



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 10:54 PM UTC

PDB ID : 7N69 / pdb_00007n69
EMDB ID : EMD-24201
Title : Pre-fusion state 2 of EEEV with localized reconstruction
Authors : Chen, C.-L.; Kuhn, R.J.; Klose, T.
Deposited on : 2021-06-07
Resolution : 14.10 Å(reported)
Based on initial model : 6MX4

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

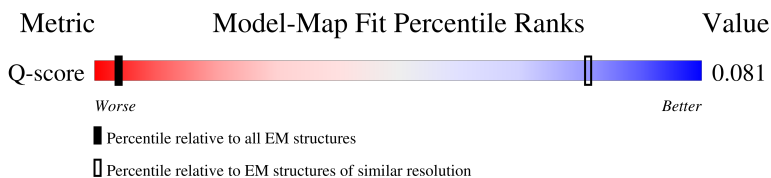
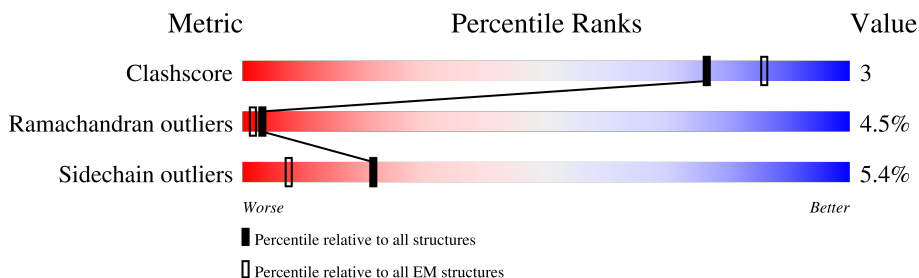
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 14.10 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.



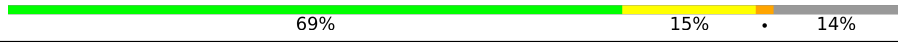
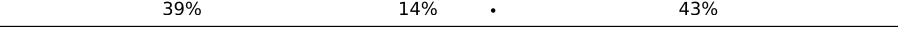
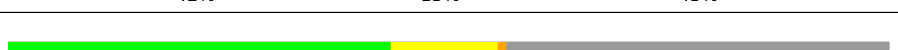
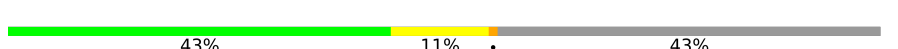
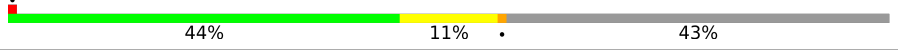
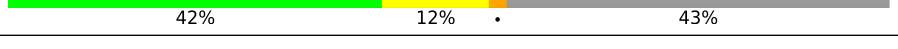
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	53 (13.60 - 14.50)

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	441	
1	C	441	
1	E	441	
1	G	441	

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Mol	Chain	Length	Quality of chain
1	I	441	
1	K	441	
2	B	420	
2	D	420	
2	F	420	
2	H	420	
2	J	420	
2	L	420	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 28686 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 Spike glycoprotein E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	381	Total	C	N	O	S	0	0
			2907	1840	485	562	20		
1	C	381	Total	C	N	O	S	0	0
			2907	1840	485	562	20		
1	E	381	Total	C	N	O	S	0	0
			2907	1840	485	562	20		
1	G	381	Total	C	N	O	S	0	0
			2907	1840	485	562	20		
1	I	381	Total	C	N	O	S	0	0
			2907	1840	485	562	20		
1	K	381	Total	C	N	O	S	0	0
			2907	1840	485	562	20		

