:86:VAL:HG13	4:W:195:LEU:HD23	2.03	0.41
4:W:253:VAL:O	4:W:256:ILE:HG12	2.21	0.41
4:W:346:THR:HG22	4:W:347:SER:H	1.85	0.41
4:Z:715:HIS:O	4:Z:719:ASN:ND2	2.52	0.41
2:U:569:GLU:CG	4:X:64:VAL:HG11	2.50	0.41
3:F:84:ASP:OD1	3:F:85:TRP:N	2.47	0.41
3:N:84:ASP:OD1	3:N:85:TRP:N	2.47	0.41
4:X:11:GLY:O	4:X:463:ARG:O	2.38	0.41
4:Z:159:SER:HA	4:Z:164:ILE:CG1	2.51	0.41
2:U:248:ASP:OD2	2:U:248:ASP:C	2.63	0.41
2:U:273:MET:HG3	2:U:392:SER:OG	2.21	0.41
3:T:98:ILE:CD1	4:V:337:ASN:OD1	2.62	0.41
4:V:92:TYR:O	4:V:96:THR:HG22	2.20	0.41
4:V:171:VAL:HG22	4:V:571:HIS:CE1	2.56	0.41
4:V:253:VAL:HA	4:V:256:ILE:HG22	2.01	0.41
4:W:81:SER:OG	4:W:83:ASP:OD1	2.26	0.41
4:X:132:LEU:C	4:X:132:LEU:HD23	2.46	0.41
4:X:606:VAL:HG21	4:X:611:LEU:HD21	2.02	0.41
2:U:153:ILE:HD12	2:U:198:ALA:O	2.21	0.41
2:U:391:LEU:HD23	2:U:391:LEU:HA	1.62	0.41
2:U:633:THR:O	2:U:634:GLU:C	2.64	0.41
3:F:55:LEU:HD22	3:F:85:TRP:CE2	2.56	0.41
3:N:55:LEU:HD22	3:N:85:TRP:CE2	2.56	0.41
3:T:5:LEU:HA	3:T:5:LEU:HD23	1.79	0.41
4:V:16:LEU:N	4:V:16:LEU:HD12	2.36	0.41
4:V:53:LEU:HD23	4:V:173:ARG:HA	2.02	0.41
4:V:169:ALA:HB3	4:V:575:ILE:HG13	2.02	0.41
4:V:350:ASP:OD1	4:V:352:MET:N	2.52	0.41
4:V:362:GLU:CD	4:V:364:TRP:HE1	2.27	0.41
4:V:683:THR:HB	4:V:765:ILE:HD12	2.02	0.41
4:V:750:LEU:HD12	4:V:750:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:402:ALA:HB3	4:W:403:PRO:HD3	2.03	0.41
4:W:509:VAL:HG13	4:W:511:ALA:H	1.85	0.41
4:X:253:VAL:O	4:X:256:ILE:HG12	2.21	0.41
4:X:580:TRP:CG	4:X:581:HIS:N	2.89	0.41
4:X:733:GLN:HE22	4:X:740:ARG:NE	2.19	0.41
4:Z:48:MET:O	4:Z:48:MET:HG3	2.21	0.41
4:Z:153:PHE:CD1	4:Z:202:LEU:HG	2.56	0.41
4:Z:586:GLU:CD	4:Z:587:PHE:H	2.29	0.41
2:U:96:ILE:HA	2:U:97:PRO:HA	1.86	0.41
2:U:548:GLY:N	2:U:594:ASP:OD1	2.52	0.41
4:V:22:ILE:CG2	4:V:23:GLY:N	2.83	0.41
4:V:711:SER:O	4:V:715:HIS:ND1	2.47	0.41
4:Z:155:CYS:O	4:Z:159:SER:HB3	2.21	0.41
4:Z:217:LYS:C	4:Z:219:ALA:H	2.29	0.41
3:E:4:TYR:OH	3:E:103:LYS:NZ	2.32	0.40
4:V:487:TYR:CZ	4:V:491:MET:SD	3.14	0.40
4:W:733:GLN:OE1	4:W:740:ARG:HA	2.21	0.40
4:X:675:LEU:HD21	4:X:750:LEU:HD13	2.02	0.40
4:Z:214:PHE:O	4:Z:218:GLY:HA2	2.21	0.40
1:x:6:DC:C2'	1:x:7:DC:H5'	2.35	0.40
2:U:95:MET:O	2:U:96:ILE:HD13	2.21	0.40
2:U:280:ASN:HD22	2:U:396:GLY:H	1.68	0.40
2:U:419:ALA:N	2:U:420:PRO:CD	2.84	0.40
2:U:517:ASN:HB3	2:U:520:SER:OG	2.21	0.40
3:T:55:LEU:HD22	3:T:85:TRP:CE2	2.56	0.40
4:V:580:TRP:CE3	4:V:581:HIS:HA	2.57	0.40
4:W:445:VAL:HA	4:W:448:ASP:OD2	2.21	0.40
4:W:482:SER:HA	4:W:485:ASN:HD22	1.85	0.40
4:W:758:MET:SD	4:W:758:MET:C	3.04	0.40
4:X:2:PHE:HB3	4:X:439:LEU:HD21	2.03	0.40
4:X:309:SER:HB3	4:X:313:LEU:H	1.85	0.40
4:X:384:GLN:CG	4:X:577:ILE:O	2.69	0.40
4:Z:624:LEU:HD23	4:Z:624:LEU:C	2.47	0.40
3:A:83:SER:CB	4:W:570:ASN:C	2.93	0.40
4:V:210:LEU:O	4:V:213:THR:HG22	2.21	0.40
4:W:535:ILE:HG13	4:W:535:ILE:O	2.21	0.40
4:X:540:ILE:HG13	4:X:551:TYR:CZ	2.56	0.40
4:Z:414:VAL:O	4:Z:418:THR:HG23	2.21	0.40
4:V:132:LEU:HD23	4:V:132:LEU:O	2.22	0.40
4:V:158:LEU:O	4:V:158:LEU:CG	2.70	0.40
4:W:107:THR:HG1	4:W:226:SER:HG	1.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:254:LEU:N	4:W:254:LEU:HD12	2.36	0.40
4:W:370:ILE:HG21	4:W:397:MET:HB3	2.04	0.40
4:X:524:THR:CG2	4:X:525:GLU:N	2.85	0.40
2:U:127:PHE:CD2	2:U:408:ILE:HG21	2.56	0.40
4:V:275:LEU:HD13	4:V:281:ILE:HG13	2.02	0.40
4:V:361:TYR:HA	4:V:440:GLY:O	2.21	0.40
4:Z:441:PHE:O	4:Z:444:VAL:HG12	2.22	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	
2	U	651/664 (98%)	599 (92%)	46 (7%)	6 (1%)	14	49
3	A	109/111 (98%)	105 (96%)	4 (4%)	0	100	100
3	B	109/111 (98%)	103 (94%)	6 (6%)	0	100	100
3	E	109/111 (98%)	105 (96%)	4 (4%)	0	100	100
3	F	109/111 (98%)	103 (94%)	6 (6%)	0	100	100
3	M	109/111 (98%)	105 (96%)	4 (4%)	0	100	100
3	N	109/111 (98%)	103 (94%)	6 (6%)	0	100	100
3	S	109/111 (98%)	105 (96%)	4 (4%)	0	100	100
3	T	109/111 (98%)	103 (94%)	6 (6%)	0	100	100
4	V	764/766 (100%)	718 (94%)	45 (6%)	1 (0%)	48	83
4	W	764/766 (100%)	719 (94%)	45 (6%)	0	100	100
4	X	764/766 (100%)	724 (95%)	40 (5%)	0	100	100
4	Z	764/766 (100%)	729 (95%)	34 (4%)	1 (0%)	48	83
All	All	4579/4616 (99%)	4321 (94%)	250 (6%)	8 (0%)	44	78

