



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 02:19 PM UTC

PDB ID : 9C3A / pdb_00009c3a
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:

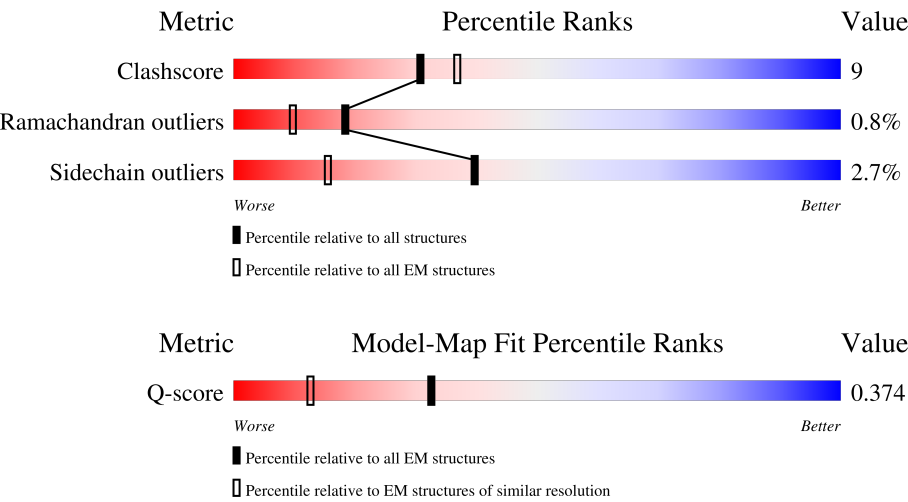
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 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.



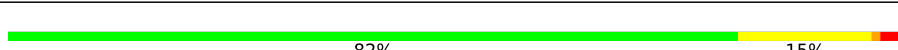
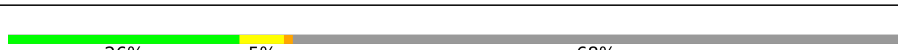
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	A	367	73%25%..
1	B	367	73%24%..
1	C	367	70%22%5%.
1	D	367	72%20%5%.

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Mol	Chain	Length	Quality of chain
1	E	367	 71% 24% . .
1	F	367	 74% 23% .
1	G	367	 79% 16% . .
1	H	367	 80% 18% . .
1	I	367	 73% 19% . . .
2	J	125	 76% 17% 5% . .
2	K	125	 84% 14% . .
2	L	125	 82% 14% . . .
2	M	125	 77% 22% .
2	N	125	 72% 22% . . .
2	O	125	 75% 22% . . .
2	P	125	 78% 21% . .
2	Q	125	 86% 10% . . .
2	R	125	 82% 15% . . .
3	S	372	 26% 5% . 68%

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		

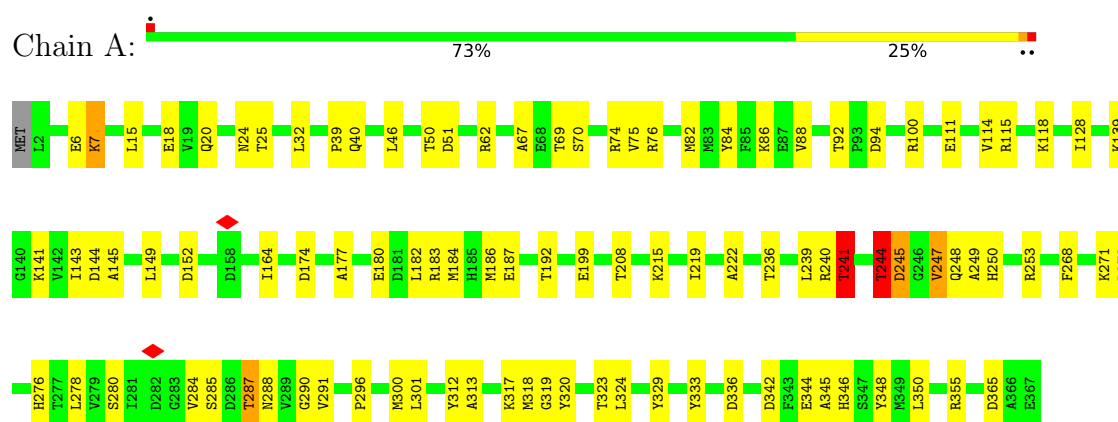
- Molecule 3 is a protein called Putative tail protein.

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

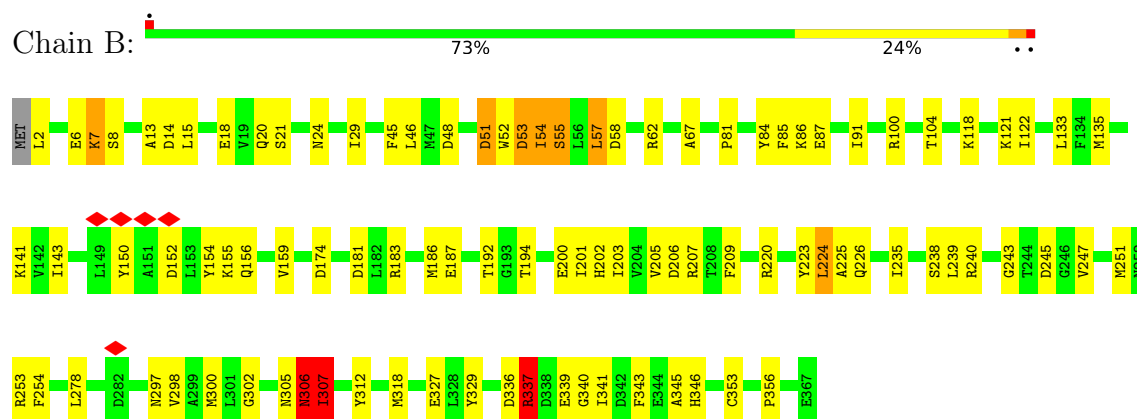
3 Residue-property plots

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.

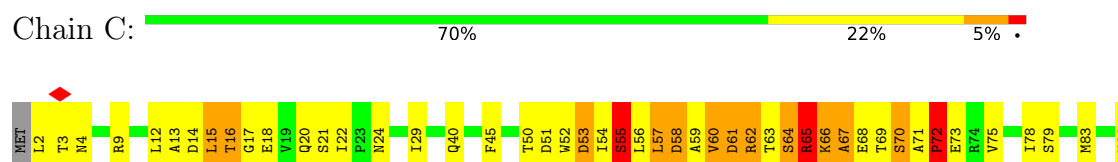
- Molecule 1: Major capsid protein

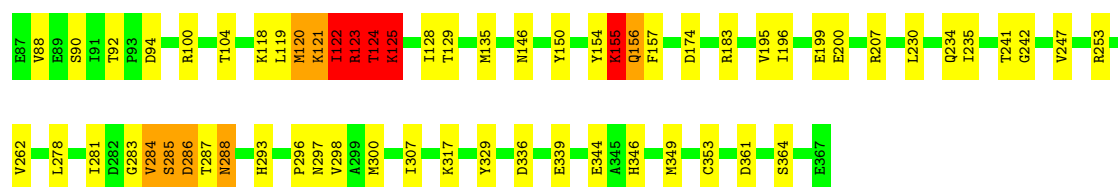


- Molecule 1: Major capsid protein

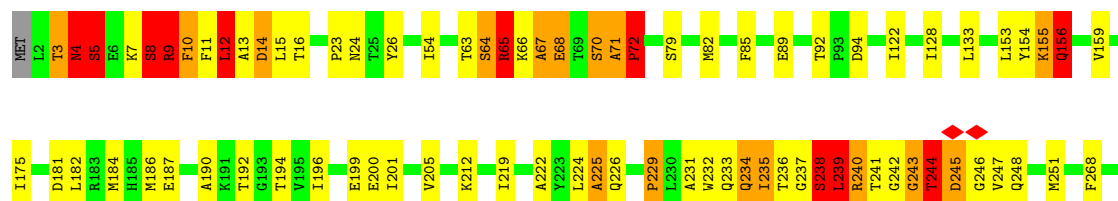


- Molecule 1: Major capsid protein

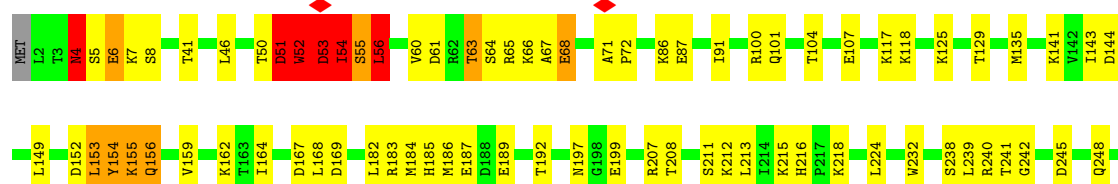




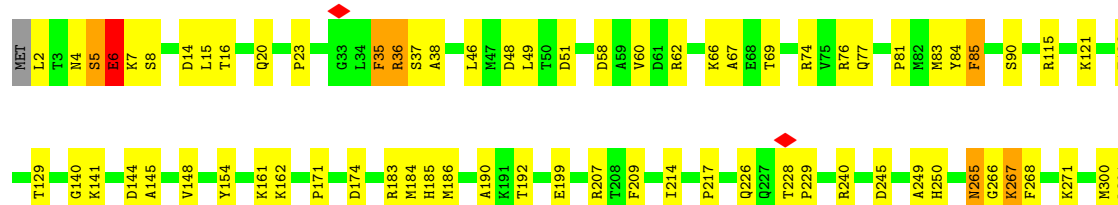
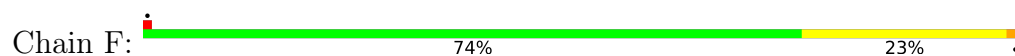
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein



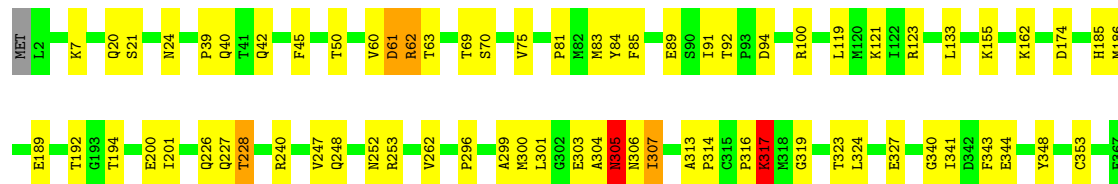
- Molecule 1: Major capsid protein

Chain G:  79% 16% ..



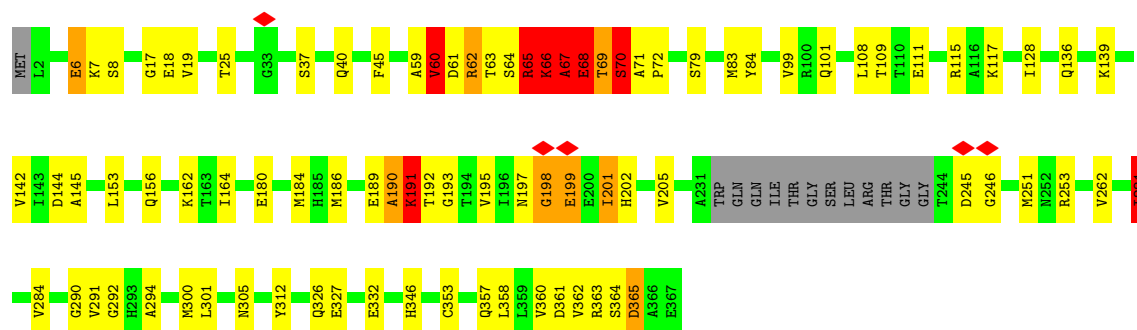
- Molecule 1: Major capsid protein

Chain H:  80% 18% ..



- Molecule 1: Major capsid protein

Chain I:  73% 19% ..



- Molecule 2: Putative structural protein

Chain J:  76% 17% 5% ..



- Molecule 2: Putative structural protein

Chain K:  84% 14% ..



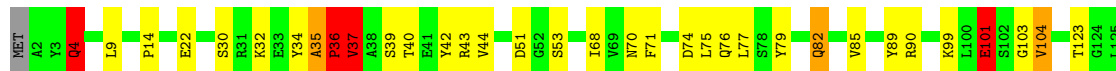
• Molecule 2: Putative structural protein

Chain L:  82% 14% ...

• Molecule 2: Putative structural protein

Chain M:  77% 22% ..

• Molecule 2: Putative structural protein

Chain N:  72% 22% ...

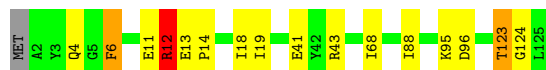
• Molecule 2: Putative structural protein

Chain O:  75% 22% ...

• Molecule 2: Putative structural protein

Chain P:  78% 21% ..

