Full wwPDB EM Validation Report ⓘ

Jan 27, 2025 – 08:33 PM EST

PDB ID	:	9C3A
EMDB ID	:	EMD-45163
Title	:	Bacteriophage Sf14 Capsid Empty Icosahedral reconstruction
Authors	:	Subramanian, S.; Kerns, H.R.; Braverman, S.G.; Doore, S.M.
Deposited on	:	2024-05-31
Resolution	:	3.10 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:

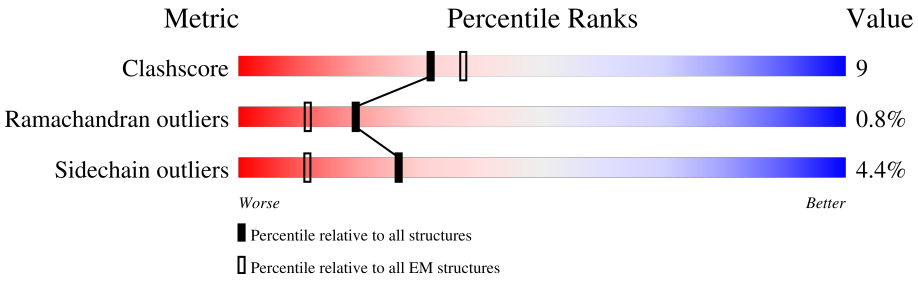
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	367	74% 24%
1	B	367	75% 23%
1	C	367	71% 22%
1	D	367	74% 19% 5%
1	E	367	70% 26%
1	F	367	75% 22%
1	G	367	81% 16%
1	H	367	81% 18%

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Mol	Chain	Length	Quality of chain
1	I	367	
2	J	125	
2	K	125	
2	L	125	
2	M	125	
2	N	125	
2	O	125	
2	P	125	
2	Q	125	
2	R	125	
3	S	372	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 35315 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	366	Total	C	N	O	S	0	0
			2911	1848	493	557	13		
1	B	366	Total	C	N	O	S	0	0
			2894	1837	490	554	13		
1	C	366	Total	C	N	O	S	0	0
			2878	1828	489	548	13		
1	D	366	Total	C	N	O	S	0	0
			2856	1810	483	551	12		
1	E	366	Total	C	N	O	S	0	0
			2876	1829	485	549	13		
1	F	366	Total	C	N	O	S	0	0
			2908	1847	491	557	13		
1	G	366	Total	C	N	O	S	0	0
			2902	1840	492	557	13		
1	H	366	Total	C	N	O	S	0	0
			2909	1847	493	556	13		
1	I	354	Total	C	N	O	S	0	0
			2788	1771	473	531	13		

- Molecule 2 is a protein called Putative structural protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	124	Total	C	N	O	S	0	0
			926	589	156	180	1		
2	K	124	Total	C	N	O	S	0	0
			943	600	158	184	1		
2	L	124	Total	C	N	O	S	0	0
			944	600	158	185	1		
2	M	124	Total	C	N	O	S	0	0
			936	594	158	183	1		
2	N	124	Total	C	N	O	S	0	0
			934	593	158	182	1		
2	O	124	Total	C	N	O	S	0	0
			933	592	158	182	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	124	Total	C	N	O	S	0	0
			928	588	157	182	1		
2	Q	124	Total	C	N	O	S	0	0
			944	600	158	185	1		
2	R	124	Total	C	N	O	S	0	0
			944	600	158	185	1		

- Molecule 3 is a protein called Putative tail protein.

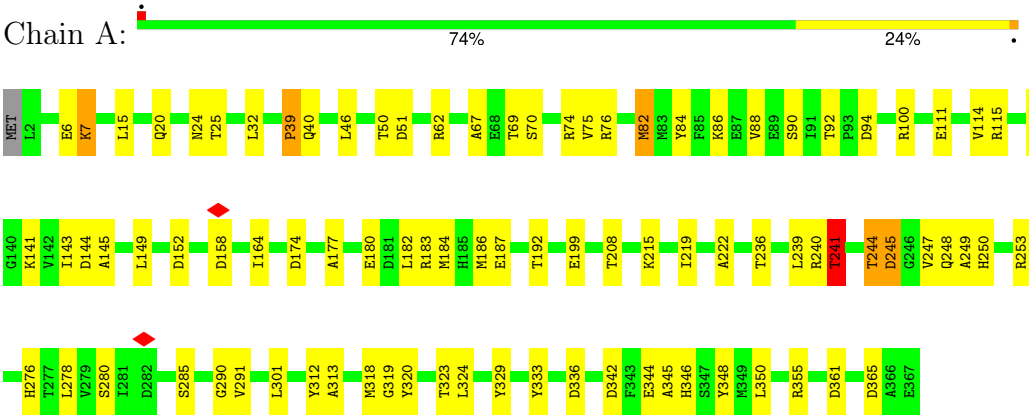
Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	120	Total	C	N	O	S	0	0
			961	630	149	179	3		

3 Residue-property plots (i)

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

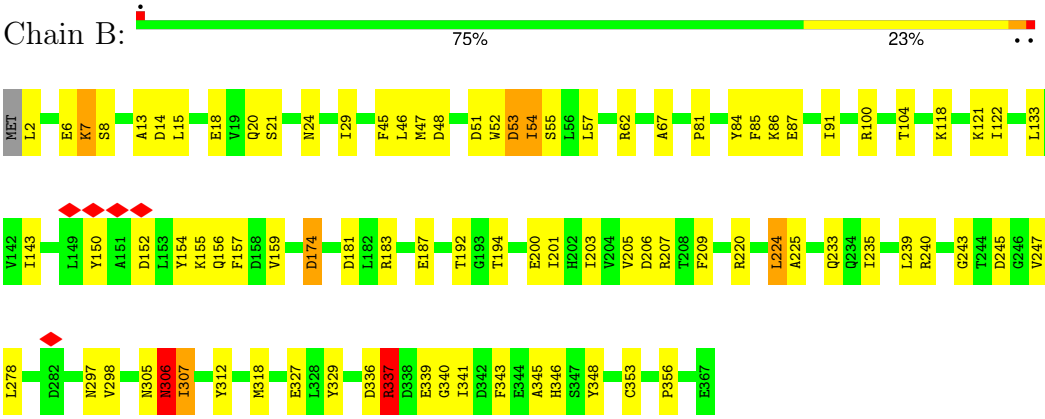
• Molecule 1: Major capsid protein

Chain A:



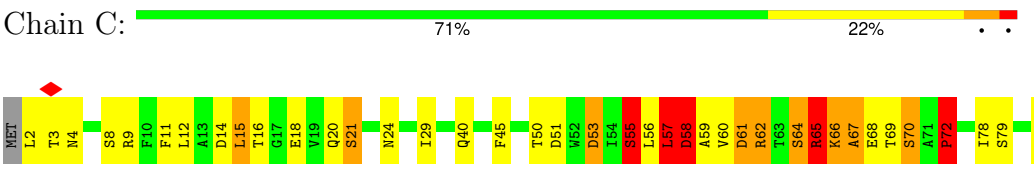
• Molecule 1: Major capsid protein

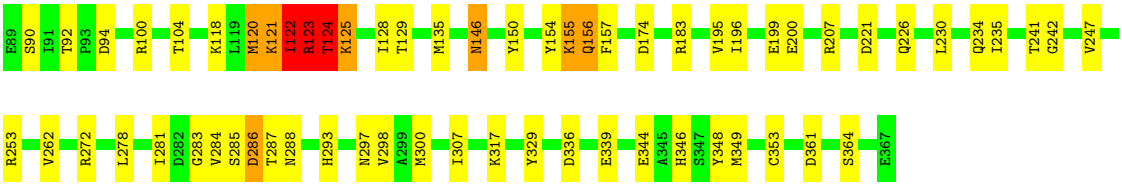
Chain B:



• Molecule 1: Major capsid protein

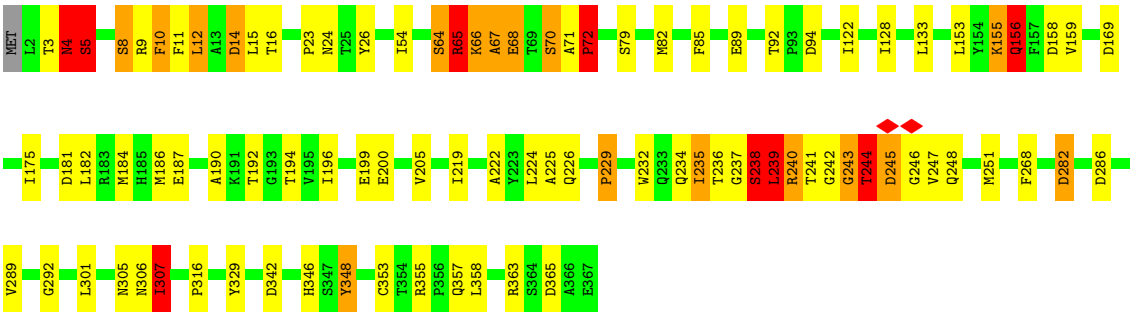
Chain C:





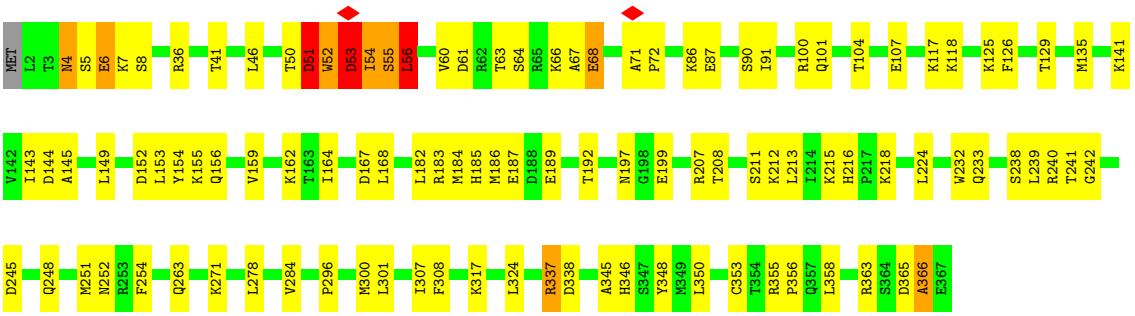
• Molecule 1: Major capsid protein

Chain D:



• Molecule 1: Major capsid protein

Chain E:

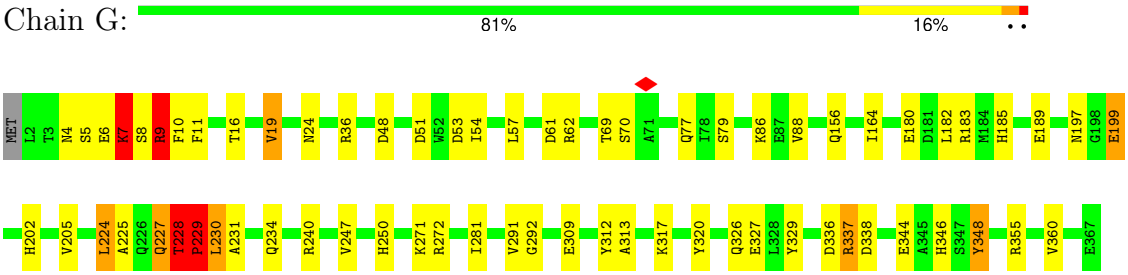


• Molecule 1: Major capsid protein

Chain F:

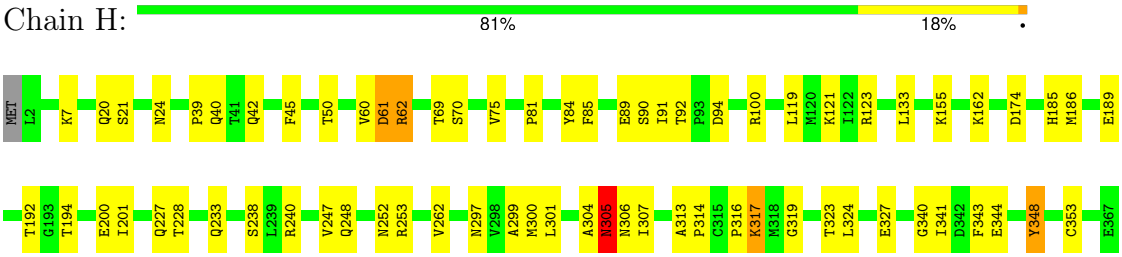
• Molecule 1: Major capsid protein

Chain G:



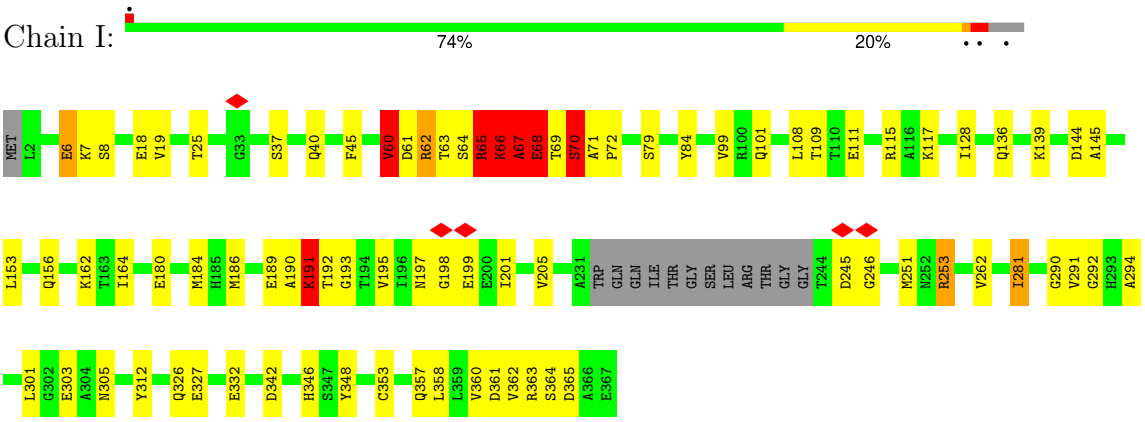
• Molecule 1: Major capsid protein

Chain H:



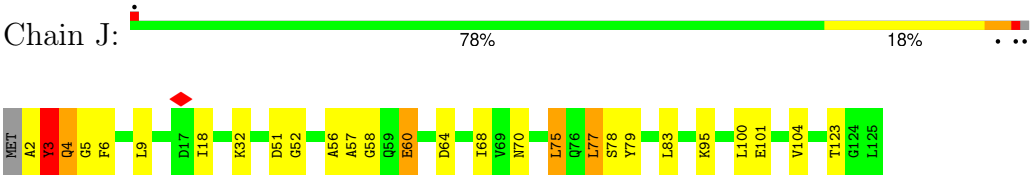
• Molecule 1: Major capsid protein

Chain I:



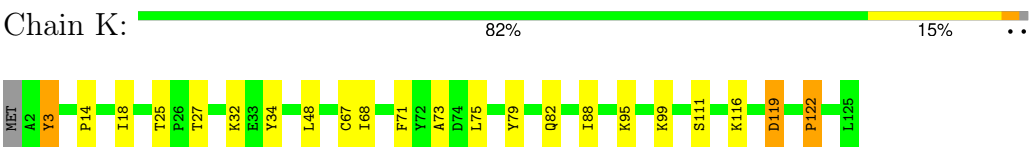
• Molecule 2: Putative structural protein

Chain J:



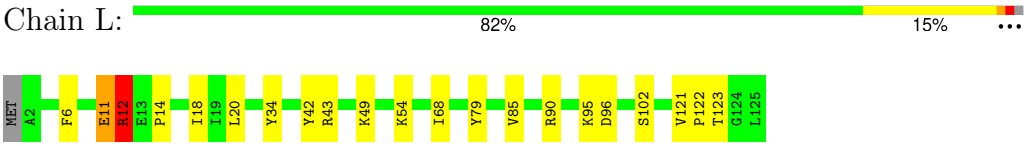
• Molecule 2: Putative structural protein

Chain K:



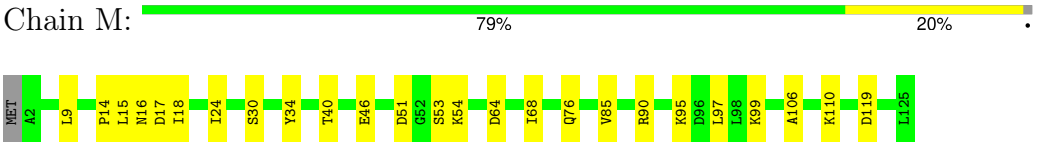
• Molecule 2: Putative structural protein

Chain L:



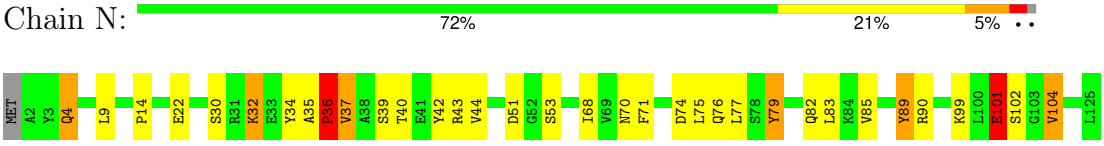
• Molecule 2: Putative structural protein

Chain M:



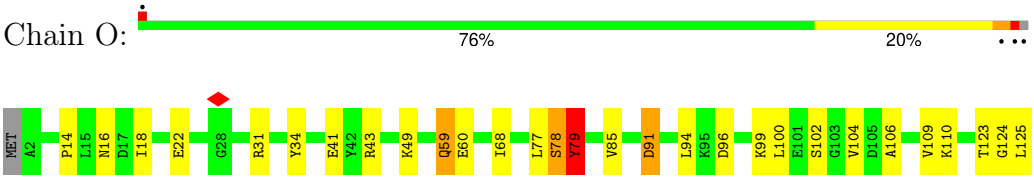
• Molecule 2: Putative structural protein