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	U	564	TYR
2	U	207	SER
2	U	630	TYR
2	U	88	ARG
2	U	663	PRO
4	V	29	LEU
2	U	2	ARG
4	Z	205	VAL

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	
2	U	552/557 (99%)	512 (93%)	40 (7%)	13	35
3	A	92/92 (100%)	92 (100%)	0	100	100
3	B	92/92 (100%)	92 (100%)	0	100	100
3	E	92/92 (100%)	92 (100%)	0	100	100
3	F	92/92 (100%)	92 (100%)	0	100	100
3	M	92/92 (100%)	92 (100%)	0	100	100
3	N	92/92 (100%)	92 (100%)	0	100	100
3	S	92/92 (100%)	92 (100%)	0	100	100
3	T	91/92 (99%)	91 (100%)	0	100	100
4	V	635/635 (100%)	611 (96%)	24 (4%)	29	51
4	W	635/635 (100%)	610 (96%)	25 (4%)	28	50
4	X	635/635 (100%)	607 (96%)	28 (4%)	25	47
4	Z	635/635 (100%)	619 (98%)	16 (2%)	42	62
All	All	3827/3833 (100%)	3694 (96%)	133 (4%)	32	53

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	U	16	MET
2	U	43	LEU
2	U	44	LEU
2	U	75	VAL
2	U	78	ASN
2	U	90	MET
2	U	113	ASP
2	U	119	VAL
2	U	143	LEU
2	U	146	ARG
2	U	154	PRO
2	U	192	LEU
2	U	202	VAL
2	U	204	ARG
2	U	206	GLN
2	U	239	GLN
2	U	289	PRO
2	U	307	ARG
2	U	308	LEU
2	U	333	PRO
2	U	351	PRO
2	U	360	SER
2	U	373	GLU
2	U	387	LEU
2	U	398	THR
2	U	404	LEU
2	U	437	ASP
2	U	480	VAL
2	U	497	LEU
2	U	519	ASN
2	U	534	SER
2	U	576	TRP
2	U	581	GLU
2	U	587	ARG
2	U	591	LEU
2	U	626	ASN
2	U	629	GLN
2	U	633	THR
2	U	649	VAL
2	U	651	VAL
4	V	10	ASN
4	V	17	THR
4	V	38	LEU

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Mol	Chain	Res	Type
4	V	69	LEU
4	V	81	SER
4	V	82	VAL
4	V	170	TYR
4	V	250	VAL
4	V	267	LYS
4	V	282	ASP
4	V	305	GLU
4	V	314	SER
4	V	337	ASN
4	V	413	PHE
4	V	417	ARG
4	V	575	ILE
4	V	577	ILE
4	V	608	GLU
4	V	621	VAL
4	V	637	TYR
4	V	683	THR
4	V	693	LEU
4	V	707	LEU
4	V	733	GLN
4	W	7	LYS
4	W	38	LEU
4	W	48	MET
4	W	71	PHE
4	W	131	ILE
4	W	135	LEU
4	W	138	LEU
4	W	150	THR
4	W	165	LEU
4	W	195	LEU
4	W	260	LEU
4	W	340	THR
4	W	390	GLU
4	W	457	VAL
4	W	464	THR
4	W	471	LEU
4	W	507	GLN
4	W	533	ASN
4	W	575	ILE
4	W	586	GLU
4	W	608	GLU

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Mol	Chain	Res	Type
4	W	628	VAL
4	W	693	LEU
4	W	707	LEU
4	W	766	ASP
4	X	9	LEU
4	X	34	LEU
4	X	36	LEU
4	X	52	LEU
4	X	53	LEU
4	X	58	LYS
4	X	138	LEU
4	X	144	GLU
4	X	158	LEU
4	X	210	LEU
4	X	227	GLN
4	X	238	GLU
4	X	253	VAL
4	X	297	MET
4	X	354	GLN
4	X	368	LYS
4	X	378	LEU
4	X	413	PHE
4	X	436	GLU
4	X	457	VAL
4	X	524	THR
4	X	525	GLU
4	X	533	ASN
4	X	577	ILE
4	X	581	HIS
4	X	608	GLU
4	X	713	ASP
4	X	748	LYS
4	Z	66	TYR
4	Z	164	ILE
4	Z	247	ASN
4	Z	313	LEU
4	Z	369	GLU
4	Z	395	ASP
4	Z	422	GLU
4	Z	433	ASN
4	Z	436	GLU
4	Z	446	GLU

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Mol	Chain	Res	Type
4	Z	502	VAL
4	Z	505	GLU
4	Z	533	ASN
4	Z	608	GLU
4	Z	618	ARG
4	Z	731	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
2	U	15	GLN
2	U	25	GLN
2	U	26	GLN
2	U	78	ASN
2	U	89	HIS
2	U	183	GLN
2	U	206	GLN
2	U	255	GLN
2	U	280	ASN
2	U	304	HIS
2	U	309	ASN
2	U	328	HIS
2	U	448	GLN
2	U	519	ASN
2	U	525	GLN
2	U	626	ASN
2	U	642	HIS
3	A	112	ASN
3	B	54	ASN
3	B	90	HIS
3	E	90	HIS
3	E	112	ASN
3	F	54	ASN
3	F	90	HIS
3	M	112	ASN
3	N	54	ASN
3	N	59	ASN
3	N	90	HIS
3	S	112	ASN
3	T	54	ASN
3	T	59	ASN
4	V	39	GLN

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Mol	Chain	Res	Type
4	V	243	ASN
4	V	279	ASN
4	V	287	ASN
4	V	381	ASN
4	V	498	ASN
4	V	552	ASN
4	V	571	HIS
4	V	630	HIS
4	W	147	HIS
4	W	156	HIS
4	W	228	HIS
4	W	295	GLN
4	W	497	HIS
4	W	513	GLN
4	W	630	HIS
4	X	72	GLN
4	X	87	ASN
4	X	156	HIS
4	X	383	ASN
4	X	384	GLN
4	X	507	GLN
4	X	692	HIS
4	X	733	GLN
4	Z	10	ASN
4	Z	351	HIS
4	Z	506	HIS
4	Z	533	ASN
4	Z	715	HIS
4	Z	719	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

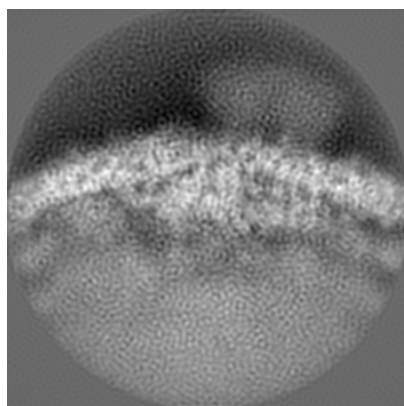
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52389. These allow visual inspection of the internal detail of the map and identification of artifacts.