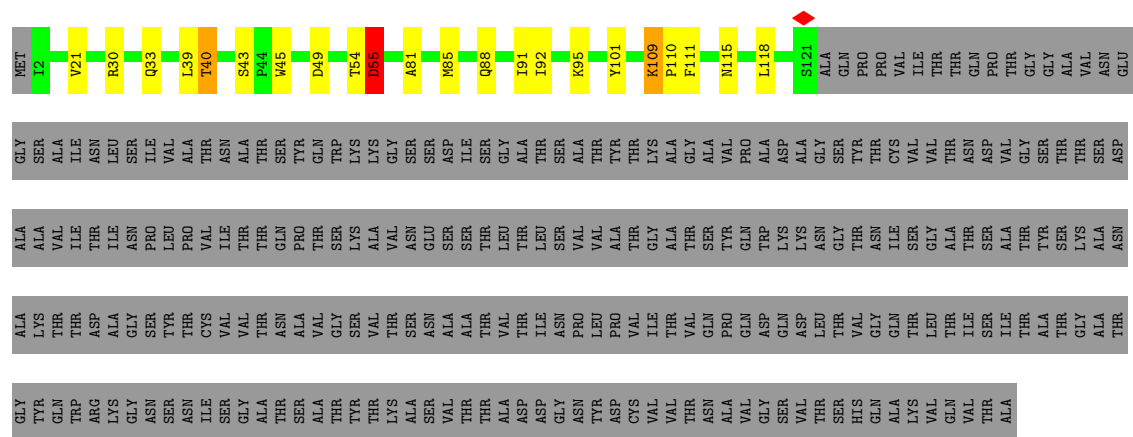
• Molecule 2: Putative structural protein

Chain Q:  86% 10% ...

• Molecule 2: Putative structural protein

Chain R:  82% 15% ...

Chain S: 26% 5% 68%



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ($\text{\AA}$)	1224.0, 1224.0, 1224.0	wwPDB
Map dimensions	1000, 1000, 1000	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	0.36	2/2972 (0.1%)	0.76	15/4021 (0.4%)
1	B	0.57	7/2955 (0.2%)	0.74	20/4001 (0.5%)
1	C	0.84	19/2939 (0.6%)	1.42	71/3979 (1.8%)
1	D	0.93	28/2915 (1.0%)	1.29	62/3949 (1.6%)
1	E	0.71	15/2937 (0.5%)	0.96	34/3978 (0.9%)
1	F	0.58	11/2969 (0.4%)	0.71	18/4017 (0.4%)
1	G	0.68	10/2962 (0.3%)	0.93	35/4009 (0.9%)
1	H	0.50	2/2970 (0.1%)	0.72	21/4019 (0.5%)
1	I	0.65	9/2846 (0.3%)	0.98	35/3851 (0.9%)
2	J	0.76	3/941 (0.3%)	1.06	14/1274 (1.1%)
2	K	0.34	1/959 (0.1%)	0.59	2/1298 (0.2%)
2	L	0.58	3/960 (0.3%)	0.68	7/1299 (0.5%)
2	M	0.29	1/951 (0.1%)	0.53	4/1287 (0.3%)
2	N	0.72	4/949 (0.4%)	1.21	11/1284 (0.9%)
2	O	0.58	2/948 (0.2%)	0.72	8/1283 (0.6%)
2	P	0.43	1/943 (0.1%)	0.73	5/1276 (0.4%)
2	Q	0.55	2/960 (0.2%)	1.08	10/1299 (0.8%)
2	R	0.47	1/960 (0.1%)	0.86	4/1299 (0.3%)
3	S	0.25	0/990	0.57	2/1351 (0.1%)
All	All	0.63	121/36026 (0.3%)	0.94	378/48774 (0.8%)

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 (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	8	SER	CA-CB	-11.38	1.35	1.53
1	D	67	ALA	CA-CB	-10.80	1.38	1.53
2	J	4	GLN	CA-CB	-10.79	1.38	1.53
1	G	228	THR	CA-C	-10.09	1.40	1.52
1	D	235	ILE	CA-CB	-9.66	1.41	1.54
1	C	64	SER	CA-CB	-9.03	1.39	1.52
1	E	8	SER	CA-CB	-8.89	1.38	1.53
1	B	8	SER	CA-CB	-8.59	1.36	1.54
1	F	308	PHE	CA-C	-8.56	1.42	1.52
2	J	3	TYR	CA-CB	-8.45	1.39	1.53
1	F	38	ALA	CA-CB	-8.14	1.43	1.53
1	C	70	SER	CA-CB	-8.11	1.39	1.53
1	G	230	LEU	C-O	-8.08	1.14	1.24
2	O	78	SER	CA-CB	-7.99	1.40	1.53
2	L	6	PHE	CA-C	-7.77	1.42	1.52
1	D	64	SER	CA-CB	-7.70	1.43	1.54
1	I	70	SER	CA-CB	-7.67	1.40	1.53
1	F	37	SER	CA-CB	-7.66	1.42	1.53
1	C	66	LYS	CA-C	7.65	1.60	1.53
2	R	3	TYR	CA-C	-7.61	1.42	1.52
1	B	226	GLN	C-O	-7.58	1.15	1.23
1	F	5	SER	CA-CB	-7.49	1.41	1.53
1	E	68	GLU	CA-CB	-7.31	1.41	1.53
1	I	64	SER	CA-CB	-7.17	1.41	1.53
1	B	52	TRP	CA-C	-7.14	1.43	1.52
1	C	66	LYS	C-N	-7.11	1.25	1.33
1	G	202	HIS	C-O	-7.10	1.16	1.24
2	N	36	PRO	CA-CB	-7.10	1.44	1.53
1	D	5	SER	CA-CB	-7.03	1.44	1.54
1	C	58	ASP	N-CA	6.84	1.55	1.46
1	B	225	ALA	CA-CB	-6.83	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	4	GLN	CA-CB	-6.82	1.42	1.53
1	D	240	ARG	CA-CB	-6.75	1.43	1.53
1	C	67	ALA	CA-CB	-6.71	1.40	1.53
1	D	70	SER	CA-CB	-6.70	1.41	1.54
1	E	154	TYR	CA-C	-6.68	1.43	1.52
1	C	154	TYR	CA-C	-6.56	1.44	1.52
2	L	123	THR	CA-C	-6.56	1.44	1.52
1	C	52	TRP	CA-C	-6.55	1.44	1.52
1	G	7	LYS	C-N	-6.42	1.24	1.33
1	D	7	LYS	C-O	-6.41	1.16	1.23
1	C	13	ALA	CA-CB	-6.40	1.43	1.54
1	B	53	ASP	C-N	-6.37	1.26	1.33
1	E	366	ALA	CA-CB	-6.34	1.41	1.53
1	F	266	GLY	CA-C	-6.33	1.46	1.52
2	J	61	ALA	CA-CB	-6.33	1.45	1.54
1	H	63	THR	C-O	-6.29	1.15	1.24
2	N	82	GLN	C-O	-6.25	1.15	1.23
1	I	190	ALA	CA-CB	-6.24	1.44	1.53
1	G	338	ASP	C-O	-6.21	1.16	1.23
2	K	122	PRO	CA-CB	-6.21	1.45	1.53
2	Q	4	GLN	C-O	-6.20	1.15	1.23
1	G	231	ALA	CA-CB	-6.16	1.43	1.53
1	D	72	PRO	CA-CB	-6.07	1.45	1.53
2	N	36	PRO	CA-C	-6.05	1.45	1.52
1	D	13	ALA	CA-CB	-6.02	1.43	1.53
1	C	72	PRO	CA-CB	-6.00	1.45	1.53
1	E	4	ASN	C-O	-5.98	1.18	1.24
1	E	64	SER	CA-CB	-5.89	1.44	1.53
1	G	7	LYS	CA-C	-5.86	1.44	1.52
1	C	63	THR	C-O	-5.86	1.16	1.24
1	I	201	ILE	C-O	-5.85	1.17	1.23
1	D	232	TRP	CA-CB	-5.84	1.45	1.52
1	E	54	ILE	CA-CB	-5.79	1.46	1.54
1	E	338	ASP	C-O	-5.79	1.16	1.24
1	E	65	ARG	CA-CB	-5.78	1.44	1.53
1	B	52	TRP	C-N	-5.72	1.26	1.33
1	F	35	PHE	CA-C	-5.69	1.45	1.52
1	I	72	PRO	CA-CB	-5.66	1.44	1.53
1	D	234	GLN	C-O	-5.63	1.16	1.24
1	D	229	PRO	CA-CB	-5.61	1.45	1.53
1	D	11	PHE	CA-C	-5.59	1.45	1.52
1	F	4	ASN	C-O	-5.58	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	5	SER	C-O	-5.57	1.17	1.24
1	G	7	LYS	CA-CB	-5.56	1.44	1.53
1	F	268	PHE	CA-C	-5.54	1.45	1.52
1	D	244	THR	C-N	5.53	1.41	1.33
1	D	11	PHE	C-O	-5.52	1.17	1.23
1	C	285	SER	CA-CB	-5.51	1.45	1.53
2	M	123	THR	CA-C	-5.51	1.45	1.52
2	N	39	SER	CA-CB	-5.50	1.45	1.53
1	D	320	TYR	CA-C	-5.49	1.45	1.52
1	D	154	TYR	CA-C	-5.49	1.40	1.52
1	D	225	ALA	CA-CB	-5.47	1.44	1.53
1	A	319	GLY	CA-C	-5.46	1.45	1.52
1	E	68	GLU	C-N	5.45	1.40	1.33
1	B	8	SER	C-O	-5.42	1.17	1.23
1	D	239	LEU	CA-C	-5.41	1.45	1.52
1	C	70	SER	C-O	-5.39	1.17	1.24
1	G	225	ALA	C-O	-5.35	1.17	1.23
1	D	71	ALA	CA-CB	-5.35	1.45	1.53
1	D	155	LYS	C-O	-5.34	1.18	1.24
1	D	304	ALA	CA-CB	-5.33	1.45	1.53
2	O	79	TYR	CA-C	-5.33	1.45	1.52
1	D	320	TYR	C-O	-5.33	1.16	1.24
1	E	63	THR	CA-C	-5.31	1.45	1.52
1	D	240	ARG	CA-C	-5.31	1.46	1.53
1	E	153	LEU	C-O	-5.31	1.16	1.24
1	D	3	THR	CA-C	-5.31	1.46	1.52
1	I	71	ALA	CA-CB	-5.30	1.45	1.53
1	C	122	ILE	C-N	-5.29	1.26	1.33
1	C	53	ASP	C-N	-5.28	1.26	1.33
1	E	68	GLU	C-O	-5.27	1.17	1.24
1	G	3	THR	CA-C	-5.27	1.45	1.52
1	I	8	SER	CA-CB	-5.27	1.43	1.53
1	C	71	ALA	CA-CB	-5.27	1.45	1.53
1	F	267	LYS	C-O	-5.24	1.17	1.23
1	I	67	ALA	C-N	-5.21	1.26	1.33
1	C	73	GLU	CA-CB	-5.20	1.45	1.53
1	D	365	ASP	C-O	-5.14	1.18	1.24
1	D	231	ALA	CA-CB	-5.12	1.46	1.53
1	H	84	TYR	CA-C	-5.11	1.46	1.52
1	F	8	SER	C-O	-5.11	1.17	1.23
1	D	63	THR	C-O	-5.10	1.17	1.24
1	A	285	SER	CA-CB	-5.06	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	13	GLU	C-O	-5.05	1.17	1.23
2	Q	14	PRO	C-O	-5.04	1.18	1.23
1	I	69	THR	CA-CB	-5.04	1.45	1.53
1	C	121	LYS	C-N	-5.02	1.26	1.33
1	C	121	LYS	CA-C	-5.01	1.45	1.52
1	E	5	SER	CA-CB	-5.01	1.45	1.53

