



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:00 AM UTC

PDB ID : 7LGH / pdb_00007lgh
EMDB ID : EMD-23324
Title : Asymmetric unit for phage Qbeta small prolate particle
Authors : Chang, J.Y.; Zhang, J.
Deposited on : 2021-01-20
Resolution : 8.90 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:

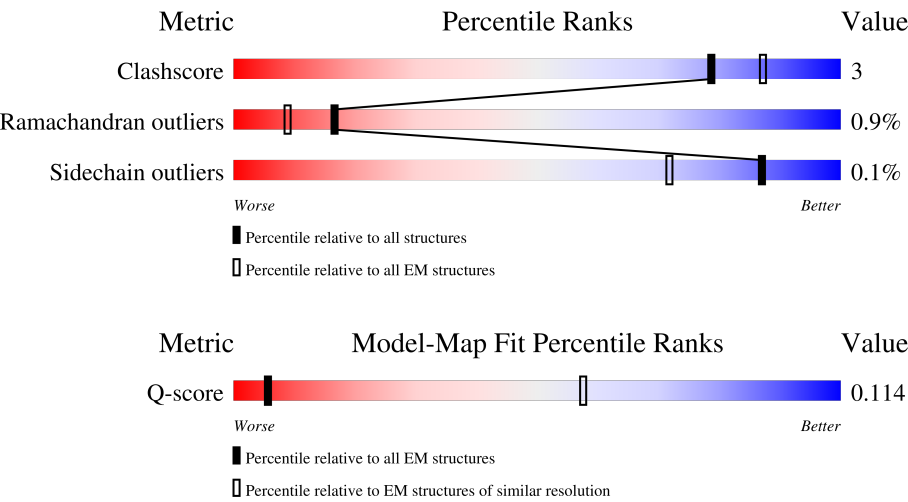
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 8.90 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	258 (8.40 - 9.40)

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	133	6% 87% 11% ..
1	B	133	10% 85% 14% ..
1	C	133	8% 79% 16% ...
1	D	133	78% 17% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	133	
1	F	133	
1	G	133	
1	H	133	
1	I	133	
1	J	133	
1	K	133	
1	L	133	
1	M	133	
1	N	133	
1	O	133	
1	P	133	
1	Q	133	
1	R	133	
1	S	133	
1	T	133	
1	U	133	
1	V	133	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 21846 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	B	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	C	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	L	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	D	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	M	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	E	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	N	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	F	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	O	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	G	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	P	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	H	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	Q	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	R	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	I	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	S	132	Total 993	C 616	N 177	O 198	S 2	0	0

Continued on next page...

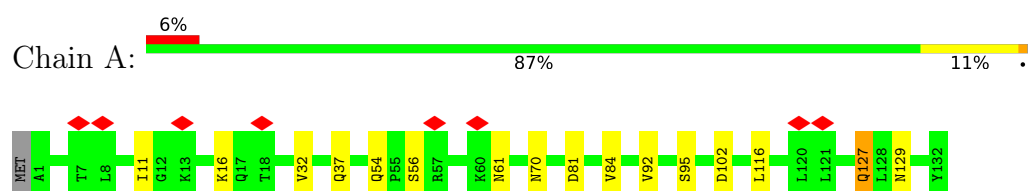
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	T	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	U	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	K	132	Total 993	C 616	N 177	O 198	S 2	0	0
1	V	132	Total 993	C 616	N 177	O 198	S 2	0	0

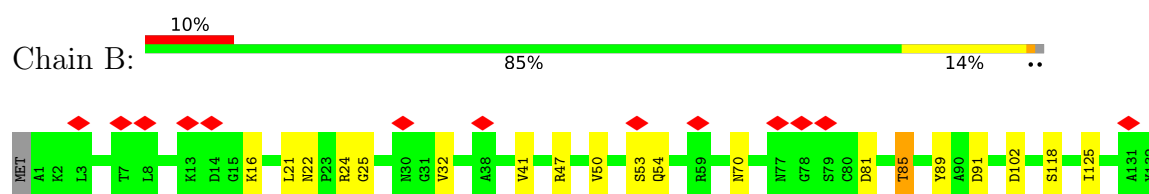
3 Residue-property plots [i](#)

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.

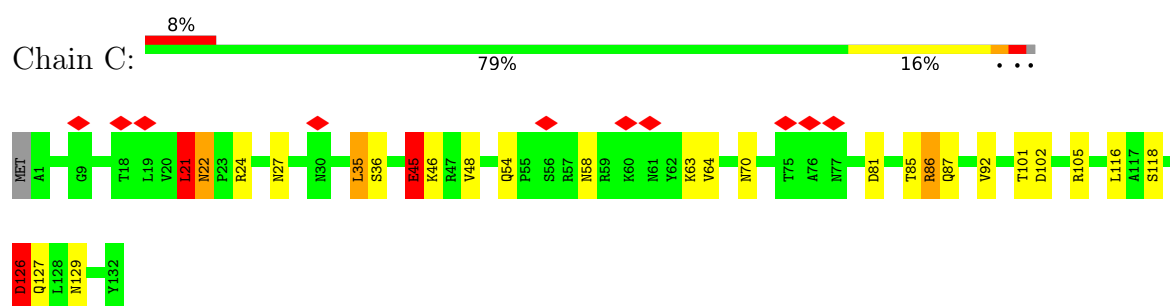
- Molecule 1: Capsid protein



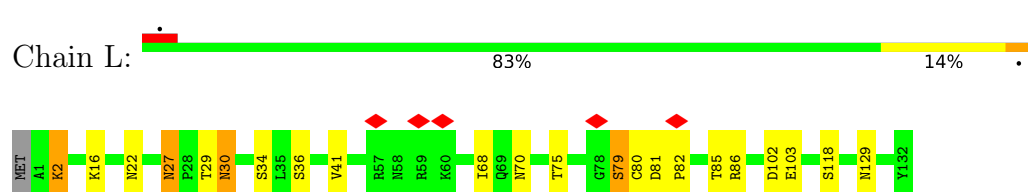
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

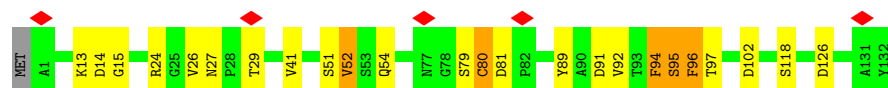
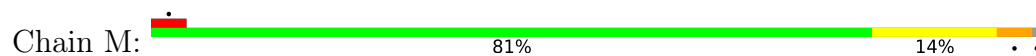


- Molecule 1: Capsid protein

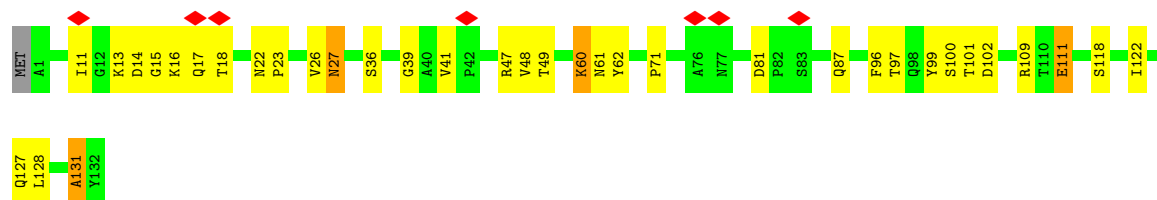




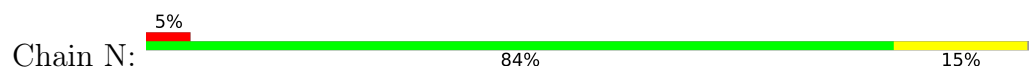
- Molecule 1: Capsid protein



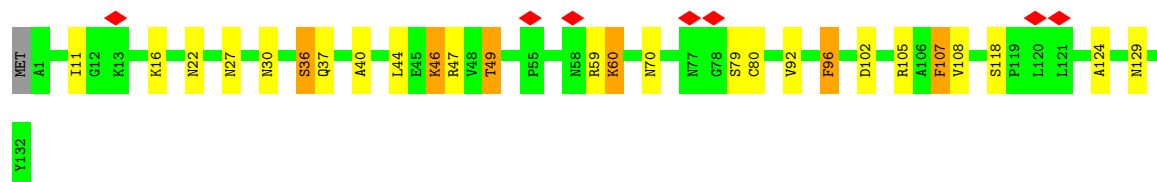
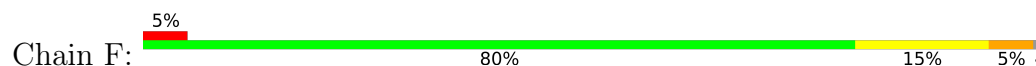
- Molecule 1: Capsid protein



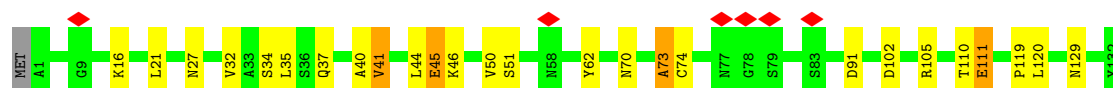
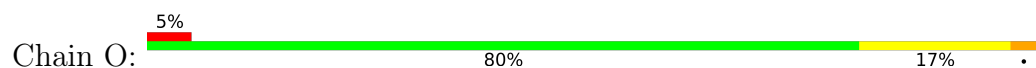
- Molecule 1: Capsid protein



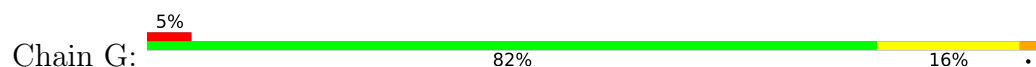
- Molecule 1: Capsid protein

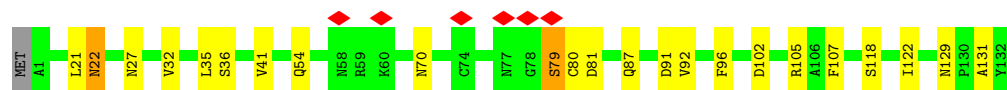


- Molecule 1: Capsid protein

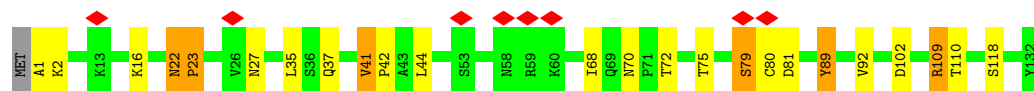
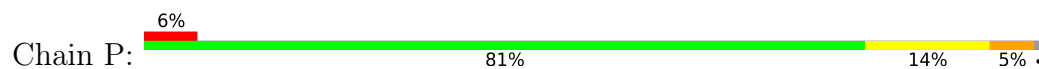


- Molecule 1: Capsid protein

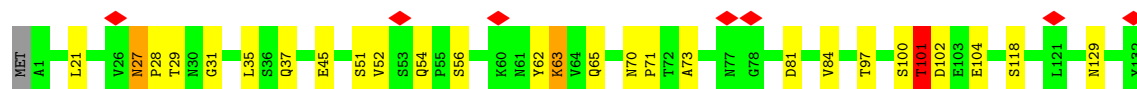
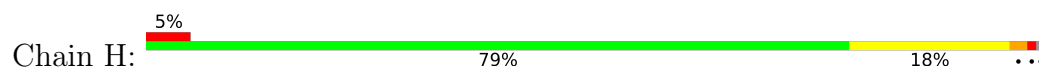




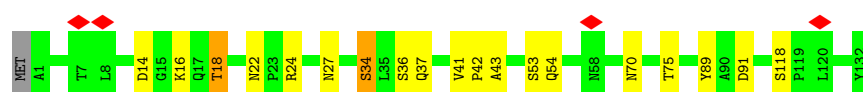
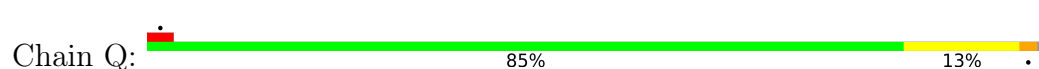
- Molecule 1: Capsid protein



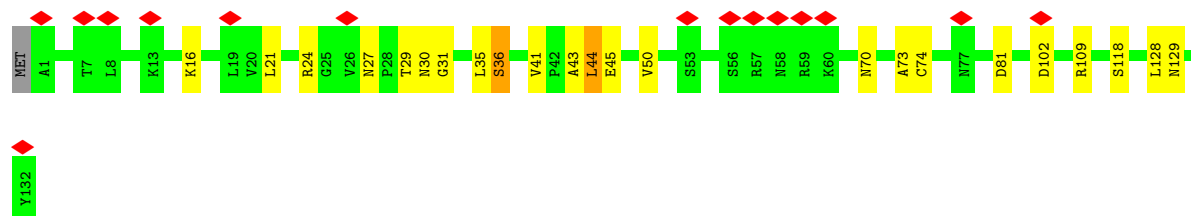
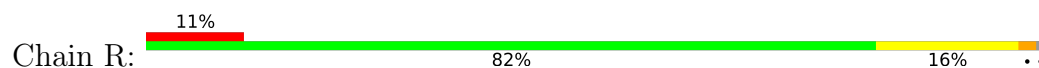
- Molecule 1: Capsid protein