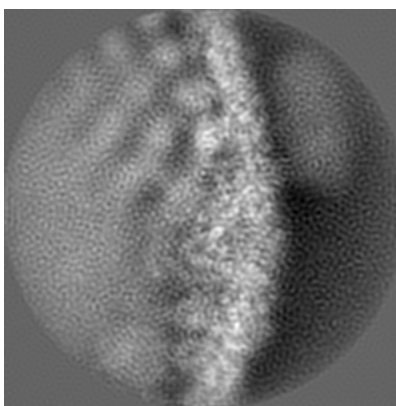
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

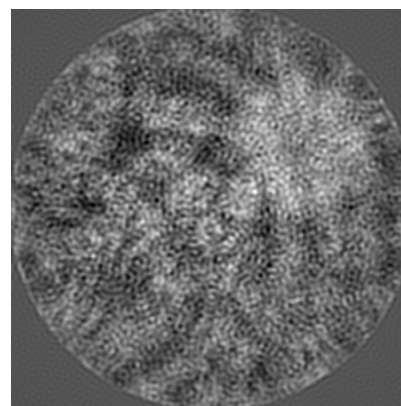
6.1.1 Primary map



X

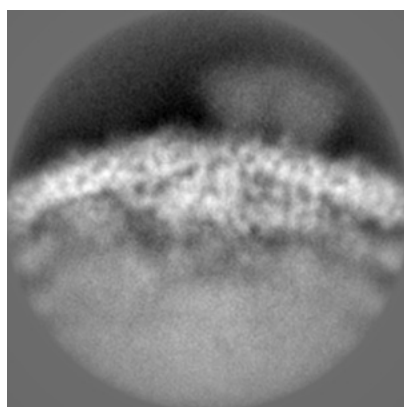


Y

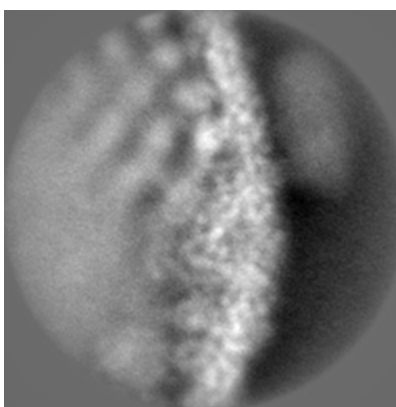


Z

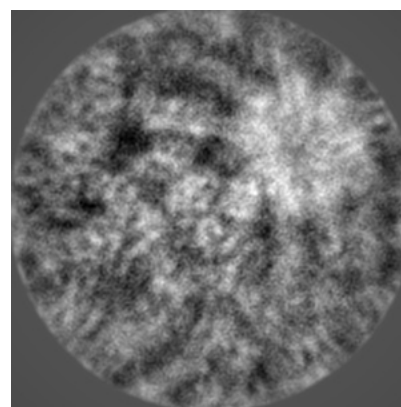
6.1.2 Raw map



X



Y

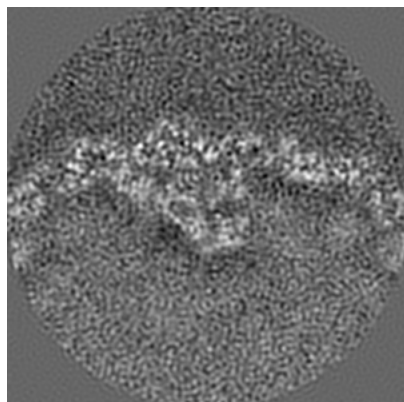


Z

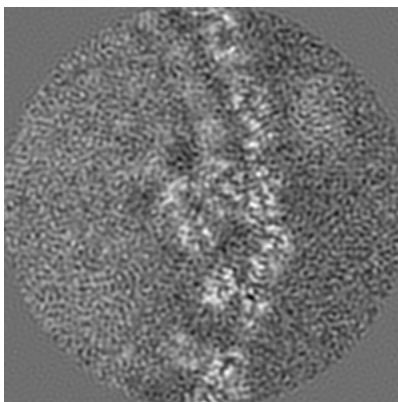
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

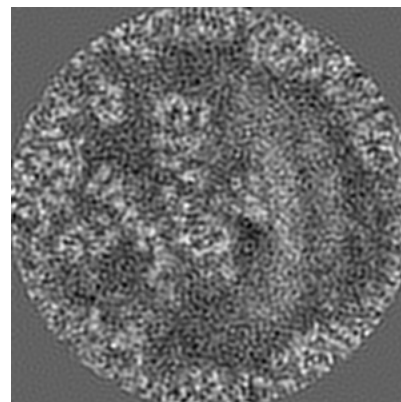
6.2.1 Primary map



X Index: 96

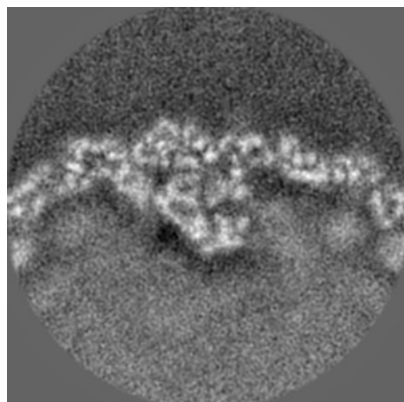


Y Index: 96

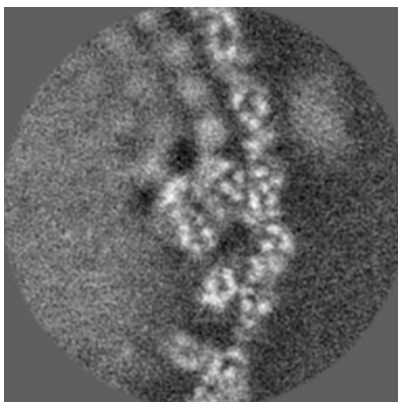


Z Index: 96

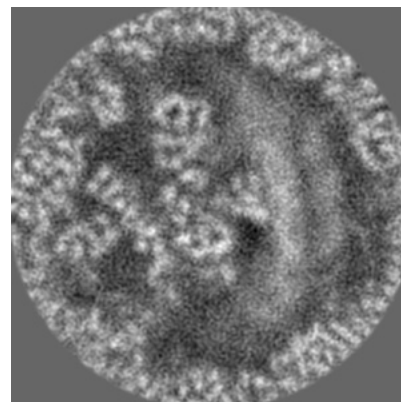
6.2.2 Raw map



X Index: 96



Y Index: 96

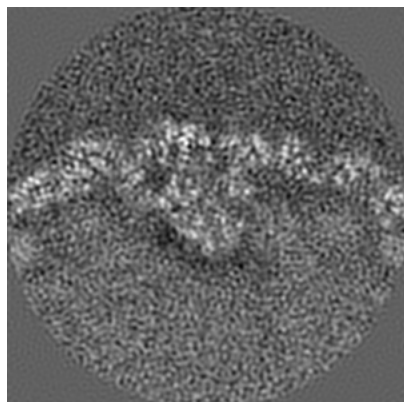


Z Index: 96

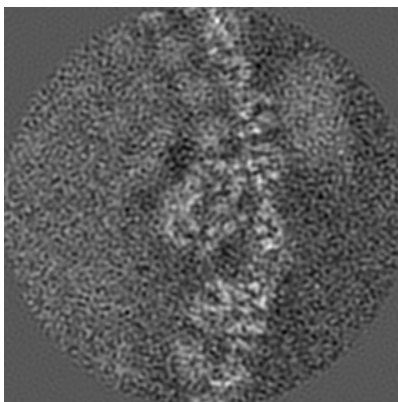
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