All (378) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	36	PRO	N-CA-CB	-26.56	79.88	103.25
1	C	57	LEU	N-CA-CB	-23.90	60.97	111.87
1	A	245	ASP	CB-CA-C	-19.86	77.00	110.56
1	C	65	ARG	N-CA-CB	-19.65	77.84	109.87
1	C	72	PRO	N-CA-CB	-19.09	83.21	103.25
2	Q	14	PRO	N-CA-CB	-18.99	85.68	103.34
1	C	121	LYS	CB-CA-C	-18.55	71.90	109.55
2	R	6	PHE	CB-CA-C	-18.27	74.22	109.66
1	D	10	PHE	N-CA-CB	-18.11	82.95	109.94
1	I	65	ARG	CB-CA-C	-17.82	74.95	110.42
1	C	120	MET	CB-CA-C	-16.22	82.74	110.64
1	D	72	PRO	N-CA-CB	-16.07	86.37	103.25
1	C	62	ARG	CB-CA-C	-15.97	82.19	109.02
1	C	51	ASP	CB-CA-C	-15.36	89.44	110.79
1	C	61	ASP	CB-CA-C	-13.83	80.23	113.15
2	R	6	PHE	CA-CB-CG	13.71	127.51	113.80
1	E	6	GLU	N-CA-CB	-13.20	88.17	110.49
1	E	56	LEU	N-CA-CB	-12.62	91.37	111.43
1	D	10	PHE	CB-CA-C	12.32	130.53	110.81
1	F	267	LYS	CB-CA-C	-12.21	90.33	109.99
1	I	72	PRO	N-CA-CB	-11.96	88.16	102.86
1	D	244	THR	N-CA-C	-11.77	85.74	110.80
2	Q	6	PHE	CA-CB-CG	11.72	125.52	113.80
2	K	122	PRO	N-CA-CB	-11.49	91.19	103.25
1	D	233	GLN	N-CA-C	-11.45	99.84	114.04
1	A	319	GLY	CA-C-N	-11.44	104.35	122.65
1	A	319	GLY	C-N-CA	-11.44	104.35	122.65
1	C	53	ASP	CA-C-N	-11.40	104.66	122.68
1	C	53	ASP	C-N-CA	-11.40	104.66	122.68
1	E	51	ASP	CB-CA-C	-11.38	94.01	110.62
1	D	305	ASN	CB-CA-C	11.28	129.75	111.24
1	A	245	ASP	CA-CB-CG	11.07	123.67	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	61	ASP	CB-CA-C	-11.06	90.48	109.83
1	C	157	PHE	N-CA-CB	-10.95	93.95	110.04
1	D	231	ALA	N-CA-C	-10.85	98.30	112.41
1	G	7	LYS	N-CA-C	-10.84	99.25	111.82
1	I	72	PRO	N-CD-CG	-10.66	87.21	103.20
2	Q	11	GLU	CB-CA-C	-10.55	89.42	110.30
2	J	60	GLU	CB-CA-C	-10.49	92.16	110.72
1	C	57	LEU	CA-C-O	-10.35	109.66	121.26
1	G	197	ASN	CB-CA-C	-10.35	90.46	109.29
1	G	9	ARG	N-CA-CB	-10.29	93.10	110.49
2	J	6	PHE	CA-C-N	10.22	137.39	122.99
2	J	6	PHE	C-N-CA	10.22	137.39	122.99
1	C	121	LYS	N-CA-C	-10.20	100.58	113.23
1	F	326	GLN	N-CA-CB	-10.19	93.97	111.69
1	D	224	LEU	N-CA-CB	-10.15	98.98	110.35
1	E	156	GLN	N-CA-C	-10.11	100.95	113.18
1	D	155	LYS	CB-CA-C	-10.03	96.22	109.16
2	N	36	PRO	CB-CG-CD	-9.95	74.25	106.10
1	G	230	LEU	N-CA-C	-9.74	100.50	111.71
1	G	229	PRO	N-CA-CB	9.71	113.45	103.25
1	D	65	ARG	N-CA-CB	-9.69	94.11	110.49
1	D	66	LYS	CA-C-O	-9.64	110.30	121.68
1	D	305	ASN	N-CA-C	-9.59	99.10	110.41
1	D	66	LYS	CB-CA-C	9.58	128.25	110.24
1	G	230	LEU	N-CA-CB	9.55	124.93	110.22
1	F	6	GLU	N-CA-CB	-9.46	96.09	109.91
1	G	199	GLU	CB-CA-C	-9.37	94.88	110.72
1	D	67	ALA	N-CA-CB	-9.30	97.12	111.35
2	P	6	PHE	CA-CB-CG	9.24	123.05	113.80
1	E	68	GLU	N-CA-CB	-9.19	94.95	110.49
1	E	308	PHE	N-CA-CB	-9.11	95.49	110.52
1	F	6	GLU	CB-CA-C	9.08	124.95	110.96
1	A	241	THR	O-C-N	-8.99	112.52	123.04
1	I	191	LYS	CB-CA-C	8.99	126.84	111.46
1	D	66	LYS	N-CA-CB	-8.96	97.61	111.05
1	A	288	ASN	CA-C-N	-8.95	110.50	122.94
1	A	288	ASN	C-N-CA	-8.95	110.50	122.94
1	C	72	PRO	N-CA-C	8.91	130.82	112.47
1	D	156	GLN	N-CA-C	-8.81	101.60	111.82
1	E	56	LEU	CA-C-N	8.78	133.97	121.42
1	E	56	LEU	C-N-CA	8.78	133.97	121.42
1	D	241	THR	N-CA-C	-8.76	92.38	108.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	GLY	N-CA-C	-8.75	102.87	114.25
1	D	11	PHE	CA-CB-CG	8.72	122.52	113.80
1	F	307	ILE	N-CA-C	-8.71	104.54	112.90
1	C	58	ASP	CB-CA-C	-8.70	93.11	110.42
1	D	10	PHE	CA-C-O	-8.70	111.59	120.90
1	H	319	GLY	CA-C-N	-8.68	108.77	122.65
1	H	319	GLY	C-N-CA	-8.68	108.77	122.65
1	C	66	LYS	N-CA-CB	-8.64	91.70	110.88
1	G	229	PRO	CA-C-N	-8.64	107.84	120.28
1	G	229	PRO	C-N-CA	-8.64	107.84	120.28
1	A	287	THR	N-CA-C	-8.63	102.93	113.97
2	N	35	ALA	O-C-N	8.57	129.02	121.39
2	Q	11	GLU	N-CA-CB	-8.54	97.86	111.43
1	C	55	SER	N-CA-C	-8.52	92.65	110.80
1	I	60	VAL	N-CA-CB	-8.49	97.23	111.23
1	H	60	VAL	O-C-N	-8.47	113.68	123.00
1	B	58	ASP	CA-CB-CG	8.44	121.03	112.60
1	C	56	LEU	CA-C-O	-8.42	108.47	120.51
1	G	202	HIS	CA-CB-CG	8.41	122.21	113.80
1	C	68	GLU	N-CA-C	-8.37	97.17	110.14
1	I	284	VAL	N-CA-CB	-8.33	102.17	111.66
1	D	229	PRO	N-CA-CB	-8.31	94.53	103.25
1	E	6	GLU	CB-CG-CD	8.30	126.70	112.60
1	F	308	PHE	N-CA-CB	-8.26	97.77	110.65
1	D	156	GLN	N-CA-CB	8.25	123.07	110.28
2	M	123	THR	CA-C-N	-8.25	112.85	121.35
2	M	123	THR	C-N-CA	-8.25	112.85	121.35
2	Q	13	GLU	N-CA-CB	-8.24	99.08	110.04
1	E	67	ALA	CA-C-O	-8.14	110.63	121.46
1	A	317	LYS	N-CA-C	-8.07	98.27	110.14
1	D	239	LEU	N-CA-C	-7.93	102.68	113.30
1	G	9	ARG	CB-CA-C	7.91	126.15	110.42
1	C	120	MET	N-CA-C	-7.88	101.83	112.94
1	G	202	HIS	CB-CA-C	-7.86	97.11	110.16
1	D	64	SER	N-CA-C	-7.86	103.91	113.97
1	G	326	GLN	N-CA-CB	-7.84	98.69	110.60
1	I	68	GLU	CA-C-N	-7.76	108.55	121.97
1	I	68	GLU	C-N-CA	-7.76	108.55	121.97
1	C	58	ASP	N-CA-CB	7.73	123.56	110.49
1	B	254	PHE	CA-C-O	-7.73	112.35	120.70
2	J	61	ALA	N-CA-C	-7.70	104.37	114.31
1	E	52	TRP	N-CA-C	-7.69	102.54	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	7	LYS	CA-C-N	-7.61	107.00	121.54
1	G	7	LYS	C-N-CA	-7.61	107.00	121.54
1	B	52	TRP	CA-CB-CG	7.60	128.04	113.60
1	G	202	HIS	CA-C-O	-7.59	112.18	120.30
1	E	302	GLY	CA-C-O	-7.58	114.76	122.26
2	O	80	HIS	N-CA-C	-7.54	101.24	111.87
1	D	243	GLY	N-CA-C	-7.52	95.36	113.18
2	J	4	GLN	CA-C-O	-7.45	112.68	121.32
1	E	68	GLU	CA-C-O	-7.41	109.92	120.51
1	F	268	PHE	CA-CB-CG	7.40	121.20	113.80
1	H	327	GLU	CB-CG-CD	-7.35	100.10	112.60
1	C	58	ASP	CA-C-N	-7.34	111.29	122.81
1	C	58	ASP	C-N-CA	-7.34	111.29	122.81
1	D	65	ARG	CB-CA-C	7.32	124.99	110.42
1	I	67	ALA	CA-C-N	-7.32	107.57	121.54
1	I	67	ALA	C-N-CA	-7.32	107.57	121.54
2	R	4	GLN	N-CA-CB	-7.26	98.22	110.49
1	D	11	PHE	N-CA-CB	-7.24	98.19	111.37
1	I	68	GLU	N-CA-CB	-7.24	98.25	110.49
2	O	123	THR	CA-C-N	-7.24	115.78	122.80
2	O	123	THR	C-N-CA	-7.24	115.78	122.80
1	E	53	ASP	CA-C-N	-7.23	108.95	121.97
1	E	53	ASP	C-N-CA	-7.23	108.95	121.97
1	C	52	TRP	CA-C-N	-7.22	109.24	121.08
1	C	52	TRP	C-N-CA	-7.22	109.24	121.08
1	I	327	GLU	CB-CG-CD	-7.22	100.33	112.60
1	C	125	LYS	N-CA-C	-7.21	95.45	110.80
1	H	317	LYS	CA-CB-CG	7.21	128.51	114.10
1	D	155	LYS	N-CA-C	-7.20	105.68	114.75
1	I	18	GLU	CB-CA-C	-7.15	95.24	109.33
1	F	327	GLU	N-CA-CB	-7.13	99.36	110.06
1	B	254	PHE	CA-CB-CG	7.12	120.92	113.80
2	J	77	LEU	N-CA-C	-7.12	99.67	110.14
1	D	14	ASP	CB-CA-C	-7.11	95.80	109.37
1	G	16	THR	N-CA-CB	-7.05	100.03	110.53
1	E	55	SER	N-CA-C	-7.03	97.94	109.40
2	P	3	TYR	CA-C-O	-7.02	111.92	122.38
2	Q	14	PRO	N-CD-CG	-7.02	92.67	103.20
1	C	123	ARG	N-CA-CB	-7.00	98.67	110.49
1	C	154	TYR	N-CA-CB	-6.99	98.67	110.49
1	I	62	ARG	N-CA-CB	6.99	121.06	110.30
1	C	53	ASP	CA-C-O	6.98	126.53	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	LYS	CA-C-O	-6.96	111.74	121.98
2	N	39	SER	CA-C-N	-6.96	113.18	122.99
2	N	39	SER	C-N-CA	-6.96	113.18	122.99
1	C	62	ARG	N-CA-CB	6.93	120.11	110.90
1	B	55	SER	N-CA-C	-6.91	101.61	110.53
1	I	190	ALA	CA-C-N	-6.90	111.58	123.25
1	I	190	ALA	C-N-CA	-6.90	111.58	123.25
1	F	266	GLY	CA-C-O	-6.90	113.85	121.71
1	G	7	LYS	CB-CA-C	-6.88	97.47	110.67
1	A	284	VAL	N-CA-CB	-6.87	103.17	111.21
1	I	326	GLN	N-CA-CB	-6.87	100.49	110.87
2	J	5	GLY	N-CA-C	-6.86	104.46	112.83
1	C	123	ARG	CA-C-O	-6.86	110.70	120.51
1	A	245	ASP	N-CA-C	-6.85	104.49	112.92
1	D	4	ASN	CB-CA-C	-6.84	96.80	110.42
1	H	305	ASN	CB-CA-C	6.84	124.03	110.42
1	E	156	GLN	CA-C-N	-6.83	111.64	122.29
1	E	156	GLN	C-N-CA	-6.83	111.64	122.29
1	B	337	ARG	CB-CA-C	6.81	123.97	110.42
2	P	4	GLN	CB-CA-C	-6.80	96.88	110.42
1	E	66	LYS	CA-C-O	-6.80	113.53	122.03
1	G	9	ARG	CA-C-N	-6.79	111.40	121.99
1	G	9	ARG	C-N-CA	-6.79	111.40	121.99
1	C	157	PHE	N-CA-C	-6.77	101.14	110.35
1	E	7	LYS	N-CA-CB	6.77	124.55	111.07
1	C	157	PHE	CA-C-O	-6.77	114.38	121.55
1	B	225	ALA	N-CA-CB	-6.76	101.94	110.45
1	F	265	ASN	N-CA-CB	-6.70	100.35	110.73
1	C	22	ILE	CA-C-N	6.69	126.61	119.85
1	C	22	ILE	C-N-CA	6.69	126.61	119.85
2	L	11	GLU	N-CA-CB	-6.67	99.94	111.55