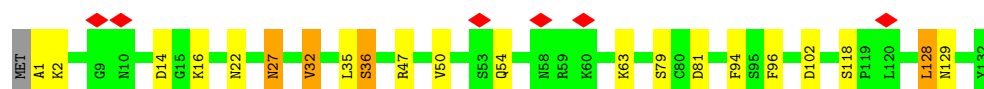
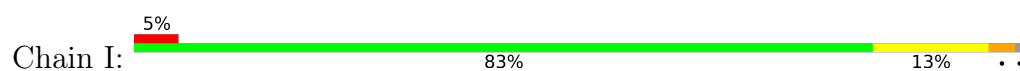
- Molecule 1: Capsid protein



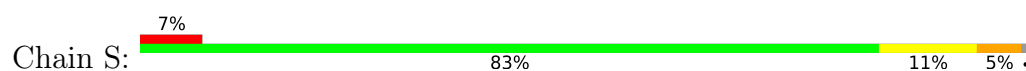
- Molecule 1: Capsid protein

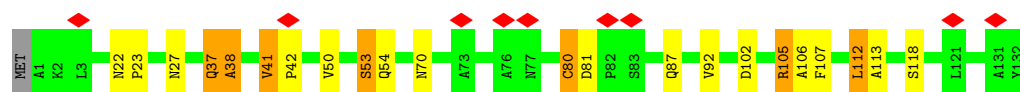


- Molecule 1: Capsid protein

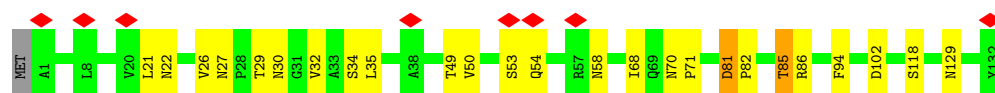
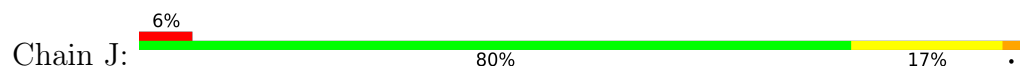


- Molecule 1: Capsid protein

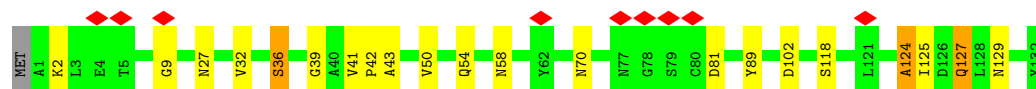
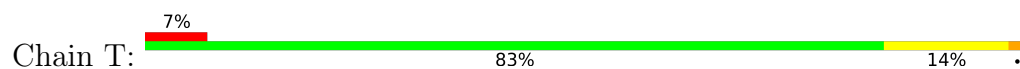




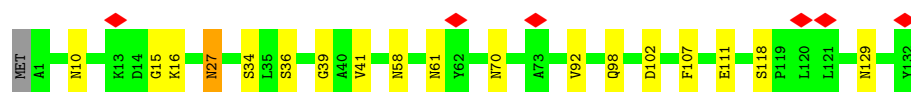
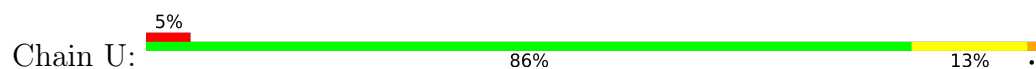
- Molecule 1: Capsid protein



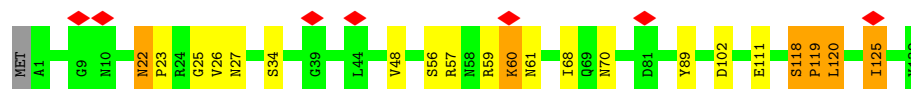
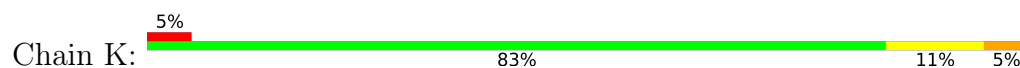
- Molecule 1: Capsid protein



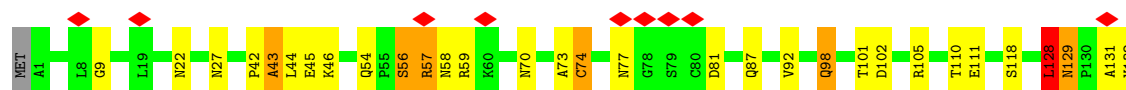
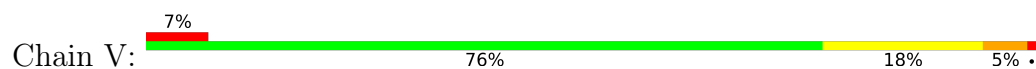
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6842	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC, FEI TECNAI F20	Depositor
Voltage (kV)	300, 200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30, 30	Depositor
Minimum defocus (nm)	Not provided, Not provided	Depositor
Maximum defocus (nm)	Not provided, Not provided	Depositor
Magnification	Not provided, Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	400.0, 400.0, 400.0	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.5, 2.5, 2.5	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	1.02	0/1007	1.67	20/1371 (1.5%)
1	B	1.01	0/1007	1.78	23/1371 (1.7%)
1	C	0.95	1/1007 (0.1%)	1.67	31/1371 (2.3%)
1	D	1.09	1/1007 (0.1%)	1.68	32/1371 (2.3%)
1	E	1.08	1/1007 (0.1%)	1.83	32/1371 (2.3%)
1	F	1.02	0/1007	1.69	27/1371 (2.0%)
1	G	0.97	0/1007	1.54	24/1371 (1.8%)
1	H	1.00	0/1007	2.14	22/1371 (1.6%)
1	I	1.04	0/1007	1.52	19/1371 (1.4%)
1	J	0.95	0/1007	1.58	25/1371 (1.8%)
1	K	1.10	2/1007 (0.2%)	1.73	27/1371 (2.0%)
1	L	1.03	0/1007	1.63	23/1371 (1.7%)
1	M	1.13	3/1007 (0.3%)	1.59	21/1371 (1.5%)
1	N	1.01	0/1007	1.50	16/1371 (1.2%)
1	O	1.06	1/1007 (0.1%)	1.66	22/1371 (1.6%)
1	P	1.06	0/1007	1.66	28/1371 (2.0%)
1	Q	1.02	0/1007	1.60	21/1371 (1.5%)
1	R	1.04	0/1007	1.55	17/1371 (1.2%)
1	S	1.08	2/1007 (0.2%)	1.63	27/1371 (2.0%)
1	T	0.97	0/1007	1.71	29/1371 (2.1%)
1	U	1.03	0/1007	1.52	20/1371 (1.5%)
1	V	0.99	0/1007	1.67	27/1371 (2.0%)
All	All	1.03	11/22154 (0.0%)	1.67	533/30162 (1.8%)

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	2
1	C	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	7
1	F	0	4
1	H	0	1
1	K	0	1
1	L	0	3
1	M	0	4
1	N	0	2
1	O	0	1
1	P	0	1
1	Q	0	5
1	S	0	3
1	T	0	5
1	U	0	2
1	V	0	3
All	All	0	47

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	127	GLN	CA-C	7.40	1.56	1.52
1	K	68	ILE	CA-CB	-6.11	1.51	1.55
1	M	96	PHE	CG-CD1	-5.95	1.26	1.38
1	K	22	ASN	CA-C	5.73	1.58	1.52
1	M	96	PHE	CA-C	5.70	1.60	1.52
1	O	41	VAL	CA-CB	-5.64	1.50	1.53
1	M	24	ARG	NE-CZ	5.50	1.39	1.33
1	S	107	PHE	CB-CG	-5.46	1.38	1.50
1	E	111	GLU	CG-CD	-5.33	1.38	1.52
1	S	23	PRO	CA-C	-5.12	1.46	1.52
1	C	35	LEU	CB-CG	5.03	1.63	1.53