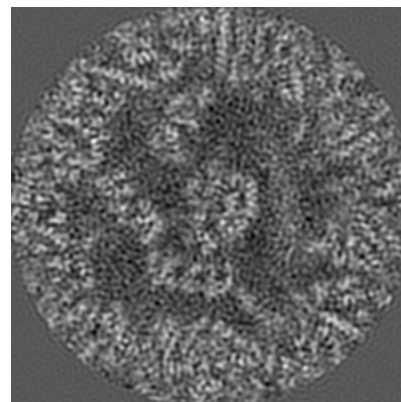
6.3.1 Primary map



X Index: 98

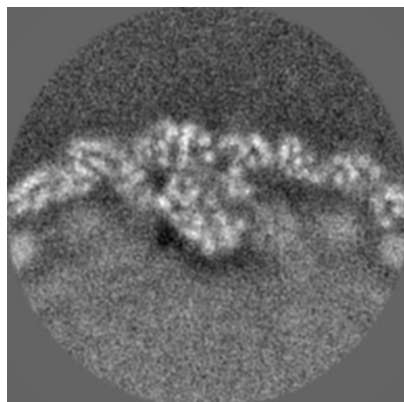


Y Index: 103

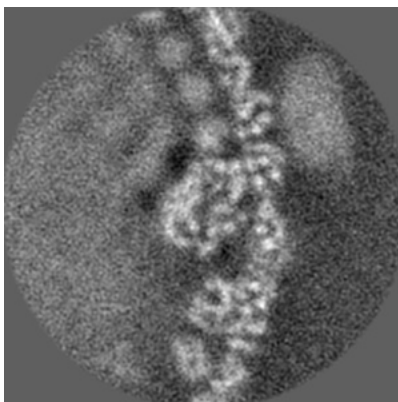


Z Index: 105

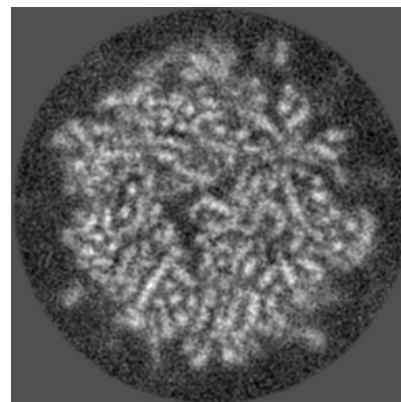
6.3.2 Raw map



X Index: 98



Y Index: 103

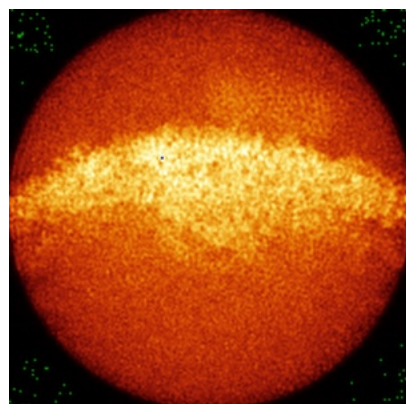


Z Index: 119

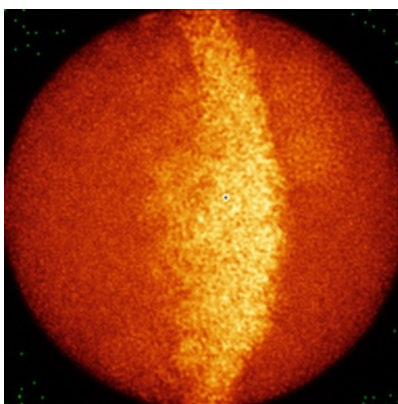
The images above show the largest variance slices of the map in three orthogonal directions.

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

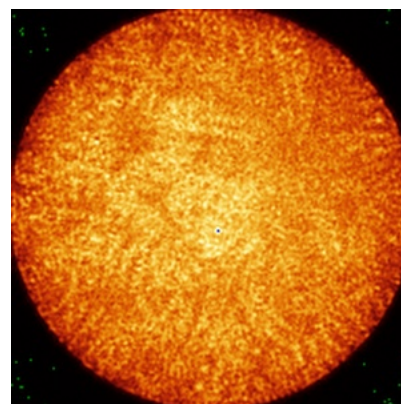
6.4.1 Primary map



X

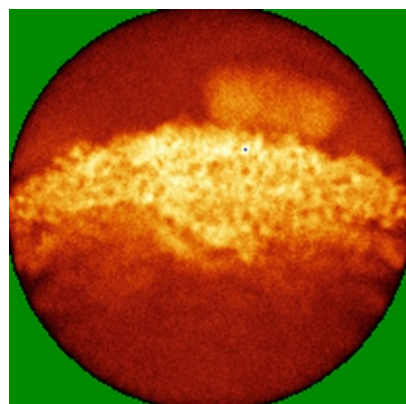


Y

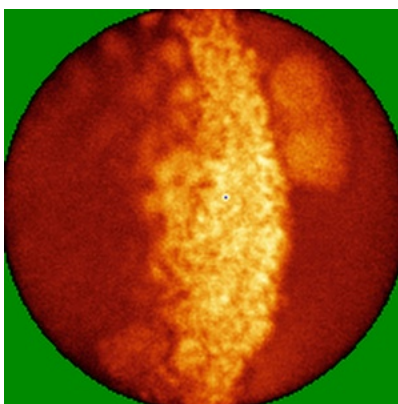


Z

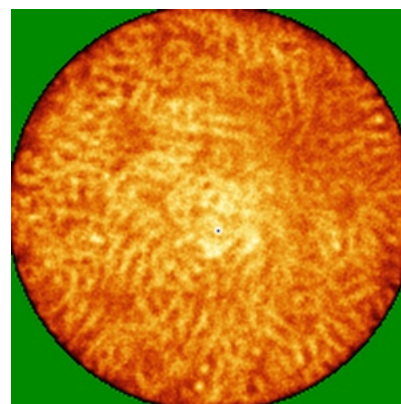
6.4.2 Raw map



X



Y

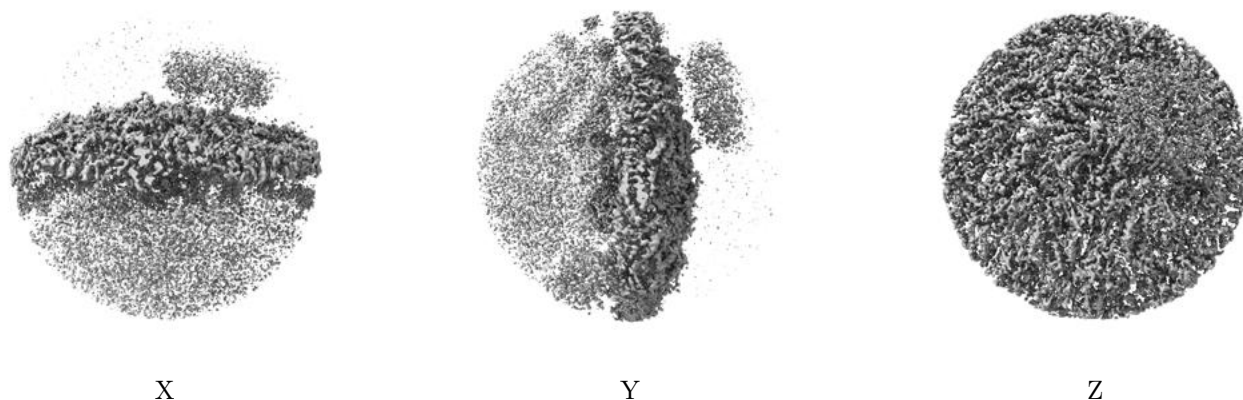


Z

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.