2	P	4	GLN	CA-C-O	-6.63	111.03	120.51
2	N	123	THR	CA-CB-OG1	-6.62	99.67	109.60
1	H	307	ILE	N-CA-CB	-6.61	102.03	112.07
1	C	156	GLN	N-CA-C	-6.60	96.75	110.80
1	I	202	HIS	CA-C-O	-6.57	113.27	120.43
1	D	239	LEU	CA-C-N	-6.56	109.06	121.66
1	D	239	LEU	C-N-CA	-6.56	109.06	121.66
1	H	317	LYS	N-CA-C	-6.55	96.84	110.80
1	C	60	VAL	O-C-N	-6.54	115.69	122.95
1	C	124	THR	OG1-CB-CG2	-6.54	96.21	109.30
1	C	66	LYS	CB-CA-C	6.54	130.06	114.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	226	GLN	N-CA-CB	-6.54	102.22	110.45
1	B	225	ALA	CA-C-O	-6.51	112.68	122.38
1	D	232	TRP	CA-C-N	6.50	133.93	122.42
1	D	232	TRP	C-N-CA	6.50	133.93	122.42
1	E	304	ALA	N-CA-C	-6.48	104.53	112.88
1	F	8	SER	CB-CA-C	-6.47	98.21	109.86
2	L	6	PHE	CA-CB-CG	6.46	120.26	113.80
1	B	7	LYS	CB-CA-C	6.45	123.22	110.65
1	D	240	ARG	CA-C-O	6.42	129.14	121.88
2	O	4	GLN	CA-C-N	-6.41	112.01	122.40
2	O	4	GLN	C-N-CA	-6.41	112.01	122.40
2	J	101	GLU	N-CA-CB	-6.40	100.57	109.97
2	J	6	PHE	CA-CB-CG	6.39	120.19	113.80
1	D	244	THR	CA-C-O	-6.38	111.39	120.51
1	B	302	GLY	O-C-N	-6.35	115.38	122.68
1	E	338	ASP	CA-CB-CG	6.34	118.94	112.60
1	E	308	PHE	CA-CB-CG	6.32	120.12	113.80
1	E	6	GLU	CA-C-N	6.30	129.87	120.17
1	E	6	GLU	C-N-CA	6.30	129.87	120.17
1	D	232	TRP	CB-CA-C	6.28	121.46	111.91
1	D	240	ARG	CB-CA-C	-6.26	97.76	111.71
1	I	71	ALA	N-CA-CB	-6.25	102.59	109.72
2	P	6	PHE	N-CA-CB	-6.24	99.71	111.00
2	J	75	LEU	N-CA-CB	6.22	119.80	110.65
1	C	62	ARG	CA-CB-CG	6.22	126.54	114.10
1	C	22	ILE	N-CA-CB	-6.21	102.52	111.21
1	G	197	ASN	N-CA-CB	6.20	119.64	110.53
1	E	7	LYS	CB-CA-C	-6.20	97.43	110.45
1	D	244	THR	N-CA-CB	6.19	120.96	110.49
1	D	155	LYS	N-CA-CB	6.13	120.10	111.15
1	D	319	GLY	N-CA-C	-6.12	106.58	114.85
1	D	154	TYR	N-CA-C	-6.12	106.18	113.21
1	C	54	ILE	O-C-N	6.11	129.82	123.04
1	C	66	LYS	CA-C-N	-6.11	108.15	122.19
1	C	66	LYS	C-N-CA	-6.11	108.15	122.19
2	N	37	VAL	N-CA-C	-6.10	100.97	109.45
1	I	66	LYS	CB-CA-C	-6.08	98.33	110.42
1	E	66	LYS	CB-CA-C	6.05	120.94	112.11
2	N	103	GLY	N-CA-C	-6.05	106.75	114.37
1	C	154	TYR	CB-CA-C	-6.03	98.42	110.42
1	C	16	THR	N-CA-CB	-6.01	101.29	110.12
1	B	53	ASP	CA-C-N	-6.00	112.00	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	ASP	C-N-CA	-6.00	112.00	120.35
1	H	155	LYS	N-CA-CB	-6.00	101.33	110.33
1	G	8	SER	O-C-N	5.99	130.56	122.59
1	H	226	GLN	CB-CA-C	5.98	119.99	110.19
1	G	281	ILE	N-CA-C	-5.96	99.83	108.17
2	Q	12	ARG	CA-CB-CG	5.95	125.99	114.10
1	D	235	ILE	CB-CA-C	-5.94	101.55	111.29
1	C	61	ASP	N-CA-CB	5.93	119.82	110.39
1	C	155	LYS	N-CA-C	-5.92	98.19	110.80
1	F	267	LYS	N-CA-C	-5.91	99.53	108.52
1	D	13	ALA	CA-C-O	-5.91	115.10	121.36
1	C	65	ARG	CA-C-O	-5.89	113.66	120.49
2	M	124	GLY	N-CA-C	5.88	119.72	110.96
1	C	284	VAL	N-CA-CB	5.87	120.91	111.23
1	I	72	PRO	N-CA-C	5.84	119.81	110.40
1	G	225	ALA	N-CA-C	-5.82	98.79	108.75
3	S	55	ASP	CB-CA-C	-5.80	103.09	111.91
1	C	65	ARG	N-CA-C	5.80	118.13	109.25
1	I	198	GLY	N-CA-C	-5.80	105.64	113.24
1	B	254	PHE	CA-C-N	5.79	131.16	123.05
1	B	254	PHE	C-N-CA	5.79	131.16	123.05
1	I	17	GLY	N-CA-C	5.79	121.38	112.81
2	J	60	GLU	N-CA-C	5.77	119.84	113.21
1	F	307	ILE	N-CA-CB	-5.73	104.86	112.26
2	Q	123	THR	CA-C-N	-5.73	114.39	121.38
2	Q	123	THR	C-N-CA	-5.73	114.39	121.38
1	I	72	PRO	CB-CG-CD	-5.72	87.79	106.10
2	L	12	ARG	CB-CA-C	-5.72	100.09	109.53
2	Q	14	PRO	CB-CG-CD	-5.72	87.80	106.10
1	D	12	LEU	N-CA-CB	-5.71	101.94	111.20
1	C	58	ASP	CA-CB-CG	5.71	118.31	112.60
1	D	11	PHE	CA-C-O	-5.70	114.45	121.11
1	C	52	TRP	N-CA-C	-5.69	100.39	109.96
1	I	59	ALA	O-C-N	-5.69	116.15	122.86
1	I	66	LYS	CA-C-N	-5.68	110.70	121.54
1	I	66	LYS	C-N-CA	-5.68	110.70	121.54
1	E	303	GLU	N-CA-C	-5.67	105.67	112.59
1	I	281	ILE	N-CA-C	-5.67	100.17	108.97
1	G	196	ILE	CA-C-O	-5.67	114.70	121.28
1	D	224	LEU	N-CA-C	-5.66	101.73	109.71
1	C	55	SER	CB-CA-C	5.65	121.67	110.42
1	C	124	THR	N-CA-CB	5.65	120.04	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	16	THR	CA-CB-OG1	-5.65	101.13	109.60
1	C	13	ALA	CA-C-O	-5.65	115.03	121.58
1	C	75	VAL	CA-C-O	-5.64	114.50	120.48
1	G	224	LEU	CB-CA-C	5.64	120.04	111.70
1	E	154	TYR	CB-CA-C	-5.63	101.83	111.46
1	C	73	GLU	N-CA-C	5.63	117.59	110.33
1	E	7	LYS	N-CA-C	-5.61	104.24	113.50
1	F	267	LYS	CA-C-O	-5.61	114.47	120.75
1	C	121	LYS	CA-C-N	-5.59	111.90	121.97
1	C	121	LYS	C-N-CA	-5.59	111.90	121.97
2	N	101	GLU	N-CA-CB	-5.59	101.04	110.49
2	R	3	TYR	CB-CA-C	-5.58	99.31	110.42
1	H	84	TYR	CB-CA-C	-5.57	98.32	109.35
2	N	4	GLN	CB-CA-C	-5.57	99.33	110.42
2	O	79	TYR	CA-CB-CG	5.57	123.92	113.90
1	G	228	THR	O-C-N	5.56	127.72	121.32
3	S	54	THR	N-CA-C	-5.56	106.42	113.43
1	D	242	GLY	CA-C-N	-5.56	110.52	121.41
1	D	242	GLY	C-N-CA	-5.56	110.52	121.41
1	E	365	ASP	CA-CB-CG	5.54	118.14	112.60
1	H	307	ILE	N-CA-C	-5.54	106.41	113.22
1	C	68	GLU	N-CA-CB	-5.50	102.38	110.85
1	D	66	LYS	CA-C-N	-5.49	112.89	122.84
1	D	66	LYS	C-N-CA	-5.49	112.89	122.84
1	H	62	ARG	CB-CG-CD	-5.48	98.69	111.30
1	B	223	TYR	O-C-N	-5.46	114.92	122.46
1	D	12	LEU	CA-C-O	-5.46	115.07	121.46
2	L	6	PHE	CB-CA-C	-5.40	100.28	110.16
1	D	8	SER	CA-C-O	-5.39	113.67	120.84
1	I	199	GLU	CA-C-N	-5.39	111.83	122.02
1	I	199	GLU	C-N-CA	-5.39	111.83	122.02
1	D	301	LEU	N-CA-C	-5.38	106.88	113.50
1	I	62	ARG	N-CA-C	-5.38	105.46	112.23
1	A	247	VAL	N-CA-CB	-5.37	101.59	110.56
1	C	68	GLU	CB-CA-C	5.37	119.37	109.71
1	H	228	THR	CA-C-N	5.36	125.43	119.32
1	H	228	THR	C-N-CA	5.36	125.43	119.32
1	I	201	ILE	N-CA-C	-5.34	99.92	107.98
1	B	8	SER	CB-CA-C	-5.33	97.73	109.56
1	C	119	LEU	CA-C-N	5.32	130.56	122.37
1	C	119	LEU	C-N-CA	5.32	130.56	122.37
1	F	305	ASN	CA-C-O	-5.32	116.24	121.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	2	ALA	CA-C-O	-5.31	111.77	120.80
1	B	52	TRP	CA-C-O	5.30	127.10	121.05
1	E	52	TRP	N-CA-CB	-5.30	102.13	110.30
1	C	66	LYS	CA-CB-CG	5.30	124.70	114.10
1	D	10	PHE	N-CA-C	-5.29	104.76	111.11
1	H	62	ARG	CB-CA-C	-5.29	99.59	110.38
2	L	7	THR	CA-C-N	-5.27	113.51	121.05
2	L	7	THR	C-N-CA	-5.27	113.51	121.05
1	G	225	ALA	CB-CA-C	-5.26	99.27	109.68
1	D	232	TRP	N-CA-C	-5.24	102.58	110.70
1	B	51	ASP	O-C-N	5.23	130.15	123.24
1	C	157	PHE	CB-CA-C	5.23	118.98	109.62
1	D	72	PRO	CB-CG-CD	-5.22	89.41	106.10
1	D	317	LYS	CA-C-O	-5.21	115.01	121.06
1	F	308	PHE	CA-CB-CG	5.21	119.02	113.80
2	N	36	PRO	N-CD-CG	-5.21	95.38	103.20
1	I	72	PRO	CA-C-O	-5.21	114.24	121.90
1	G	225	ALA	CA-C-O	-5.21	114.14	120.54
1	A	244	THR	N-CA-C	-5.20	99.72	110.80
2	J	3	TYR	CA-C-N	-5.20	113.31	123.13
2	J	3	TYR	C-N-CA	-5.20	113.31	123.13
2	L	13	GLU	N-CA-CB	-5.20	102.19	110.03
1	C	75	VAL	N-CA-CB	-5.17	104.22	111.25
1	D	232	TRP	N-CA-CB	-5.14	102.37	110.49
1	B	307	ILE	N-CA-CB	-5.14	102.75	111.23
2	O	4	GLN	N-CA-CB	-5.14	102.98	110.53
1	C	288	ASN	N-CA-C	-5.12	106.34	112.59
2	K	122	PRO	CB-CG-CD	-5.12	89.71	106.10
1	C	17	GLY	CA-C-O	-5.12	115.97	121.35
1	G	327	GLU	CA-C-O	-5.12	115.43	120.70
1	A	244	THR	N-CA-CB	5.12	119.14	110.49
1	E	56	LEU	CB-CG-CD1	-5.12	95.35	110.70
2	O	79	TYR	N-CA-C	-5.12	107.04	113.28
1	D	9	ARG	N-CA-CB	5.11	119.13	110.49
1	D	240	ARG	CA-C-N	-5.10	115.22	122.41
1	D	240	ARG	C-N-CA	-5.10	115.22	122.41
1	G	282	ASP	CA-C-N	-5.07	116.23	123.08
1	G	282	ASP	C-N-CA	-5.07	116.23	123.08
1	I	65	ARG	N-CA-CB	-5.07	101.92	110.49
1	E	336	ASP	CA-CB-CG	5.07	117.67	112.60
2	M	123	THR	N-CA-C	-5.07	100.19	108.76
1	C	64	SER	N-CA-C	-5.05	97.70	107.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	61	ASP	CA-CB-CG	5.04	117.64	112.60
1	G	197	ASN	N-CA-C	-5.04	107.30	113.50
1	I	365	ASP	CA-CB-CG	5.04	117.64	112.60
1	F	35	PHE	CA-CB-CG	5.03	118.83	113.80
1	H	307	ILE	CA-C-N	5.03	130.09	123.05
1	H	307	ILE	C-N-CA	5.03	130.09	123.05
1	H	327	GLU	CA-C-O	-5.03	114.66	120.24
1	F	6	GLU	CA-C-O	-5.02	115.73	121.00
1	D	231	ALA	CA-C-O	-5.01	113.88	119.95
1	B	253	ARG	CA-C-O	-5.01	114.12	120.28