Chain N:



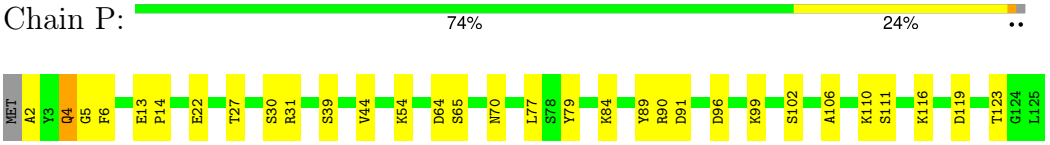
• Molecule 2: Putative structural protein

Chain O:



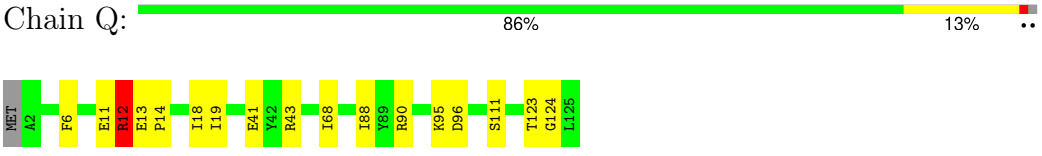
• Molecule 2: Putative structural protein

Chain P:



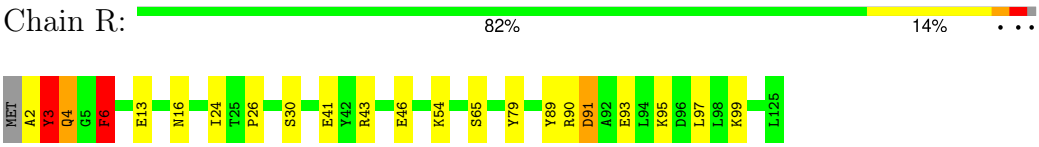
• Molecule 2: Putative structural protein

Chain Q:



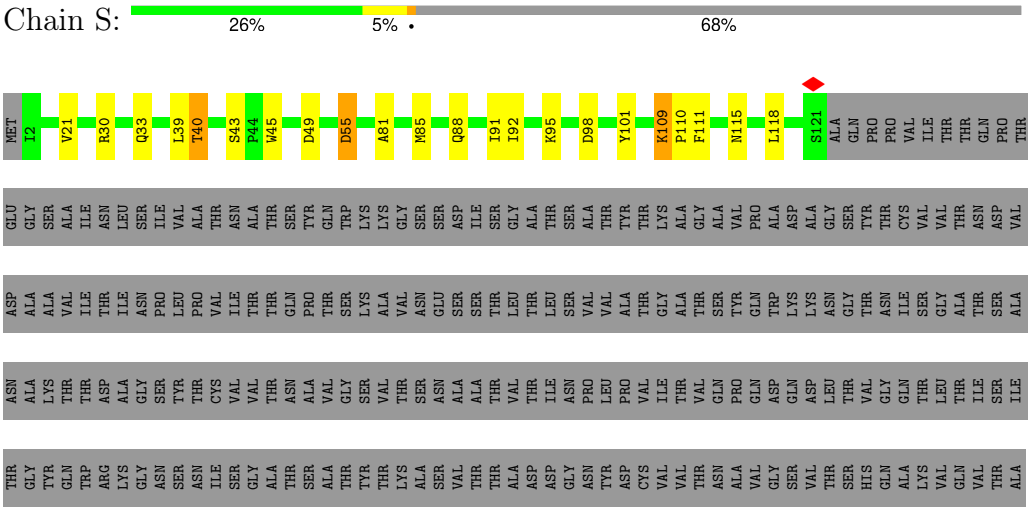
• Molecule 2: Putative structural protein

Chain R:



• Molecule 3: Putative tail protein

Chain S:


26%
5%
68%
MET I2 V21 R30 Q33 L39 T40 S43 P44 W45 D49 D55 A81 M85 Q88 I91 I92 K95 D98 Y101 K109 P110 F111 N115 L118 S121 ALA GLN PRO PRO VAL ILE THR THR GLN PRO THR GLY GLY ALA VAL ASN
GLU GLY SER ALA ILE ASN LEU SER ILE VAL ALA THR ASN ALA THR SER TYR GLN TRP LYS LYS GLY SER SER ASP ILE SER GLY ALA THR SER ALA THR THR TYR THR LYS ALA GLY ALA VAL PRO ALA ASP ALA GLY SER TYR THR CYS VAL VAL THR ASN ASP VAL GLY SER THR THR SER
ASP ALA ALA VAL ILE THR ILE ASN PRO LEU PRO VAL ILE THR THR GLN PRO THR SER LYS ALA VAL ASN GLU SER SER THR LEU THR LEU SER VAL VAL ALA THR GLY ALA THR SER TYR GLN TRP LYS LYS ASN GLY THR ASN ILE SER GLY ALA THR SER ALA THR TYR SER LYS ALA
ASN ALA LYS THR THR ASP ALA GLY SER TYR THR CYS VAL VAL THR ASN ALA VAL GLY SER VAL THR SER ASN ALA ALA THR VAL THR ILE ASN PRO LEU PRO VAL ILE THR VAL GLN PRO GLN ASP GLN ASP LEU THR VAL GLY GLN THR LEU THR ILE SER ILE THR ALA THR GLY ALA
THR GLY TYR GLN TRP ARG LYS GLY ASN SER ASN ILE SER GLY ALA THR SER ALA THR TYR THR LYS ALA SER VAL THR THR ALA ASP ASP GLY ASN TYR ASP CYS VAL VAL THR ASN ALA VAL GLY SER VAL THR SER HIS GLN ALA LYS VAL GLN VAL THR ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98511	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	33	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.923	Depositor
Minimum map value	-2.864	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.249	Depositor
Recommended contour level	0.651	Depositor
Map size (Å)	1224.0, 1224.0, 1224.0	wwPDB
Map dimensions	1000, 1000, 1000	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.224, 1.224, 1.224	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	0.35	1/2972 (0.0%)	0.66	3/4021 (0.1%)
1	B	0.47	1/2955 (0.0%)	0.70	6/4001 (0.1%)
1	C	0.62	4/2939 (0.1%)	1.22	34/3979 (0.9%)
1	D	0.67	5/2915 (0.2%)	1.04	28/3949 (0.7%)
1	E	0.56	6/2937 (0.2%)	0.81	13/3978 (0.3%)
1	F	0.48	3/2969 (0.1%)	0.68	9/4017 (0.2%)
1	G	0.50	0/2962	0.80	17/4009 (0.4%)
1	H	0.40	0/2970	0.68	10/4019 (0.2%)
1	I	0.53	3/2846 (0.1%)	0.86	15/3851 (0.4%)
2	J	0.59	2/941 (0.2%)	0.88	4/1274 (0.3%)
2	K	0.34	0/959	0.61	1/1298 (0.1%)
2	L	0.44	0/960	0.64	3/1299 (0.2%)
2	M	0.30	0/951	0.52	0/1287
2	N	0.58	2/949 (0.2%)	0.96	6/1284 (0.5%)
2	O	0.50	1/948 (0.1%)	0.62	1/1283 (0.1%)
2	P	0.40	1/943 (0.1%)	0.66	2/1276 (0.2%)
2	Q	0.44	0/960	0.91	7/1299 (0.5%)
2	R	0.39	0/960	0.83	4/1299 (0.3%)
3	S	0.30	0/990	0.52	0/1351
All	All	0.50	29/36026 (0.1%)	0.82	163/48774 (0.3%)

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	1
1	B	0	1
1	C	0	3
1	D	0	2
1	E	0	1
1	F	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	3
1	H	0	1
1	I	0	2
2	L	0	2
2	Q	0	1
3	S	0	1
All	All	0	19

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	8	SER	CA-CB	-11.87	1.35	1.52
1	B	8	SER	CA-CB	-11.28	1.36	1.52
1	E	8	SER	CA-CB	-9.97	1.38	1.52
1	C	64	SER	CA-CB	-8.82	1.39	1.52
1	C	70	SER	CA-CB	-8.79	1.39	1.52
2	O	78	SER	CA-CB	-8.24	1.40	1.52
1	I	70	SER	CA-CB	-8.17	1.40	1.52
1	C	21	SER	CA-CB	-8.13	1.40	1.52
1	D	70	SER	CA-CB	-7.80	1.41	1.52
1	F	5	SER	CA-CB	-7.78	1.41	1.52
1	I	64	SER	CA-CB	-7.73	1.41	1.52
2	J	4	GLN	CA-CB	-7.20	1.38	1.53
1	F	37	SER	CA-CB	-7.02	1.42	1.52
2	J	3	TYR	CA-CB	-6.71	1.39	1.53
1	D	64	SER	CA-CB	-6.57	1.43	1.52
1	D	67	ALA	CA-CB	-6.52	1.38	1.52
1	I	8	SER	CA-CB	-6.45	1.43	1.52
1	E	55	SER	CA-CB	-6.12	1.43	1.52
1	E	64	SER	CA-CB	-6.03	1.44	1.52
1	D	5	SER	CA-CB	-5.93	1.44	1.52
1	D	235	ILE	CA-CB	-5.88	1.41	1.54
1	A	285	SER	CA-CB	-5.87	1.44	1.52
1	C	67	ALA	CA-CB	-5.83	1.40	1.52
1	E	68	GLU	CA-CB	-5.83	1.41	1.53
2	P	4	GLN	CA-CB	-5.45	1.42	1.53
1	E	5	SER	CA-CB	-5.30	1.45	1.52
2	N	39	SER	CA-CB	-5.19	1.45	1.52
1	E	366	ALA	CA-CB	-5.12	1.41	1.52
2	N	102	SER	CA-CB	-5.12	1.45	1.52

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	57	LEU	N-CA-CB	-24.72	60.97	110.40
2	N	36	PRO	N-CA-CB	-19.52	79.88	103.30
1	C	121	LYS	CB-CA-C	-19.25	71.90	110.40
1	C	65	ARG	N-CA-CB	-18.20	77.84	110.60
2	R	6	PHE	CB-CA-C	-18.09	74.22	110.40
1	I	65	ARG	CB-CA-C	-17.73	74.95	110.40
1	C	72	PRO	N-CA-CB	-16.74	83.21	103.30
1	A	245	ASP	CB-CA-C	-16.70	77.00	110.40
1	D	10	PHE	N-CA-CB	-15.36	82.95	110.60
1	C	61	ASP	CB-CA-C	-15.09	80.23	110.40
2	Q	14	PRO	N-CA-CB	-14.69	85.68	103.30
1	C	62	ARG	CB-CA-C	-14.11	82.19	110.40
1	D	72	PRO	N-CA-CB	-14.11	86.37	103.30
1	C	120	MET	CB-CA-C	-13.83	82.74	110.40
1	I	72	PRO	N-CA-CB	-12.62	88.16	103.30
1	E	6	GLU	N-CA-CB	-12.46	88.17	110.60
1	I	72	PRO	N-CD-CG	-10.66	87.21	103.20
1	C	66	LYS	N-CA-CB	-10.50	91.70	110.60
2	Q	11	GLU	CB-CA-C	-10.49	89.42	110.40
1	C	51	ASP	CB-CA-C	-10.48	89.44	110.40
2	K	122	PRO	N-CA-CB	-10.09	91.19	103.30
1	D	10	PHE	CB-CA-C	10.06	130.53	110.40
1	F	267	LYS	CB-CA-C	-10.03	90.33	110.40
1	G	197	ASN	CB-CA-C	-9.97	90.46	110.40
1	H	61	ASP	CB-CA-C	-9.96	90.48	110.40
1	C	66	LYS	CB-CA-C	9.83	130.06	110.40
1	G	9	ARG	N-CA-CB	-9.72	93.10	110.60
1	D	305	ASN	CB-CA-C	9.67	129.75	110.40
1	E	56	LEU	N-CA-CB	-9.52	91.37	110.40
1	D	244	THR	N-CA-C	-9.36	85.74	111.00
1	D	67	ALA	N-CA-CB	-9.27	97.12	110.10
1	C	157	PHE	N-CA-CB	-9.25	93.95	110.60
1	F	326	GLN	N-CA-CB	-9.24	93.97	110.60
1	E	56	LEU	CB-CG-CD1	-9.21	95.35	111.00
1	D	65	ARG	N-CA-CB	-9.16	94.11	110.60
2	J	60	GLU	CB-CA-C	-9.12	92.16	110.40
1	D	66	LYS	CB-CA-C	8.93	128.25	110.40
1	E	68	GLU	N-CA-CB	-8.69	94.95	110.60
1	C	58	ASP	CB-CA-C	-8.64	93.11	110.40
1	G	229	PRO	N-CA-CB	8.46	113.45	103.30
1	E	308	PHE	N-CA-CB	-8.39	95.49	110.60
2	N	36	PRO	CB-CG-CD	-8.27	74.25	106.50
1	I	191	LYS	CB-CA-C	8.22	126.84	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	51	ASP	CB-CA-C	-8.20	94.01	110.40
1	F	6	GLU	N-CA-CB	-8.06	96.09	110.60
1	G	9	ARG	CB-CA-C	7.88	126.15	110.40
1	G	199	GLU	CB-CA-C	-7.76	94.88	110.40
1	E	7	LYS	N-CA-CB	7.75	124.55	110.60
1	I	18	GLU	CB-CA-C	-7.58	95.24	110.40
1	B	52	TRP	CA-CB-CG	7.54	128.04	113.70
1	D	229	PRO	N-CA-CB	-7.31	94.53	103.30
1	D	14	ASP	CB-CA-C	-7.30	95.80	110.40
1	D	65	ARG	CB-CA-C	7.29	124.99	110.40
1	F	6	GLU	CB-CA-C	7.27	124.95	110.40
1	G	230	LEU	N-CA-CB	7.27	124.93	110.40
1	D	301	LEU	CB-CG-CD1	-7.23	98.70	111.00
1	D	66	LYS	N-CA-CB	-7.22	97.61	110.60
1	G	225	ALA	CB-CA-C	-7.22	99.27	110.10
1	C	58	ASP	N-CA-CB	7.20	123.56	110.60
1	C	72	PRO	N-CA-C	7.20	130.82	112.10
1	F	308	PHE	N-CA-CB	-7.13	97.77	110.60
1	D	243	GLY	N-CA-C	-7.10	95.36	113.10
1	D	155	LYS	CB-CA-C	-7.09	96.22	110.40
2	Q	11	GLU	N-CA-CB	-7.08	97.86	110.60
2	Q	14	PRO	N-CD-CG	-7.02	92.67	103.20
1	A	319	GLY	C-N-CA	-6.94	104.35	121.70
1	D	156	GLN	N-CA-CB	6.93	123.07	110.60
1	D	11	PHE	N-CA-CB	-6.90	98.19	110.60
1	D	241	THR	N-CA-C	-6.90	92.38	111.00
2	R	4	GLN	N-CA-CB	-6.88	98.22	110.60
1	H	317	LYS	CA-CB-CG	6.87	128.51	113.40
1	I	68	GLU	N-CA-CB	-6.86	98.25	110.60
1	C	53	ASP	C-N-CA	-6.82	104.66	121.70
1	H	305	ASN	CB-CA-C	6.82	124.03	110.40
1	D	4	ASN	CB-CA-C	-6.80	96.80	110.40
1	C	55	SER	N-CA-C	-6.80	92.65	111.00
1	B	337	ARG	CB-CA-C	6.79	123.97	110.40
2	P	4	GLN	CB-CA-C	-6.76	96.88	110.40
1	G	202	HIS	CB-CA-C	-6.64	97.11	110.40
1	C	123	ARG	N-CA-CB	-6.63	98.67	110.60
1	C	154	TYR	N-CA-CB	-6.63	98.67	110.60
1	G	326	GLN	N-CA-CB	-6.62	98.69	110.60
1	B	8	SER	CB-CA-C	-6.51	97.73	110.10
1	I	60	VAL	N-CA-CB	-6.49	97.23	111.50
1	E	7	LYS	CB-CA-C	-6.48	97.43	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	7	LYS	CB-CA-C	-6.47	97.47	110.40
1	B	7	LYS	CB-CA-C	6.41	123.22	110.40
2	Q	13	GLU	N-CA-CB	-6.40	99.08	110.60
1	D	240	ARG	CB-CA-C	-6.32	97.76	110.40
1	F	328	LEU	CB-CG-CD1	-6.31	100.28	111.00
1	A	241	THR	O-C-N	-6.28	112.52	123.20
2	J	6	PHE	C-N-CA	6.28	137.39	121.70
1	F	8	SER	CB-CA-C	-6.26	98.21	110.10
1	F	327	GLU	N-CA-CB	-6.25	99.36	110.60
1	C	55	SER	CB-CA-C	6.09	121.67	110.10
2	P	6	PHE	N-CA-CB	-6.05	99.71	110.60
1	H	84	TYR	CB-CA-C	-6.04	98.32	110.40
1	I	66	LYS	CB-CA-C	-6.03	98.33	110.40
1	D	240	ARG	CA-C-N	-6.00	103.99	117.20
1	C	124	THR	OG1-CB-CG2	-5.99	96.21	110.00
1	C	154	TYR	CB-CA-C	-5.99	98.42	110.40
1	C	62	ARG	CA-CB-CG	5.97	126.54	113.40
2	L	11	GLU	N-CA-CB	-5.92	99.94	110.60
1	G	7	LYS	CA-C-N	-5.91	104.20	117.20
1	G	7	LYS	C-N-CA	-5.88	107.00	121.70
1	B	225	ALA	N-CA-CB	-5.83	101.94	110.10
1	I	62	ARG	N-CA-CB	5.81	121.06	110.60
1	C	125	LYS	N-CA-C	-5.76	95.45	111.00
2	Q	12	ARG	CA-CB-CG	5.72	125.99	113.40
1	D	224	LEU	N-CA-CB	-5.71	98.98	110.40
1	F	265	ASN	N-CA-CB	-5.70	100.35	110.60
2	R	6	PHE	CA-CB-CG	5.67	127.51	113.90
1	I	67	ALA	C-N-CA	-5.65	107.57	121.70
1	H	60	VAL	O-C-N	-5.63	113.68	122.70
1	I	326	GLN	N-CA-CB	-5.62	100.49	110.60
1	D	242	GLY	C-N-CA	-5.61	110.52	122.30
1	D	244	THR	N-CA-CB	5.61	120.96	110.30
2	J	101	GLU	N-CA-CB	-5.57	100.57	110.60
2	R	3	TYR	CB-CA-C	-5.55	99.31	110.40
1	G	229	PRO	C-N-CA	-5.54	107.84	121.70
1	C	56	LEU	CA-C-O	-5.54	108.47	120.10
2	O	79	TYR	CA-CB-CG	5.54	123.92	113.40
2	N	4	GLN	CB-CA-C	-5.53	99.33	110.40
1	D	232	TRP	CB-CA-C	5.53	121.46	110.40
2	J	77	LEU	CB-CG-CD1	-5.53	101.60	111.00
1	C	66	LYS	C-N-CA	-5.42	108.15	121.70
1	G	16	THR	N-CA-CB	-5.41	100.03	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	62	ARG	CB-CA-C	-5.40	99.59	110.40
1	I	71	ALA	N-CA-CB	-5.36	102.59	110.10
2	N	101	GLU	N-CA-CB	-5.31	101.04	110.60
1	E	67	ALA	N-CA-CB	-5.30	102.67	110.10
1	C	62	ARG	N-CA-CB	5.29	120.11	110.60
1	D	155	LYS	N-CA-CB	5.28	120.10	110.60
1	C	156	GLN	N-CA-C	-5.28	96.75	111.00
1	E	66	LYS	CB-CA-C	5.27	120.94	110.40
1	I	68	GLU	C-N-CA	-5.26	108.55	121.70
1	H	317	LYS	N-CA-C	-5.25	96.84	111.00
1	H	327	GLU	CB-CG-CD	-5.22	100.10	114.20
1	C	70	SER	N-CA-CB	-5.22	102.68	110.50
2	N	36	PRO	N-CD-CG	-5.21	95.38	103.20
1	C	57	LEU	CA-C-N	5.21	128.66	117.20
1	I	67	ALA	CB-CA-C	-5.19	102.31	110.10
1	G	224	LEU	CB-CA-C	5.18	120.04	110.20
1	H	319	GLY	C-N-CA	-5.17	108.77	121.70
2	N	83	LEU	CB-CG-CD1	-5.17	102.22	111.00
2	L	12	ARG	CB-CA-C	-5.15	100.09	110.40
1	H	155	LYS	N-CA-CB	-5.15	101.33	110.60
1	I	327	GLU	CB-CG-CD	-5.14	100.33	114.20
1	C	66	LYS	CA-CB-CG	5.13	124.70	113.40
1	C	124	THR	N-CA-CB	5.13	120.04	110.30
1	C	61	ASP	N-CA-CB	5.12	119.82	110.60
1	C	68	GLU	N-CA-C	-5.12	97.17	111.00
1	E	67	ALA	CB-CA-C	5.12	117.78	110.10
1	B	53	ASP	CA-C-N	-5.10	105.98	117.20
1	E	53	ASP	C-N-CA	-5.10	108.95	121.70
1	G	202	HIS	CA-CB-CG	5.06	122.21	113.60
2	L	6	PHE	CB-CA-C	-5.06	100.28	110.40
1	D	239	LEU	C-N-CA	-5.06	109.06	121.70
1	E	68	GLU	CA-C-N	5.04	128.30	117.20
1	C	122	ILE	CA-C-N	-5.04	106.12	117.20
2	Q	14	PRO	CA-N-CD	5.03	118.74	111.70
1	G	197	ASN	N-CA-CB	5.02	119.64	110.60
1	D	235	ILE	CB-CA-C	-5.02	101.55	111.60