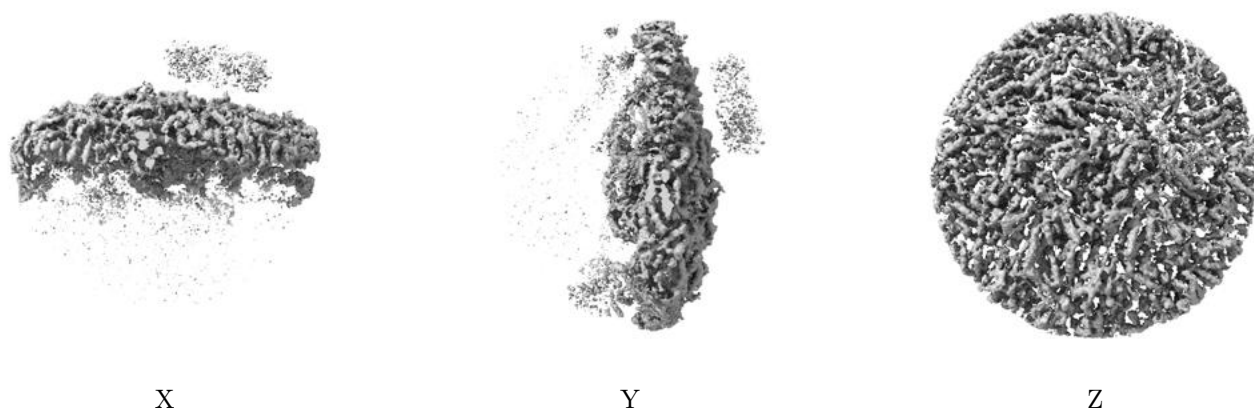
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.045. 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.

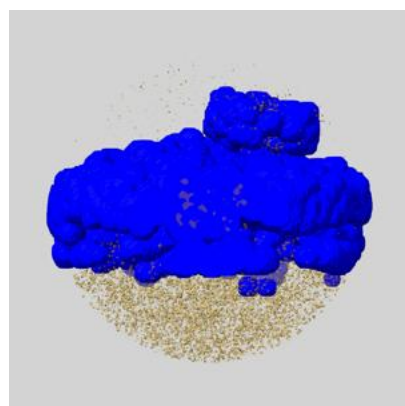
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

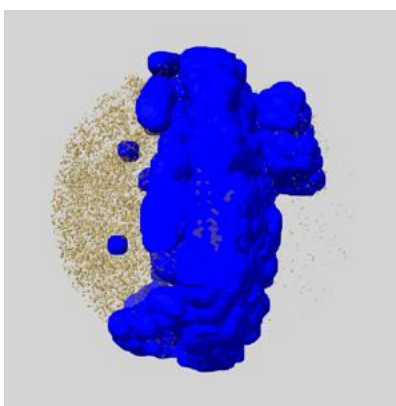
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

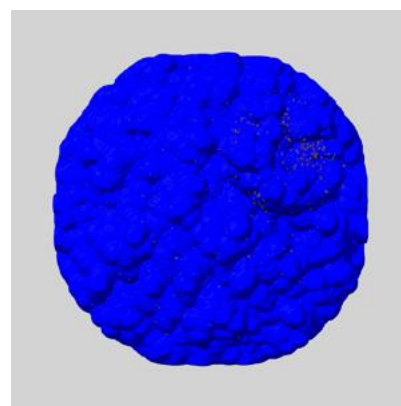
6.6.1 emd_52389_msk_1.map [i](#)