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	THR	Mainchain
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

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	67	0
1	B	2894	0	2824	71	0
1	C	2878	0	2799	68	0
1	D	2856	0	2747	64	0
1	E	2876	0	2797	76	0
1	F	2908	0	2849	69	0
1	G	2902	0	2829	51	0
1	H	2909	0	2856	41	0
1	I	2788	0	2701	43	0
2	J	926	0	913	24	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
2	P	928	0	913	21	0
2	Q	944	0	940	7	0
2	R	944	0	940	23	0
3	S	961	0	905	14	0
All	All	35315	0	34529	620	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 (620) 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	1.04
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
1:I:68:GLU:O	1:I:69:THR:C	2.15	0.83
2:R:2:ALA:O	2:R:3:TYR:C	2.21	0.83
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:D:8:SER:O	1:D:10:PHE:N	2.15	0.79
1:G:7:LYS:O	1:G:8:SER:C	2.18	0.77
1:G:229:PRO:O	1:G:230:LEU:C	2.25	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:2:ALA:CB	2:P:5:GLY:HA3	2.16	0.76
1:E:186:MET:HG2	1:E:300:MET:HE1	1.67	0.75
1:C:122:ILE:O	1:C:123:ARG:C	2.25	0.75
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:D:184:MET:HE1	1:E:207:ARG:HE	1.54	0.72
2:O:124:GLY:O	2:O:125:LEU:C	2.32	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: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:G:296:PRO:HB3	1:G:300:MET:HE2	1.73	0.71
1:C:66:LYS:O	1:C:67:ALA:HB2	1.91	0.70
1:I:186:MET:HE2	1:I:201:ILE:HG23	1.73	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
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:A:296:PRO:HB3	1:A:300:MET:HE2	1.75	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:305:ASN:O	1:B:306:ASN:C	2.38	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:A:139:LYS:NZ	1:A:278:LEU:O	2.25	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
1:G:8:SER:C	1:G:10:PHE:N	2.56	0.63
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:B:307:ILE:HG13	1:B:353:CYS:SG	2.40	0.62
1:E:184:MET:HE1	1:F:207:ARG:HD3	1.82	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:G:8:SER:O	1:G:9:ARG:C	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:29:ILE:HG13	1:C:135:MET:HG2	1.83	0.60
1:C:296:PRO:HB3	1:C:300:MET:HE2	1.83	0.60
1:C:317:LYS:HE2	1:C:346:HIS:HE1	1.65	0.60
1:G:227:GLN:C	1:G:229:PRO:N	2.55	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:B:336:ASP:O	1:B:337:ARG:C	2.44	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:I:191:LYS:C	1:I:193:GLY:H	2.10	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:C:286:ASP:C	1:C:288:ASN:H	2.11	0.59
1:B:62:ARG:HG2	2:P:84:LYS:HB2	1.84	0.58
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:D:186:MET:HE2	1:D:201:ILE:HG21	1.84	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:G:186:MET:HG3	1:G:300:MET:HE1	1.85	0.57
1:D:307:ILE:HG23	1:D:353:CYS:SG	2.44	0.57
1:H:296:PRO:HB3	1:H:300:MET:HE2	1.87	0.57
2:O:91:ASP:OD2	2:O:91:ASP:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:8:SER:C	1:D:10:PHE:N	2.63	0.57
1:A:51:ASP:HB3	1:B:21:SER:HB2	1.86	0.56
1:H:83:MET:HE1	1:H:133:LEU:HD22	1.87	0.56
1:D:68:GLU:HB2	1:E:271:LYS:HZ1	1.66	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:I:294:ALA:HB3	1:I:360:VAL:HG23	1.88	0.56
1:G:337:ARG:O	1:G:338:ASP:C	2.49	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:8:SER:C	1:G:10:PHE:H	2.15	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:C:65:ARG:C	1:C:66:LYS:HG2	2.32	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:D:199:GLU:OE1	1:E:238:SER:OG	2.24	0.55
2:O:78:SER:OG	2:O:79:TYR:N	2.38	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:22:GLU:OE2	2:N:30:SER:OG	2.24	0.54
1:D:244:THR:O	1:D:245:ASP:C	2.50	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: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:D:153:LEU:C	1:D:155:LYS:H	2.15	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:D:68:GLU:HB2	1:E:271:LYS:HZ3	1.70	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:H:304:ALA:O	1:H:305:ASN:HB2	2.06	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
1:D:175:ILE:HD12	1:D:219:ILE:HD11	1.90	0.53
1:B:340:GLY:C	1:B:341:ILE:HD13	2.34	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:B:53:ASP:O	1:B:54:ILE:C	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:8:SER:C	1:D:10:PHE:H	2.16	0.51
1:I:197:ASN:O	1:I:198:GLY:C	2.52	0.51
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: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:70:SER:HB2	1:H:121:LYS:HE2	1.93	0.51
1:G:229:PRO:C	1:G:231:ALA:N	2.63	0.51
1:I:300:MET:HE2	1:I:300:MET:HA	1.92	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
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
1:F:184:MET:HA	1:F:184:MET:HE2	1.93	0.51
2:P:2:ALA:CB	2:P:5:GLY:CA	2.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:58:GLY:C	2:J:60:GLU:H	2.19	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:I:197:ASN:C	1:I:199:GLU:N	2.65	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: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:E:101:GLN:O	1:E:104:THR:HG22	2.12	0.49
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:MET:HE1	1:B:207:ARG:HG3	1.95	0.48
1:E:52:TRP:O	1:E:53:ASP:C	2.56	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: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:C:125:LYS:O	1:C:129:THR:OG1	2.24	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
1:I:191:LYS:C	1:I:193:GLY:N	2.69	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
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
2:J:2:ALA:O	2:J:3:TYR:C	2.57	0.47
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:A:241:THR:HG1	1:A:253:ARG:HE	1.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:J:56:ALA:O	2:J:57:ALA:C	2.59	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
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
2:K:48:LEU:HD11	2:K:67:CYS:HB2	1.98	0.46
1:F:186:MET:HG2	1:F:300:MET:HE1	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:4:ASN:CG	1:D:5:SER:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:R:13:GLU:OE1	2:R:72:TYR:OH	2.31	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
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
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
2:N:51:ASP:OD1	2:N:53:SER:OG	2.24	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:E:167:ASP:CG	1:E:366:ALA:HB2	2.41	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
2:M:119:ASP:CG	2:N:90:ARG:HH22	2.22	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:D:244:THR:C	1:D:245:ASP:O	2.60	0.45
1:F:171:PRO:HB3	1:F:217:PRO:HG2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:205:VAL:HG13	1:B:209:PHE:HB3	1.97	0.44
1:D:8:SER:O	1:D:9:ARG:C	2.60	0.44
1:E:241:THR:OG1	1:E:242:GLY:N	2.50	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:J:101:GLU:O	2:J:102:SER:C	2.61	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:E:155:LYS:HZ2	1:E:155:LYS:HG2	1.67	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:I:83:MET:HE1	1:I:142:VAL:HG12	2.00	0.44
1:C:286:ASP:C	1:C:288:ASN:N	2.75	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: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
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:A:199:GLU:OE2	1:B:238:SER:OG	2.25	0.43
1:E:159:VAL:HG21	1:E:356:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:52:TRP:C	1:E:52:TRP:CD1	2.95	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
1:A:219:ILE:H	1:A:219:ILE:HG12	1.66	0.43
1:E:54:ILE:O	1:F:121:LYS:NZ	2.40	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
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:A:248:GLN:NE2	1:F:184:MET:HE1	2.35	0.42
1:D:153:LEU:C	1:D:155:LYS:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:84:TYR:OH	1:I:346:HIS:ND1	2.52	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:184:MET:HE3	1:I:184:MET:HB3	1.95	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:D:212:LYS:HZ2	1:D:212:LYS:HG2	1.79	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: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:9:ARG:O	1:D:10:PHE:C	2.63	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:B:186:MET:HB3	1:B:300:MET:HE1	2.03	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
1:E:317:LYS:HE3	1:E:346:HIS:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:312:TYR:CE1	1:F:349:MET:HB3	2.56	0.41
2:J:51:ASP:OD2	2:J:51:ASP:C	2.63	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
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:16:THR:O	1:F:16:THR:OG1	2.39	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: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:J:17:ASP:OD1	2:J:17:ASP:C	2.65	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
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%)	36	67
1	B	364/367 (99%)	347 (95%)	16 (4%)	1 (0%)	36	67
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	47
1	F	364/367 (99%)	350 (96%)	14 (4%)	0	100	100
1	G	364/367 (99%)	347 (95%)	13 (4%)	4 (1%)	11	39
1	H	364/367 (99%)	358 (98%)	5 (1%)	1 (0%)	36	67
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	47
2	K	122/125 (98%)	118 (97%)	3 (2%)	1 (1%)	16	47
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%)	7	30
2	O	122/125 (98%)	119 (98%)	3 (2%)	0	100	100
2	P	122/125 (98%)	118 (97%)	3 (2%)	1 (1%)	16	47
2	Q	122/125 (98%)	117 (96%)	5 (4%)	0	100	100
2	R	122/125 (98%)	117 (96%)	4 (3%)	1 (1%)	16	47
3	S	118/372 (32%)	111 (94%)	6 (5%)	1 (1%)	16	47
All	All	4478/4800 (93%)	4252 (95%)	188 (4%)	38 (1%)	18	47

All (38) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	309 (98%)	5 (2%)	55	75
1	B	310/317 (98%)	303 (98%)	7 (2%)	44	70
1	C	305/317 (96%)	292 (96%)	13 (4%)	26	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	300/317 (95%)	283 (94%)	17 (6%)	18	49
1	E	305/317 (96%)	294 (96%)	11 (4%)	31	62
1	F	313/317 (99%)	306 (98%)	7 (2%)	45	71
1	G	311/317 (98%)	302 (97%)	9 (3%)	37	66
1	H	314/317 (99%)	307 (98%)	7 (2%)	45	71
1	I	295/317 (93%)	284 (96%)	11 (4%)	30	61
2	J	92/99 (93%)	91 (99%)	1 (1%)	65	78
2	K	96/99 (97%)	95 (99%)	1 (1%)	68	79
2	L	97/99 (98%)	96 (99%)	1 (1%)	68	79
2	M	95/99 (96%)	94 (99%)	1 (1%)	65	78
2	N	94/99 (95%)	89 (95%)	5 (5%)	20	51
2	O	95/99 (96%)	94 (99%)	1 (1%)	65	78
2	P	93/99 (94%)	93 (100%)	0	100	100
2	Q	97/99 (98%)	95 (98%)	2 (2%)	47	71
2	R	97/99 (98%)	96 (99%)	1 (1%)	68	79
3	S	100/307 (33%)	98 (98%)	2 (2%)	48	72
All	All	3723/4051 (92%)	3621 (97%)	102 (3%)	40	67

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	18	GLU
1	A	245	ASP
1	A	287	THR
1	A	318	MET
1	B	54	ILE
1	B	55	SER
1	B	57	LEU
1	B	202	HIS
1	B	224	LEU
1	B	306	ASN
1	B	307	ILE
1	C	14	ASP
1	C	15	LEU
1	C	20	GLN

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Mol	Chain	Res	Type
1	C	50	THR
1	C	55	SER
1	C	61	ASP
1	C	69	THR
1	C	70	SER
1	C	72	PRO
1	C	120	MET
1	C	125	LYS
1	C	155	LYS
1	C	285	SER
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	229	PRO
1	D	234	GLN
1	D	236	THR
1	D	238	SER
1	D	239	LEU
1	D	244	THR
1	D	307	ILE
1	E	4	ASN
1	E	6	GLU
1	E	50	THR
1	E	51	ASP
1	E	52	TRP
1	E	55	SER
1	E	56	LEU
1	E	155	LYS
1	E	156	GLN
1	E	169	ASP
1	E	307	ILE
1	F	6	GLU
1	F	7	LYS
1	F	36	ARG
1	F	85	PHE

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Mol	Chain	Res	Type
1	F	267	LYS
1	F	305	ASN
1	F	328	LEU
1	G	5	SER
1	G	6	GLU
1	G	9	ARG
1	G	19	VAL
1	G	201	ILE
1	G	224	LEU
1	G	227	GLN
1	G	228	THR
1	G	336	ASP
1	H	61	ASP
1	H	227	GLN
1	H	228	THR
1	H	248	GLN
1	H	303	GLU
1	H	306	ASN
1	H	317	LYS
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	281	ILE
2	J	75	LEU
2	K	122	PRO
2	L	12	ARG
2	M	104	VAL
2	N	4	GLN
2	N	36	PRO
2	N	37	VAL
2	N	101	GLU
2	N	104	VAL
2	O	79	TYR
2	Q	6	PHE
2	Q	12	ARG

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Mol	Chain	Res	Type
2	R	6	PHE
3	S	49	ASP
3	S	55	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	276	HIS
1	B	202	HIS
1	C	42	GLN
1	C	276	HIS
1	C	346	HIS
1	D	265	ASN
1	E	24	ASN
1	E	216	HIS
1	E	288	ASN
1	E	322	ASN
1	F	227	GLN
1	F	250	HIS
1	F	263	GLN
1	F	265	ASN
1	G	24	ASN
1	G	77	GLN
1	G	136	GLN
1	G	226	GLN
1	H	42	GLN
1	H	77	GLN
1	H	136	GLN
1	H	226	GLN
1	H	227	GLN
1	H	248	GLN
1	H	252	ASN
1	H	276	HIS
1	H	305	ASN
1	H	306	ASN
1	H	346	HIS
1	I	24	ASN
1	I	97	GLN
1	I	101	GLN
1	I	248	GLN
1	I	305	ASN

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Mol	Chain	Res	Type
2	K	29	HIS
2	K	82	GLN
2	L	62	GLN
2	L	82	GLN
2	N	4	GLN
2	O	16	ASN
2	P	62	GLN
2	Q	82	GLN
3	S	33	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

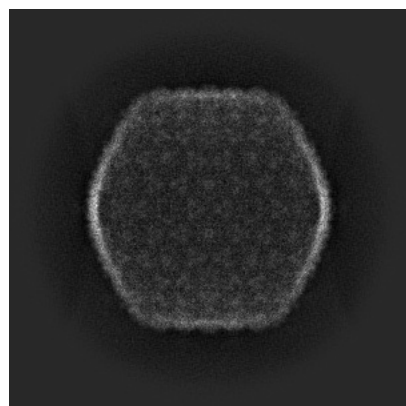
6 Map visualisation [i](#)