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	THR	Mainchain

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Mol	Chain	Res	Type	Group
1	B	337	ARG	Sidechain
1	C	12	LEU	Mainchain
1	C	283	GLY	Mainchain
1	C	65	ARG	Sidechain
1	D	244	THR	Mainchain
1	D	65	ARG	Sidechain
1	E	337	ARG	Sidechain
1	F	36	ARG	Sidechain
1	G	228	THR	Mainchain
1	G	337	ARG	Sidechain
1	G	7	LYS	Mainchain
1	H	62	ARG	Sidechain
1	I	65	ARG	Sidechain
1	I	66	LYS	Mainchain
2	L	12	ARG	Sidechain
2	L	122	PRO	Mainchain
2	Q	12	ARG	Sidechain
3	S	109	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2911	0	2855	64	0
1	B	2894	0	2824	69	0
1	C	2878	0	2799	67	0
1	D	2856	0	2747	61	0
1	E	2876	0	2797	73	0
1	F	2908	0	2849	65	0
1	G	2902	0	2829	49	0
1	H	2909	0	2856	39	0
1	I	2788	0	2701	40	0
2	J	926	0	913	21	0
2	K	943	0	937	11	0
2	L	944	0	940	11	0
2	M	936	0	930	18	0
2	N	934	0	925	24	0
2	O	933	0	929	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	928	0	913	21	0
2	Q	944	0	940	7	0
2	R	944	0	940	22	0
3	S	961	0	905	14	0
All	All	35315	0	34529	595	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 9.