X



Y

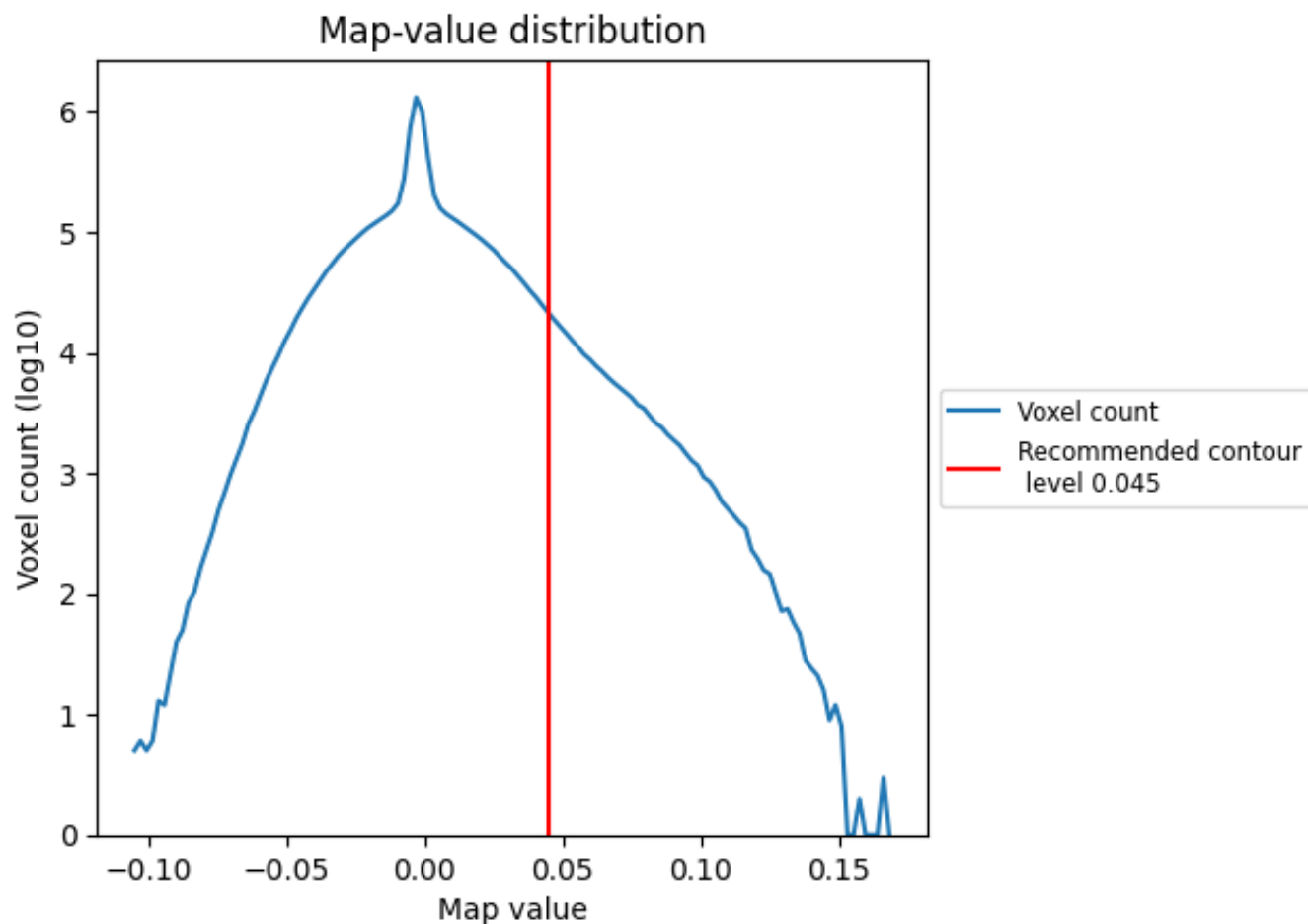


Z

7 Map analysis [i](#)

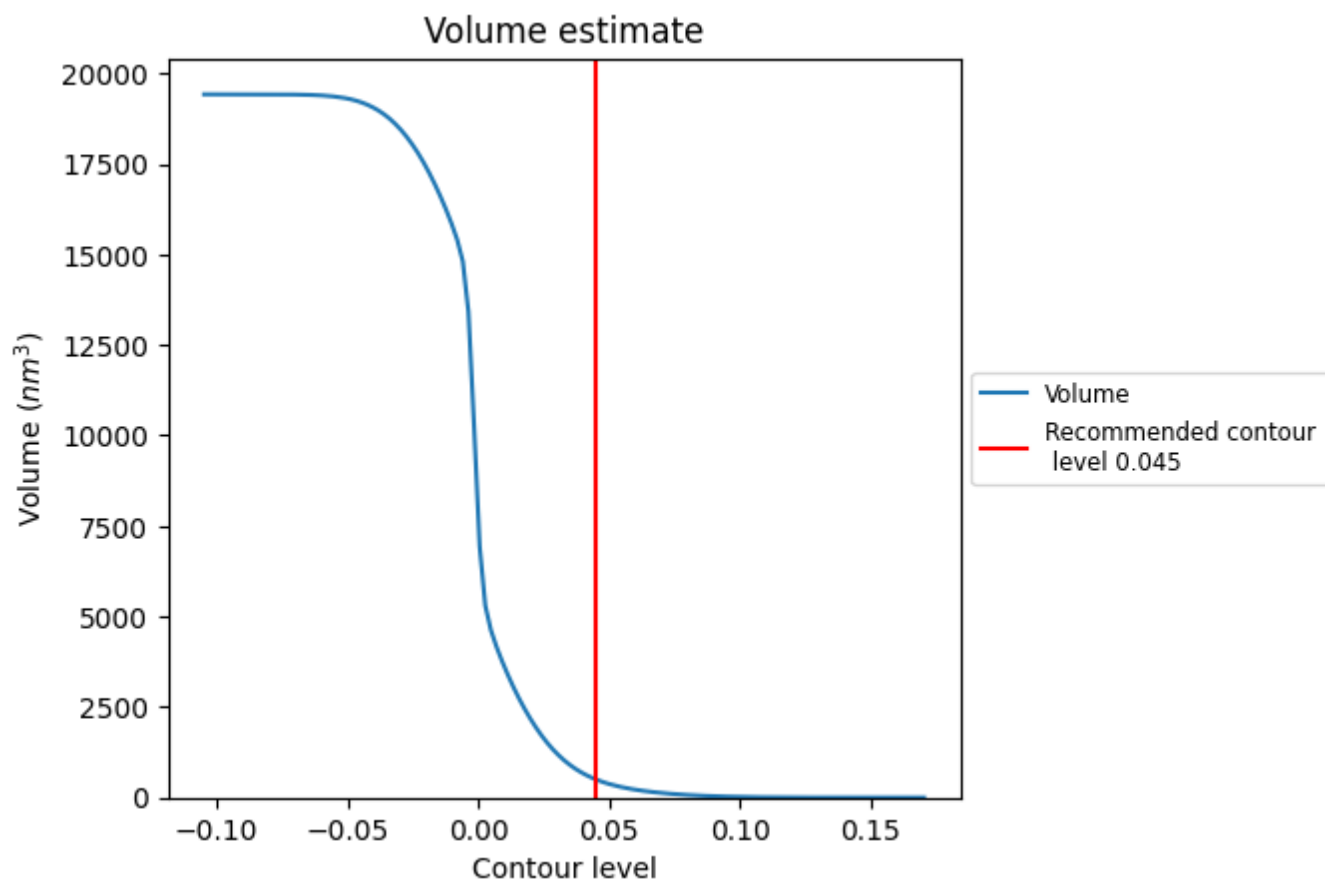
This section contains the results of statistical analysis of the map.

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.

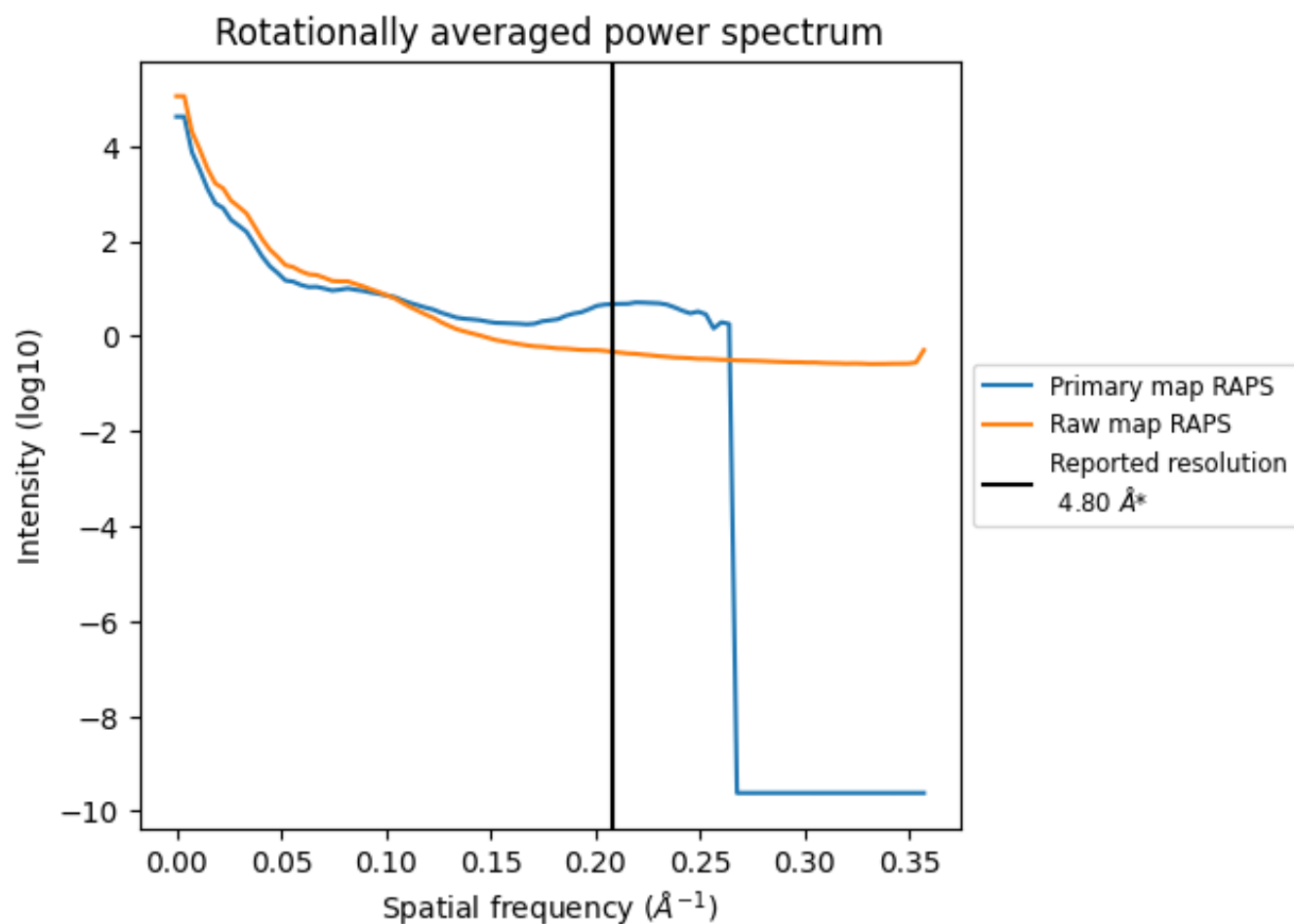
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 501 nm³; this corresponds to an approximate mass of 453 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 ⓘ