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

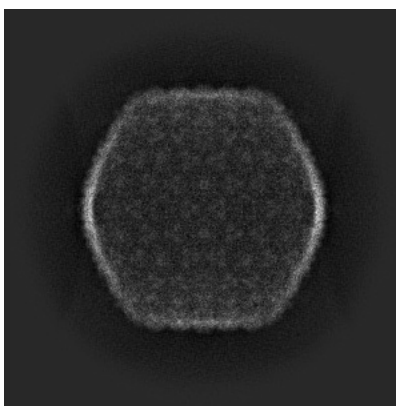
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

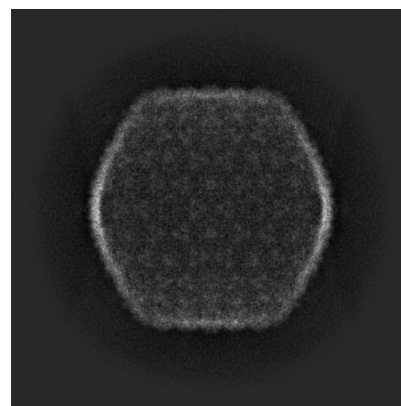
6.1.1 Primary map



X

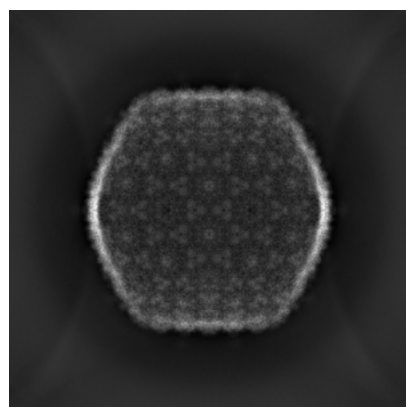


Y

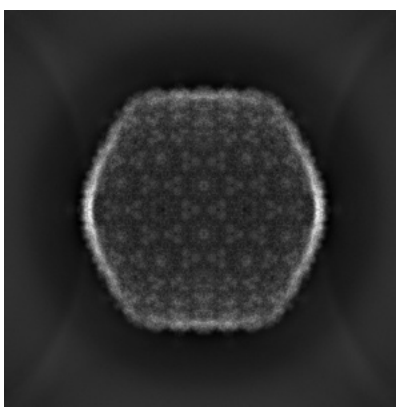


Z

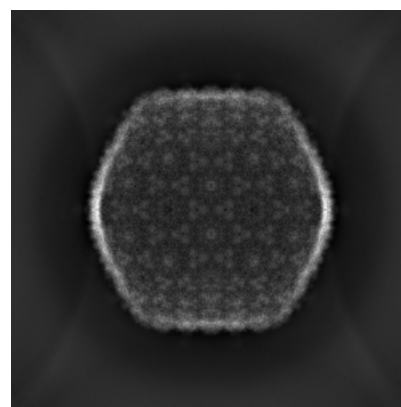
6.1.2 Raw map



X



Y

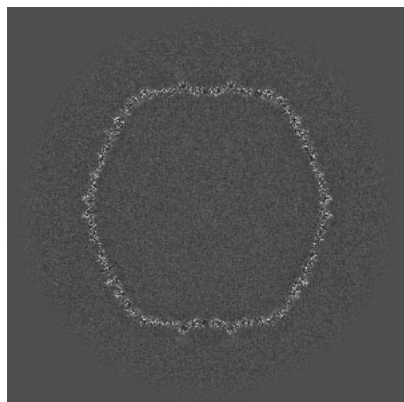


Z

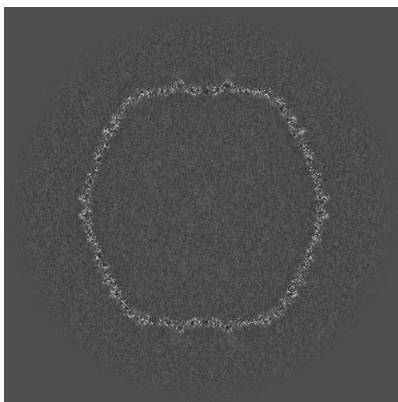
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

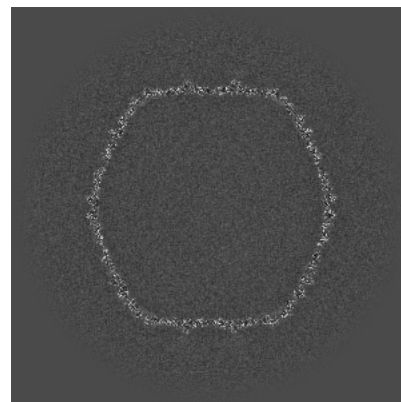
6.2.1 Primary map



X Index: 500



Y Index: 500



Z Index: 500

6.2.2 Raw map



X Index: 500



Y Index: 500

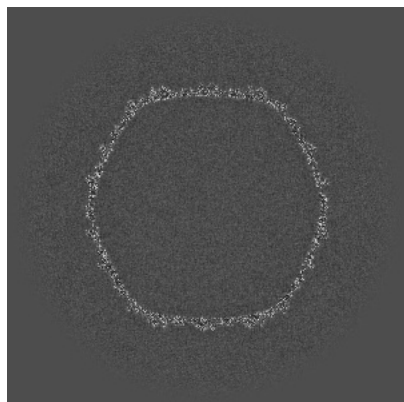


Z Index: 500

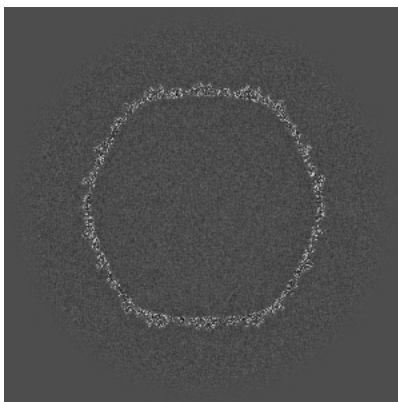
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

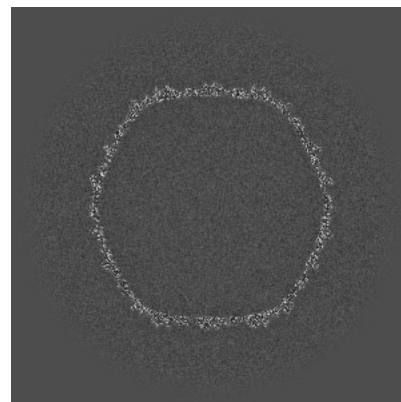
6.3.1 Primary map



X Index: 547

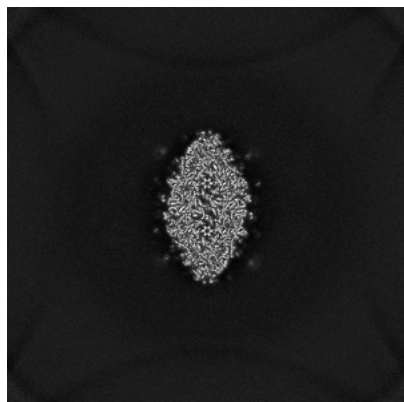


Y Index: 453

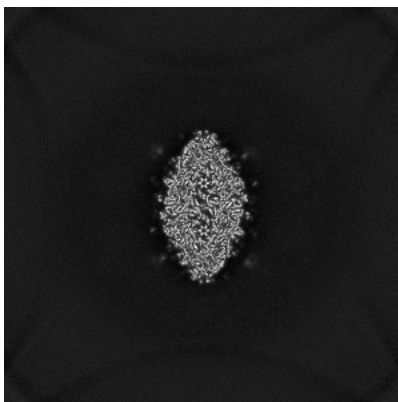


Z Index: 546

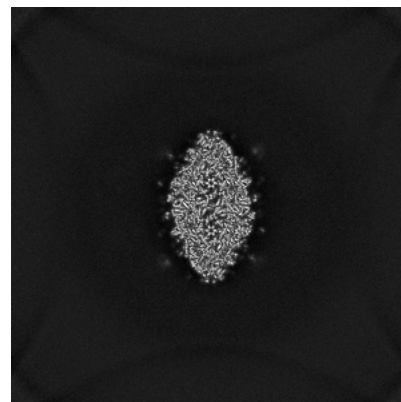
6.3.2 Raw map



X Index: 218



Y Index: 218

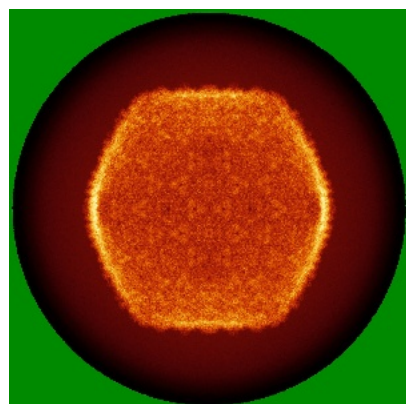


Z Index: 781

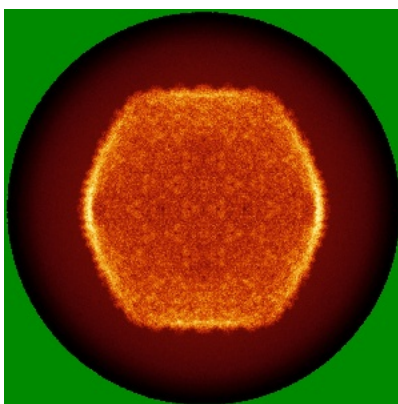
The images above show the largest variance slices of the map in three orthogonal directions.

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

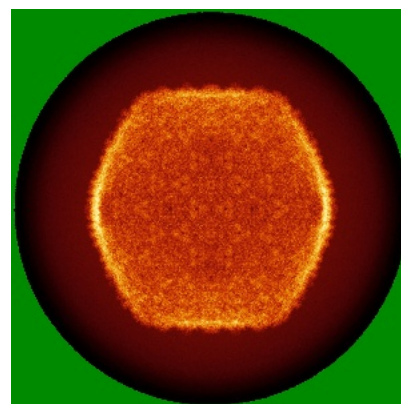
6.4.1 Primary map



X

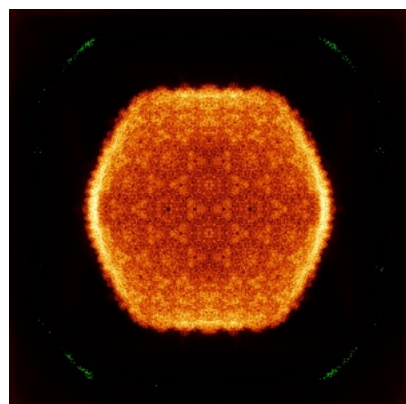


Y

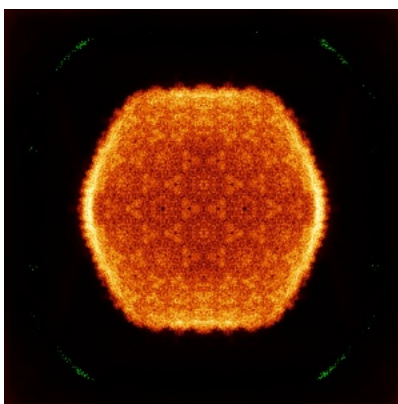


Z

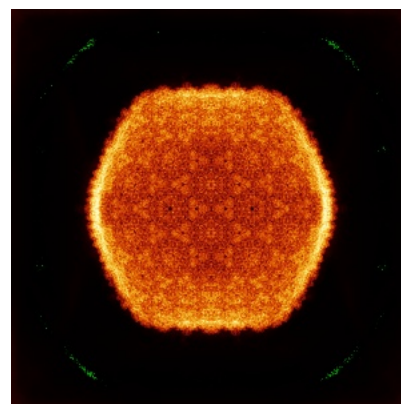
6.4.2 Raw map



X



Y

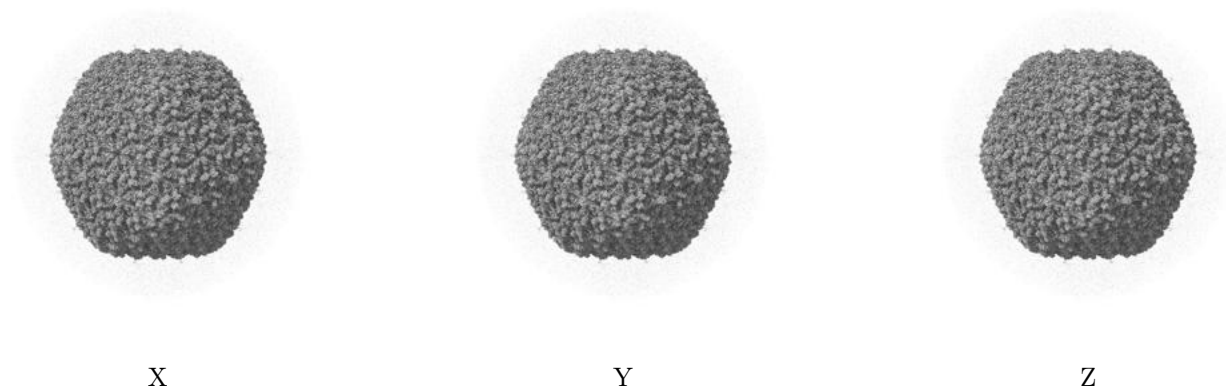


Z

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.