All (595) 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:D:243:GLY:C	1:D:245:ASP:N	2.02	1.00
1:D:243:GLY:C	1:D:245:ASP:H	1.65	0.94
1:G:8:SER:O	1:G:10:PHE:N	2.04	0.90
1:G:227:GLN:O	1:G:229:PRO:N	2.08	0.85
1:E:53:ASP:HA	1:F:23:PRO:HG3	1.59	0.84
1:I:190:ALA:HB2	1:I:358:LEU:HD21	1.58	0.84
2:J:2:ALA:HB1	2:J:5:GLY:H	1.42	0.81
2:M:16:ASN:ND2	2:M:68:ILE:O	2.14	0.81
1:B:156:GLN:CB	2:R:6:PHE:HB3	2.12	0.80
1:D:68:GLU:HB2	1:E:271:LYS:NZ	1.97	0.79
1:I:68:GLU:O	1:I:69:THR:C	2.15	0.79
1:D:8:SER:O	1:D:10:PHE:N	2.15	0.79
2:R:2:ALA:O	2:R:3:TYR:C	2.21	0.78
2:P:2:ALA:CB	2:P:5:GLY:HA3	2.16	0.76
2:K:14:PRO:HG3	2:K:99:LYS:HE2	1.69	0.75
2:P:2:ALA:HB1	2:P:5:GLY:HA3	1.68	0.74
1:B:62:ARG:NH1	1:C:150:TYR:OH	2.22	0.73
1:G:7:LYS:O	1:G:8:SER:C	2.18	0.72
1:I:290:GLY:H	1:I:364:SER:HB3	1.55	0.72
1:A:183:ARG:HD2	1:A:199:GLU:HG2	1.71	0.72
1:G:229:PRO:O	1:G:230:LEU:C	2.25	0.71
1:C:122:ILE:O	1:C:124:THR:N	2.24	0.71
2:L:95:LYS:HB3	2:L:123:THR:HG21	1.71	0.71
1:A:20:GLN:O	1:F:355:ARG:NH2	2.24	0.71
1:E:300:MET:HG2	1:E:301:LEU:HG	1.73	0.71
1:C:66:LYS:O	1:C:67:ALA:HB2	1.91	0.70
1:C:122:ILE:O	1:C:123:ARG:C	2.25	0.70
2:N:14:PRO:HG3	2:N:99:LYS:HE2	1.74	0.70
1:G:227:GLN:HG3	1:G:231:ALA:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:301:LEU:HD13	1:F:307:ILE:HD11	1.74	0.69
1:B:135:MET:HG2	1:B:278:LEU:HB3	1.75	0.69
1:E:183:ARG:HD3	1:E:199:GLU:HG3	1.73	0.69
1:I:281:ILE:HD12	1:I:291:VAL:HG13	1.74	0.69
1:H:92:THR:HG22	1:H:94:ASP:H	1.58	0.68
1:D:187:GLU:HA	1:D:196:ILE:HD11	1.73	0.68
2:M:34:TYR:HB2	2:M:85:VAL:HG13	1.75	0.68
2:J:2:ALA:CB	2:J:5:GLY:H	2.07	0.68
2:O:124:GLY:O	2:O:125:LEU:C	2.32	0.68
2:O:18:ILE:HG22	2:O:94:LEU:HB3	1.75	0.68
2:M:30:SER:HA	2:M:90:ARG:HB2	1.76	0.67
1:A:139:LYS:NZ	1:A:278:LEU:O	2.25	0.67
2:L:18:ILE:HD11	2:L:68:ILE:HG22	1.77	0.67
1:G:281:ILE:HD12	1:G:291:VAL:HG22	1.75	0.67
2:J:2:ALA:HB1	2:J:5:GLY:N	2.08	0.67
1:I:60:VAL:HG21	1:I:66:LYS:HA	1.76	0.67
1:I:153:LEU:HD21	1:I:353:CYS:H	1.58	0.67
1:A:39:PRO:HB2	1:A:324:LEU:HD22	1.76	0.67
1:E:87:GLU:HB3	1:E:345:ALA:HB3	1.76	0.67
2:M:34:TYR:OH	2:M:64:ASP:OD1	2.11	0.66
1:G:329:TYR:HB2	1:G:346:HIS:HB2	1.78	0.66
1:D:181:ASP:OD1	1:E:207:ARG:NH1	2.29	0.66
1:C:88:VAL:HG12	1:C:344:GLU:HG2	1.77	0.66
1:D:92:THR:HG22	1:D:94:ASP:H	1.60	0.66
1:A:355:ARG:NH2	1:B:20:GLN:O	2.27	0.66
2:K:119:ASP:OD1	2:L:90:ARG:NH2	2.29	0.65
2:M:46:GLU:HG2	2:M:99:LYS:HB2	1.78	0.65
1:H:85:PHE:CZ	1:H:133:LEU:HD11	2.31	0.65
1:E:240:ARG:HG3	1:E:252:ASN:HB3	1.79	0.65
2:O:100:LEU:HD11	2:O:109:VAL:HG21	1.79	0.64
1:E:52:TRP:O	1:E:54:ILE:N	2.31	0.64
2:O:49:LYS:NZ	2:O:59:GLN:OE1	2.31	0.64
1:C:9:ARG:O	1:H:100:ARG:NH1	2.29	0.63
1:H:50:THR:HG22	1:H:75:VAL:HG13	1.80	0.63
2:R:2:ALA:O	2:R:4:GLN:N	2.31	0.63
2:R:30:SER:HA	2:R:90:ARG:HB2	1.78	0.63
1:D:329:TYR:HB2	1:D:346:HIS:HB2	1.79	0.63
1:B:297:ASN:OD1	1:B:298:VAL:N	2.32	0.63
1:H:24:ASN:HB2	1:H:247:VAL:HG22	1.79	0.63
1:B:29:ILE:HG13	1:B:135:MET:SD	2.39	0.63
1:C:146:ASN:O	1:C:146:ASN:ND2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:ASP:O	1:C:288:ASN:N	2.33	0.62
1:H:69:THR:HG22	1:H:70:SER:H	1.64	0.62
1:I:111:GLU:OE2	1:I:115:ARG:NH2	2.32	0.62
1:D:68:GLU:HB2	1:E:271:LYS:HZ1	1.63	0.62
1:B:307:ILE:HG13	1:B:353:CYS:SG	2.40	0.62
1:D:71:ALA:HB1	1:D:72:PRO:HD2	1.82	0.62
1:H:40:GLN:HG2	1:H:42:GLN:H	1.63	0.61
2:M:119:ASP:OD2	2:N:90:ARG:NH2	2.32	0.61
1:G:77:GLN:HB3	2:N:9:LEU:HB2	1.82	0.61
1:C:195:VAL:HG22	1:D:246:GLY:H	1.66	0.61
1:F:81:PRO:HG3	2:J:4:GLN:CB	2.31	0.61
1:B:339:GLU:HG3	2:M:24:ILE:HD12	1.83	0.61
1:C:339:GLU:HG3	2:R:24:ILE:HD12	1.83	0.61
1:A:111:GLU:OE2	1:A:115:ARG:NH1	2.32	0.60
1:E:183:ARG:NH1	1:E:199:GLU:OE2	2.34	0.60
1:B:305:ASN:O	1:B:306:ASN:C	2.38	0.60
1:D:67:ALA:HB1	1:E:86:LYS:O	2.02	0.60
2:O:22:GLU:OE2	2:O:31:ARG:NH1	2.34	0.60
1:A:100:ARG:NH2	1:F:48:ASP:OD2	2.33	0.60
1:E:135:MET:HG2	1:E:278:LEU:HB3	1.82	0.60
1:H:200:GLU:HG2	1:H:299:ALA:HB3	1.83	0.60
2:J:83:LEU:HD23	2:J:83:LEU:H	1.66	0.60
1:B:159:VAL:HG21	1:B:356:PRO:HG2	1.84	0.60
2:O:60:GLU:OE1	2:O:60:GLU:N	2.33	0.60
1:I:186:MET:HE2	1:I:201:ILE:HD12	1.84	0.60
1:C:29:ILE:HG13	1:C:135:MET:HG2	1.83	0.60
1:C:317:LYS:HE2	1:C:346:HIS:HE1	1.65	0.60
1:H:119:LEU:O	1:H:123:ARG:HG2	2.02	0.59
1:E:153:LEU:O	1:E:356:PRO:HG3	2.02	0.59
1:B:57:LEU:HD12	1:C:128:ILE:HG13	1.83	0.59
1:H:316:PRO:O	1:H:317:LYS:HG2	2.03	0.59
1:C:297:ASN:OD1	1:C:298:VAL:N	2.36	0.59
1:G:69:THR:HG22	1:G:70:SER:H	1.66	0.59
1:C:135:MET:HG3	1:C:278:LEU:HD23	1.84	0.59
1:G:180:GLU:OE2	1:H:240:ARG:NH2	2.35	0.59
1:I:68:GLU:O	1:I:70:SER:N	2.35	0.59
2:N:34:TYR:HB2	2:N:85:VAL:HG13	1.84	0.59
2:J:32:LYS:NZ	2:J:64:ASP:OD2	2.35	0.59
1:B:91:ILE:HD12	1:B:343:PHE:HE2	1.68	0.59
1:C:57:LEU:HD12	1:D:128:ILE:HG22	1.84	0.59
1:B:62:ARG:HG2	2:P:84:LYS:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:TYR:HB2	1:B:346:HIS:HB2	1.85	0.58
1:D:226:GLN:HG3	1:E:232:TRP:CD1	2.38	0.58
1:C:336:ASP:HB2	2:R:24:ILE:HD11	1.85	0.58
2:L:34:TYR:HB2	2:L:85:VAL:HG13	1.86	0.58
2:L:49:LYS:NZ	2:L:54:LYS:O	2.36	0.58
1:C:123:ARG:O	1:C:124:THR:OG1	2.17	0.58
1:G:8:SER:C	1:G:10:PHE:N	2.56	0.58
1:A:236:THR:OG1	1:F:226:GLN:NE2	2.34	0.58
1:B:45:PHE:HB2	1:C:16:THR:CG2	2.34	0.58
1:C:92:THR:HG22	1:C:94:ASP:H	1.68	0.58
1:F:245:ASP:OD1	1:F:245:ASP:N	2.34	0.58
1:E:60:VAL:HG22	1:F:85:PHE:HD2	1.69	0.57
1:D:307:ILE:HG23	1:D:353:CYS:SG	2.44	0.57
2:O:91:ASP:OD2	2:O:91:ASP:N	2.36	0.57
1:C:183:ARG:NH1	1:C:199:GLU:OE1	2.37	0.57
1:C:329:TYR:HB2	1:C:346:HIS:HB2	1.86	0.57
1:D:159:VAL:HG21	1:D:357:GLN:HB3	1.86	0.57
1:E:154:TYR:HD1	1:E:159:VAL:HG23	1.69	0.57
1:G:7:LYS:O	1:G:9:ARG:N	2.36	0.57
1:D:184:MET:HE1	1:E:207:ARG:HE	1.70	0.57
1:A:51:ASP:HB3	1:B:21:SER:HB2	1.86	0.56
2:O:78:SER:OG	2:O:79:TYR:N	2.38	0.56
1:B:305:ASN:O	1:B:307:ILE:N	2.38	0.56
2:R:95:LYS:HB3	2:R:97:LEU:HD12	1.87	0.56
1:B:152:ASP:H	1:B:155:LYS:HE3	1.69	0.56
1:E:239:LEU:HD11	1:E:254:PHE:HD1	1.70	0.56
1:F:183:ARG:NH1	1:F:199:GLU:OE2	2.38	0.56
1:G:8:SER:O	1:G:9:ARG:C	2.42	0.56
1:I:294:ALA:HB3	1:I:360:VAL:HG23	1.88	0.56
1:E:46:LEU:HB2	1:F:15:LEU:HD12	1.88	0.56
1:A:180:GLU:OE2	1:B:240:ARG:NH2	2.33	0.56
1:G:57:LEU:HD22	1:H:85:PHE:HD2	1.69	0.56
2:N:44:VAL:HG23	2:N:68:ILE:HA	1.86	0.56
1:E:4:ASN:N	1:E:4:ASN:OD1	2.38	0.55
1:H:174:ASP:OD1	1:H:174:ASP:N	2.36	0.55
2:J:18:ILE:HD11	2:J:68:ILE:HG22	1.87	0.55
1:F:154:TYR:CZ	1:F:161:LYS:HD3	2.42	0.55
1:H:304:ALA:O	1:H:305:ASN:HB2	2.06	0.55
1:D:199:GLU:OE1	1:E:238:SER:OG	2.24	0.55
1:C:241:THR:OG1	1:C:242:GLY:N	2.40	0.55
2:L:96:ASP:H	2:L:123:THR:HG23	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:101:TYR:HD2	3:S:115:ASN:HB3	1.71	0.55
1:C:100:ARG:NH1	1:C:104:THR:O	2.38	0.55
1:D:238:SER:O	1:D:238:SER:OG	2.22	0.55
1:G:227:GLN:C	1:G:229:PRO:N	2.55	0.55
3:S:39:LEU:O	3:S:40:THR:OG1	2.21	0.55
1:E:208:THR:HG22	1:E:212:LYS:HD2	1.87	0.55
1:F:2:LEU:HB3	1:F:14:ASP:HA	1.89	0.55
2:P:65:SER:HB3	2:P:89:TYR:HB3	1.88	0.55
1:B:336:ASP:O	1:B:337:ARG:C	2.44	0.55
2:N:37:VAL:HG23	2:N:40:THR:CB	2.37	0.55
1:G:164:ILE:HD13	1:G:182:LEU:HB2	1.89	0.54
3:S:30:ARG:HD3	3:S:85:MET:HG3	1.89	0.54
2:J:70:ASN:HB2	2:J:79:TYR:HB2	1.90	0.54
2:N:22:GLU:OE2	2:N:30:SER:OG	2.24	0.54
1:I:191:LYS:C	1:I:193:GLY:H	2.10	0.54
1:A:84:TYR:OH	1:A:346:HIS:ND1	2.39	0.54
1:C:293:HIS:ND1	1:C:361:ASP:OD1	2.28	0.54
1:I:162:LYS:HB3	1:I:360:VAL:HG12	1.90	0.54
1:F:183:ARG:HD3	1:F:199:GLU:HG3	1.88	0.54
1:G:230:LEU:O	1:G:234:GLN:HG3	2.08	0.54
1:C:286:ASP:C	1:C:288:ASN:H	2.11	0.54
1:G:164:ILE:HD12	1:G:360:VAL:HG11	1.90	0.54
1:H:307:ILE:HG22	1:H:353:CYS:SG	2.47	0.54
1:B:67:ALA:HB2	1:C:86:LYS:HD3	1.89	0.54
2:J:2:ALA:HB1	2:J:5:GLY:CA	2.38	0.54
1:G:79:SER:O	1:G:156:GLN:NE2	2.41	0.54
2:L:96:ASP:H	2:L:123:THR:CG2	2.21	0.54
1:C:230:LEU:O	1:C:234:GLN:HG2	2.08	0.54
1:E:100:ARG:NH1	1:E:104:THR:O	2.41	0.54
1:E:192:THR:HG21	1:E:301:LEU:HD22	1.90	0.54
1:F:342:ASP:N	1:F:342:ASP:OD2	2.39	0.54
1:G:86:LYS:NZ	2:R:26:PRO:O	2.38	0.54
1:F:190:ALA:HB2	1:F:358:LEU:HD21	1.89	0.54
2:N:37:VAL:HG23	2:N:40:THR:HB	1.90	0.54
1:A:336:ASP:OD1	1:A:336:ASP:N	2.40	0.53
1:I:245:ASP:HB2	1:I:251:MET:SD	2.48	0.53
1:A:244:THR:HA	1:A:248:GLN:O	2.08	0.53
1:D:307:ILE:HD11	1:D:355:ARG:HB2	1.88	0.53
1:F:77:GLN:HG2	2:J:9:LEU:HD12	1.91	0.53
1:D:244:THR:CG2	1:D:248:GLN:HG2	2.38	0.53
1:E:248:GLN:HE21	1:E:251:MET:HG2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ILE:HD12	1:D:219:ILE:HD11	1.90	0.53
1:E:355:ARG:NH2	1:F:20:GLN:O	2.41	0.53
1:B:48:ASP:O	1:C:18:GLU:HA	2.09	0.53
1:A:24:ASN:HB3	1:A:247:VAL:HG21	1.90	0.52
1:C:174:ASP:N	1:C:174:ASP:OD1	2.38	0.52
1:I:79:SER:O	1:I:156:GLN:NE2	2.42	0.52
1:D:128:ILE:HD12	1:D:268:PHE:CE1	2.44	0.52
2:N:30:SER:HA	2:N:90:ARG:HB2	1.90	0.52
3:S:81:ALA:O	3:S:85:MET:HG2	2.10	0.52
1:B:150:TYR:CE2	2:R:2:ALA:HA	2.44	0.52
1:E:184:MET:SD	1:F:265:ASN:ND2	2.82	0.52
2:L:11:GLU:HG3	2:L:12:ARG:N	2.23	0.52
2:P:44:VAL:O	2:P:99:LYS:NZ	2.41	0.52
2:M:14:PRO:HG3	2:M:99:LYS:HE2	1.90	0.52
2:P:14:PRO:HG3	2:P:99:LYS:HE2	1.91	0.52
1:B:45:PHE:HB2	1:C:16:THR:HG23	1.90	0.52
1:D:8:SER:C	1:D:10:PHE:N	2.63	0.52
1:E:284:VAL:O	1:E:284:VAL:HG23	2.09	0.52
1:F:144:ASP:OD1	1:F:145:ALA:N	2.42	0.52
1:I:144:ASP:OD1	1:I:145:ALA:N	2.42	0.52
1:B:150:TYR:CD2	2:R:2:ALA:HA	2.44	0.52
1:B:224:LEU:HD13	1:B:235:ILE:HD12	1.92	0.52
1:D:205:VAL:HG12	1:D:292:GLY:HA3	1.91	0.52
1:A:128:ILE:HD12	1:A:268:PHE:CE1	2.44	0.52
1:E:60:VAL:HG11	1:F:83:MET:HB2	1.92	0.52
1:B:200:GLU:HB3	1:B:297:ASN:HB3	1.92	0.52
1:G:183:ARG:NH1	1:G:199:GLU:OE1	2.43	0.52
2:N:70:ASN:HB2	2:N:79:TYR:HB2	1.91	0.52
1:C:53:ASP:HA	1:D:23:PRO:HG3	1.93	0.51
1:G:7:LYS:CB	1:G:11:PHE:HD2	2.23	0.51
2:K:25:THR:HG22	2:K:27:THR:H	1.75	0.51
3:S:33:GLN:NE2	3:S:110:PRO:HA	2.25	0.51
1:D:54:ILE:HD11	1:E:125:LYS:HB2	1.92	0.51
2:R:41:GLU:OE1	2:R:43:ARG:NH2	2.44	0.51
1:A:24:ASN:HB3	1:A:247:VAL:CG2	2.40	0.51
1:C:8:SER:HG	1:C:11:PHE:HD2	1.57	0.51
1:G:337:ARG:O	1:G:338:ASP:C	2.49	0.51
1:F:85:PHE:CE1	1:F:347:SER:HB3	2.46	0.51
2:Q:18:ILE:HD11	2:Q:68:ILE:HG22	1.93	0.51
1:C:58:ASP:OD1	1:C:59:ALA:N	2.41	0.51
1:G:8:SER:C	1:G:10:PHE:H	2.15	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:SER:HB2	1:H:121:LYS:HE2	1.93	0.51
1:I:301:LEU:HB2	1:I:305:ASN:HB2	1.93	0.51
1:A:241:THR:OG1	1:A:253:ARG:NE	2.31	0.51
1:C:65:ARG:C	1:C:66:LYS:HG2	2.32	0.51
2:J:2:ALA:HB1	2:J:5:GLY:HA3	1.93	0.51
3:S:33:GLN:HE22	3:S:110:PRO:HA	1.75	0.51
1:D:286:ASP:HB3	1:D:289:VAL:HG22	1.93	0.51
1:E:164:ILE:HD13	1:E:182:LEU:HB2	1.91	0.51
2:P:2:ALA:CB	2:P:5:GLY:CA	2.89	0.51
1:E:54:ILE:O	1:F:121:LYS:NZ	2.40	0.50
1:G:205:VAL:HG12	1:G:292:GLY:HA3	1.92	0.50
1:A:192:THR:HG21	1:A:301:LEU:HD22	1.93	0.50
1:C:83:MET:HG2	1:C:349:MET:O	2.11	0.50
1:D:222:ALA:HA	1:E:224:LEU:HD11	1.93	0.50
1:A:280:SER:HA	1:A:291:VAL:HG21	1.92	0.50
1:D:192:THR:HG23	1:D:194:THR:H	1.75	0.50
1:I:66:LYS:O	1:I:67:ALA:HB2	2.10	0.50
2:O:16:ASN:ND2	2:O:68:ILE:O	2.44	0.50
2:R:6:PHE:N	2:R:6:PHE:CD2	2.80	0.50
3:S:95:LYS:HD3	3:S:118:LEU:HD13	1.93	0.50
1:G:53:ASP:OD2	1:G:54:ILE:N	2.43	0.50
1:A:240:ARG:O	1:A:250:HIS:HB3	2.12	0.50
1:B:156:GLN:CB	2:R:6:PHE:CB	2.88	0.50
1:I:281:ILE:HD11	1:I:361:ASP:HB3	1.92	0.50
1:C:183:ARG:HD3	1:C:199:GLU:HG2	1.92	0.50
1:D:244:THR:O	1:D:245:ASP:O	2.30	0.50
1:I:40:GLN:NE2	1:I:45:PHE:HB3	2.27	0.50
1:C:60:VAL:HG21	1:C:66:LYS:HB2	1.94	0.50
1:D:363:ARG:HB3	1:D:365:ASP:OD1	2.11	0.50
1:C:3:THR:HG23	1:C:4:ASN:H	1.76	0.50
2:O:100:LEU:HD12	2:O:104:VAL:HG11	1.94	0.50
1:D:244:THR:O	1:D:245:ASP:C	2.50	0.49
1:G:185:HIS:CE1	1:G:189:GLU:HG3	2.47	0.49
1:I:189:GLU:HB3	1:I:357:GLN:HG3	1.94	0.49
2:P:96:ASP:HB3	2:P:123:THR:HG22	1.94	0.49
1:E:296:PRO:HB3	1:E:300:MET:SD	2.52	0.49
1:F:90:SER:HA	1:F:342:ASP:HA	1.94	0.49
1:B:181:ASP:OD1	1:C:207:ARG:NH2	2.37	0.49
1:I:101:GLN:NE2	1:I:108:LEU:O	2.45	0.49
1:D:68:GLU:HB2	1:E:271:LYS:HZ3	1.73	0.49
1:E:101:GLN:O	1:E:104:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:LEU:N	1:B:13:ALA:O	2.45	0.49
1:C:200:GLU:HB2	1:C:300:MET:HB2	1.95	0.49
1:D:153:LEU:C	1:D:155:LYS:H	2.15	0.49
2:M:51:ASP:OD1	2:M:53:SER:OG	2.24	0.49
1:C:79:SER:O	1:C:156:GLN:NE2	2.45	0.49
1:C:94:ASP:OD2	2:R:16:ASN:ND2	2.46	0.49
1:F:84:TYR:OH	1:F:346:HIS:ND1	2.43	0.49
2:P:2:ALA:HB1	2:P:5:GLY:CA	2.40	0.49
1:A:313:ALA:HB3	1:A:348:TYR:CD2	2.48	0.49
1:E:56:LEU:HD11	1:F:271:LYS:CA	2.43	0.49
1:H:314:PRO:HG3	1:H:323:THR:O	2.12	0.49
1:D:8:SER:C	1:D:10:PHE:H	2.16	0.48
1:E:240:ARG:HA	1:E:252:ASN:HA	1.95	0.48
1:D:244:THR:O	1:D:244:THR:OG1	2.18	0.48
1:E:149:LEU:HD21	1:E:152:ASP:HB2	1.94	0.48
1:F:35:PHE:HB3	1:F:310:VAL:HG23	1.94	0.48
2:P:91:ASP:N	2:P:91:ASP:OD1	2.47	0.48
1:A:271:LYS:NZ	1:F:58:ASP:OD1	2.46	0.48
1:B:53:ASP:O	1:B:54:ILE:C	2.46	0.48
1:C:24:ASN:HB2	1:C:247:VAL:HG22	1.94	0.48
1:H:185:HIS:CE1	1:H:189:GLU:HG3	2.48	0.48
1:I:164:ILE:HB	1:I:362:VAL:HG12	1.95	0.48
2:N:42:TYR:HB2	2:N:71:PHE:HB3	1.94	0.48
2:P:22:GLU:OE1	2:P:31:ARG:NH1	2.47	0.48
1:B:340:GLY:C	1:B:341:ILE:HD13	2.34	0.48
1:D:85:PHE:CZ	1:D:133:LEU:HD11	2.49	0.48
1:E:183:ARG:O	1:E:187:GLU:HG3	2.14	0.48
1:E:216:HIS:HE1	1:E:218:LYS:HD2	1.77	0.48
1:I:37:SER:HB2	1:I:312:TYR:HE2	1.78	0.48
2:J:2:ALA:CB	2:J:5:GLY:N	2.74	0.48
2:R:91:ASP:OD1	2:R:91:ASP:N	2.47	0.48
1:A:86:LYS:HD3	1:F:67:ALA:HB2	1.94	0.48
1:B:48:ASP:OD1	1:B:48:ASP:N	2.47	0.48
1:E:61:ASP:OD1	1:F:85:PHE:HA	2.14	0.48
1:B:312:TYR:CZ	1:B:327:GLU:HG3	2.49	0.48