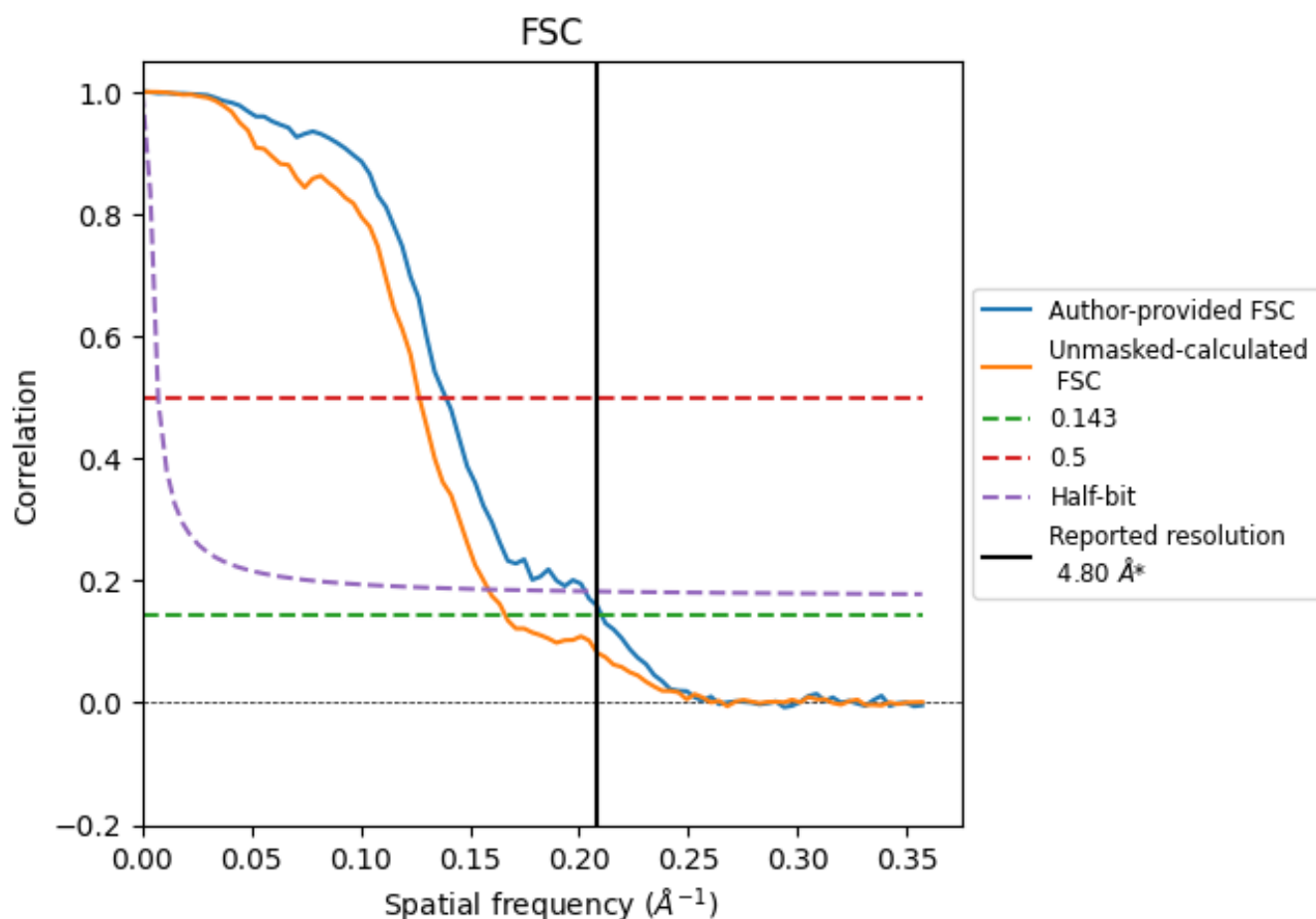


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.208 \AA^{-1}

8.2 Resolution estimates [i](#)

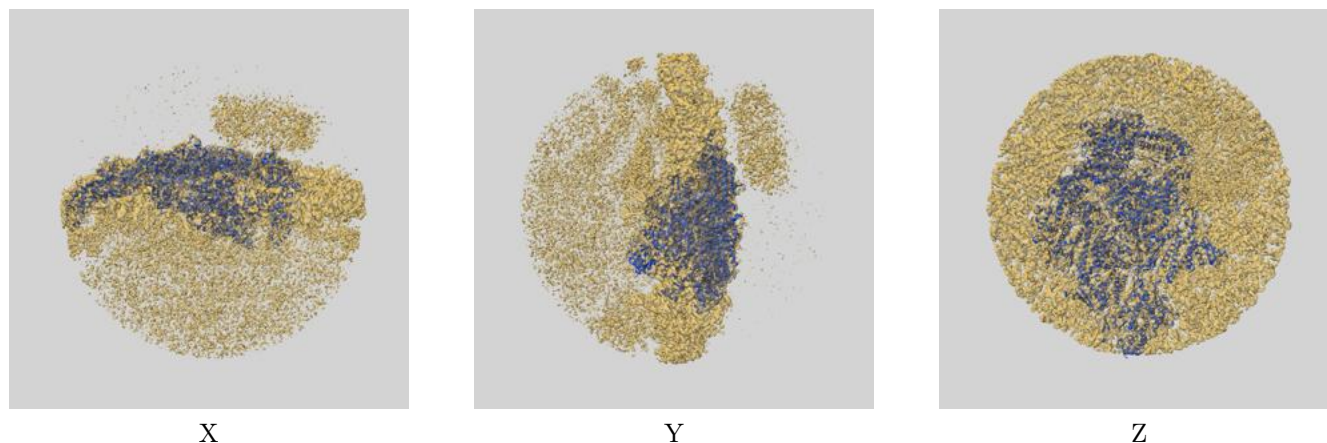
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.75	7.19	4.93
Unmasked-calculated*	6.01	7.89	6.31

*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 6.01 differs from the reported value 4.8 by more than 10 %