All (533) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	56	SER	CA-C-O	-34.79	82.92	121.19
1	H	56	SER	O-C-N	30.52	160.41	122.87
1	B	21	LEU	CA-C-N	23.69	154.54	121.61
1	B	21	LEU	C-N-CA	23.69	154.54	121.61
1	H	37	GLN	CA-C-N	21.83	151.60	120.82
1	H	37	GLN	C-N-CA	21.83	151.60	120.82
1	A	61	ASN	CA-C-N	18.83	154.65	121.89
1	A	61	ASN	C-N-CA	18.83	154.65	121.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	116	LEU	CA-C-N	18.48	153.04	122.54
1	C	116	LEU	C-N-CA	18.48	153.04	122.54
1	E	131	ALA	CA-C-N	18.00	154.10	121.70
1	E	131	ALA	C-N-CA	18.00	154.10	121.70
1	M	96	PHE	CA-CB-CG	17.50	131.30	113.80
1	V	128	LEU	CA-C-N	16.82	151.97	121.70
1	V	128	LEU	C-N-CA	16.82	151.97	121.70
1	T	2	LYS	CA-C-N	16.76	153.54	121.54
1	T	2	LYS	C-N-CA	16.76	153.54	121.54
1	G	129	ASN	N-CA-C	11.89	124.58	109.72
1	K	60	LYS	CA-C-N	11.36	142.15	121.70
1	K	60	LYS	C-N-CA	11.36	142.15	121.70
1	D	127	GLN	CA-C-O	-10.85	112.93	119.55
1	F	60	LYS	CA-C-N	10.42	140.46	121.70
1	F	60	LYS	C-N-CA	10.42	140.46	121.70
1	Q	36	SER	N-CA-C	10.17	122.77	108.74
1	P	22	ASN	CB-CA-C	9.80	119.88	110.17
1	O	50	VAL	CA-C-N	9.61	138.99	121.70
1	O	50	VAL	C-N-CA	9.61	138.99	121.70
1	T	58	ASN	N-CA-C	-9.33	102.71	114.56
1	P	110	THR	N-CA-C	-9.16	101.87	113.23
1	E	127	GLN	N-CA-C	-9.12	99.89	112.30
1	O	40	ALA	CA-C-N	8.88	125.84	120.24
1	O	40	ALA	C-N-CA	8.88	125.84	120.24
1	T	41	VAL	N-CA-C	-8.80	100.33	108.95
1	S	37	GLN	CA-C-N	8.76	137.47	121.70
1	S	37	GLN	C-N-CA	8.76	137.47	121.70
1	O	37	GLN	N-CA-C	8.74	123.75	113.18
1	E	96	PHE	N-CA-C	8.69	122.70	109.23
1	M	96	PHE	CA-C-N	8.65	137.27	121.70
1	M	96	PHE	C-N-CA	8.65	137.27	121.70
1	J	94	PHE	CA-CB-CG	8.63	122.43	113.80
1	P	89	TYR	N-CA-C	8.62	119.62	108.24
1	K	118	SER	CA-C-N	8.42	129.24	119.47
1	K	118	SER	C-N-CA	8.42	129.24	119.47
1	D	118	SER	CA-C-N	8.40	128.13	119.56
1	D	118	SER	C-N-CA	8.40	128.13	119.56
1	D	62	TYR	N-CA-C	8.40	121.37	111.71
1	P	81	ASP	CA-C-N	8.36	128.30	120.03
1	P	81	ASP	C-N-CA	8.36	128.30	120.03
1	B	91	ASP	CA-CB-CG	8.33	120.93	112.60
1	N	41	VAL	CA-C-N	8.29	128.02	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	41	VAL	C-N-CA	8.29	128.02	119.56
1	P	27	ASN	CA-C-N	8.27	128.47	119.87
1	P	27	ASN	C-N-CA	8.27	128.47	119.87
1	K	120	LEU	CA-C-O	-8.26	111.72	120.55
1	E	60	LYS	CA-C-N	8.25	136.54	121.70
1	E	60	LYS	C-N-CA	8.25	136.54	121.70
1	H	70	ASN	CA-C-N	8.25	128.25	119.76
1	H	70	ASN	C-N-CA	8.25	128.25	119.76
1	K	22	ASN	CA-C-N	8.22	128.17	120.03
1	K	22	ASN	C-N-CA	8.22	128.17	120.03
1	Q	34	SER	CA-C-O	-8.20	112.13	121.81
1	R	31	GLY	N-CA-C	8.19	121.35	111.93
1	B	70	ASN	CA-C-N	8.17	128.19	119.78
1	B	70	ASN	C-N-CA	8.17	128.19	119.78
1	R	50	VAL	N-CA-C	8.14	119.84	108.12
1	L	86	ARG	N-CA-C	-8.13	99.04	110.50
1	M	52	VAL	CA-C-O	-8.12	111.67	118.98
1	G	27	ASN	CA-C-N	8.11	127.83	119.56
1	G	27	ASN	C-N-CA	8.11	127.83	119.56
1	C	126	ASP	N-CA-C	-8.09	93.57	110.80
1	F	102	ASP	CA-CB-CG	8.07	120.67	112.60
1	P	72	THR	CA-C-N	7.93	131.69	120.28
1	P	72	THR	C-N-CA	7.93	131.69	120.28
1	E	122	ILE	N-CA-C	-7.89	102.40	111.00
1	R	44	LEU	CA-C-N	7.88	135.89	121.70
1	R	44	LEU	C-N-CA	7.88	135.89	121.70
1	D	45	GLU	CA-C-N	-7.88	111.11	122.77
1	D	45	GLU	C-N-CA	-7.88	111.11	122.77
1	Q	75	THR	N-CA-C	-7.87	94.03	110.80
1	V	46	LYS	N-CA-C	-7.84	99.21	110.59
1	H	81	ASP	CA-C-N	7.84	127.86	119.78
1	H	81	ASP	C-N-CA	7.84	127.86	119.78
1	L	70	ASN	CA-C-N	7.82	127.97	120.31
1	L	70	ASN	C-N-CA	7.82	127.97	120.31
1	S	112	LEU	CA-C-O	-7.79	112.29	120.55
1	E	22	ASN	CA-C-N	7.79	128.26	119.93
1	E	22	ASN	C-N-CA	7.79	128.26	119.93
1	E	81	ASP	CA-C-N	7.67	127.62	120.03
1	E	81	ASP	C-N-CA	7.67	127.62	120.03
1	J	70	ASN	CA-C-N	7.62	127.57	120.03
1	J	70	ASN	C-N-CA	7.62	127.57	120.03
1	A	129	ASN	CA-C-N	7.60	129.34	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ASN	C-N-CA	7.60	129.34	119.84
1	V	27	ASN	CA-C-N	7.59	127.23	119.56
1	V	27	ASN	C-N-CA	7.59	127.23	119.56
1	J	29	THR	N-CA-C	-7.58	102.95	111.07
1	I	27	ASN	CA-C-N	7.57	127.28	119.56
1	I	27	ASN	C-N-CA	7.57	127.28	119.56
1	P	22	ASN	CA-C-N	7.56	128.02	119.93
1	P	22	ASN	C-N-CA	7.56	128.02	119.93
1	S	27	ASN	CA-C-N	7.54	127.18	119.56
1	S	27	ASN	C-N-CA	7.54	127.18	119.56
1	S	53	SER	CA-C-N	7.50	135.19	121.70
1	S	53	SER	C-N-CA	7.50	135.19	121.70
1	F	27	ASN	CA-C-N	7.49	127.66	119.87
1	F	27	ASN	C-N-CA	7.49	127.66	119.87
1	T	129	ASN	CA-C-N	7.49	127.45	120.03
1	T	129	ASN	C-N-CA	7.49	127.45	120.03
1	B	54	GLN	CA-C-N	7.44	127.39	120.03
1	B	54	GLN	C-N-CA	7.44	127.39	120.03
1	L	30	ASN	N-CA-C	7.44	119.01	108.74
1	G	87	GLN	CA-C-N	7.42	135.06	121.70
1	G	87	GLN	C-N-CA	7.42	135.06	121.70
1	F	46	LYS	N-CA-C	7.42	119.43	108.60
1	P	44	LEU	N-CA-C	-7.41	104.49	113.97
1	V	70	ASN	CA-C-N	7.38	127.96	120.14
1	V	70	ASN	C-N-CA	7.38	127.96	120.14
1	R	81	ASP	N-CA-C	7.37	126.11	109.81
1	J	50	VAL	N-CA-C	7.36	118.72	108.12
1	M	118	SER	CA-C-N	7.35	127.06	119.56
1	M	118	SER	C-N-CA	7.35	127.06	119.56
1	P	109	ARG	CA-C-O	-7.35	113.04	120.90
1	T	36	SER	CA-C-O	-7.33	113.38	121.23
1	C	86	ARG	CA-C-N	7.32	134.88	121.70
1	C	86	ARG	C-N-CA	7.32	134.88	121.70
1	F	107	PHE	CA-C-O	-7.31	112.80	120.55
1	E	127	GLN	CA-C-N	7.30	131.18	120.95
1	E	127	GLN	C-N-CA	7.30	131.18	120.95
1	D	129	ASN	CA-C-N	7.28	128.94	119.84
1	D	129	ASN	C-N-CA	7.28	128.94	119.84
1	O	46	LYS	N-CA-C	7.26	121.68	110.20
1	C	54	GLN	CA-C-N	7.26	127.21	120.03
1	C	54	GLN	C-N-CA	7.26	127.21	120.03
1	L	129	ASN	CA-CB-CG	7.22	119.82	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	41	VAL	CA-C-N	7.22	127.25	119.89
1	P	41	VAL	C-N-CA	7.22	127.25	119.89
1	F	37	GLN	N-CA-C	-7.19	99.17	109.96
1	D	52	VAL	CA-C-N	7.17	134.60	121.70
1	D	52	VAL	C-N-CA	7.17	134.60	121.70
1	T	125	ILE	N-CA-C	7.17	118.48	111.67
1	T	118	SER	CA-C-N	7.15	127.76	119.47
1	T	118	SER	C-N-CA	7.15	127.76	119.47
1	N	41	VAL	N-CA-C	7.14	115.22	108.15
1	R	41	VAL	CA-C-N	7.14	127.13	119.28
1	R	41	VAL	C-N-CA	7.14	127.13	119.28
1	C	70	ASN	CA-C-N	7.11	127.53	119.92
1	C	70	ASN	C-N-CA	7.11	127.53	119.92
1	O	129	ASN	CA-C-N	7.11	127.11	119.78
1	O	129	ASN	C-N-CA	7.11	127.11	119.78
1	K	70	ASN	CA-C-N	7.11	127.07	120.03
1	K	70	ASN	C-N-CA	7.11	127.07	120.03
1	S	22	ASN	CA-C-N	7.09	127.05	120.03
1	S	22	ASN	C-N-CA	7.09	127.05	120.03
1	U	129	ASN	CA-C-N	7.07	128.67	119.84
1	U	129	ASN	C-N-CA	7.07	128.67	119.84
1	R	70	ASN	CA-C-N	7.06	126.98	119.85
1	R	70	ASN	C-N-CA	7.06	126.98	119.85
1	E	100	SER	N-CA-C	-7.06	101.73	110.41
1	K	27	ASN	CA-C-N	7.05	126.75	119.56
1	K	27	ASN	C-N-CA	7.05	126.75	119.56
1	U	41	VAL	CA-C-N	7.04	126.74	119.56
1	U	41	VAL	C-N-CA	7.04	126.74	119.56
1	Q	53	SER	N-CA-C	7.03	120.04	110.55
1	O	27	ASN	CA-C-N	7.01	126.64	119.56
1	O	27	ASN	C-N-CA	7.01	126.64	119.56
1	F	60	LYS	N-CA-C	7.00	125.72	110.80
1	S	70	ASN	CA-C-N	7.00	126.92	119.85
1	S	70	ASN	C-N-CA	7.00	126.92	119.85
1	S	80	CYS	CA-C-O	-7.00	112.04	120.65
1	K	60	LYS	N-CA-C	7.00	125.71	110.80
1	A	95	SER	CA-C-N	6.94	133.37	121.29
1	A	95	SER	C-N-CA	6.94	133.37	121.29
1	B	53	SER	N-CA-C	6.93	119.87	108.99
1	O	120	LEU	N-CA-C	-6.91	103.19	111.69
1	K	34	SER	N-CA-C	6.90	119.65	109.24
1	U	36	SER	N-CA-C	6.88	119.22	108.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	GLN	CA-C-N	6.87	134.06	121.70
1	A	37	GLN	C-N-CA	6.87	134.06	121.70
1	P	92	VAL	CB-CA-C	-6.87	101.57	110.98
1	G	54	GLN	CA-C-N	6.86	126.82	120.03
1	G	54	GLN	C-N-CA	6.86	126.82	120.03
1	P	70	ASN	CA-C-N	6.85	126.81	120.03
1	P	70	ASN	C-N-CA	6.85	126.81	120.03
1	F	70	ASN	CA-C-N	6.85	126.81	120.03
1	F	70	ASN	C-N-CA	6.85	126.81	120.03
1	E	71	PRO	N-CA-C	-6.82	100.53	111.03
1	A	32	VAL	N-CA-C	6.80	117.68	107.75
1	S	87	GLN	N-CA-C	6.78	119.15	107.28
1	A	54	GLN	CA-C-N	6.77	126.75	119.78
1	A	54	GLN	C-N-CA	6.77	126.75	119.78
1	J	54	GLN	CA-C-N	6.76	126.79	119.89
1	J	54	GLN	C-N-CA	6.76	126.79	119.89
1	H	29	THR	N-CA-C	-6.76	98.24	108.52
1	G	118	SER	CA-C-N	6.75	127.30	119.47
1	G	118	SER	C-N-CA	6.75	127.30	119.47
1	N	70	ASN	CA-C-N	6.74	126.71	120.03
1	N	70	ASN	C-N-CA	6.74	126.71	120.03
1	I	81	ASP	CA-C-N	6.73	126.71	119.78
1	I	81	ASP	C-N-CA	6.73	126.71	119.78
1	T	70	ASN	CA-C-N	6.73	126.64	119.85
1	T	70	ASN	C-N-CA	6.73	126.64	119.85
1	D	131	ALA	CA-C-O	-6.71	112.39	122.38
1	F	36	SER	CA-C-O	-6.71	113.80	121.58
1	R	36	SER	N-CA-C	6.70	118.39	108.60
1	Q	43	ALA	N-CA-C	-6.70	105.11	113.28
1	M	52	VAL	N-CA-C	6.69	120.23	113.47
1	I	22	ASN	CA-C-N	6.69	126.45	119.76
1	I	22	ASN	C-N-CA	6.69	126.45	119.76
1	O	32	VAL	N-CA-C	6.69	117.48	107.51
1	T	27	ASN	CA-C-N	6.67	126.37	119.56
1	T	27	ASN	C-N-CA	6.67	126.37	119.56
1	M	27	ASN	CA-C-N	6.67	126.35	119.82
1	M	27	ASN	C-N-CA	6.67	126.35	119.82
1	A	92	VAL	CB-CA-C	-6.66	101.85	110.98
1	U	34	SER	N-CA-C	-6.65	101.95	110.53
1	D	87	GLN	CA-C-O	-6.63	113.45	121.28
1	C	27	ASN	CA-C-N	6.63	127.16	119.47
1	C	27	ASN	C-N-CA	6.63	127.16	119.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	22	ASN	N-CA-C	6.63	119.11	109.04
1	O	37	GLN	CA-C-N	6.60	133.58	121.70
1	O	37	GLN	C-N-CA	6.60	133.58	121.70
1	T	54	GLN	CA-C-N	6.59	126.97	119.92
1	T	54	GLN	C-N-CA	6.59	126.97	119.92
1	G	41	VAL	CA-C-N	6.57	126.27	119.56
1	G	41	VAL	C-N-CA	6.57	126.27	119.56
1	Q	18	THR	CA-C-N	-6.57	113.94	123.00
1	Q	18	THR	C-N-CA	-6.57	113.94	123.00
1	F	118	SER	CA-C-N	6.55	127.07	119.47
1	F	118	SER	C-N-CA	6.55	127.07	119.47
1	H	84	VAL	N-CA-C	6.54	117.48	109.30
1	J	53	SER	CA-C-N	6.54	133.47	121.70
1	J	53	SER	C-N-CA	6.54	133.47	121.70
1	V	56	SER	CA-C-N	6.53	133.45	121.70
1	V	56	SER	C-N-CA	6.53	133.45	121.70
1	C	35	LEU	CA-C-N	6.52	133.43	121.70
1	C	35	LEU	C-N-CA	6.52	133.43	121.70
1	H	52	VAL	N-CA-C	6.51	117.22	108.11
1	J	129	ASN	CA-C-N	6.50	126.47	120.03
1	J	129	ASN	C-N-CA	6.50	126.47	120.03
1	L	118	SER	CA-C-N	6.49	126.18	119.56
1	L	118	SER	C-N-CA	6.49	126.18	119.56
1	N	81	ASP	CA-C-N	6.49	127.02	120.14
1	N	81	ASP	C-N-CA	6.49	127.02	120.14
1	G	70	ASN	CA-C-N	6.49	126.45	120.03
1	G	70	ASN	C-N-CA	6.49	126.45	120.03
1	D	61	ASN	N-CA-C	6.46	119.27	110.35
1	T	36	SER	O-C-N	-6.46	116.51	123.42
1	S	105	ARG	CA-C-O	-6.44	113.59	120.42
1	Q	54	GLN	CA-C-N	6.43	126.39	120.03
1	Q	54	GLN	C-N-CA	6.43	126.39	120.03
1	G	129	ASN	CA-C-N	6.40	126.77	119.92
1	G	129	ASN	C-N-CA	6.40	126.77	119.92
1	D	61	ASN	CA-C-N	6.39	129.49	120.28
1	D	61	ASN	C-N-CA	6.39	129.49	120.28
1	Q	70	ASN	CA-C-N	6.39	126.31	119.85
1	Q	70	ASN	C-N-CA	6.39	126.31	119.85
1	G	79	SER	N-CA-C	6.39	118.48	108.96
1	V	129	ASN	CA-C-N	6.36	126.31	119.76
1	V	129	ASN	C-N-CA	6.36	126.31	119.76
1	C	118	SER	CA-C-N	6.36	126.84	119.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	118	SER	C-N-CA	6.36	126.84	119.47
1	U	118	SER	CA-C-N	6.35	126.84	119.47
1	U	118	SER	C-N-CA	6.35	126.84	119.47
1	V	118	SER	CA-C-N	6.34	126.83	119.47
1	V	118	SER	C-N-CA	6.34	126.83	119.47
1	K	118	SER	CB-CA-C	6.34	118.73	109.48