1:H:40:GLN:OE1	1:H:45:PHE:HB3	2.13	0.48
3:S:109:LYS:HB3	3:S:110:PRO:CD	2.44	0.48
1:D:200:GLU:O	1:D:200:GLU:HG3	2.14	0.48
1:I:191:LYS:HB3	1:I:191:LYS:HE3	1.35	0.48
1:A:236:THR:OG1	1:A:236:THR:O	2.29	0.48
1:B:51:ASP:HB3	1:C:21:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ASP:HB3	1:B:251:MET:SD	2.53	0.48
1:D:243:GLY:O	1:D:245:ASP:N	2.24	0.48
1:B:206:ASP:OD2	1:B:207:ARG:N	2.46	0.47
1:E:104:THR:HG21	1:E:107:GLU:HB3	1.95	0.47
1:A:15:LEU:HD12	1:F:46:LEU:HB2	1.95	0.47
1:C:125:LYS:O	1:C:129:THR:OG1	2.24	0.47
1:B:174:ASP:OD1	1:B:174:ASP:N	2.40	0.47
1:B:183:ARG:O	1:B:187:GLU:HG3	2.15	0.47
1:D:67:ALA:HB2	1:E:86:LYS:HG2	1.96	0.47
1:F:329:TYR:HB2	1:F:346:HIS:HB2	1.95	0.47
1:B:6:GLU:O	1:B:7:LYS:HB2	2.15	0.47
1:A:70:SER:HB2	1:B:121:LYS:HE2	1.95	0.47
1:D:237:GLY:O	1:D:239:LEU:N	2.47	0.47
1:D:240:ARG:CB	1:D:251:MET:O	2.63	0.47
1:E:337:ARG:O	1:E:338:ASP:HB2	2.14	0.47
2:M:18:ILE:HG22	2:M:97:LEU:HD12	1.96	0.47
2:N:35:ALA:HA	2:N:36:PRO:HD3	1.80	0.47
2:O:41:GLU:OE1	2:O:43:ARG:NH2	2.48	0.47
2:P:30:SER:HA	2:P:90:ARG:HB2	1.95	0.47
1:D:24:ASN:HB3	1:D:247:VAL:HG22	1.96	0.47
1:F:83:MET:HG2	1:F:349:MET:O	2.14	0.47
1:I:190:ALA:HB1	1:I:192:THR:HG23	1.97	0.47
1:I:197:ASN:O	1:I:198:GLY:C	2.52	0.47
2:J:51:ASP:OD2	2:J:52:GLY:N	2.48	0.46
3:S:55:ASP:OD1	3:S:55:ASP:N	2.44	0.46
2:Q:41:GLU:OE1	2:Q:43:ARG:NH1	2.48	0.46
1:A:46:LEU:HD22	2:M:9:LEU:HD11	1.97	0.46
1:B:24:ASN:HB3	1:B:247:VAL:HG11	1.98	0.46
1:C:64:SER:O	1:C:64:SER:OG	2.22	0.46
2:Q:18:ILE:HA	2:Q:95:LYS:HG3	1.97	0.46
1:D:182:LEU:O	1:D:186:MET:HG2	2.15	0.46
1:F:228:THR:N	1:F:229:PRO:HD3	2.30	0.46
1:H:162:LYS:HD3	1:H:185:HIS:ND1	2.29	0.46
2:L:42:TYR:O	2:L:43:ARG:NH1	2.48	0.46
1:E:168:LEU:HD22	1:E:213:LEU:HA	1.98	0.46
1:G:229:PRO:C	1:G:231:ALA:N	2.63	0.46
2:N:76:GLN:HG3	2:R:2:ALA:HB3	1.97	0.46
1:B:2:LEU:HD23	1:B:14:ASP:HA	1.98	0.46
1:B:81:PRO:HG3	2:R:3:TYR:CE2	2.50	0.46
1:E:186:MET:HG3	1:E:358:LEU:HD22	1.97	0.46
1:I:197:ASN:C	1:I:199:GLU:N	2.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:48:LEU:HD11	2:K:67:CYS:HB2	1.98	0.46
1:G:228:THR:O	1:G:228:THR:OG1	2.25	0.46
2:O:96:ASP:H	2:O:123:THR:HG23	1.79	0.46
1:B:46:LEU:O	1:C:16:THR:OG1	2.30	0.46
1:D:26:TYR:CE2	1:D:247:VAL:HG21	2.51	0.46
1:G:36:ARG:NH1	1:G:309:GLU:OE2	2.47	0.46
1:G:317:LYS:HB2	1:G:320:TYR:HD1	1.79	0.46
1:D:184:MET:CE	1:E:207:ARG:HE	2.28	0.46
2:J:58:GLY:C	2:J:60:GLU:H	2.19	0.46
2:Q:19:ILE:HD11	2:Q:88:ILE:HG13	1.97	0.46
1:A:249:ALA:O	1:A:250:HIS:ND1	2.48	0.46
1:E:125:LYS:O	1:E:129:THR:HG23	2.16	0.46
1:E:252:ASN:OD1	1:E:263:GLN:HB3	2.15	0.46
1:F:51:ASP:OD1	1:F:74:ARG:NH2	2.48	0.46
2:Q:95:LYS:HB3	2:Q:123:THR:HG21	1.97	0.46
1:A:25:THR:HB	1:A:128:ILE:HD11	1.98	0.45
1:B:192:THR:HG23	1:B:194:THR:H	1.80	0.45
1:E:162:LYS:HD2	1:E:185:HIS:CG	2.51	0.45
1:F:69:THR:HB	2:J:123:THR:HG23	1.98	0.45
1:I:191:LYS:C	1:I:193:GLY:N	2.69	0.45
2:L:14:PRO:HD2	2:L:43:ARG:HD2	1.98	0.45
1:A:272:ARG:NH2	1:F:58:ASP:OD2	2.50	0.45
1:A:333:TYR:HB2	1:A:342:ASP:HB2	1.98	0.45
1:I:6:GLU:H	1:I:6:GLU:HG2	1.37	0.45
1:B:87:GLU:HB3	1:B:345:ALA:HB3	1.96	0.45
1:D:64:SER:O	1:D:65:ARG:HB2	2.17	0.45
1:D:282:ASP:OD2	1:D:282:ASP:N	2.49	0.45
2:N:51:ASP:OD1	2:N:53:SER:OG	2.24	0.45
1:A:82:MET:HB3	1:A:350:LEU:HB2	1.98	0.45
1:A:222:ALA:HB2	1:B:220:ARG:NH2	2.31	0.45
1:D:79:SER:O	1:D:156:GLN:NE2	2.50	0.45
1:I:25:THR:HB	1:I:128:ILE:HD11	1.97	0.45
1:A:320:TYR:O	1:A:323:THR:OG1	2.33	0.45
1:D:82:MET:HB2	1:D:348:TYR:CE1	2.51	0.45
1:G:54:ILE:HD12	1:H:121:LYS:HE3	1.98	0.45
1:I:180:GLU:O	1:I:184:MET:HG2	2.17	0.45
1:B:118:LYS:O	1:B:122:ILE:HG12	2.17	0.45
1:E:51:ASP:OD1	1:E:51:ASP:N	2.50	0.45
1:E:91:ILE:HG22	1:E:118:LYS:HE3	1.99	0.45
1:A:88:VAL:HG12	1:A:344:GLU:HG2	1.97	0.45
1:E:241:THR:OG1	1:E:242:GLY:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:PRO:HB3	1:F:217:PRO:HG2	1.98	0.45
1:A:184:MET:HE1	1:B:207:ARG:HG3	1.99	0.45
1:D:10:PHE:N	1:D:10:PHE:CD1	2.81	0.45
1:H:253:ARG:HG2	1:H:262:VAL:HG22	1.99	0.45
2:P:13:GLU:HB3	2:P:70:ASN:ND2	2.32	0.45
1:A:164:ILE:HD13	1:A:182:LEU:HB2	1.99	0.45
1:G:355:ARG:NH2	1:H:20:GLN:O	2.44	0.45
1:A:6:GLU:O	1:A:7:LYS:HB2	2.17	0.45
1:A:313:ALA:HB3	1:A:348:TYR:HD2	1.81	0.45
1:E:363:ARG:HB3	1:E:365:ASP:OD1	2.17	0.45
1:I:205:VAL:HG12	1:I:292:GLY:HA3	1.99	0.45
2:R:65:SER:HB3	2:R:89:TYR:HB3	1.98	0.45
1:A:40:GLN:N	1:A:312:TYR:O	2.45	0.44
1:C:90:SER:O	1:C:118:LYS:NZ	2.50	0.44
1:F:6:GLU:H	1:F:6:GLU:HG2	0.96	0.44
1:G:312:TYR:CZ	1:G:327:GLU:HG3	2.52	0.44
2:K:3:TYR:CE1	2:M:76:GLN:HG3	2.53	0.44
1:A:241:THR:HG1	1:A:253:ARG:HE	1.57	0.44
1:B:205:VAL:HG13	1:B:209:PHE:HB3	1.97	0.44
2:N:74:ASP:OD1	2:N:75:LEU:N	2.50	0.44
1:I:136:GLN:OE1	1:I:139:LYS:NZ	2.44	0.44
2:N:32:LYS:HB3	2:N:89:TYR:CD1	2.52	0.44
1:A:365:ASP:OD1	1:A:365:ASP:N	2.47	0.44
1:F:5:SER:OG	1:F:6:GLU:N	2.50	0.44
2:N:32:LYS:HD3	2:N:34:TYR:CZ	2.53	0.44
2:N:77:LEU:HD23	2:N:77:LEU:HA	1.82	0.44
2:O:14:PRO:HG3	2:O:99:LYS:HE2	1.98	0.44
2:R:46:GLU:HG2	2:R:99:LYS:HB2	1.99	0.44
1:A:46:LEU:HB2	1:B:15:LEU:HD23	1.98	0.44
1:C:45:PHE:HB2	1:D:16:THR:HG23	1.98	0.44
1:A:268:PHE:O	1:A:276:HIS:N	2.44	0.44
1:B:15:LEU:HD23	1:B:15:LEU:HA	1.80	0.44
1:F:363:ARG:NH2	1:F:365:ASP:OD2	2.38	0.44
1:G:228:THR:O	1:G:229:PRO:CB	2.64	0.44
1:C:364:SER:O	1:C:364:SER:OG	2.34	0.44
2:J:100:LEU:HD22	2:J:104:VAL:HG11	2.00	0.44
1:B:318:MET:SD	1:H:340:GLY:HA2	2.58	0.44
1:E:52:TRP:O	1:E:53:ASP:C	2.56	0.44
1:I:253:ARG:HG3	1:I:262:VAL:HG22	2.00	0.44
2:K:68:ILE:HD13	2:K:88:ILE:HG13	2.00	0.44
2:L:20:LEU:HD12	2:L:121:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:THR:HG23	1:A:290:GLY:HA2	1.99	0.44
1:C:253:ARG:HG2	1:C:262:VAL:HG22	2.00	0.44
1:H:81:PRO:HG3	2:O:77:LEU:HD11	1.99	0.44
2:N:42:TYR:O	2:N:43:ARG:HD3	2.17	0.44
1:E:159:VAL:HG21	1:E:356:PRO:HG2	2.00	0.43
2:N:82:GLN:HE21	2:N:82:GLN:HB3	1.45	0.43
1:G:61:ASP:OD1	1:G:62:ARG:N	2.51	0.43
2:P:27:THR:HB	2:R:93:GLU:OE1	2.18	0.43
3:S:43:SER:O	3:S:45:TRP:HD1	2.01	0.43
1:B:100:ARG:NH1	1:B:104:THR:O	2.50	0.43
1:C:235:ILE:HD13	1:C:235:ILE:HA	1.84	0.43
1:I:245:ASP:OD1	1:I:246:GLY:N	2.50	0.43
2:J:75:LEU:HD12	2:J:77:LEU:HB2	2.00	0.43
2:P:77:LEU:HD23	2:P:77:LEU:HA	1.89	0.43
2:P:89:TYR:CZ	2:P:90:ARG:HG3	2.54	0.43
1:A:62:ARG:H	2:N:82:GLN:NE2	2.16	0.43
1:B:141:LYS:HD2	1:B:143:ILE:HD11	2.00	0.43
1:B:154:TYR:HD1	1:B:159:VAL:HG23	1.83	0.43
1:C:40:GLN:HE22	1:C:45:PHE:HD1	1.67	0.43
1:E:162:LYS:HD2	1:E:185:HIS:ND1	2.34	0.43
1:F:77:GLN:HB3	2:J:9:LEU:HB2	2.00	0.43
2:K:32:LYS:HD3	2:K:34:TYR:CZ	2.54	0.43
2:M:106:ALA:O	2:M:110:LYS:HG2	2.18	0.43
1:A:114:VAL:O	1:A:118:LYS:HG2	2.19	0.43
1:A:144:ASP:OD2	1:A:145:ALA:N	2.51	0.43
1:F:14:ASP:N	1:F:14:ASP:OD1	2.48	0.43
1:F:209:PHE:CD1	1:F:364:SER:HB3	2.54	0.43
1:G:51:ASP:HB3	1:H:21:SER:HB2	2.01	0.43
2:J:2:ALA:O	2:J:3:TYR:C	2.57	0.43
1:A:219:ILE:H	1:A:219:ILE:HG12	1.66	0.43
1:F:144:ASP:HB2	1:F:148:VAL:HG22	2.00	0.43
1:F:214:ILE:HD13	1:F:214:ILE:HA	1.83	0.43
1:G:19:VAL:HG22	1:G:19:VAL:O	2.19	0.43
1:G:48:ASP:OD2	1:H:100:ARG:NH2	2.52	0.43
1:G:230:LEU:O	1:G:234:GLN:CG	2.67	0.43
1:I:363:ARG:NE	1:I:365:ASP:OD1	2.45	0.43
2:N:37:VAL:HG22	2:N:42:TYR:OH	2.17	0.43
1:C:86:LYS:HG3	1:C:346:HIS:CD2	2.54	0.43
1:D:12:LEU:HD12	1:D:12:LEU:HA	1.90	0.43
1:F:140:GLY:HA3	1:F:154:TYR:CE2	2.54	0.42
1:G:230:LEU:HD12	1:G:230:LEU:HA	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ALA:HB2	1:B:86:LYS:HD3	2.00	0.42
2:P:44:VAL:HG23	2:P:70:ASN:OD1	2.19	0.42
1:F:49:LEU:HB2	1:F:76:ARG:HB2	2.01	0.42
1:F:162:LYS:O	1:F:360:VAL:HG23	2.20	0.42
1:A:74:ARG:NH1	1:A:76:ARG:HD3	2.35	0.42
1:E:56:LEU:HD11	1:F:271:LYS:HA	2.00	0.42
1:G:240:ARG:O	1:G:250:HIS:HB3	2.20	0.42
1:H:313:ALA:HB3	1:H:348:TYR:CD2	2.54	0.42
1:A:69:THR:HG22	1:A:70:SER:H	1.83	0.42
1:A:141:LYS:HB3	1:A:143:ILE:HD13	2.00	0.42
1:E:71:ALA:HA	1:E:72:PRO:HD3	1.90	0.42
1:E:245:ASP:OD1	1:E:248:GLN:HG2	2.20	0.42
1:F:115:ARG:NH1	1:F:332:GLU:OE2	2.51	0.42
1:H:186:MET:HG3	1:H:201:ILE:HD11	2.02	0.42
1:I:115:ARG:NH1	1:I:332:GLU:OE2	2.47	0.42
1:E:197:ASN:HA	1:F:249:ALA:HB3	2.02	0.42
1:F:141:LYS:HB3	1:F:141:LYS:HE3	1.73	0.42
2:R:46:GLU:OE1	2:R:54:LYS:HE2	2.20	0.42
1:F:192:THR:HG21	1:F:301:LEU:HD22	2.02	0.42
1:G:86:LYS:HG3	1:G:346:HIS:CD2	2.55	0.42
1:E:154:TYR:CE1	1:E:356:PRO:HB2	2.54	0.42
2:K:116:LYS:HB3	2:K:116:LYS:HE3	1.73	0.42
2:O:34:TYR:N	2:O:85:VAL:O	2.52	0.42
3:S:21:VAL:HG12	3:S:91:ILE:HG21	2.02	0.42
1:B:18:GLU:OE1	1:B:20:GLN:NE2	2.52	0.42
1:B:84:TYR:OH	1:B:346:HIS:ND1	2.34	0.42
1:F:307:ILE:HG22	1:F:353:CYS:SG	2.60	0.42
1:G:57:LEU:HD22	1:H:85:PHE:CD2	2.52	0.42
2:Q:96:ASP:H	2:Q:123:THR:HG23	1.85	0.42
1:A:50:THR:HG22	1:A:75:VAL:HG23	2.02	0.42
1:A:186:MET:H	1:A:186:MET:HG2	1.55	0.42
1:B:45:PHE:HB2	1:C:16:THR:HG21	2.02	0.42
1:E:144:ASP:OD1	1:E:145:ALA:N	2.53	0.42
1:H:240:ARG:HG2	1:H:252:ASN:ND2	2.35	0.42
2:M:54:LYS:H	2:M:54:LYS:HG2	1.63	0.42
1:A:187:GLU:OE2	1:B:240:ARG:NH1	2.53	0.41
1:F:69:THR:HG21	2:J:95:LYS:HG2	2.01	0.41
1:F:171:PRO:HG2	3:S:101:TYR:CD1	2.55	0.41
1:H:91:ILE:HB	1:H:341:ILE:HG13	2.02	0.41
1:H:240:ARG:HE	1:H:252:ASN:HD21	1.66	0.41
1:I:84:TYR:OH	1:I:346:HIS:ND1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:LEU:HD23	1:C:15:LEU:HA	1.63	0.41
1:H:300:MET:HG2	1:H:301:LEU:HG	2.01	0.41
2:J:56:ALA:O	2:J:57:ALA:C	2.59	0.41
1:B:6:GLU:HG3	2:K:75:LEU:HD21	2.02	0.41
1:D:190:ALA:HA	1:D:358:LEU:HD21	2.02	0.41
1:E:63:THR:HG22	1:F:316:PRO:HG3	2.01	0.41
2:M:15:LEU:HD23	2:M:15:LEU:HA	1.89	0.41
2:P:27:THR:HG22	2:P:27:THR:O	2.20	0.41
1:B:239:LEU:HB3	1:B:240:ARG:H	1.70	0.41
1:C:78:ILE:HB	1:C:156:GLN:OE1	2.20	0.41
1:F:37:SER:O	1:F:37:SER:OG	2.38	0.41
1:H:317:LYS:NZ	1:H:344:GLU:OE1	2.53	0.41
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.86	0.41
1:D:4:ASN:CG	1:D:5:SER:H	2.24	0.41
1:G:271:LYS:HG2	2:Q:124:GLY:HA3	2.01	0.41
1:H:7:LYS:HE2	1:H:7:LYS:HB2	1.82	0.41
1:C:307:ILE:HD12	1:C:353:CYS:SG	2.61	0.41
1:D:89:GLU:HB2	1:D:122:ILE:HD11	2.03	0.41
1:E:211:SER:O	1:E:215:LYS:HB2	2.21	0.41
1:E:245:ASP:HB3	1:E:251:MET:SD	2.60	0.41
3:S:88:GLN:O	3:S:92:ILE:HG13	2.21	0.41
1:A:324:LEU:HD23	1:A:324:LEU:HA	1.96	0.41
1:B:85:PHE:CZ	1:B:133:LEU:HD11	2.55	0.41
1:C:2:LEU:HD12	1:C:2:LEU:HA	1.90	0.41
1:C:62:ARG:HG2	1:D:316:PRO:HG3	2.03	0.41
1:E:141:LYS:HE2	1:E:143:ILE:HD11	2.03	0.41
1:F:185:HIS:NE2	1:F:357:GLN:O	2.44	0.41
1:G:88:VAL:HG12	1:G:344:GLU:HG2	2.01	0.41
2:O:106:ALA:O	2:O:110:LYS:HG2	2.20	0.41
1:F:60:VAL:HG11	1:F:66:LYS:O	2.21	0.41
1:F:62:ARG:H	2:K:82:GLN:NE2	2.18	0.41
1:G:313:ALA:HB3	1:G:348:TYR:CD2	2.56	0.41
1:H:89:GLU:HB3	1:H:343:PHE:HD2	1.86	0.41
1:A:32:LEU:HD23	1:A:32:LEU:HA	1.92	0.41
1:A:92:THR:HG22	1:A:94:ASP:H	1.86	0.41
1:B:156:GLN:CB	2:R:6:PHE:CG	3.04	0.41
1:C:21:SER:O	1:C:21:SER:OG	2.34	0.41
1:C:121:LYS:HB3	1:C:121:LYS:HE3	1.63	0.41
1:C:317:LYS:HE2	1:C:346:HIS:CE1	2.52	0.41
1:D:289:VAL:HG12	1:D:365:ASP:HB3	2.03	0.41
1:E:41:THR:HG22	1:E:324:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:LYS:HE3	1:E:346:HIS:HE1	1.86	0.41
1:F:312:TYR:CE1	1:F:349:MET:HB3	2.56	0.41
2:N:101:GLU:H	2:N:104:VAL:HG11	1.86	0.41
3:S:109:LYS:O	3:S:111:PHE:N	2.54	0.41
1:A:174:ASP:HB3	1:A:177:ALA:HB3	2.03	0.41
1:B:87:GLU:OE2	1:B:87:GLU:HA	2.21	0.41
1:C:281:ILE:HG22	1:C:284:VAL:HG23	2.03	0.41
1:D:66:LYS:O	1:D:67:ALA:HB2	2.20	0.41
1:E:167:ASP:CG	1:E:366:ALA:HB2	2.41	0.41
2:K:18:ILE:HA	2:K:95:LYS:HD2	2.02	0.41
1:C:196:ILE:HD13	1:C:196:ILE:HA	1.92	0.40
1:E:117:LYS:HG3	1:E:118:LYS:N	2.36	0.40
1:H:39:PRO:HB2	1:H:324:LEU:HD12	2.02	0.40
1:B:243:GLY:O	1:B:251:MET:HG3	2.21	0.40
1:F:126:PHE:HA	1:F:129:THR:HG22	2.04	0.40
1:F:240:ARG:HD2	1:F:250:HIS:O	2.21	0.40
1:H:192:THR:HG23	1:H:194:THR:H	1.86	0.40
1:I:117:LYS:HB3	1:I:117:LYS:HE3	1.89	0.40
2:P:106:ALA:O	2:P:110:LYS:HG2	2.21	0.40
1:A:215:LYS:HE3	1:F:174:ASP:OD2	2.20	0.40
1:B:201:ILE:HG13	1:B:203:ILE:HG13	2.03	0.40
1:E:185:HIS:CE1	1:E:189:GLU:HG3	2.56	0.40
1:I:99:VAL:O	1:I:109:THR:HG22	2.21	0.40
2:M:119:ASP:CG	2:N:90:ARG:HH22	2.22	0.40
2:P:54:LYS:H	2:P:54:LYS:HG2	1.58	0.40
1:A:329:TYR:O	1:A:345:ALA:HA	2.22	0.40
1:G:24:ASN:HB3	1:G:247:VAL:HG21	2.03	0.40
2:P:64:ASP:O	2:P:116:LYS:HE2	2.21	0.40
1:A:149:LEU:HD21	1:A:152:ASP:HB2	2.03	0.40
1:C:29:ILE:HD13	1:C:29:ILE:HA	1.94	0.40
1:D:244:THR:C	1:D:245:ASP:O	2.60	0.40
2:M:17:ASP:O	2:M:95:LYS:HE3	2.22	0.40
2:M:40:THR:HG22	2:M:54:LYS:HE3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	364/367 (99%)	352 (97%)	11 (3%)	1 (0%)	37	68
1	B	364/367 (99%)	347 (95%)	16 (4%)	1 (0%)	37	68
1	C	364/367 (99%)	337 (93%)	19 (5%)	8 (2%)	5	24
1	D	364/367 (99%)	336 (92%)	20 (6%)	8 (2%)	5	24
1	E	364/367 (99%)	342 (94%)	19 (5%)	3 (1%)	16	48
1	F	364/367 (99%)	350 (96%)	14 (4%)	0	100	100
1	G	364/367 (99%)	347 (95%)	13 (4%)	4 (1%)	12	39
1	H	364/367 (99%)	358 (98%)	5 (1%)	1 (0%)	37	68
1	I	350/367 (95%)	329 (94%)	16 (5%)	5 (1%)	9	34
2	J	122/125 (98%)	111 (91%)	10 (8%)	1 (1%)	16	48
2	K	122/125 (98%)	118 (97%)	3 (2%)	1 (1%)	16	48
2	L	122/125 (98%)	117 (96%)	5 (4%)	0	100	100
2	M	122/125 (98%)	113 (93%)	9 (7%)	0	100	100
2	N	122/125 (98%)	113 (93%)	7 (6%)	2 (2%)	8	31
2	O	122/125 (98%)	119 (98%)	3 (2%)	0	100	100
2	P	122/125 (98%)	118 (97%)	3 (2%)	1 (1%)	16	48
2	Q	122/125 (98%)	117 (96%)	5 (4%)	0	100	100
2	R	122/125 (98%)	117 (96%)	4 (3%)	1 (1%)	16	48
3	S	118/372 (32%)	111 (94%)	6 (5%)	1 (1%)	16	48
All	All	4478/4800 (93%)	4252 (95%)	188 (4%)	38 (1%)	19	48