9 Map-model fit [i](#)

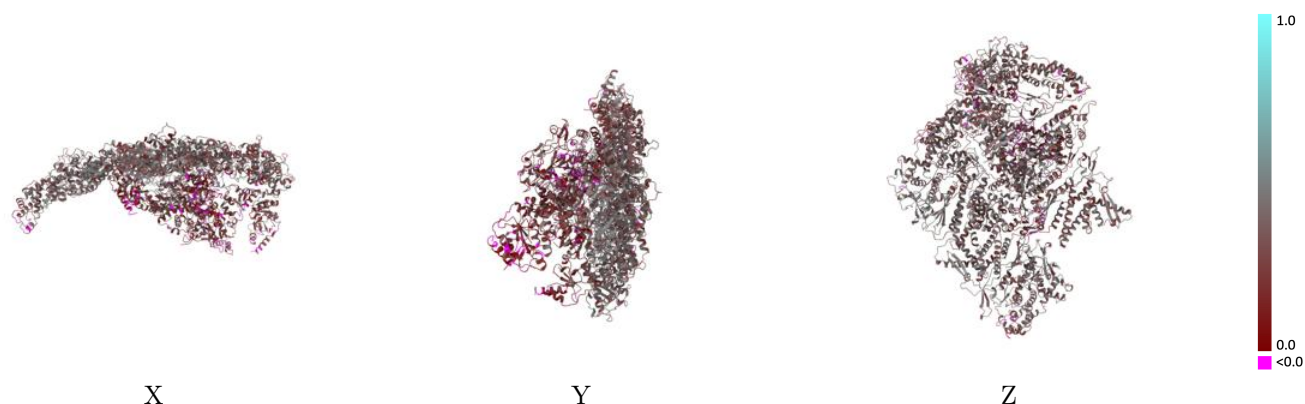
This section contains information regarding the fit between EMDB map EMD-52389 and PDB model 9I7W. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



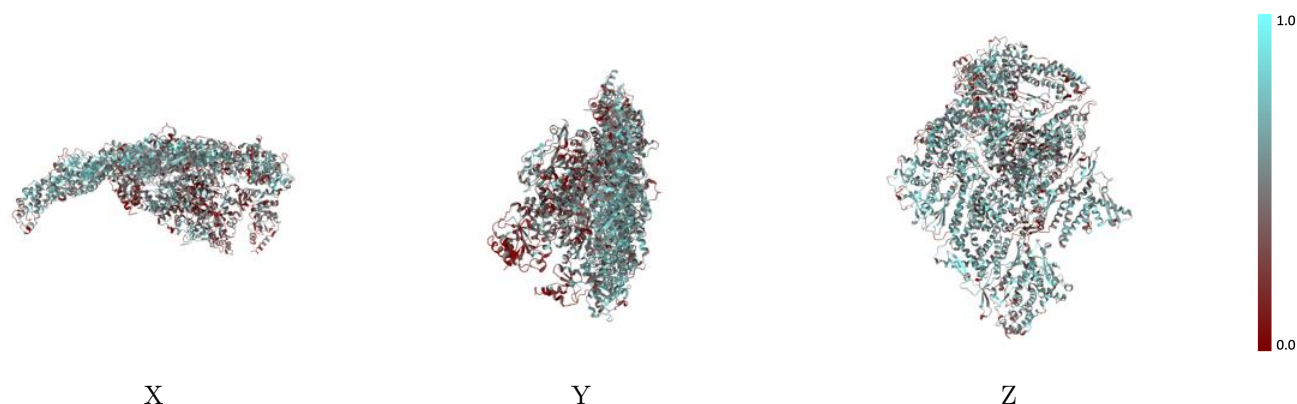
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



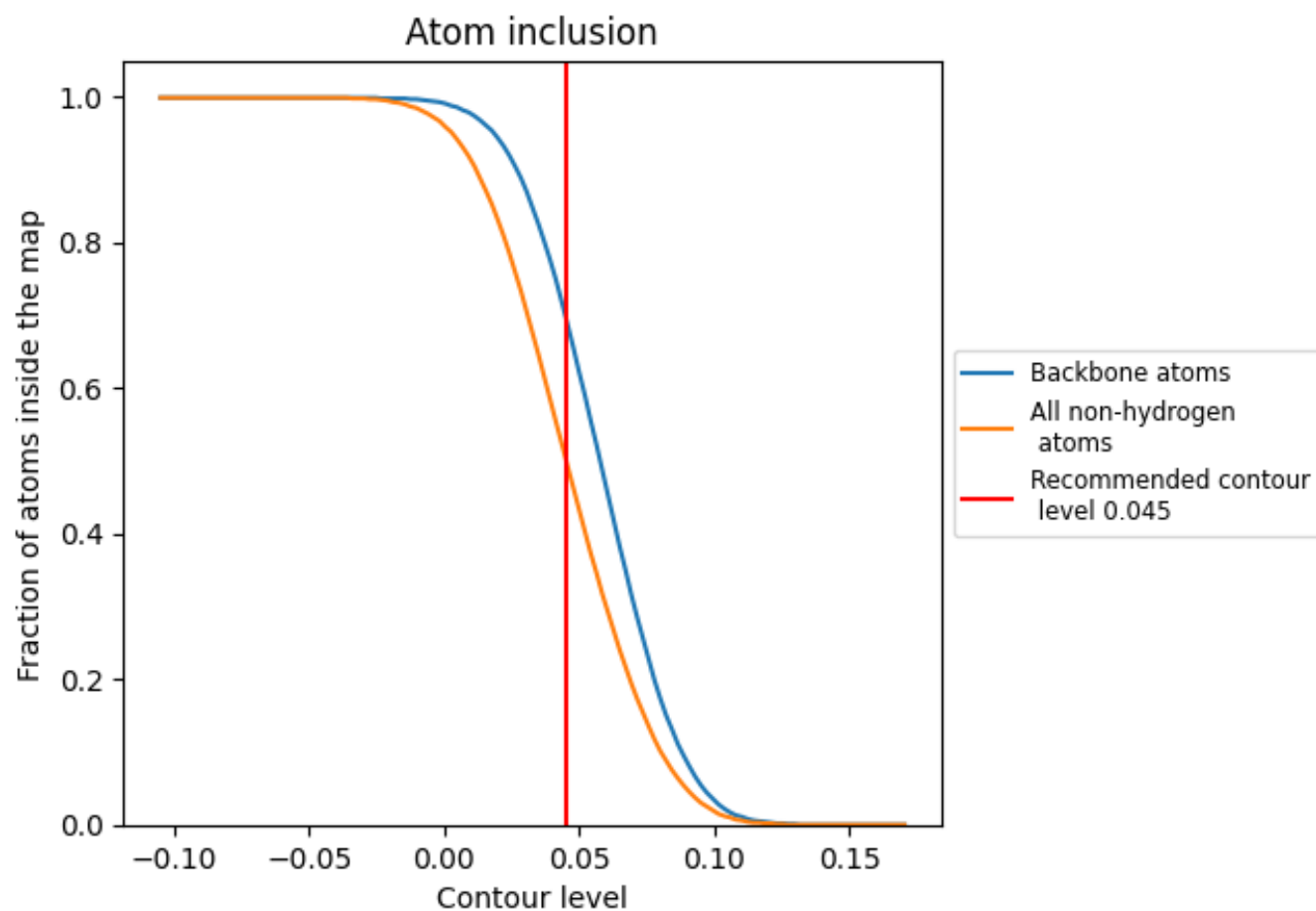
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).































9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5030	 0.3360
A	 0.5480	 0.3390
B	 0.3590	 0.2360
E	 0.4210	 0.2660
F	 0.2910	 0.1860
M	 0.4020	 0.2530
N	 0.2620	 0.1660
S	 0.3160	 0.1840
T	 0.3270	 0.2480
U	 0.4300	 0.2390
V	 0.5480	 0.3770
W	 0.6010	 0.4100
X	 0.5350	 0.3780
Z	 0.5540	 0.3820
x	 0.0320	 -0.0680