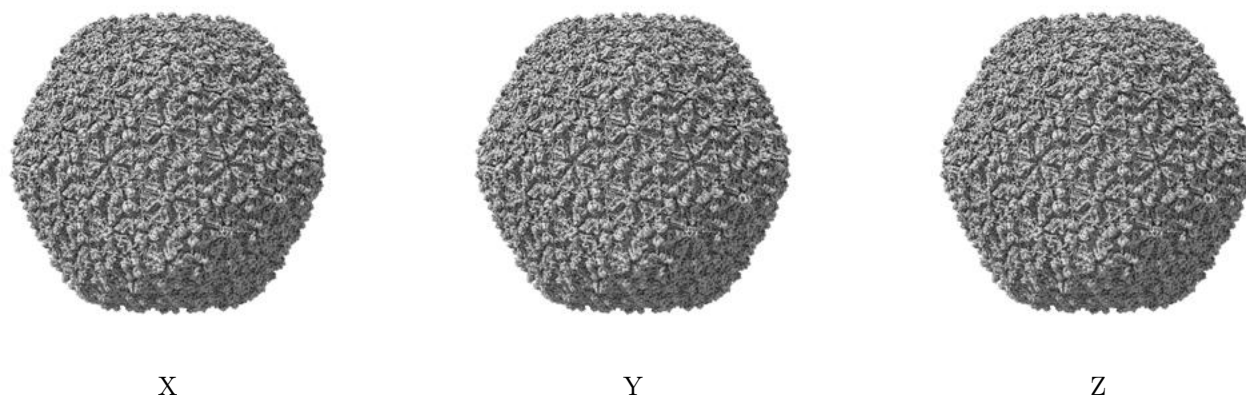
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

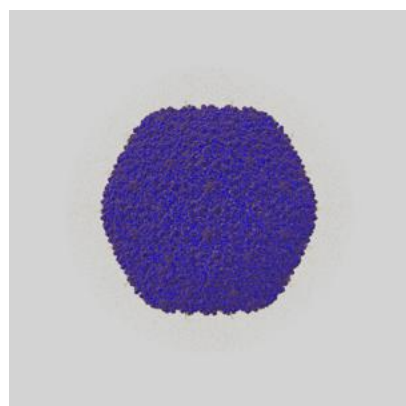
6.6 Mask visualisation [i](#)

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

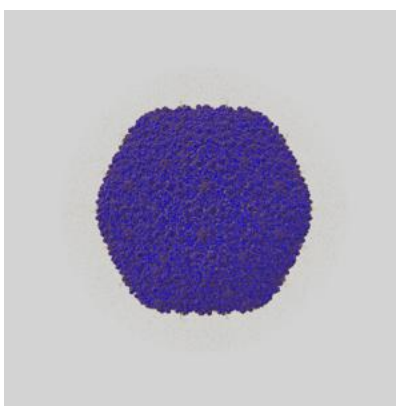
A mask typically either:

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

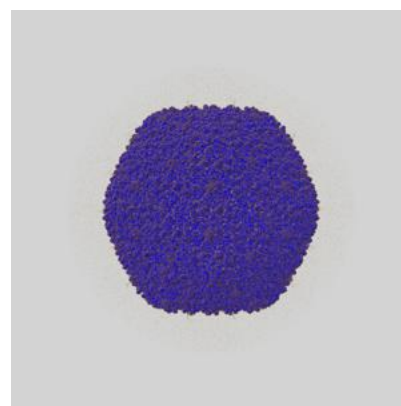
6.6.1 emd_45163_msk_1.map [i](#)



X



Y

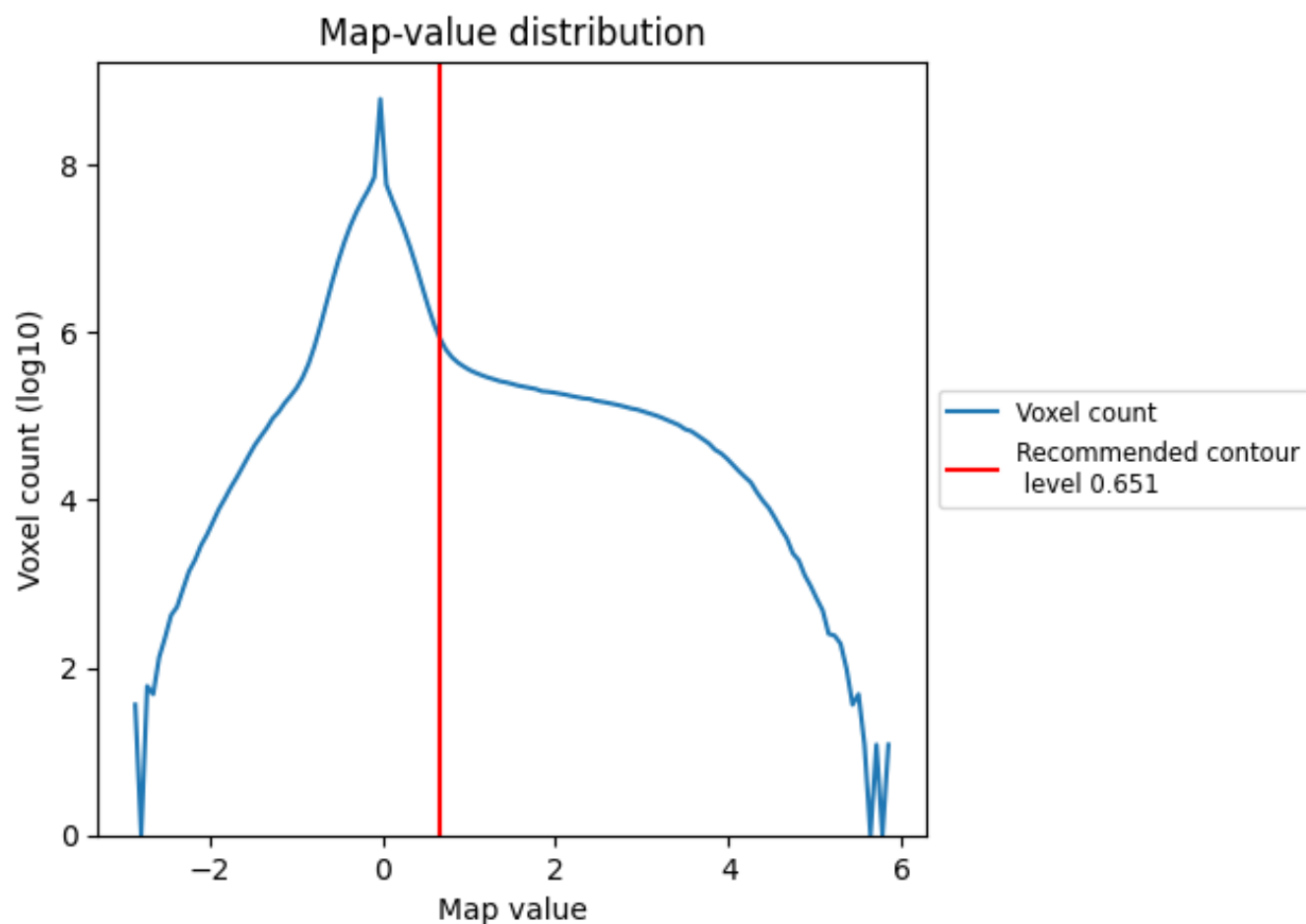


Z

7 Map analysis [i](#)

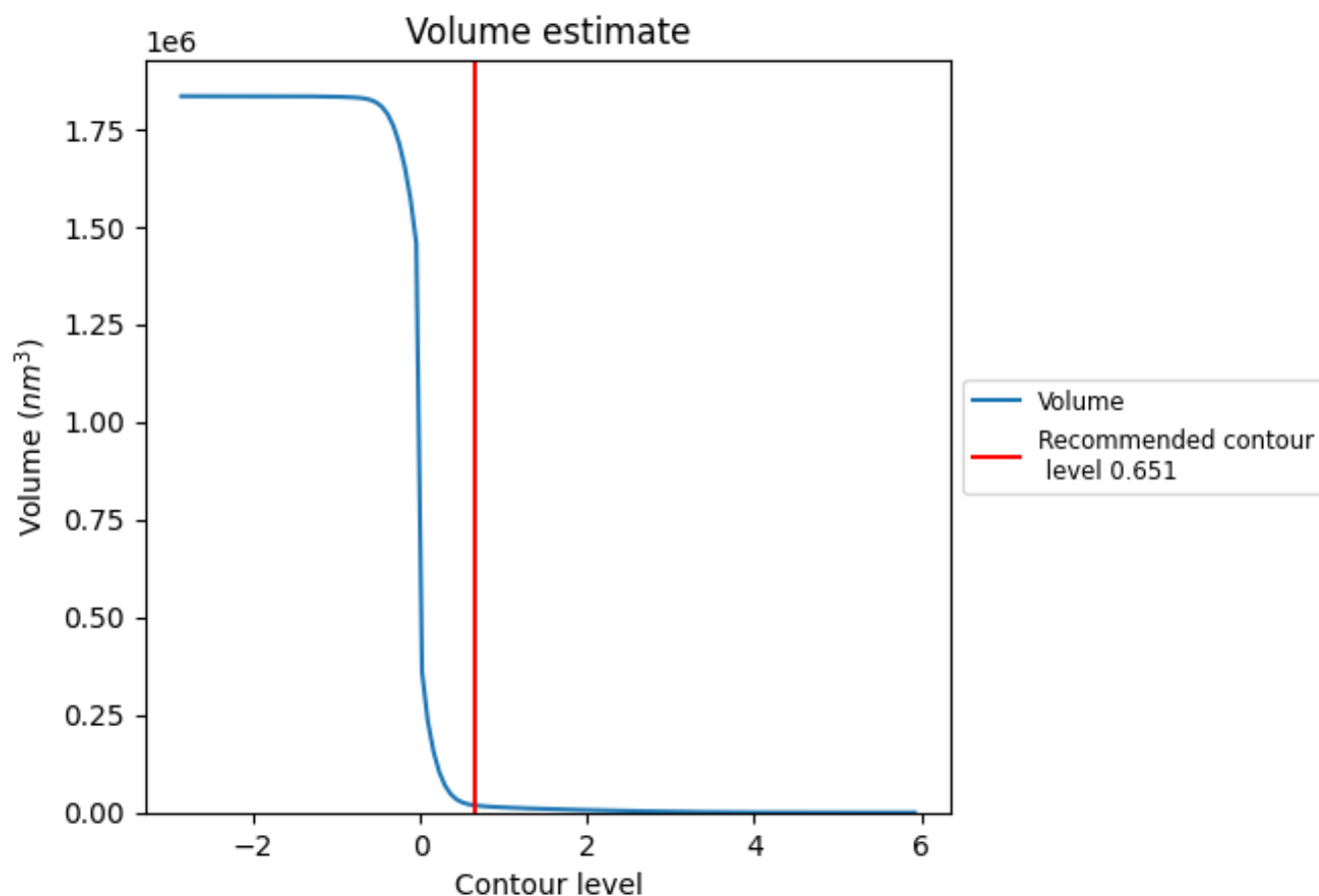
This section contains the results of statistical analysis of the map.

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.