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	123	ARG
1	C	124	THR

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Mol	Chain	Res	Type
1	D	9	ARG
1	D	225	ALA
1	D	245	ASP
1	E	53	ASP
1	G	228	THR
1	G	229	PRO
1	H	305	ASN
1	I	68	GLU
2	N	4	GLN
2	N	101	GLU
1	D	4	ASN
1	D	235	ILE
1	D	306	ASN
1	G	9	ARG
1	I	65	ARG
1	I	66	LYS
1	I	67	ALA
2	P	4	GLN
1	C	122	ILE
1	C	287	THR
1	E	68	GLU
1	G	4	ASN
2	K	73	ALA
2	R	3	TYR
1	A	244	THR
1	B	306	ASN
1	C	72	PRO
1	C	286	ASP
1	D	238	SER
3	S	40	THR
1	C	55	SER
1	C	155	LYS
2	J	3	TYR
1	I	195	VAL
1	D	307	ILE
1	E	54	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	314/317 (99%)	306 (98%)	8 (2%)	42	69
1	B	310/317 (98%)	299 (96%)	11 (4%)	31	61
1	C	305/317 (96%)	286 (94%)	19 (6%)	15	43
1	D	300/317 (95%)	278 (93%)	22 (7%)	11	37
1	E	305/317 (96%)	288 (94%)	17 (6%)	17	46
1	F	313/317 (99%)	301 (96%)	12 (4%)	28	59
1	G	311/317 (98%)	301 (97%)	10 (3%)	34	63
1	H	314/317 (99%)	303 (96%)	11 (4%)	31	61
1	I	295/317 (93%)	280 (95%)	15 (5%)	20	49
2	J	92/99 (93%)	90 (98%)	2 (2%)	47	71
2	K	96/99 (97%)	90 (94%)	6 (6%)	15	42
2	L	97/99 (98%)	94 (97%)	3 (3%)	35	63
2	M	95/99 (96%)	95 (100%)	0	100	100
2	N	94/99 (95%)	88 (94%)	6 (6%)	14	42
2	O	95/99 (96%)	91 (96%)	4 (4%)	25	56
2	P	93/99 (94%)	88 (95%)	5 (5%)	18	47
2	Q	97/99 (98%)	93 (96%)	4 (4%)	26	57
2	R	97/99 (98%)	93 (96%)	4 (4%)	26	57
3	S	100/307 (33%)	97 (97%)	3 (3%)	36	64
All	All	3723/4051 (92%)	3561 (96%)	162 (4%)	26	54

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	39	PRO
1	A	82	MET
1	A	90	SER
1	A	158	ASP
1	A	245	ASP
1	A	318	MET
1	A	361	ASP
1	B	47	MET
1	B	54	ILE

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Mol	Chain	Res	Type
1	B	55	SER
1	B	157	PHE
1	B	174	ASP
1	B	224	LEU
1	B	233	GLN
1	B	272	ARG
1	B	306	ASN
1	B	307	ILE
1	B	348	TYR
1	C	14	ASP
1	C	15	LEU
1	C	20	GLN
1	C	50	THR
1	C	55	SER
1	C	57	LEU
1	C	58	ASP
1	C	61	ASP
1	C	69	THR
1	C	70	SER
1	C	72	PRO
1	C	120	MET
1	C	146	ASN
1	C	155	LYS
1	C	221	ASP
1	C	226	GLN
1	C	272	ARG
1	C	285	SER
1	C	348	TYR
1	D	3	THR
1	D	5	SER
1	D	8	SER
1	D	12	LEU
1	D	14	ASP
1	D	15	LEU
1	D	68	GLU
1	D	70	SER
1	D	72	PRO
1	D	156	GLN
1	D	158	ASP
1	D	169	ASP
1	D	229	PRO
1	D	234	GLN

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Mol	Chain	Res	Type
1	D	236	THR
1	D	238	SER
1	D	239	LEU
1	D	244	THR
1	D	282	ASP
1	D	307	ILE
1	D	342	ASP
1	D	348	TYR
1	E	4	ASN
1	E	6	GLU
1	E	36	ARG
1	E	50	THR
1	E	51	ASP
1	E	52	TRP
1	E	55	SER
1	E	56	LEU
1	E	90	SER
1	E	126	PHE
1	E	155	LYS
1	E	156	GLN
1	E	233	GLN
1	E	307	ILE
1	E	348	TYR
1	E	350	LEU
1	E	353	CYS
1	F	6	GLU
1	F	7	LYS
1	F	36	ARG
1	F	47	MET
1	F	85	PHE
1	F	156	GLN
1	F	233	GLN
1	F	267	LYS
1	F	305	ASN
1	F	328	LEU
1	F	342	ASP
1	F	348	TYR
1	G	5	SER
1	G	6	GLU
1	G	9	ARG
1	G	19	VAL
1	G	224	LEU

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Mol	Chain	Res	Type
1	G	227	GLN
1	G	228	THR
1	G	272	ARG
1	G	336	ASP
1	G	348	TYR
1	H	61	ASP
1	H	90	SER
1	H	227	GLN
1	H	228	THR
1	H	233	GLN
1	H	238	SER
1	H	248	GLN
1	H	297	ASN
1	H	305	ASN
1	H	306	ASN
1	H	348	TYR
1	I	6	GLU
1	I	7	LYS
1	I	19	VAL
1	I	60	VAL
1	I	61	ASP
1	I	62	ARG
1	I	63	THR
1	I	65	ARG
1	I	70	SER
1	I	191	LYS
1	I	253	ARG
1	I	281	ILE
1	I	303	GLU
1	I	342	ASP
1	I	348	TYR
2	J	75	LEU
2	J	78	SER
2	K	3	TYR
2	K	71	PHE
2	K	79	TYR
2	K	111	SER
2	K	119	ASP
2	K	122	PRO
2	L	12	ARG
2	L	79	TYR
2	L	102	SER

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Mol	Chain	Res	Type
2	N	32	LYS
2	N	36	PRO
2	N	37	VAL
2	N	79	TYR
2	N	89	TYR
2	N	104	VAL
2	O	59	GLN
2	O	79	TYR
2	O	91	ASP
2	O	102	SER
2	P	39	SER
2	P	79	TYR
2	P	102	SER
2	P	111	SER
2	P	119	ASP
2	Q	6	PHE
2	Q	12	ARG
2	Q	90	ARG
2	Q	111	SER
2	R	6	PHE
2	R	13	GLU
2	R	79	TYR
2	R	91	ASP
3	S	49	ASP
3	S	55	ASP
3	S	98	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	346	HIS
1	F	263	GLN
1	G	226	GLN
1	H	252	ASN
1	H	305	ASN
1	H	306	ASN
1	H	346	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

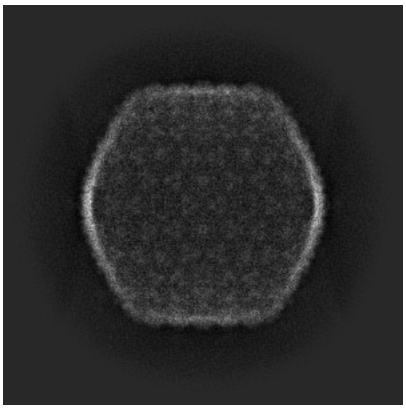
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45163. These allow visual inspection of the internal detail of the map and identification of artifacts.

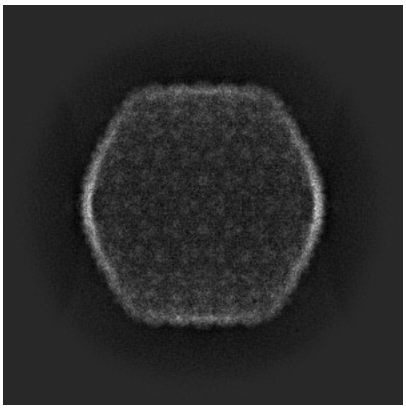
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

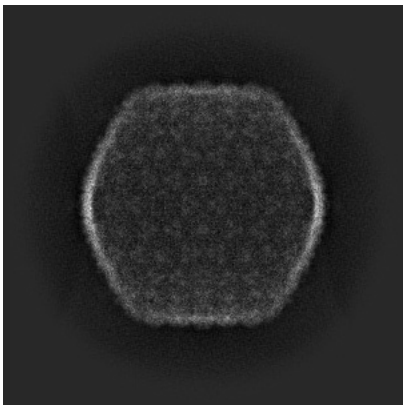
6.1.1 Primary map



X

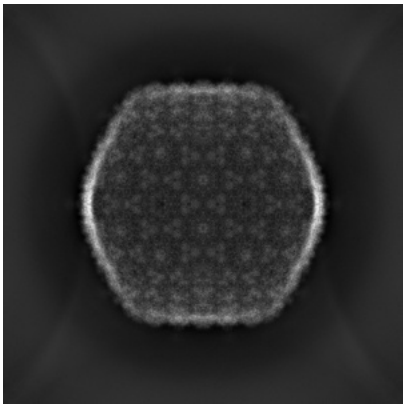


Y

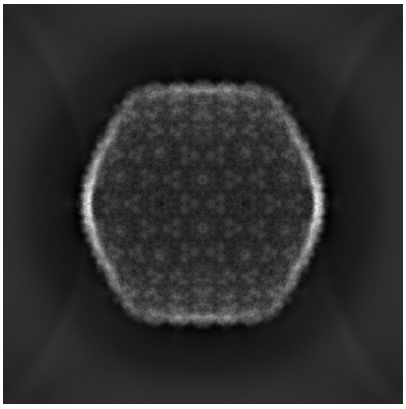


Z

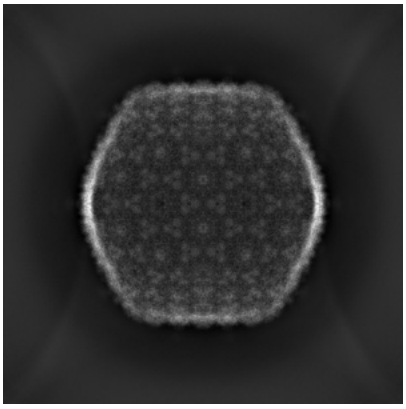
6.1.2 Raw map



X



Y

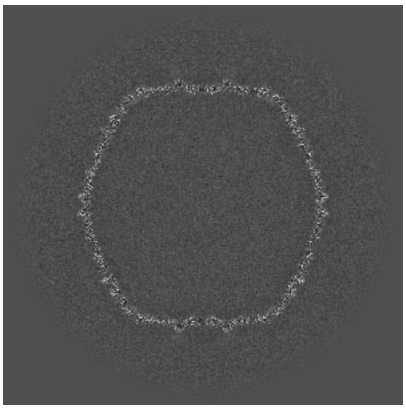


Z

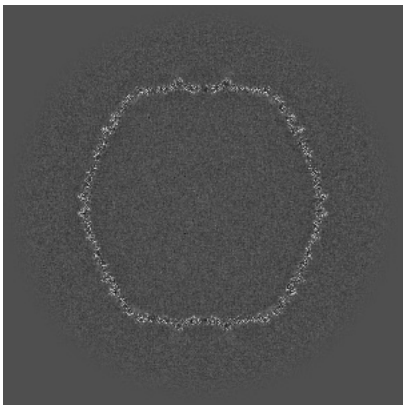
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

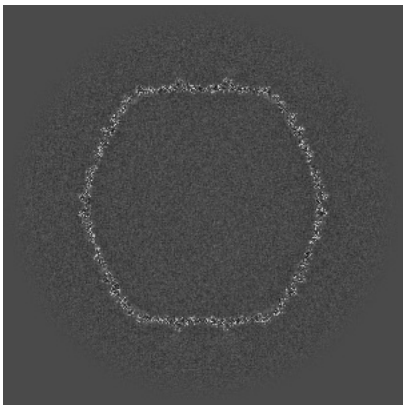
6.2.1 Primary map



X Index: 500



Y Index: 500

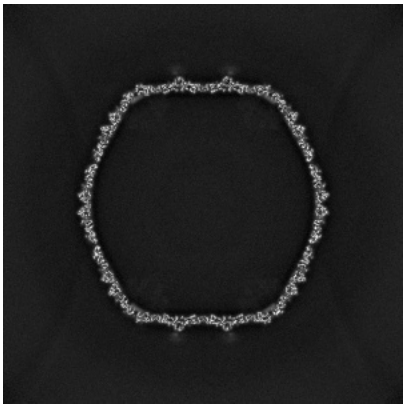


Z Index: 500

6.2.2 Raw map

X Index: 500

Y Index: 500

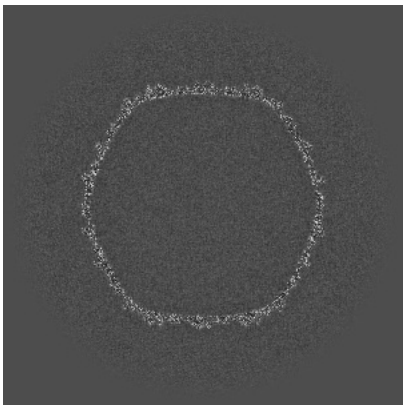


Z Index: 500

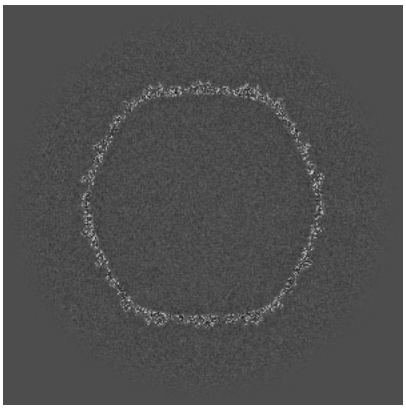
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