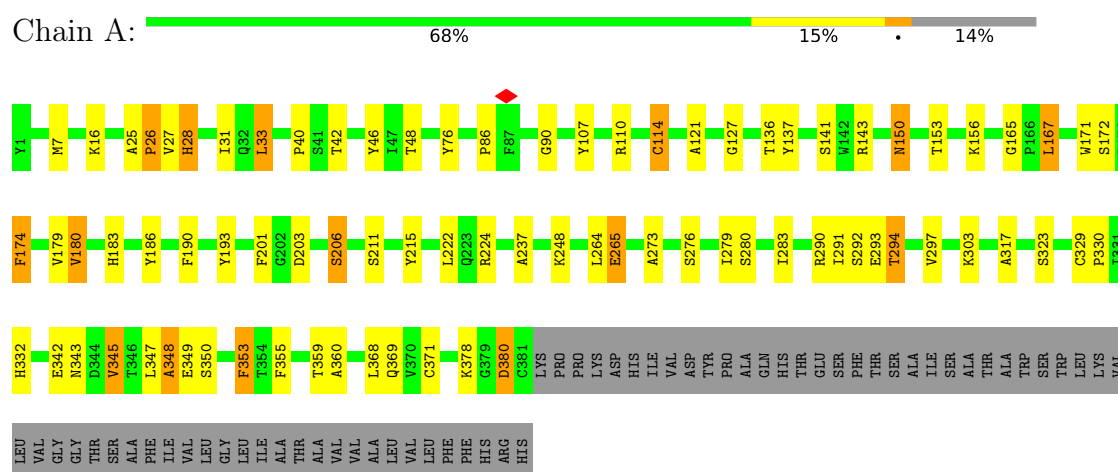
- Molecule 2 is a protein called Spike glycoprotein E2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	238	Total	C	N	O	S	0	0
			1874	1179	348	336	11		
2	D	238	Total	C	N	O	S	0	0
			1874	1179	348	336	11		
2	F	238	Total	C	N	O	S	0	0
			1874	1179	348	336	11		
2	H	238	Total	C	N	O	S	0	0
			1874	1179	348	336	11		
2	J	238	Total	C	N	O	S	0	0
			1874	1179	348	336	11		
2	L	238	Total	C	N	O	S	0	0
			1874	1179	348	336	11		

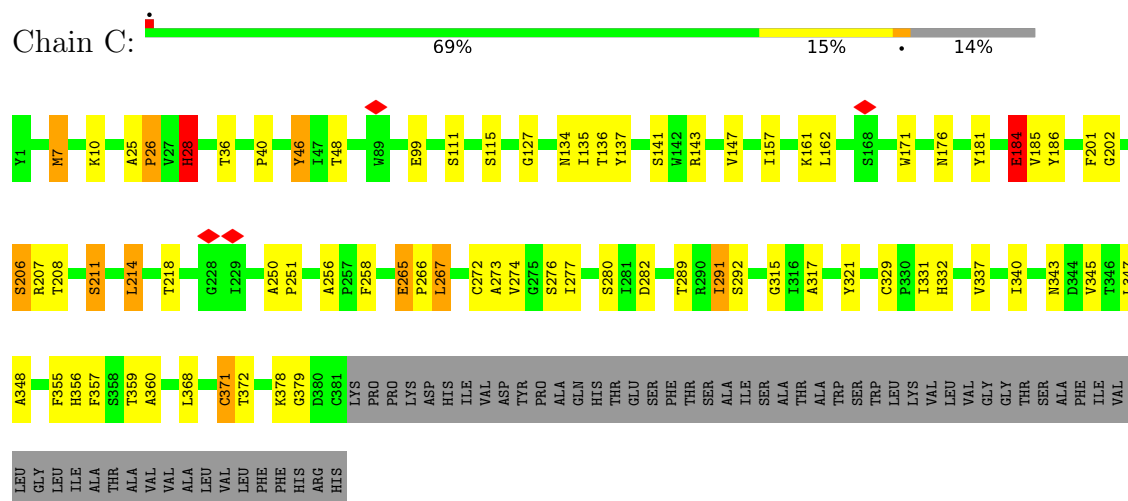
3 Residue-property plots [i](#)