1	P	79	SER	CB-CA-C	-6.33	109.29	116.63
1	P	23	PRO	N-CA-CB	-6.31	97.51	103.19
1	B	41	VAL	CA-C-N	6.30	126.78	119.47
1	B	41	VAL	C-N-CA	6.30	126.78	119.47
1	O	111	GLU	N-CA-C	-6.30	104.42	111.28
1	Q	91	ASP	CA-CB-CG	6.29	118.89	112.60
1	F	16	LYS	N-CA-C	6.28	119.01	108.02
1	C	21	LEU	CA-C-O	-6.27	112.02	119.35
1	M	91	ASP	CA-CB-CG	6.26	118.86	112.60
1	L	41	VAL	CA-C-N	6.25	125.94	119.56
1	L	41	VAL	C-N-CA	6.25	125.94	119.56
1	S	92	VAL	CB-CA-C	-6.25	102.42	110.98
1	I	128	LEU	CA-C-N	6.24	132.93	121.70
1	I	128	LEU	C-N-CA	6.24	132.93	121.70
1	L	68	ILE	N-CA-C	6.23	116.83	107.80
1	R	27	ASN	CA-C-N	6.22	125.90	119.56
1	R	27	ASN	C-N-CA	6.22	125.90	119.56
1	G	131	ALA	N-CA-C	6.21	119.27	109.39
1	M	89	TYR	N-CA-C	6.21	118.74	108.99
1	N	97	THR	N-CA-C	-6.20	105.51	114.12
1	T	50	VAL	N-CA-C	6.19	117.04	108.12
1	Q	41	VAL	CA-C-N	6.18	125.80	119.56
1	Q	41	VAL	C-N-CA	6.18	125.80	119.56
1	P	23	PRO	N-CA-C	6.17	121.31	111.26
1	C	45	GLU	CA-C-N	-6.17	114.83	122.84
1	C	45	GLU	C-N-CA	-6.17	114.83	122.84
1	N	50	VAL	N-CA-C	6.16	116.74	108.11
1	S	113	ALA	N-CA-C	-6.16	104.11	111.69
1	Q	37	GLN	N-CA-C	6.14	120.47	112.92
1	D	50	VAL	N-CA-C	6.13	116.95	108.12
1	L	81	ASP	CB-CA-C	-6.13	104.10	110.17
1	P	109	ARG	CA-C-N	-6.13	110.87	121.66
1	P	109	ARG	C-N-CA	-6.13	110.87	121.66
1	I	54	GLN	CA-C-N	6.13	126.09	119.78
1	I	54	GLN	C-N-CA	6.13	126.09	119.78
1	L	16	LYS	N-CA-C	6.13	121.42	113.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	81	ASP	CA-C-N	6.12	126.09	120.03
1	M	81	ASP	C-N-CA	6.12	126.09	120.03
1	D	47	ARG	N-CA-C	6.10	118.98	109.52
1	E	109	ARG	CB-CA-C	-6.09	101.31	110.88
1	F	59	ARG	CA-C-N	6.09	133.17	121.54
1	F	59	ARG	C-N-CA	6.09	133.17	121.54
1	U	16	LYS	N-CA-C	6.08	121.63	113.72
1	U	111	GLU	N-CA-C	-6.07	104.67	111.28
1	F	22	ASN	CA-C-N	6.06	125.97	119.85
1	F	22	ASN	C-N-CA	6.06	125.97	119.85
1	U	70	ASN	CA-C-N	6.03	125.94	119.85
1	U	70	ASN	C-N-CA	6.03	125.94	119.85
1	S	50	VAL	N-CA-C	6.03	116.69	107.77
1	I	63	LYS	N-CA-C	6.01	119.00	109.50
1	N	107	PHE	CA-CB-CG	-6.01	107.79	113.80
1	R	109	ARG	CB-CA-C	-6.01	100.81	110.79
1	E	128	LEU	N-CA-C	6.00	118.96	109.96
1	G	92	VAL	N-CA-C	5.97	116.47	108.11
1	D	16	LYS	N-CA-C	5.97	120.58	112.88
1	B	118	SER	CA-C-N	5.97	125.65	119.56
1	B	118	SER	C-N-CA	5.97	125.65	119.56
1	B	16	LYS	N-CA-C	5.96	121.47	113.72
1	U	58	ASN	N-CA-C	-5.95	100.25	109.24
1	M	92	VAL	CB-CA-C	-5.94	102.77	110.84
1	L	2	LYS	CA-C-O	-5.93	113.99	120.81
1	L	2	LYS	CA-C-N	-5.93	115.13	122.84
1	L	2	LYS	C-N-CA	-5.93	115.13	122.84
1	C	63	LYS	N-CA-C	5.92	117.86	108.79
1	N	16	LYS	N-CA-C	5.92	121.29	112.94
1	E	36	SER	N-CA-C	5.92	117.24	108.60
1	H	101	THR	CA-C-O	-5.92	112.05	120.51
1	A	95	SER	N-CA-C	5.91	119.16	110.59
1	P	110	THR	N-CA-CB	5.91	119.65	110.44
1	M	54	GLN	CA-C-N	5.91	125.88	120.03
1	M	54	GLN	C-N-CA	5.91	125.88	120.03
1	O	73	ALA	N-CA-C	5.90	117.71	111.28
1	S	81	ASP	CA-C-N	5.90	126.39	120.14
1	S	81	ASP	C-N-CA	5.90	126.39	120.14
1	Q	27	ASN	CA-C-N	5.89	125.51	119.56
1	Q	27	ASN	C-N-CA	5.89	125.51	119.56
1	F	92	VAL	N-CA-C	5.89	116.36	108.11
1	G	32	VAL	N-CA-C	5.89	116.29	107.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	45	GLU	CA-C-O	-5.89	114.23	120.71
1	S	41	VAL	CA-C-N	5.88	125.59	119.82
1	S	41	VAL	C-N-CA	5.88	125.59	119.82
1	F	129	ASN	CA-C-N	5.88	125.85	120.03
1	F	129	ASN	C-N-CA	5.88	125.85	120.03
1	M	51	SER	N-CA-C	-5.86	101.81	110.48
1	A	81	ASP	CA-C-N	5.85	125.87	119.90
1	A	81	ASP	C-N-CA	5.85	125.87	119.90
1	J	34	SER	N-CA-C	5.83	118.91	109.40
1	H	97	THR	N-CA-C	-5.82	103.03	110.53
1	M	94	PHE	N-CA-C	5.81	116.22	108.38
1	Q	118	SER	CA-C-N	5.80	125.48	119.56
1	Q	118	SER	C-N-CA	5.80	125.48	119.56
1	J	118	SER	CA-C-N	5.80	126.20	119.47
1	J	118	SER	C-N-CA	5.80	126.20	119.47
1	H	118	SER	CA-C-N	5.80	126.20	119.47
1	H	118	SER	C-N-CA	5.80	126.20	119.47
1	V	58	ASN	N-CA-C	5.79	119.64	112.58
1	C	81	ASP	CA-C-N	5.76	126.25	120.14
1	C	81	ASP	C-N-CA	5.76	126.25	120.14
1	F	108	VAL	N-CA-C	-5.76	104.91	110.72
1	T	36	SER	CA-C-N	-5.76	109.38	121.64
1	T	36	SER	C-N-CA	-5.76	109.38	121.64
1	L	75	THR	N-CA-C	5.75	118.44	109.52
1	C	129	ASN	CA-C-N	5.73	127.00	119.84
1	C	129	ASN	C-N-CA	5.73	127.00	119.84
1	M	95	SER	N-CA-C	5.72	117.49	108.96
1	E	60	LYS	N-CA-C	-5.72	99.40	109.02
1	D	22	ASN	CA-C-N	5.70	125.46	119.76
1	D	22	ASN	C-N-CA	5.70	125.46	119.76
1	B	125	ILE	N-CA-C	5.70	117.08	111.67
1	G	122	ILE	N-CA-C	-5.69	106.16	111.45
1	D	73	ALA	N-CA-C	5.68	116.89	108.60
1	D	54	GLN	CA-C-N	5.67	125.58	119.85
1	D	54	GLN	C-N-CA	5.67	125.58	119.85
1	S	81	ASP	N-CA-C	5.67	117.42	108.23
1	I	35	LEU	N-CA-C	-5.67	105.04	112.41
1	J	22	ASN	CA-C-N	5.67	125.43	119.76
1	J	22	ASN	C-N-CA	5.67	125.43	119.76
1	J	68	ILE	N-CA-C	5.66	116.01	107.80
1	I	50	VAL	N-CA-C	5.66	116.75	107.24
1	J	26	VAL	CA-C-O	-5.66	116.21	120.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	GLN	CA-C-O	-5.66	112.92	119.14
1	T	42	PRO	N-CA-C	5.65	120.36	111.38
1	H	129	ASN	CA-C-N	5.64	125.66	119.90
1	H	129	ASN	C-N-CA	5.64	125.66	119.90
1	S	106	ALA	N-CA-C	-5.64	105.12	112.23
1	U	39	GLY	CA-C-N	5.62	128.38	120.28
1	U	39	GLY	C-N-CA	5.62	128.38	120.28
1	E	87	GLN	N-CA-C	5.61	118.55	109.40
1	N	118	SER	CA-C-N	5.61	125.28	119.56
1	N	118	SER	C-N-CA	5.61	125.28	119.56
1	G	81	ASP	CA-C-N	5.61	125.56	119.78
1	G	81	ASP	C-N-CA	5.61	125.56	119.78
1	H	54	GLN	CA-C-N	5.61	125.56	119.78
1	H	54	GLN	C-N-CA	5.61	125.56	119.78
1	O	34	SER	N-CA-C	5.61	118.38	109.24
1	L	27	ASN	N-CA-C	5.60	122.19	109.81
1	T	89	TYR	N-CA-C	5.60	117.36	108.79
1	O	16	LYS	N-CA-C	5.60	120.39	113.50
1	C	126	ASP	CA-CB-CG	5.59	118.19	112.60
1	O	70	ASN	CA-C-N	5.58	125.51	119.76
1	O	70	ASN	C-N-CA	5.58	125.51	119.76
1	B	89	TYR	N-CA-C	5.57	117.74	108.99
1	E	49	THR	N-CA-C	5.57	117.81	108.73
1	K	102	ASP	CA-CB-CG	5.57	118.17	112.60
1	V	57	ARG	CA-C-N	5.56	130.74	122.74
1	V	57	ARG	C-N-CA	5.56	130.74	122.74
1	B	22	ASN	CA-C-N	5.55	125.87	119.93
1	B	22	ASN	C-N-CA	5.55	125.87	119.93
1	D	127	GLN	O-C-N	-5.55	115.72	120.71
1	M	41	VAL	N-CA-C	5.54	113.63	108.15
1	E	118	SER	CA-C-N	5.53	125.88	119.47
1	E	118	SER	C-N-CA	5.53	125.88	119.47
1	D	32	VAL	N-CA-C	5.53	116.06	107.99
1	V	46	LYS	CA-C-N	5.52	131.64	121.70
1	V	46	LYS	C-N-CA	5.52	131.64	121.70
1	A	56	SER	N-CA-C	5.52	115.69	108.07
1	L	34	SER	N-CA-C	5.52	118.00	110.55
1	T	32	VAL	N-CA-C	5.51	115.82	108.11
1	B	50	VAL	N-CA-C	5.51	115.79	107.75
1	K	26	VAL	N-CA-C	5.49	115.46	107.88
1	L	36	SER	N-CA-C	5.48	117.13	108.96
1	P	118	SER	CA-C-N	5.47	125.82	119.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	118	SER	C-N-CA	5.47	125.82	119.47
1	K	111	GLU	N-CA-C	-5.46	105.48	111.82
1	T	124	ALA	CA-C-N	-5.46	116.13	122.63
1	T	124	ALA	C-N-CA	-5.46	116.13	122.63
1	K	89	TYR	N-CA-C	5.46	116.58	108.60
1	E	16	LYS	N-CA-C	5.46	118.88	110.42
1	A	16	LYS	N-CA-C	5.45	119.19	112.54
1	K	125	ILE	CA-C-N	5.43	132.28	122.02
1	K	125	ILE	C-N-CA	5.43	132.28	122.02
1	J	30	ASN	N-CA-C	-5.42	99.68	108.41
1	V	22	ASN	CA-C-N	5.42	125.37	119.78
1	V	22	ASN	C-N-CA	5.42	125.37	119.78
1	T	127	GLN	CA-C-O	-5.42	112.97	119.15
1	V	54	GLN	CA-C-N	5.42	125.36	119.78
1	V	54	GLN	C-N-CA	5.42	125.36	119.78
1	B	32	VAL	N-CA-C	5.41	115.37	107.37
1	C	126	ASP	CA-C-N	-5.40	113.20	120.82
1	C	126	ASP	C-N-CA	-5.40	113.20	120.82
1	C	92	VAL	N-CA-CB	-5.39	104.88	111.67
1	K	119	PRO	N-CA-C	5.39	121.63	113.81
1	F	96	PHE	CA-CB-CG	-5.39	108.41	113.80
1	U	27	ASN	CA-C-N	5.38	125.72	119.47
1	U	27	ASN	C-N-CA	5.38	125.72	119.47
1	K	48	VAL	N-CA-C	5.37	115.59	107.75
1	E	27	ASN	CA-C-N	5.37	125.44	119.32
1	E	27	ASN	C-N-CA	5.37	125.44	119.32
1	F	49	THR	CA-C-N	-5.36	115.37	122.98
1	F	49	THR	C-N-CA	-5.36	115.37	122.98
1	E	47	ARG	N-CA-C	5.36	118.17	109.06
1	V	98	GLN	CA-C-O	-5.36	112.25	119.11
1	S	106	ALA	CA-C-N	5.35	127.39	120.44
1	S	106	ALA	C-N-CA	5.35	127.39	120.44
1	G	107	PHE	CA-CB-CG	5.35	119.15	113.80
1	S	118	SER	CA-C-N	5.35	125.02	119.56
1	S	118	SER	C-N-CA	5.35	125.02	119.56
1	V	81	ASP	CA-C-N	5.35	125.29	119.78
1	V	81	ASP	C-N-CA	5.35	125.29	119.78
1	T	81	ASP	CA-C-N	5.34	125.10	119.76
1	T	81	ASP	C-N-CA	5.34	125.10	119.76
1	V	87	GLN	N-CA-C	5.33	117.87	108.75
1	D	85	THR	N-CA-C	5.33	118.34	110.46
1	Q	22	ASN	N-CA-C	5.33	121.58	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	127	GLN	CA-C-N	5.32	131.28	121.70
1	D	127	GLN	C-N-CA	5.32	131.28	121.70
1	U	107	PHE	CA-CB-CG	5.32	119.12	113.80
1	H	73	ALA	N-CA-C	5.30	118.74	110.32
1	R	16	LYS	N-CA-C	5.29	120.41	112.94
1	I	79	SER	N-CA-C	5.29	117.23	109.24
1	E	48	VAL	CA-C-N	5.29	129.81	122.77
1	E	48	VAL	C-N-CA	5.29	129.81	122.77
1	F	11	ILE	N-CA-C	5.27	115.55	108.17
1	L	82	PRO	N-CA-C	-5.27	103.00	111.38
1	G	91	ASP	CA-CB-CG	5.25	117.85	112.60
1	H	31	GLY	CA-C-N	-5.23	114.58	122.01
1	H	31	GLY	C-N-CA	-5.23	114.58	122.01
1	D	89	TYR	CA-CB-CG	5.23	123.31	113.90
1	O	50	VAL	CA-C-O	-5.22	115.01	120.76
1	I	16	LYS	N-CA-C	5.21	119.64	113.28
1	J	81	ASP	CA-C-N	5.21	125.51	119.47
1	J	81	ASP	C-N-CA	5.21	125.51	119.47
1	E	41	VAL	N-CA-C	5.20	120.12	108.88
1	Q	89	TYR	N-CA-C	5.19	117.13	108.99
1	J	58	ASN	CA-C-N	5.18	129.50	122.19
1	J	58	ASN	C-N-CA	5.18	129.50	122.19
1	A	11	ILE	N-CA-C	5.17	115.76	108.36
1	K	59	ARG	CA-C-N	5.17	131.42	121.54
1	K	59	ARG	C-N-CA	5.17	131.42	121.54
1	B	47	ARG	N-CA-C	5.17	117.25	109.23
1	J	86	ARG	N-CA-C	5.17	117.73	110.23
1	B	85	THR	CA-C-O	-5.16	113.39	119.48
1	A	84	VAL	N-CA-C	5.16	116.00	108.58
1	D	27	ASN	CA-C-N	5.15	124.82	119.56
1	D	27	ASN	C-N-CA	5.15	124.82	119.56
1	N	101	THR	N-CA-C	5.15	117.84	109.24
1	K	120	LEU	O-C-N	-5.15	115.94	122.17
1	I	118	SER	CA-C-N	5.14	125.43	119.47
1	I	118	SER	C-N-CA	5.14	125.43	119.47
1	C	22	ASN	CA-C-N	5.13	126.25	119.84
1	C	22	ASN	C-N-CA	5.13	126.25	119.84
1	N	92	VAL	N-CA-C	5.13	115.15	107.51
1	O	91	ASP	CA-CB-CG	5.12	117.72	112.60
1	K	25	GLY	N-CA-C	-5.11	105.21	112.37
1	R	43	ALA	N-CA-C	5.11	116.44	110.41
1	V	92	VAL	N-CA-CB	-5.11	105.23	111.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	24	ARG	N-CA-C	5.10	117.14	109.23
1	E	23	PRO	N-CA-C	5.10	119.57	111.26
1	N	36	SER	N-CA-C	5.10	116.59	108.79
1	P	16	LYS	N-CA-C	5.10	119.77	113.50
1	B	81	ASP	CA-C-N	5.08	124.98	119.85
1	B	81	ASP	C-N-CA	5.08	124.98	119.85
1	J	85	THR	N-CA-C	5.08	115.24	108.23
1	I	36	SER	N-CA-C	5.08	119.19	112.89
1	I	32	VAL	N-CA-C	5.08	115.89	108.58
1	D	45	GLU	CA-C-O	-5.07	114.42	120.56
1	U	92	VAL	CA-C-N	-5.07	114.85	122.81
1	U	92	VAL	C-N-CA	-5.07	114.85	122.81
1	L	22	ASN	CA-C-N	5.06	124.97	119.76
1	L	22	ASN	C-N-CA	5.06	124.97	119.76
1	M	118	SER	N-CA-C	5.05	116.25	109.83
1	P	81	ASP	N-CA-C	5.04	116.04	109.64
1	R	118	SER	CA-C-N	5.03	125.31	119.47
1	R	118	SER	C-N-CA	5.03	125.31	119.47
1	T	124	ALA	CA-C-O	-5.03	112.51	119.05
1	L	85	THR	CB-CA-C	-5.02	104.92	112.09
1	E	48	VAL	N-CA-C	5.01	115.12	108.11