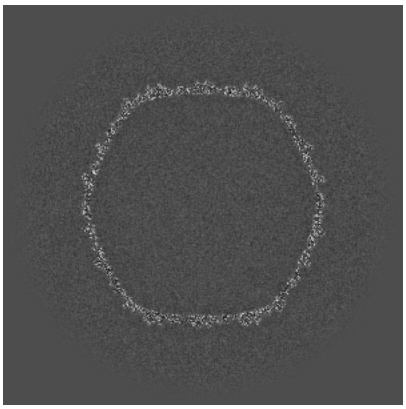
6.3.1 Primary map



X Index: 547

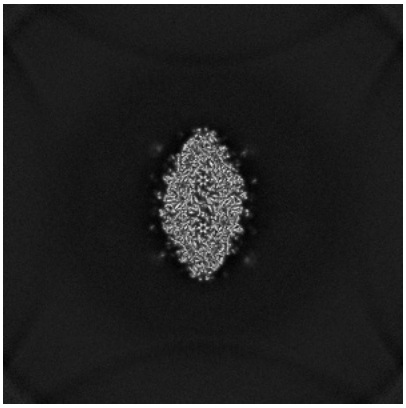


Y Index: 453

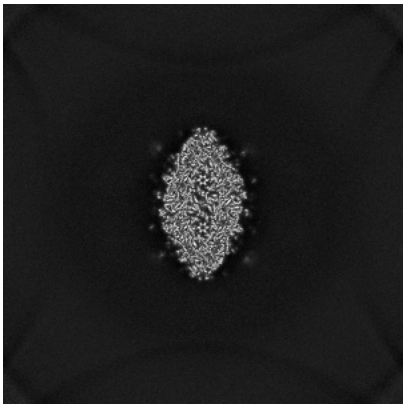


Z Index: 546

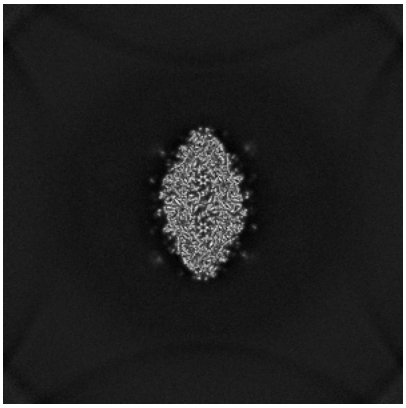
6.3.2 Raw map



X Index: 218



Y Index: 218

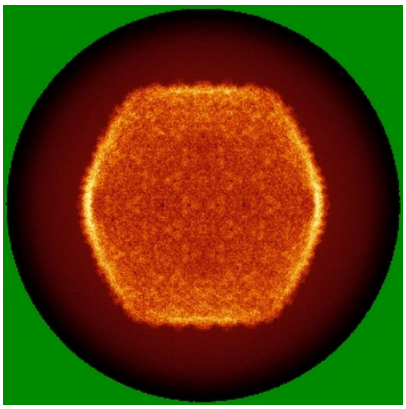


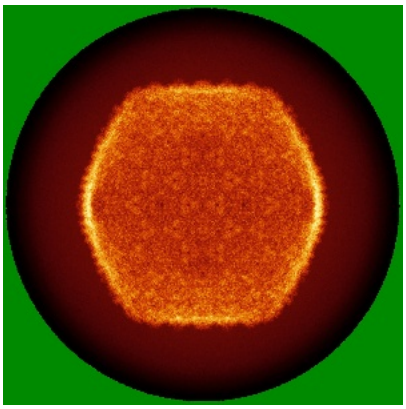
Z Index: 781

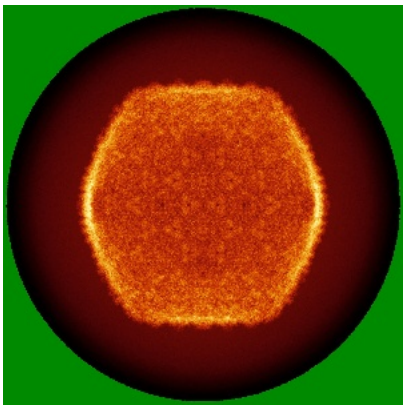
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

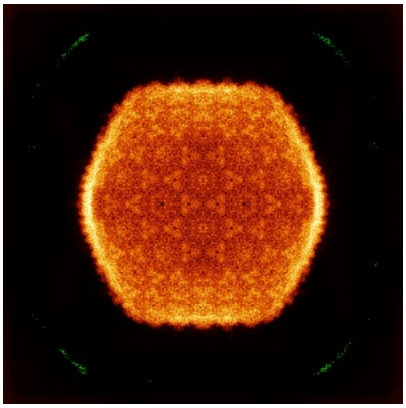
6.4.1 Primary map

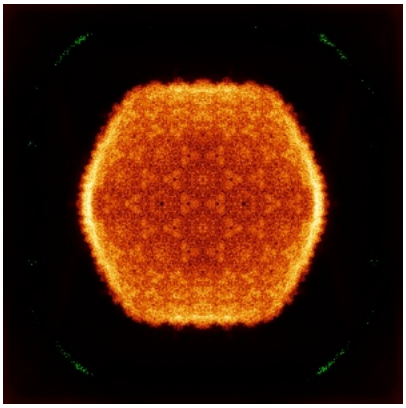

X

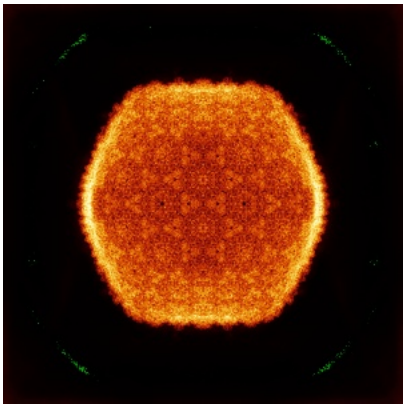

Y


Z

6.4.2 Raw map


X


Y


Z

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

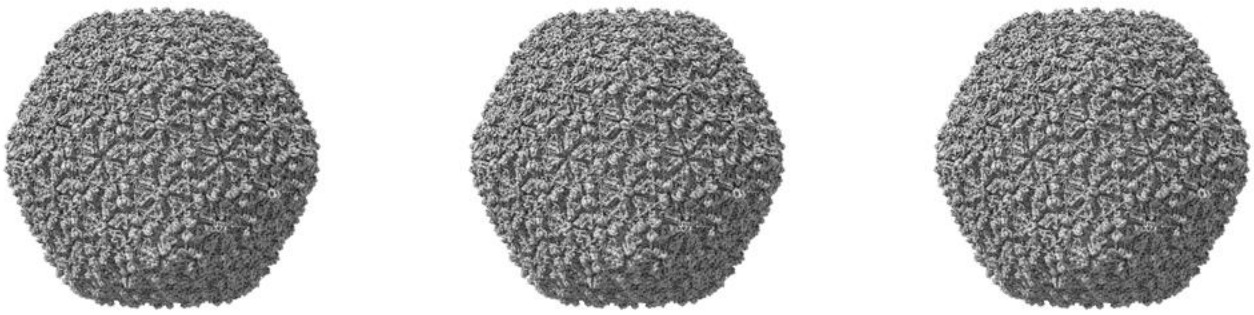
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.651. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

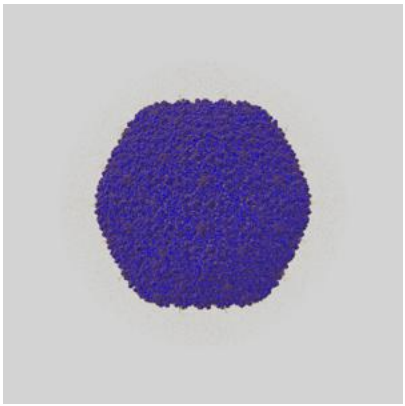
6.6 Mask visualisation (i)

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

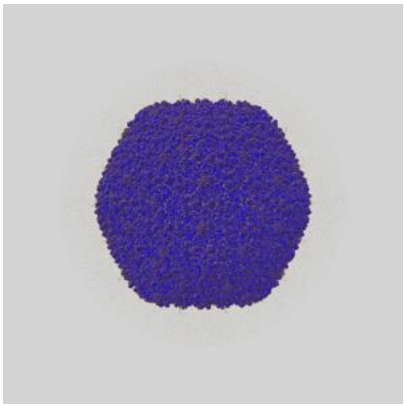
A mask typically either:

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

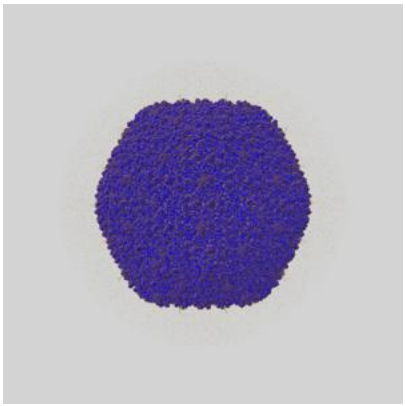
6.6.1 emd_45163_msk_1.map (i)



X



Y

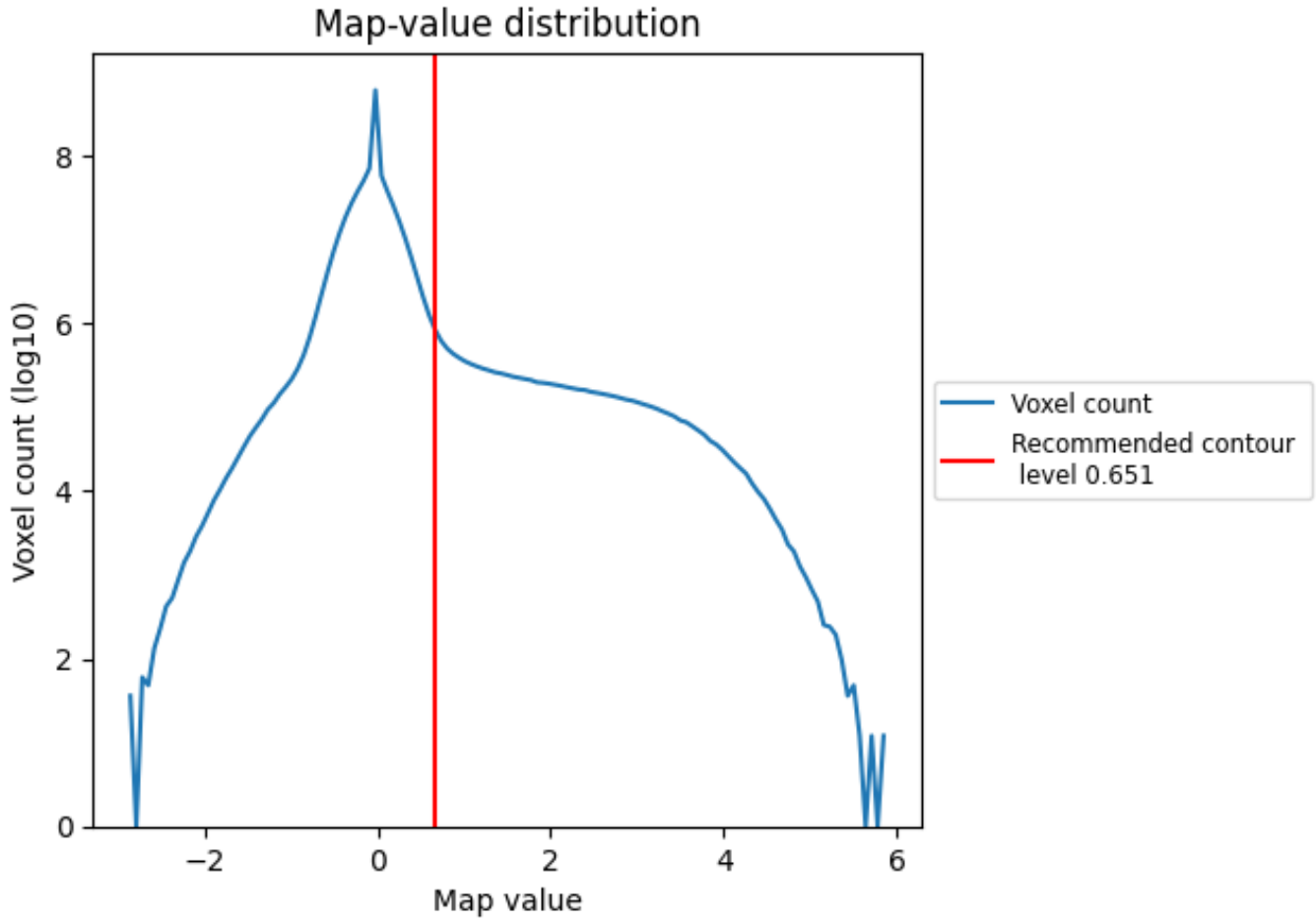


Z

7 Map analysis

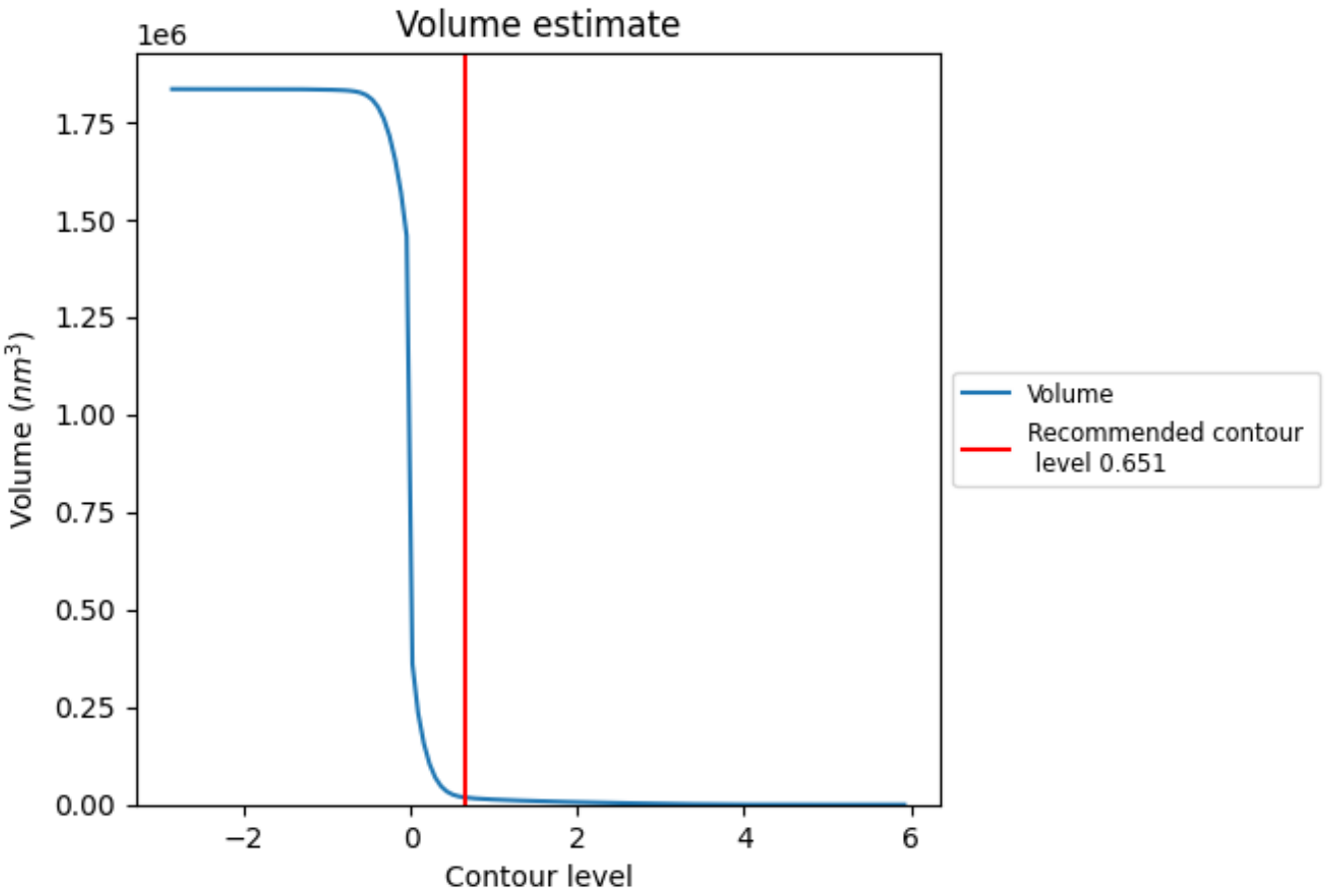
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