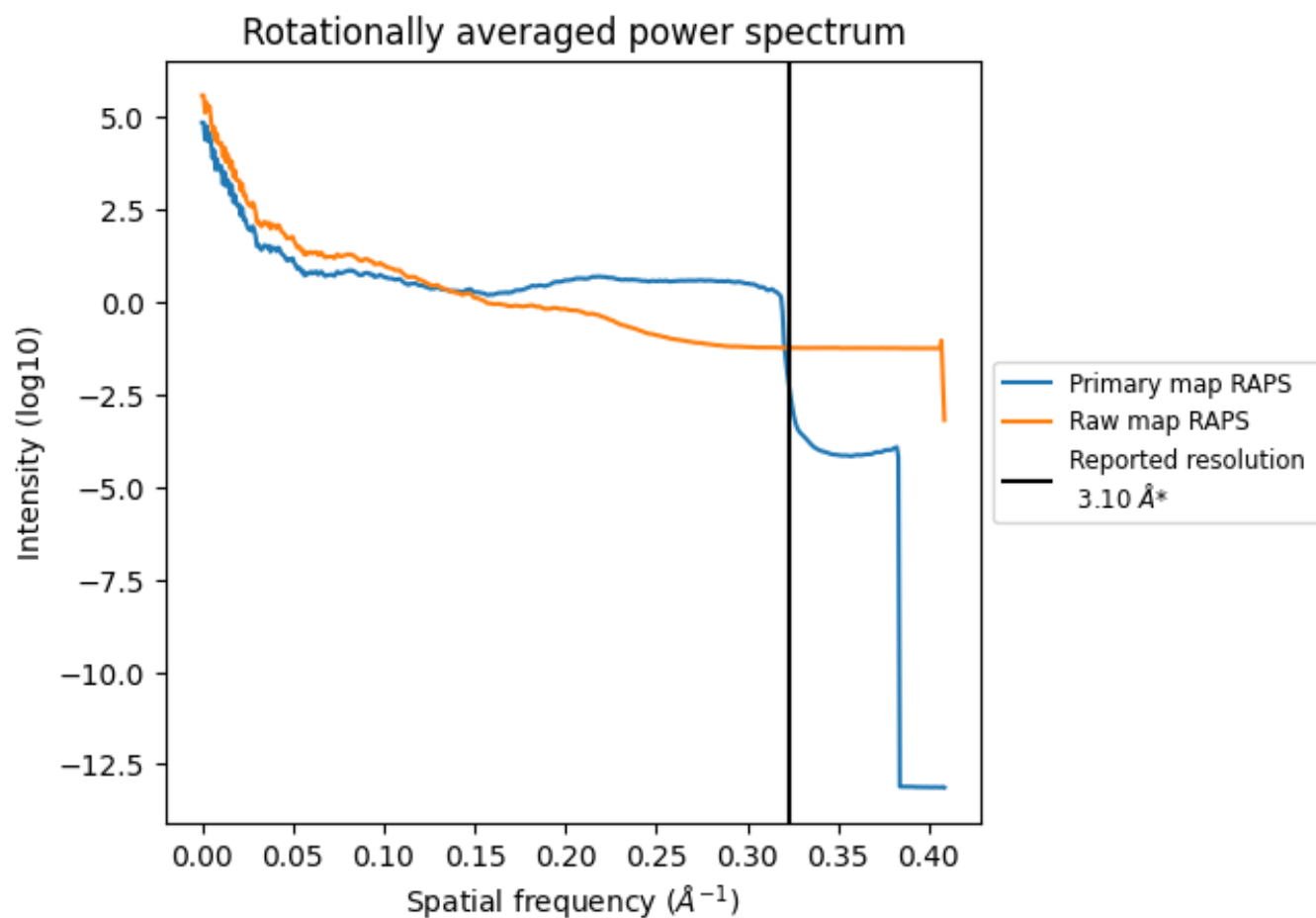
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 18437 nm³; 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 ⓘ

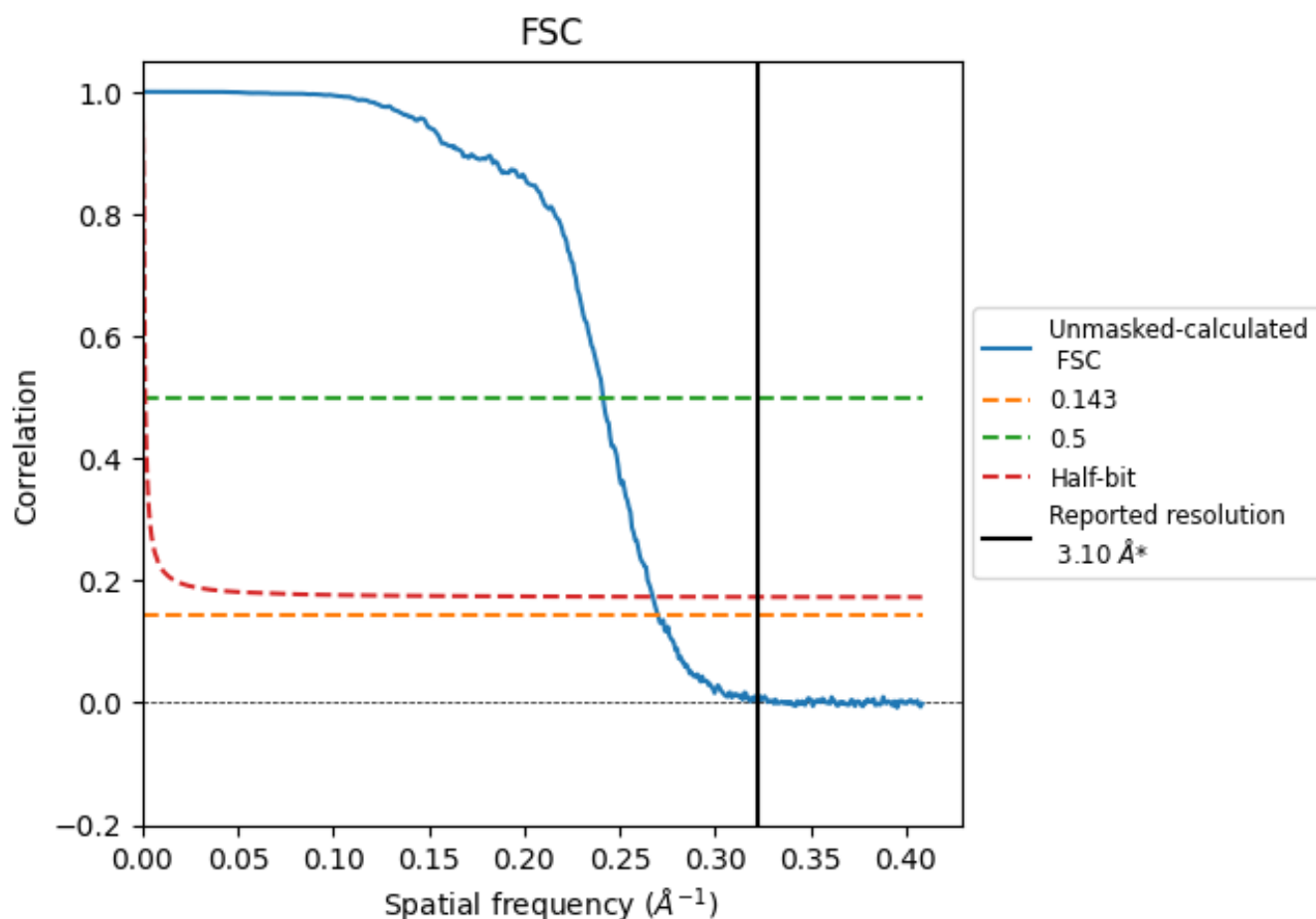


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	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 [i](#)

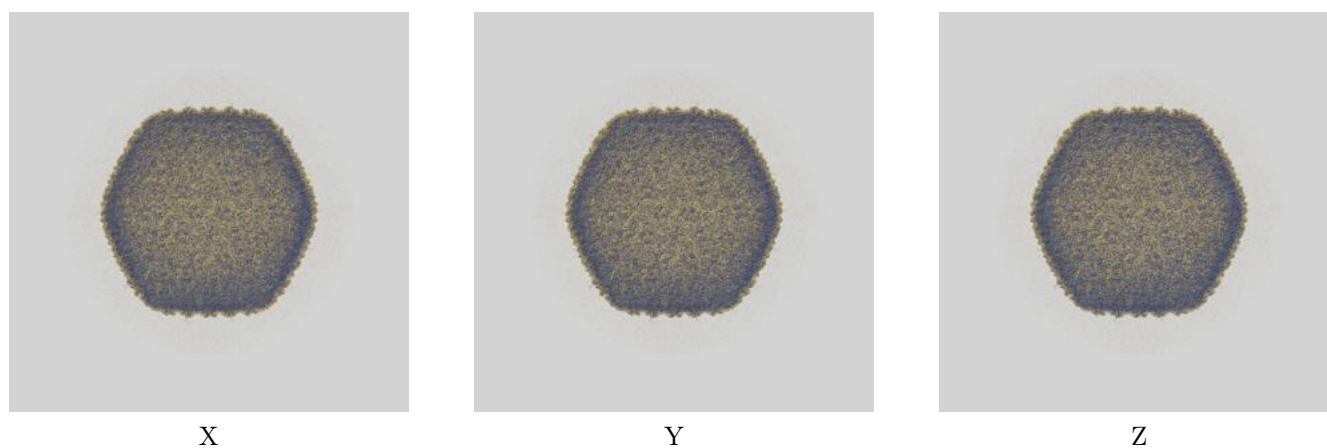
This section contains information regarding the fit between EMDB map EMD-45163 and PDB model 9C3A. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)



9.1.2 Map-model assembly overlay [i](#)



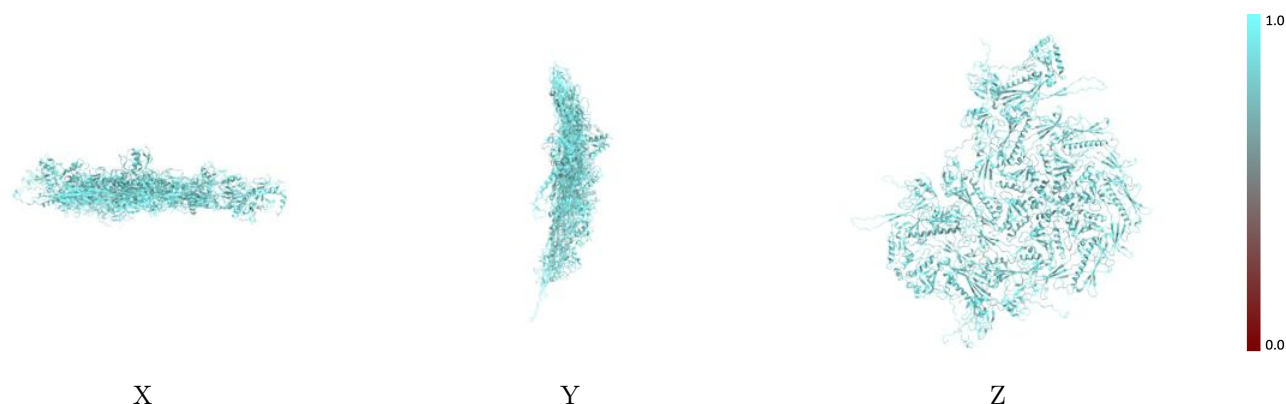
The images above show the 3D surface view of the map at the recommended contour level 0.651 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



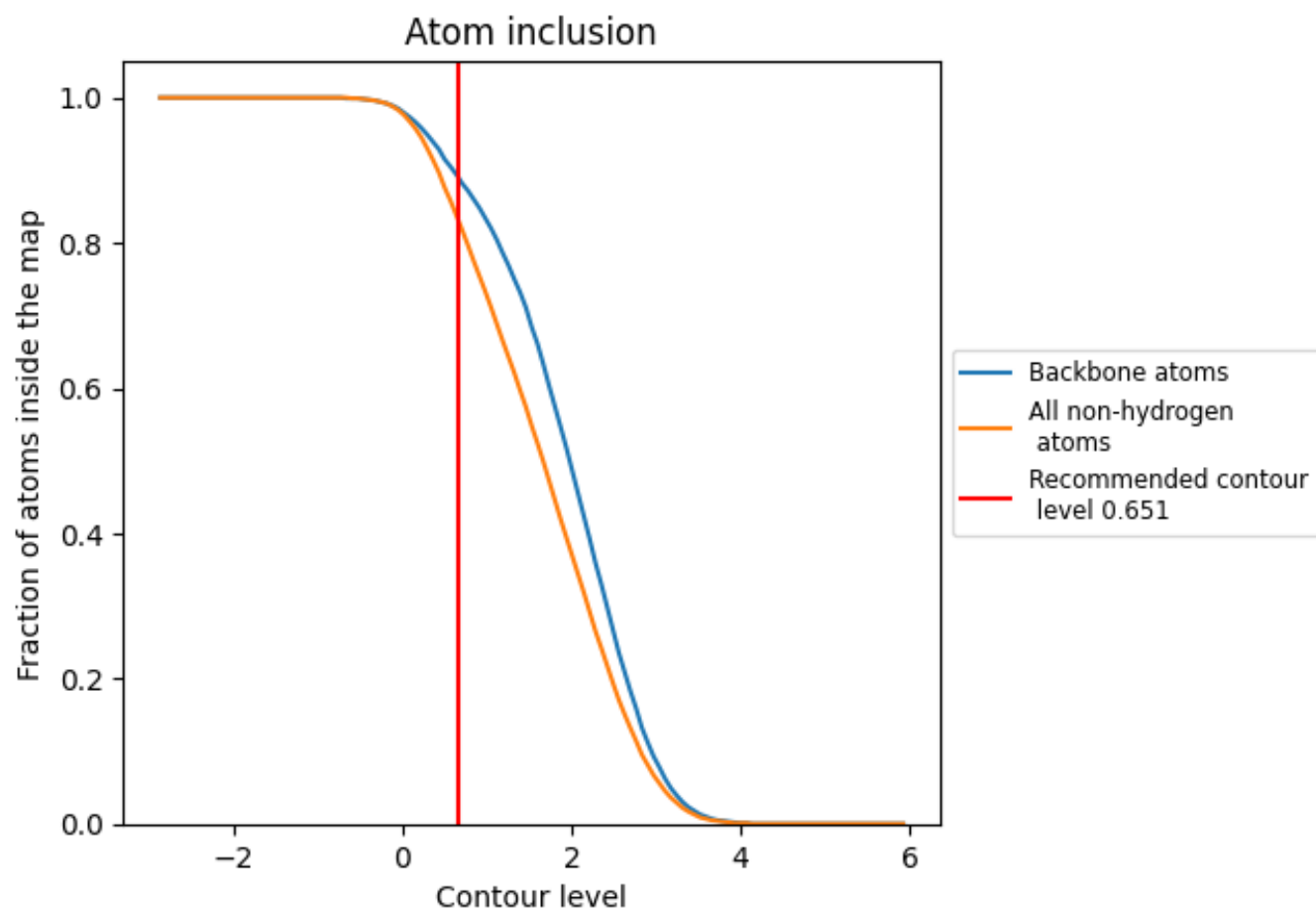
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [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 (0.651).

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