There are no chirality outliers.

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	GLN	Mainchain
1	B	24	ARG	Mainchain
1	B	85	THR	Mainchain
1	C	21	LEU	Mainchain
1	C	45	GLU	Mainchain
1	D	127	GLN	Peptide,Mainchain
1	D	131	ALA	Mainchain
1	D	45	GLU	Mainchain
1	D	79	SER	Peptide,Mainchain
1	D	87	GLN	Mainchain
1	F	107	PHE	Mainchain
1	F	30	ASN	Peptide,Mainchain
1	F	36	SER	Mainchain
1	H	101	THR	Mainchain
1	K	120	LEU	Mainchain
1	L	103	GLU	Peptide,Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	L	2	LYS	Mainchain
1	M	29	THR	Peptide,Mainchain
1	M	52	VAL	Peptide,Mainchain
1	N	38	ALA	Peptide,Mainchain
1	O	119	PRO	Mainchain
1	P	109	ARG	Mainchain
1	Q	18	THR	Peptide,Mainchain
1	Q	34	SER	Peptide,Mainchain
1	Q	42	PRO	Mainchain
1	S	105	ARG	Mainchain
1	S	112	LEU	Mainchain
1	S	80	CYS	Mainchain
1	T	124	ALA	Mainchain
1	T	127	GLN	Mainchain
1	T	36	SER	Mainchain
1	T	9	GLY	Peptide,Mainchain
1	U	61	ASN	Peptide,Mainchain
1	V	9	GLY	Peptide,Mainchain
1	V	98	GLN	Mainchain

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	993	0	1006	2	0
1	B	993	0	1007	1	0
1	C	993	0	1007	9	0
1	D	993	0	1006	6	0
1	E	993	0	1007	11	0
1	F	993	0	1006	5	0
1	G	993	0	1006	6	0
1	H	993	0	1006	8	0
1	I	993	0	1007	7	0
1	J	993	0	1007	8	0
1	K	993	0	1007	4	0
1	L	993	0	1006	3	0
1	M	993	0	1006	7	0
1	N	993	0	1007	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	993	0	1006	9	0
1	P	993	0	1006	8	0
1	Q	993	0	1007	1	0
1	R	993	0	1006	8	0
1	S	993	0	1006	4	0
1	T	993	0	1007	2	0
1	U	993	0	1008	4	0
1	V	993	0	1007	12	0
All	All	21846	0	22144	122	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 3.