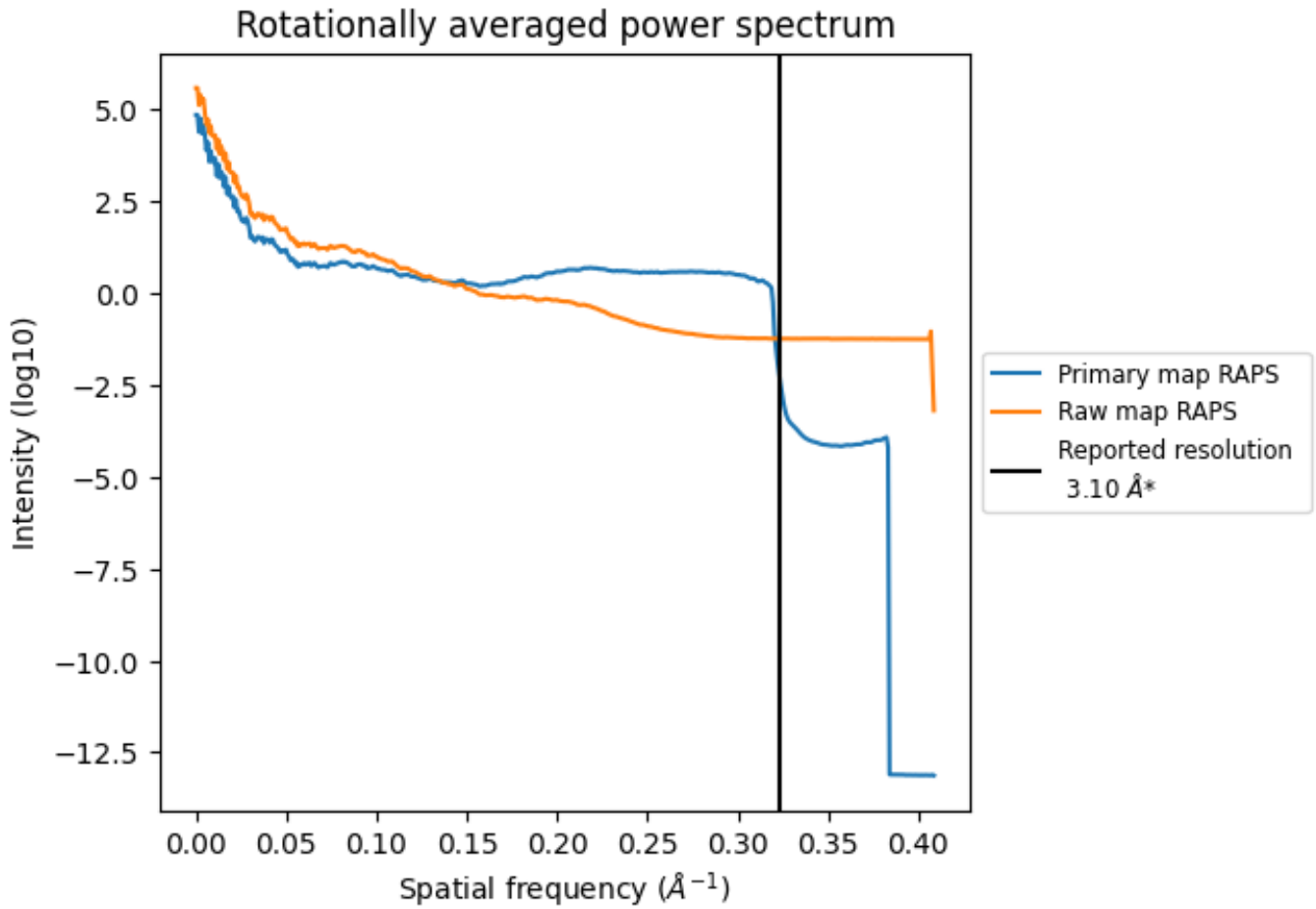
7.2 Volume estimate



The volume at the recommended contour level is 18437 nm^3; this corresponds to an approximate mass of 16655 kDa.

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

7.3 Rotationally averaged power spectrum (i)

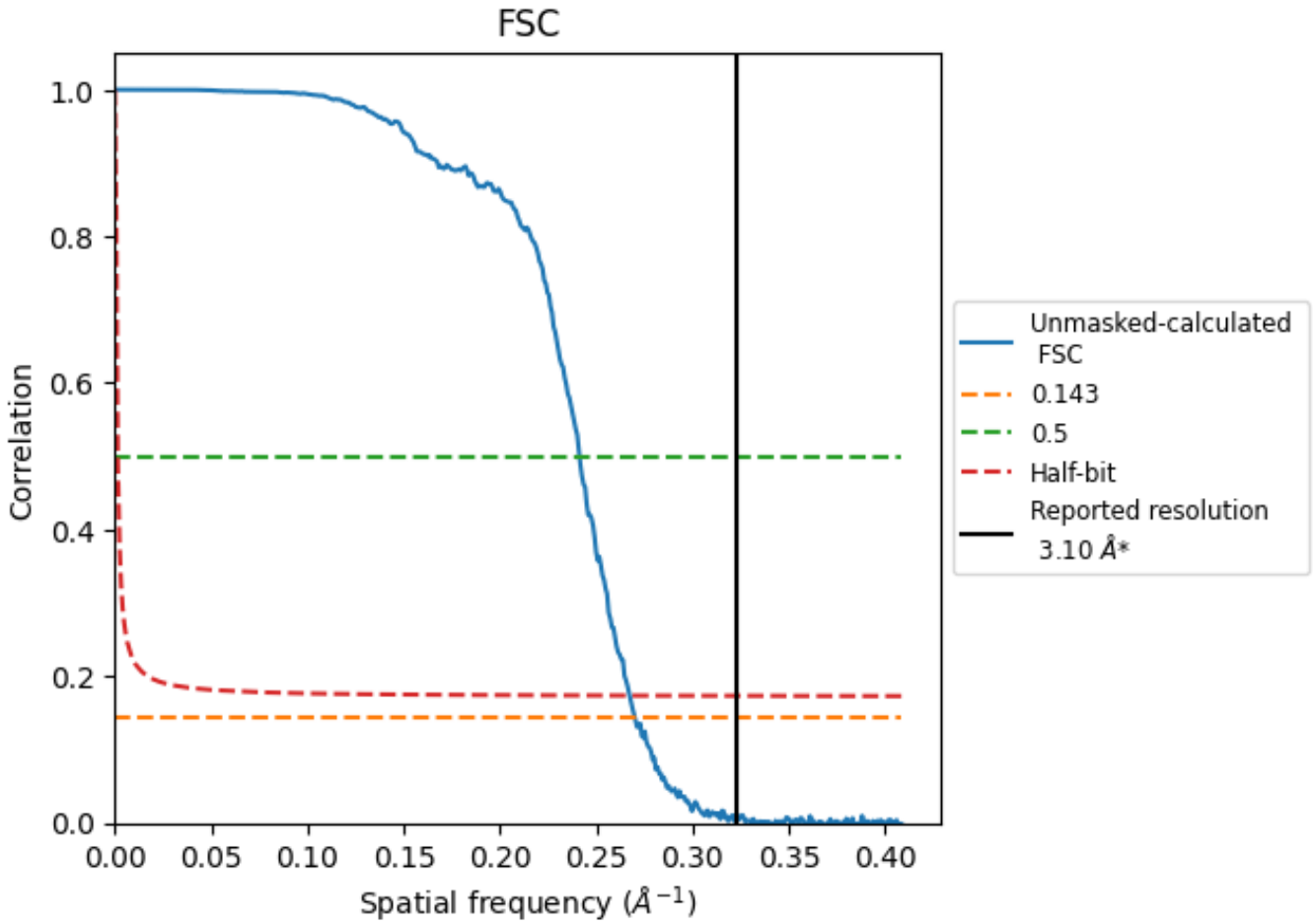


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.70	4.14	3.74

*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 3.70 differs from the reported value 3.1 by more than 10 %

9 Map-model fit

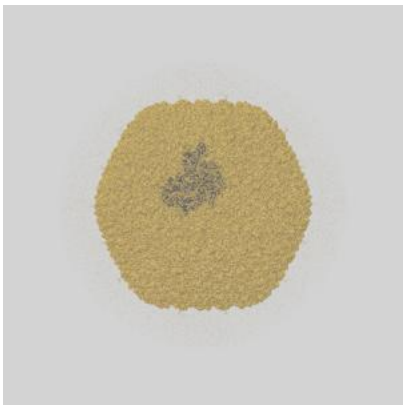
This section contains information regarding the fit between EMDB map EMD-45163 and PDB model 9C3A. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay

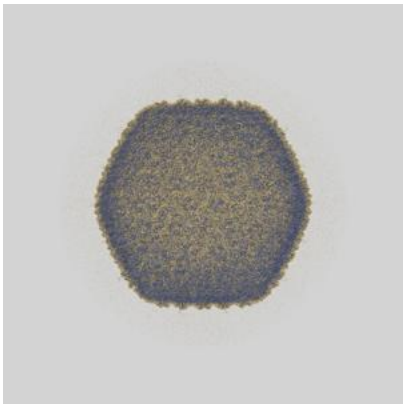
X

Y

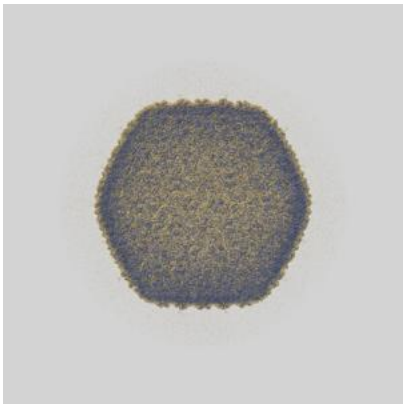


Z

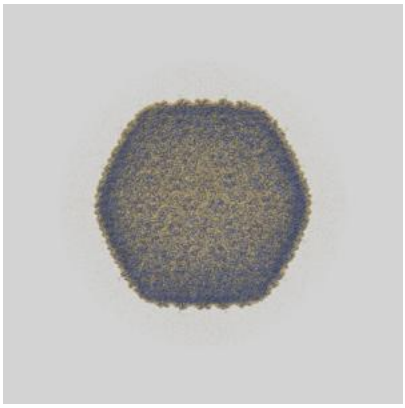
9.1.2 Map-model assembly overlay



X



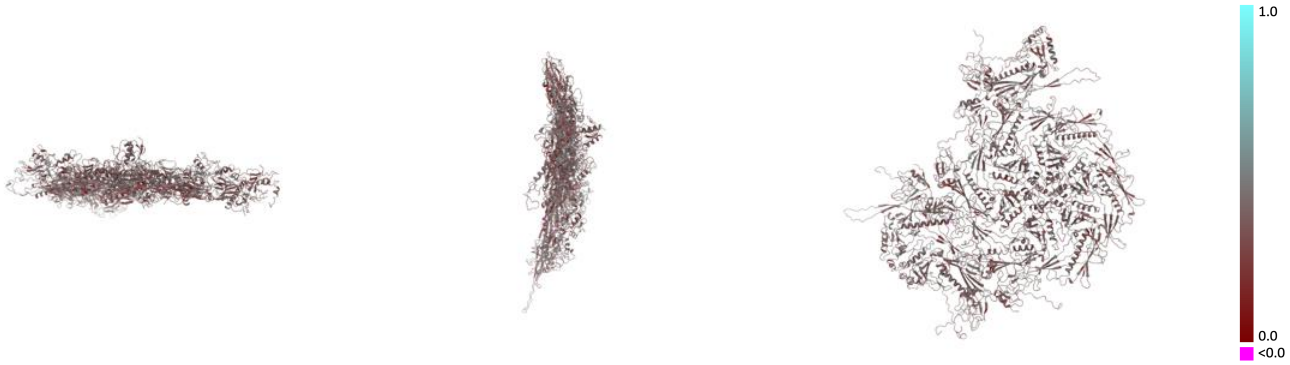
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.651 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

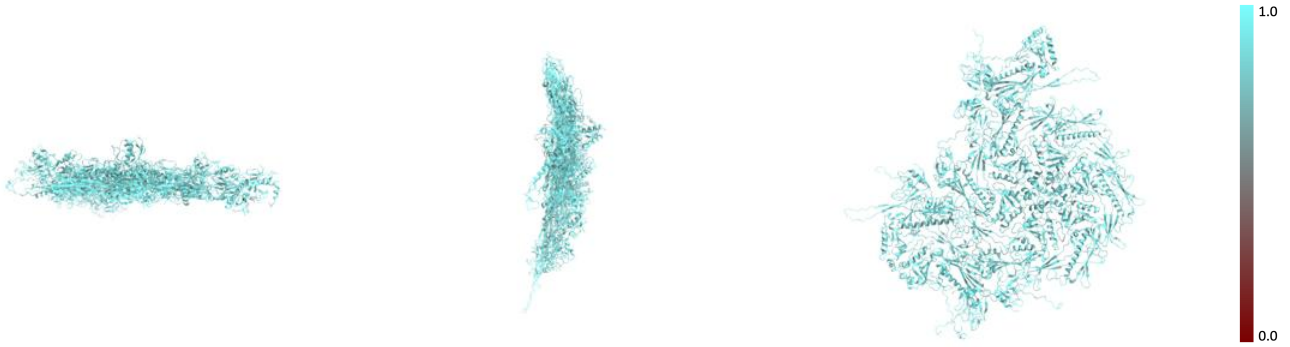
9.2 Q-score mapped to coordinate model



X Y Z

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

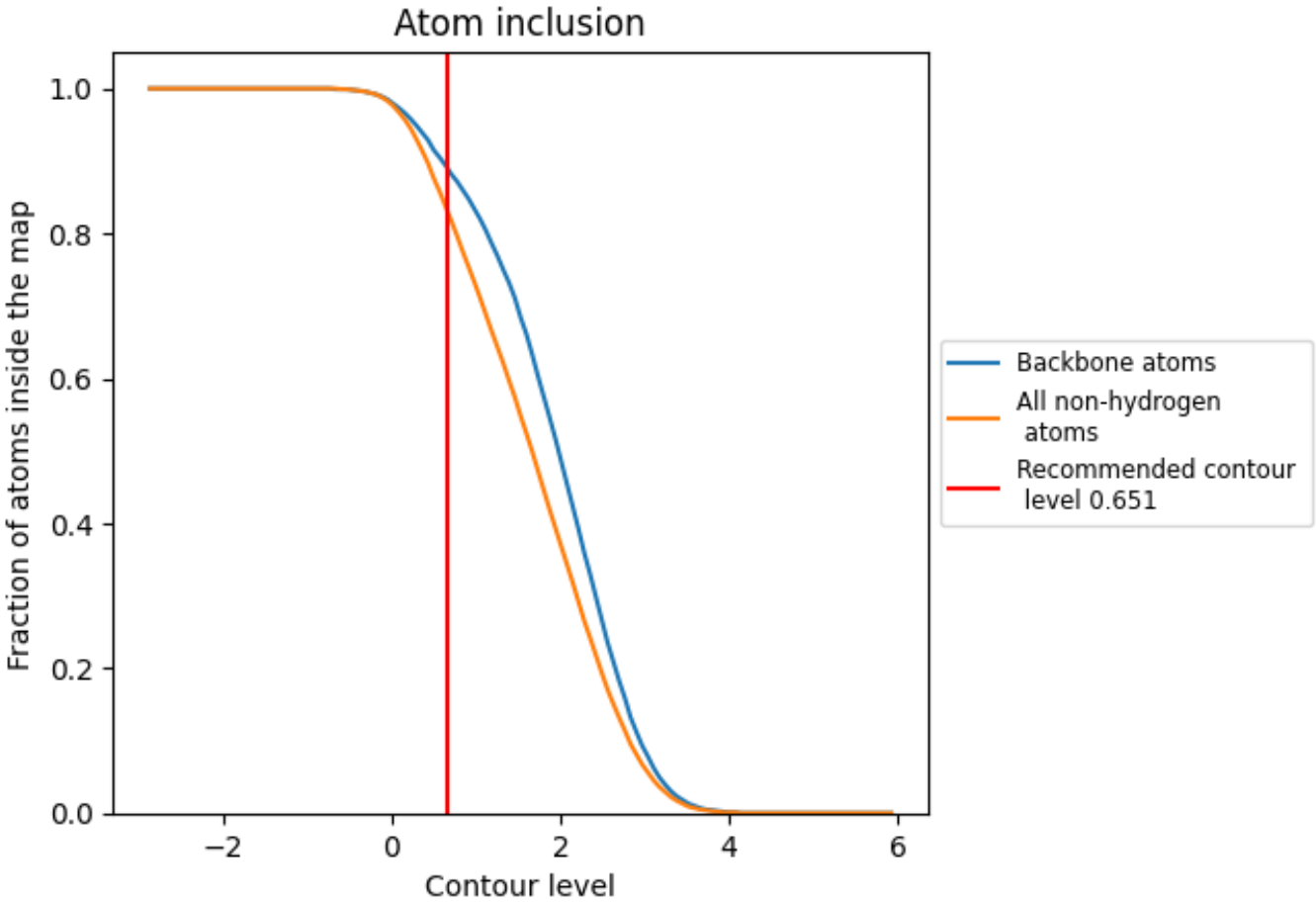
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.651).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 83% 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 (0.651) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8340	0.3740
A	0.8290	0.3760
B	0.8310	0.3640
C	0.8390	0.3730
D	0.8370	0.3720
E	0.8480	0.3680
F	0.8260	0.3720
G	0.8420	0.3760
H	0.8270	0.3700
I	0.8260	0.3730
J	0.8470	0.3990
K	0.8490	0.3820
L	0.8190	0.3620
M	0.8330	0.3610
N	0.8500	0.3970
O	0.8280	0.3810
P	0.8460	0.3930
Q	0.8430	0.3840
R	0.8180	0.3720
S	0.7970	0.3690