All (122) 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:M:96:PHE:HB3	1:M:97:THR:C	2.22	0.65
1:R:44:LEU:H	1:R:45:GLU:HB2	1.62	0.63
1:B:102:ASP:N	1:B:102:ASP:OD1	2.34	0.60
1:M:13:LYS:NZ	1:M:126:ASP:OD2	2.35	0.59
1:V:102:ASP:N	1:V:102:ASP:OD1	2.36	0.58
1:G:79:SER:OG	1:G:80:CYS:N	2.33	0.58
1:F:47:ARG:NH1	1:F:49:THR:OG1	2.38	0.57
1:L:79:SER:OG	1:L:80:CYS:N	2.36	0.56
1:V:42:PRO:O	1:V:43:ALA:C	2.50	0.55
1:L:102:ASP:N	1:L:102:ASP:OD1	2.39	0.55
1:J:102:ASP:N	1:J:102:ASP:OD1	2.38	0.55
1:E:13:LYS:NZ	1:N:102:ASP:OD2	2.36	0.55
1:R:73:ALA:O	1:R:74:CYS:C	2.46	0.55
1:M:102:ASP:OD1	1:M:102:ASP:N	2.39	0.54
1:R:128:LEU:O	1:R:129:ASN:C	2.51	0.54
1:O:110:THR:O	1:O:111:GLU:C	2.51	0.54
1:R:24:ARG:NE	1:R:36:SER:OG	2.40	0.54
1:O:102:ASP:N	1:O:102:ASP:OD1	2.41	0.53
1:H:101:THR:OG1	1:H:102:ASP:N	2.42	0.53
1:R:102:ASP:N	1:R:102:ASP:OD1	2.39	0.53
1:G:102:ASP:N	1:G:102:ASP:OD1	2.38	0.53
1:H:51:SER:OG	1:H:65:GLN:N	2.42	0.52
1:A:102:ASP:OD1	1:A:102:ASP:N	2.41	0.51
1:G:21:LEU:O	1:G:22:ASN:C	2.52	0.51
1:J:21:LEU:HB3	1:J:35:LEU:HB3	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ARG:HA	1:C:87:GLN:HB2	1.93	0.51
1:T:102:ASP:OD1	1:T:102:ASP:N	2.40	0.50
1:V:56:SER:OG	1:V:59:ARG:N	2.45	0.50
1:E:26:VAL:O	1:E:27:ASN:C	2.53	0.50
1:P:22:ASN:HB3	1:P:37:GLN:HB2	1.93	0.50
1:I:36:SER:HA	1:I:47:ARG:HB3	1.93	0.50
1:D:62:TYR:OH	1:D:105:ARG:NH1	2.45	0.50
1:H:21:LEU:HB3	1:H:35:LEU:HB3	1.94	0.49
1:I:1:ALA:O	1:I:2:LYS:C	2.53	0.49
1:C:35:LEU:HB3	1:C:36:SER:HA	1.94	0.49
1:J:81:ASP:N	1:J:82:PRO:HD3	2.27	0.49
1:K:118:SER:HB3	1:K:119:PRO:HD2	1.95	0.48
1:H:101:THR:HG23	1:H:104:GLU:H	1.78	0.48
1:E:14:ASP:OD1	1:E:15:GLY:N	2.46	0.48
1:S:102:ASP:OD1	1:S:102:ASP:N	2.47	0.48
1:F:124:ALA:O	1:O:62:TYR:OH	2.24	0.48
1:S:53:SER:HA	1:S:54:GLN:HB2	1.96	0.48
1:C:64:VAL:HG23	1:C:105:ARG:HH22	1.79	0.48
1:V:56:SER:HB2	1:V:57:ARG:HB2	1.96	0.47
1:K:118:SER:HB3	1:K:119:PRO:CD	2.43	0.47
1:D:56:SER:OG	1:D:57:ARG:N	2.49	0.46
1:C:126:ASP:O	1:C:127:GLN:C	2.55	0.46
1:H:45:GLU:O	1:H:71:PRO:HD2	2.16	0.46
1:V:73:ALA:O	1:V:74:CYS:C	2.58	0.46
1:C:45:GLU:OE1	1:C:46:LYS:NZ	2.49	0.46
1:P:102:ASP:N	1:P:102:ASP:OD1	2.47	0.46
1:I:27:ASN:HB3	1:I:32:VAL:HB	1.98	0.46
1:M:14:ASP:OD1	1:M:15:GLY:N	2.48	0.46
1:V:110:THR:O	1:V:111:GLU:C	2.57	0.46
1:O:44:LEU:O	1:O:45:GLU:HB2	2.16	0.46
1:E:97:THR:HG22	1:E:99:TYR:H	1.80	0.45
1:N:54:GLN:HB2	1:N:55:PRO:HD2	1.96	0.45
1:D:107:PHE:CD1	1:D:107:PHE:C	2.94	0.45
1:F:79:SER:OG	1:F:80:CYS:N	2.49	0.45
1:O:41:VAL:HA	1:O:44:LEU:O	2.15	0.45
1:H:100:SER:O	1:H:101:THR:C	2.59	0.45
1:P:68:ILE:O	1:P:89:TYR:HB2	2.16	0.45
1:R:44:LEU:N	1:R:45:GLU:HB2	2.31	0.45
1:I:14:ASP:OD1	1:I:14:ASP:N	2.47	0.45
1:R:21:LEU:HB3	1:R:35:LEU:HB3	1.99	0.45
1:G:21:LEU:HB3	1:G:35:LEU:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:37:GLN:HA	1:S:38:ALA:HB3	1.97	0.44
1:J:27:ASN:ND2	1:U:27:ASN:O	2.50	0.44
1:E:39:GLY:O	1:O:105:ARG:NH2	2.49	0.44
1:I:128:LEU:HB3	1:I:129:ASN:HA	1.99	0.44
1:H:27:ASN:N	1:H:28:PRO:CD	2.81	0.44
1:H:62:TYR:O	1:H:63:LYS:HB2	2.18	0.44
1:K:22:ASN:HA	1:K:23:PRO:HD3	1.86	0.43
1:M:94:PHE:CG	1:M:95:SER:N	2.87	0.43
1:F:40:ALA:O	1:F:44:LEU:HG	2.18	0.43
1:O:73:ALA:O	1:O:74:CYS:C	2.61	0.43
1:P:1:ALA:O	1:P:2:LYS:C	2.60	0.43
1:V:128:LEU:HB2	1:V:129:ASN:CA	2.48	0.43
1:I:102:ASP:OD1	1:I:102:ASP:N	2.51	0.43
1:U:102:ASP:OD1	1:U:102:ASP:N	2.46	0.43
1:S:41:VAL:N	1:S:42:PRO:HD2	2.34	0.43
1:V:43:ALA:O	1:V:45:GLU:N	2.51	0.43
1:M:96:PHE:HB3	1:M:97:THR:CA	2.47	0.43
1:L:29:THR:OG1	1:L:30:ASN:N	2.50	0.43
1:E:17:GLN:HB3	1:E:18:THR:HB	2.01	0.43
1:J:32:VAL:CG1	1:J:49:THR:HB	2.48	0.43
1:E:111:GLU:OE1	1:N:46:LYS:NZ	2.49	0.43
1:A:70:ASN:OD1	1:A:70:ASN:C	2.62	0.43
1:D:91:ASP:C	1:D:91:ASP:OD1	2.62	0.42
1:J:81:ASP:N	1:J:82:PRO:CD	2.82	0.42
1:V:77:ASN:OD1	1:V:77:ASN:N	2.50	0.42
1:I:94:PHE:HB3	1:I:96:PHE:CZ	2.55	0.42
1:P:79:SER:OG	1:P:80:CYS:N	2.52	0.42
1:D:132:TYR:OXT	1:P:2:LYS:NZ	2.53	0.42
1:E:101:THR:OG1	1:E:102:ASP:N	2.52	0.42
1:V:101:THR:O	1:V:105:ARG:HD3	2.20	0.42
1:D:101:THR:OG1	1:D:102:ASP:N	2.52	0.42
1:G:96:PHE:CD2	1:G:105:ARG:HG2	2.55	0.42
1:R:29:THR:O	1:R:30:ASN:C	2.62	0.42
1:Q:14:ASP:OD2	1:Q:16:LYS:NZ	2.50	0.42
1:P:23:PRO:HA	1:P:35:LEU:HA	2.02	0.42
1:J:71:PRO:HB2	1:J:85:THR:CG2	2.50	0.42
1:M:79:SER:OG	1:M:80:CYS:N	2.53	0.41
1:E:62:TYR:CD2	1:N:128:LEU:HD22	2.55	0.41
1:U:10:ASN:HB3	1:U:15:GLY:O	2.20	0.41
1:U:98:GLN:OE1	1:U:98:GLN:N	2.52	0.41
1:E:60:LYS:HB3	1:E:61:ASN:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:41:VAL:HA	1:P:42:PRO:HD3	1.87	0.41
1:N:21:LEU:HB3	1:N:35:LEU:HB3	2.02	0.41
1:F:96:PHE:CG	1:F:105:ARG:HG2	2.55	0.41
1:J:81:ASP:N	1:J:81:ASP:OD1	2.47	0.41
1:K:56:SER:OG	1:K:57:ARG:N	2.54	0.41
1:O:110:THR:O	1:O:110:THR:HG22	2.20	0.41
1:V:131:ALA:O	1:V:132:TYR:HB2	2.21	0.41
1:E:11:ILE:O	1:N:110:THR:OG1	2.37	0.41
1:C:35:LEU:HD22	1:C:48:VAL:H	1.86	0.40
1:O:21:LEU:HB3	1:O:35:LEU:HB3	2.03	0.40
1:C:21:LEU:O	1:C:22:ASN:C	2.65	0.40
1:C:85:THR:OG1	1:C:86:ARG:N	2.54	0.40
1:C:101:THR:OG1	1:C:102:ASP:N	2.54	0.40
1:V:128:LEU:HB2	1:V:129:ASN:HA	2.03	0.40
1:G:105:ARG:NH2	1:T:39:GLY:O	2.54	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	130/133 (98%)	121 (93%)	8 (6%)	1 (1%)	16	54
1	B	130/133 (98%)	125 (96%)	4 (3%)	1 (1%)	16	54
1	C	130/133 (98%)	118 (91%)	10 (8%)	2 (2%)	8	40
1	D	130/133 (98%)	120 (92%)	10 (8%)	0	100	100
1	E	130/133 (98%)	125 (96%)	4 (3%)	1 (1%)	16	54
1	F	130/133 (98%)	126 (97%)	3 (2%)	1 (1%)	16	54
1	G	130/133 (98%)	121 (93%)	7 (5%)	2 (2%)	8	40
1	H	130/133 (98%)	124 (95%)	3 (2%)	3 (2%)	5	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	J	130/133 (98%)	124 (95%)	6 (5%)	0	100	100
1	K	130/133 (98%)	124 (95%)	3 (2%)	3 (2%)	5	28
1	L	130/133 (98%)	121 (93%)	7 (5%)	2 (2%)	8	40
1	M	130/133 (98%)	124 (95%)	5 (4%)	1 (1%)	16	54
1	N	130/133 (98%)	124 (95%)	6 (5%)	0	100	100
1	O	130/133 (98%)	121 (93%)	7 (5%)	2 (2%)	8	40
1	P	130/133 (98%)	121 (93%)	8 (6%)	1 (1%)	16	54
1	Q	130/133 (98%)	117 (90%)	13 (10%)	0	100	100
1	R	130/133 (98%)	124 (95%)	6 (5%)	0	100	100
1	S	130/133 (98%)	126 (97%)	3 (2%)	1 (1%)	16	54
1	T	130/133 (98%)	126 (97%)	3 (2%)	1 (1%)	16	54
1	U	130/133 (98%)	124 (95%)	6 (5%)	0	100	100
1	V	130/133 (98%)	121 (93%)	5 (4%)	4 (3%)	3	22
All	All	2860/2926 (98%)	2699 (94%)	135 (5%)	26 (1%)	16	51

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	GLY
1	C	126	ASP
1	H	101	THR
1	V	43	ALA
1	V	44	LEU
1	A	116	LEU
1	C	58	ASN
1	E	131	ALA
1	O	51	SER
1	P	75	THR
1	V	74	CYS
1	F	60	LYS
1	K	60	LYS
1	K	125	ILE
1	M	80	CYS
1	O	45	GLU
1	G	36	SER
1	S	38	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	V	128	LEU
1	L	79	SER
1	H	63	LYS
1	T	43	ALA
1	K	61	ASN
1	G	22	ASN
1	H	27	ASN
1	L	27	ASN

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	110/111 (99%)	110 (100%)	0	100	100
1	B	110/111 (99%)	110 (100%)	0	100	100
1	C	110/111 (99%)	110 (100%)	0	100	100
1	D	110/111 (99%)	110 (100%)	0	100	100
1	E	110/111 (99%)	110 (100%)	0	100	100
1	F	110/111 (99%)	109 (99%)	1 (1%)	70	79
1	G	110/111 (99%)	110 (100%)	0	100	100
1	H	110/111 (99%)	110 (100%)	0	100	100
1	I	110/111 (99%)	110 (100%)	0	100	100
1	J	110/111 (99%)	110 (100%)	0	100	100
1	K	110/111 (99%)	110 (100%)	0	100	100
1	L	110/111 (99%)	110 (100%)	0	100	100
1	M	110/111 (99%)	109 (99%)	1 (1%)	70	79
1	N	110/111 (99%)	110 (100%)	0	100	100
1	O	110/111 (99%)	110 (100%)	0	100	100
1	P	110/111 (99%)	110 (100%)	0	100	100
1	Q	110/111 (99%)	109 (99%)	1 (1%)	70	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	110/111 (99%)	110 (100%)	0	100	100
1	S	110/111 (99%)	110 (100%)	0	100	100
1	T	110/111 (99%)	110 (100%)	0	100	100
1	U	110/111 (99%)	110 (100%)	0	100	100
1	V	110/111 (99%)	110 (100%)	0	100	100
All	All	2420/2442 (99%)	2417 (100%)	3 (0%)	87	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	26	VAL
1	F	46	LYS
1	Q	24	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	C	37	GLN
1	L	70	ASN
1	L	87	GLN
1	D	65	GLN
1	M	65	GLN
1	E	61	ASN
1	E	69	GLN
1	E	87	GLN
1	F	77	ASN
1	O	22	ASN
1	G	65	GLN
1	G	87	GLN
1	S	127	GLN
1	J	70	ASN
1	U	127	GLN
1	U	129	ASN
1	K	65	GLN
1	V	22	ASN
1	V	65	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.

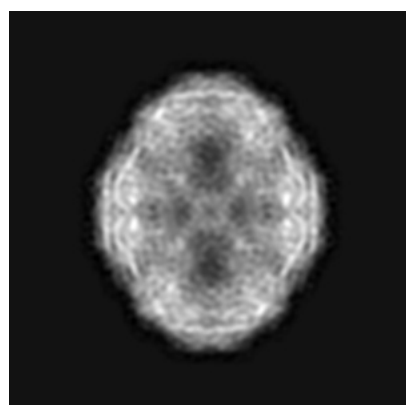
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23324. These allow visual inspection of the internal detail of the map and identification of artifacts.

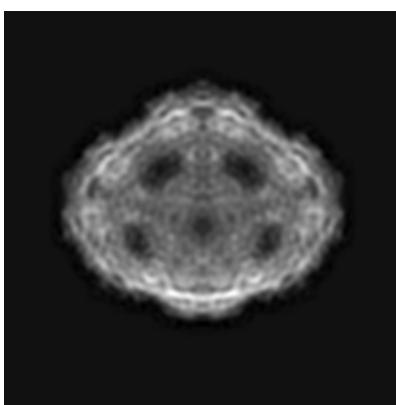
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

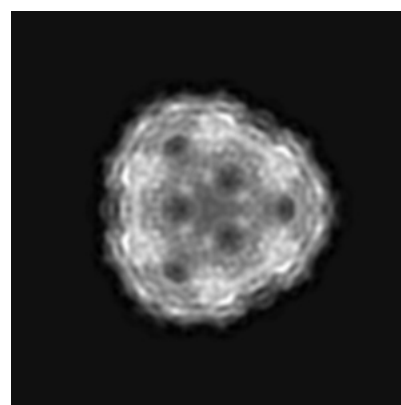
6.1.1 Primary map



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: 80



Y Index: 80

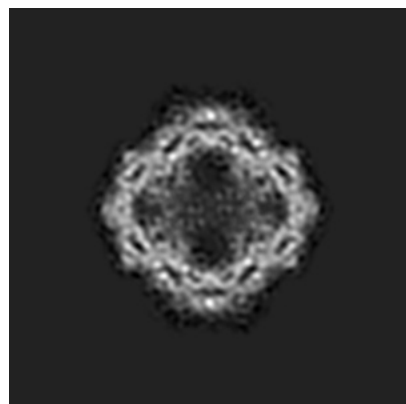


Z Index: 80

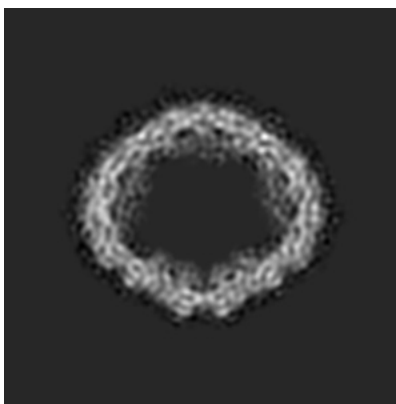
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 52



Y Index: 100

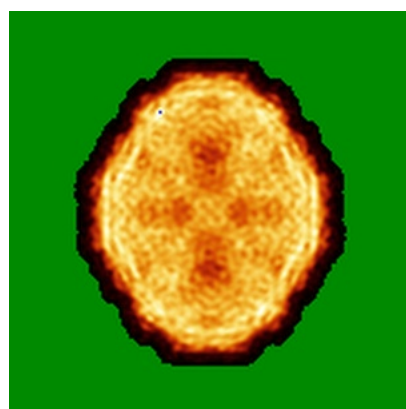


Z Index: 87

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

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

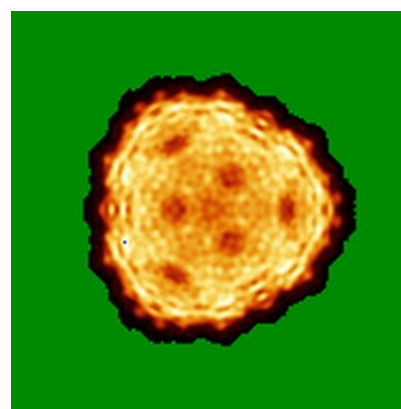
6.4.1 Primary map



X



Y

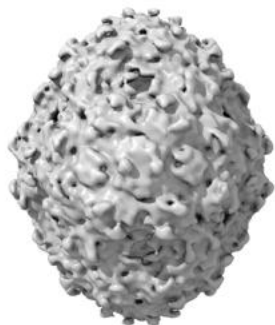


Z

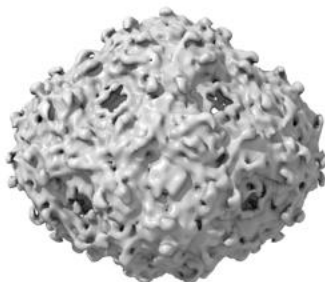
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

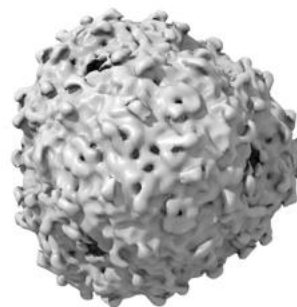
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

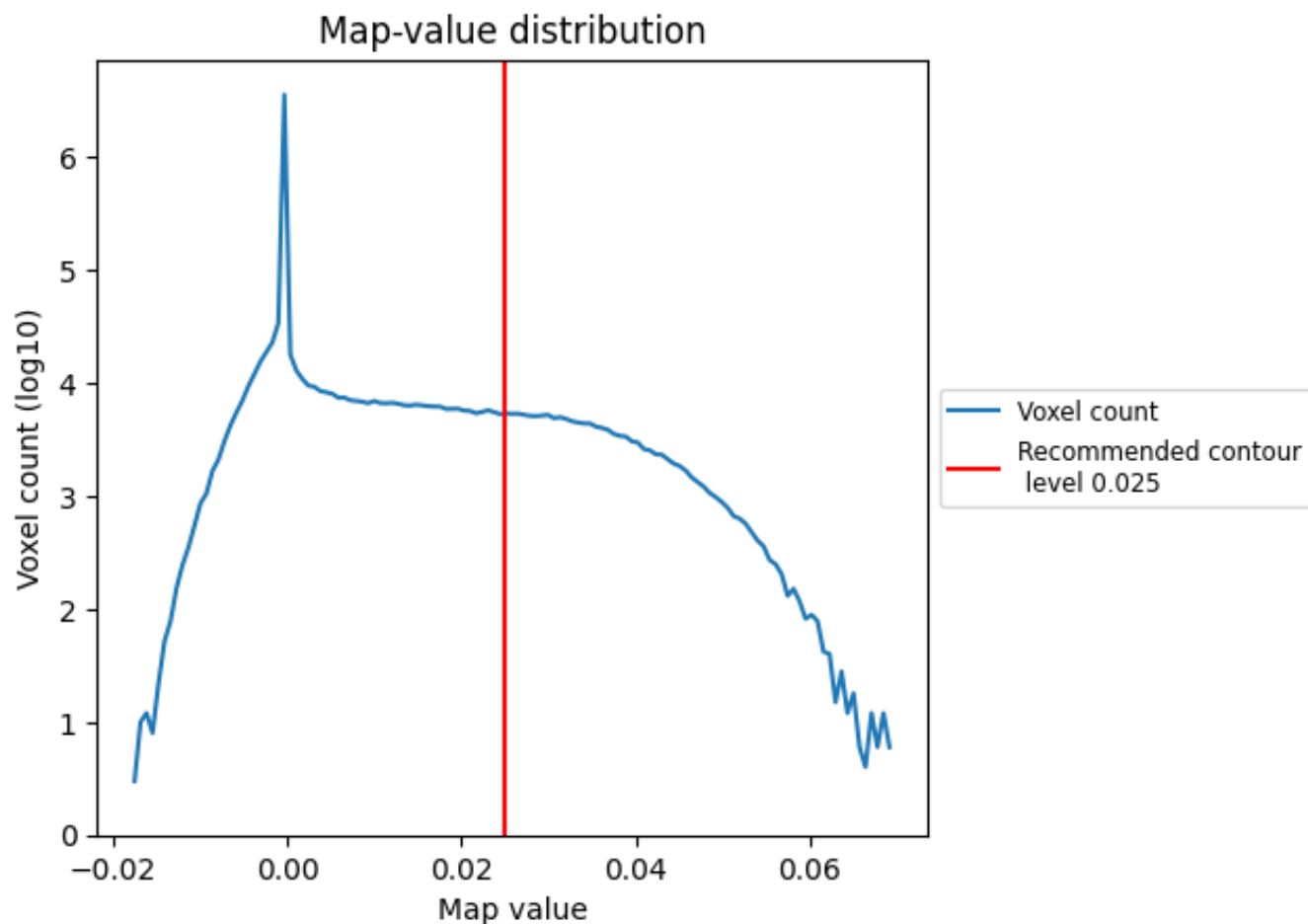
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

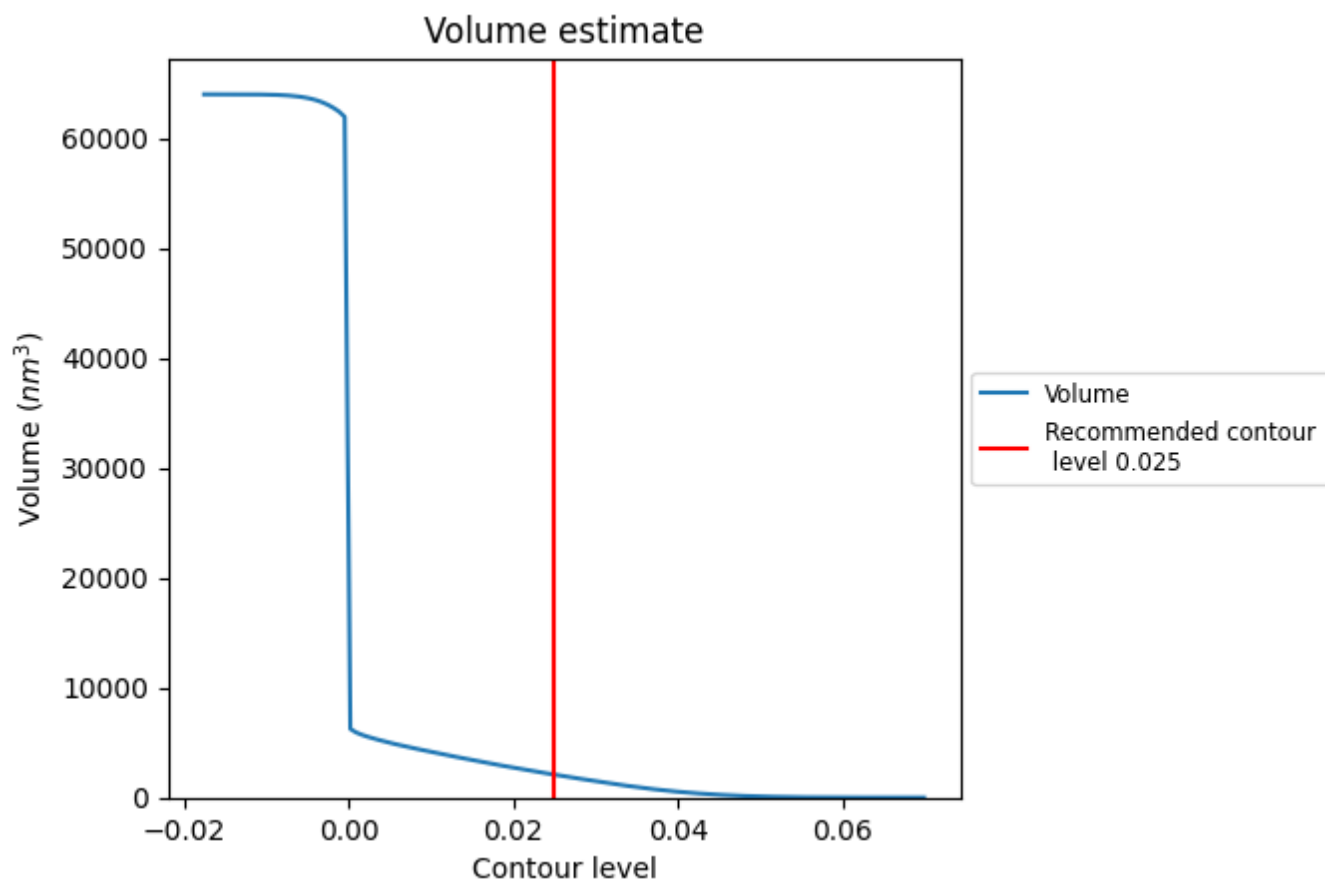
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

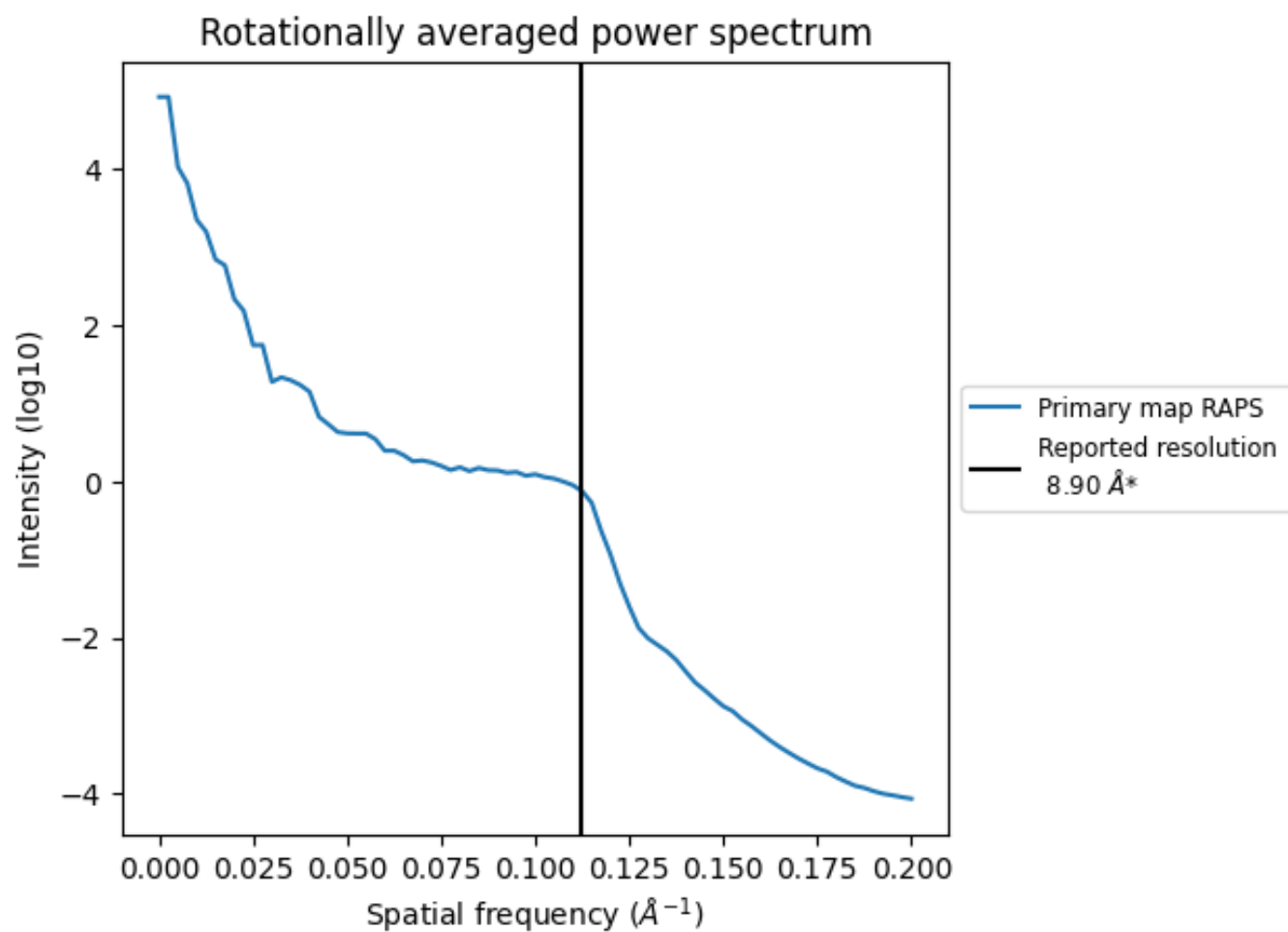
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2084 nm³; this corresponds to an approximate mass of 1882 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 ⓘ

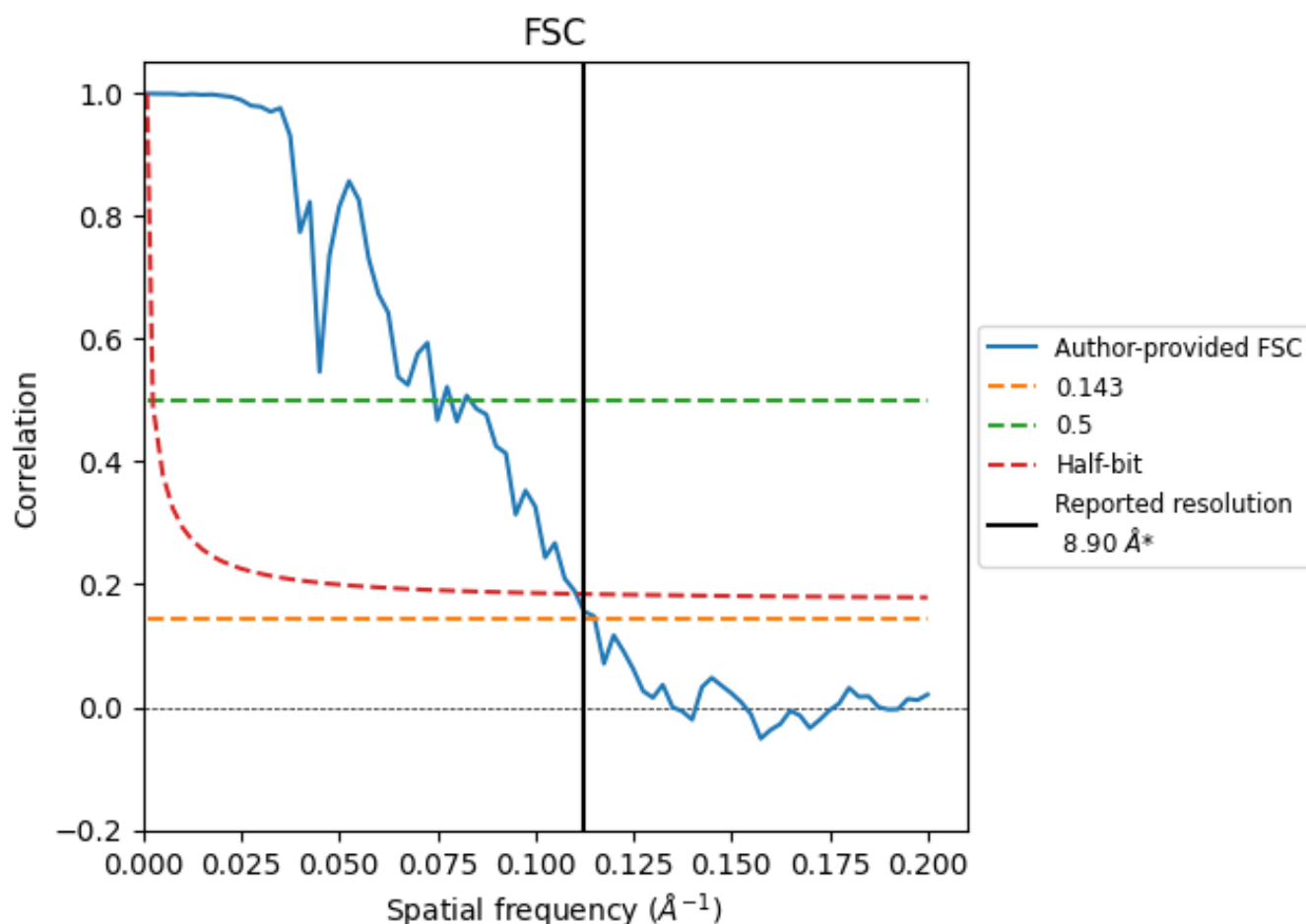


*Reported resolution corresponds to spatial frequency of 0.112 Å⁻¹

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 0.112 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.90	-	-
Author-provided FSC curve	8.68	13.44	9.06
Unmasked-calculated*	-	-	-

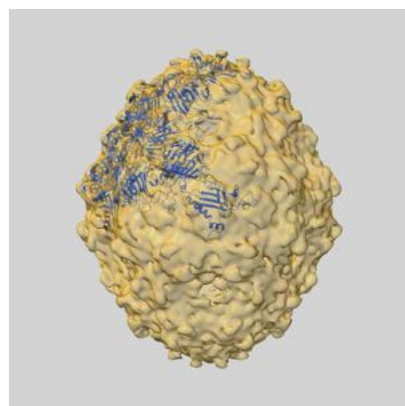
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

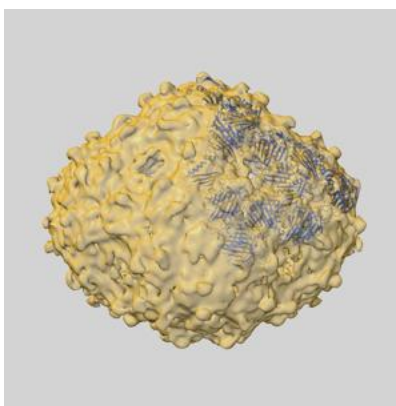
This section contains information regarding the fit between EMDB map EMD-23324 and PDB model 7LGH. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

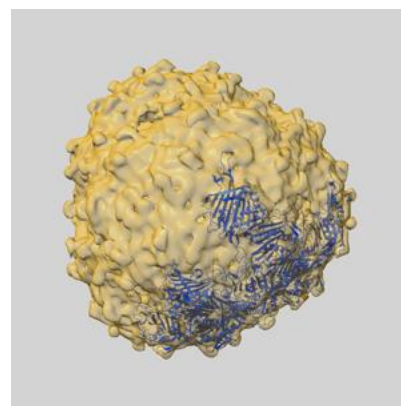
9.1.1 Map-model overlay [i](#)



X

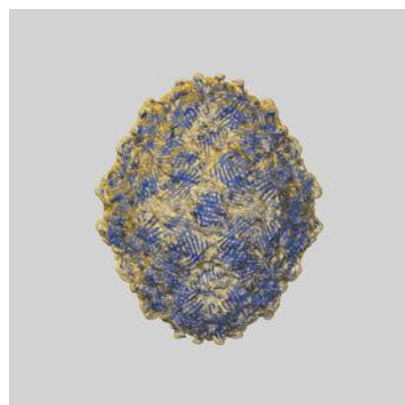


Y

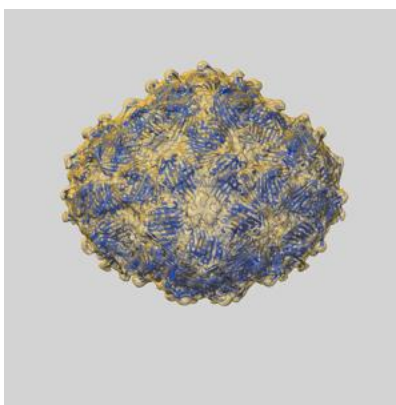


Z

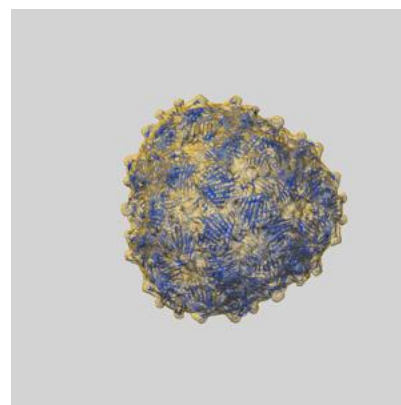
9.1.2 Map-model assembly overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

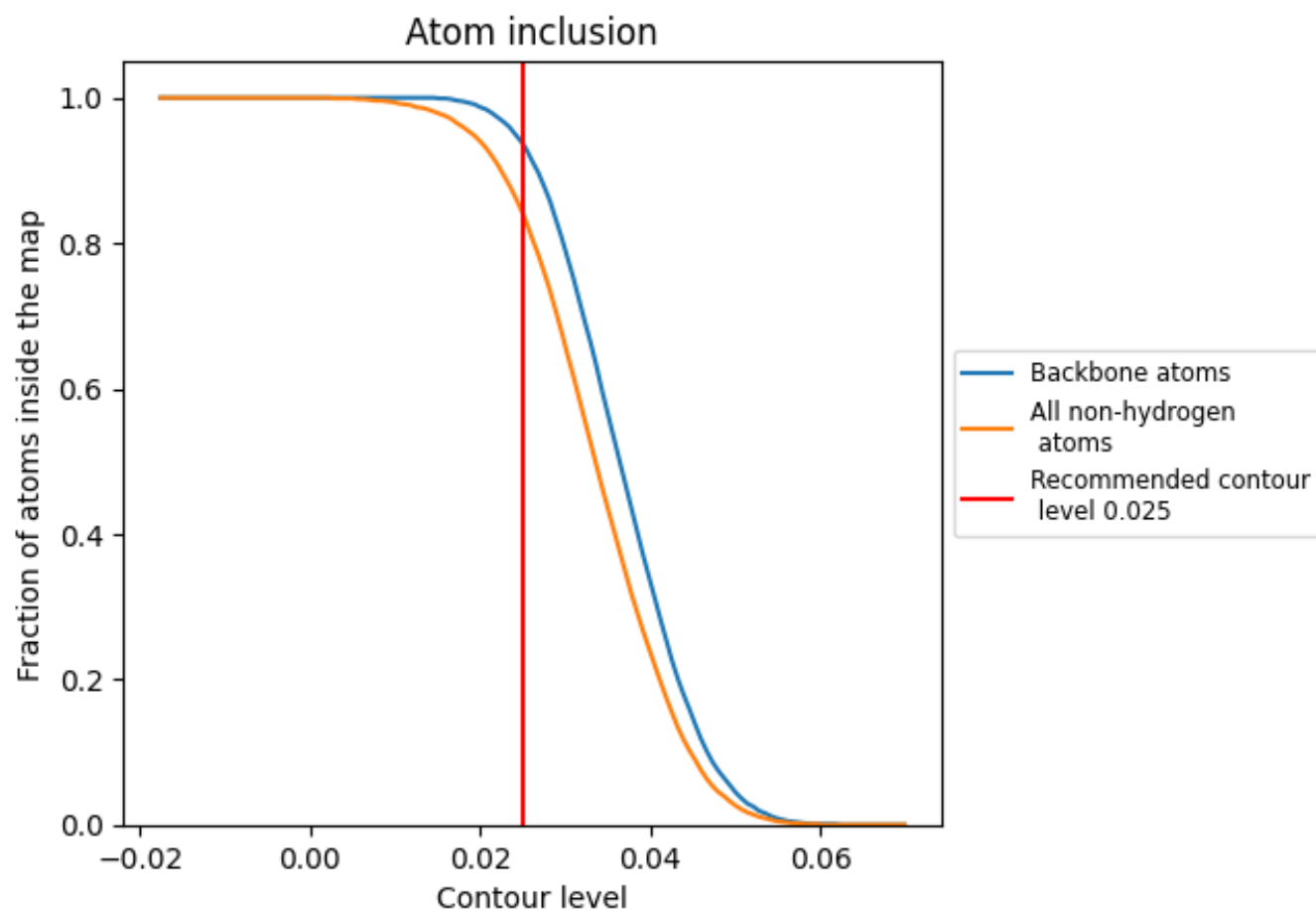


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 84% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8410	 0.1140
A	 0.8460	 0.1130
B	 0.7850	 0.1070
C	 0.8300	 0.1180
D	 0.8800	 0.1240
E	 0.8550	 0.1270
F	 0.8660	 0.1140
G	 0.8520	 0.1280
H	 0.8570	 0.1250
I	 0.8430	 0.1150
J	 0.8310	 0.1060
K	 0.8460	 0.1170
L	 0.8400	 0.1020
M	 0.8570	 0.1250
N	 0.8610	 0.0960
O	 0.8430	 0.1180
P	 0.8350	 0.1070
Q	 0.8660	 0.1340
R	 0.7860	 0.0950
S	 0.8470	 0.1220
T	 0.8250	 0.0970
U	 0.8430	 0.0980
V	 0.8110	 0.1220