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: Spike glycoprotein E1



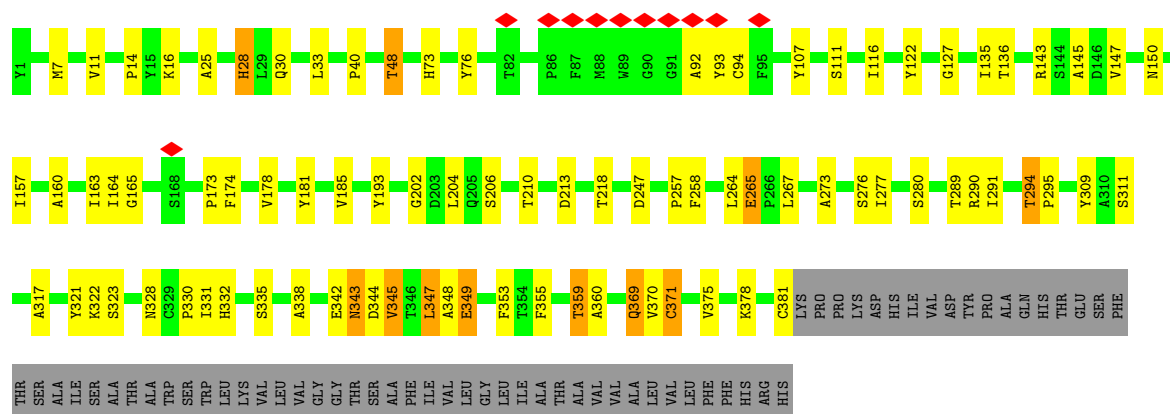
• Molecule 1: Spike glycoprotein E1



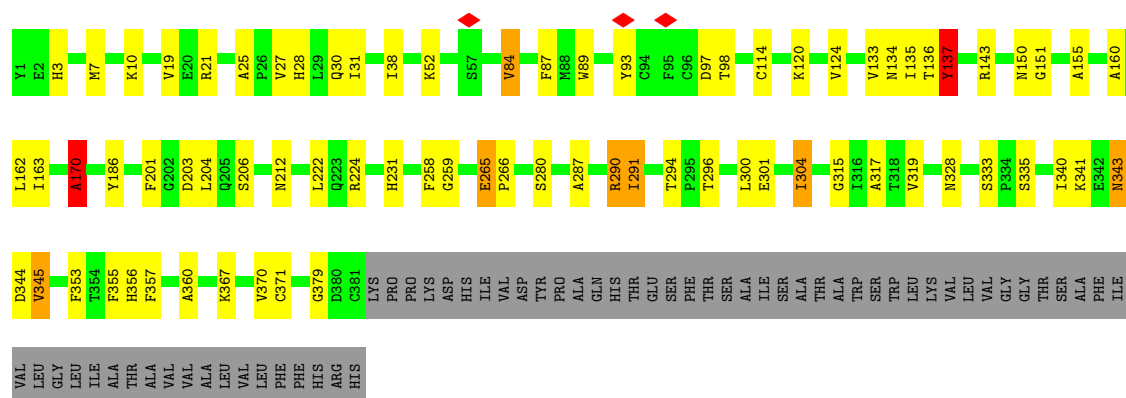
• Molecule 1: Spike glycoprotein E1



- Molecule 1: Spike glycoprotein E1



- Molecule 1: Spike glycoprotein E1



- Molecule 1: Spike glycoprotein E1



Response	Percentage
Current government is the best	43%
Opposition is the best	12%
Neither is the best	43%



Device Type	Percentage
Smartphones	43%
Tablets	11%
Other mobile devices	43%

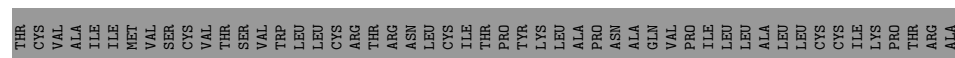
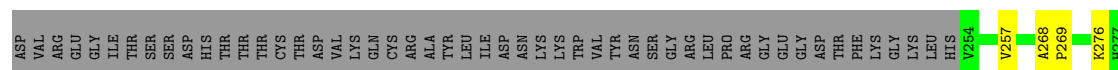
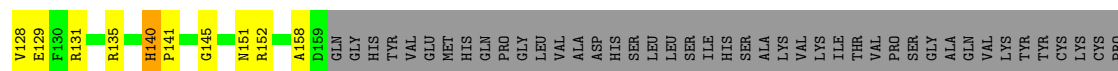


Frequency	Percentage
Daily	44%
Weekly	11%
Monthly	0%
Never	43%





Chain L: 42% 12% 43%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	192060	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.010	Depositor
Minimum map value	-3.203	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	503.424, 503.424, 503.424	wwPDB
Map dimensions	144, 144, 144	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.496, 3.496, 3.496	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	1.27	0/2984	1.55	31/4070 (0.8%)
1	C	1.26	0/2984	1.55	26/4070 (0.6%)
1	E	1.28	0/2984	1.57	34/4070 (0.8%)
1	G	1.25	0/2984	1.57	31/4070 (0.8%)
1	I	1.26	0/2984	1.56	32/4070 (0.8%)
1	K	1.24	0/2984	1.52	28/4070 (0.7%)
2	B	1.29	0/1930	1.74	49/2630 (1.9%)
2	D	1.31	0/1930	1.74	33/2630 (1.3%)
2	F	1.29	0/1930	1.65	36/2630 (1.4%)
2	H	1.30	0/1930	1.64	31/2630 (1.2%)
2	J	1.28	0/1930	1.66	31/2630 (1.2%)
2	L	1.30	1/1930 (0.1%)	1.68	32/2630 (1.2%)
All	All	1.27	1/29484 (0.0%)	1.61	394/40200 (1.0%)

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	2
1	C	0	4
1	E	0	4
1	G	0	4
1	I	0	2
1	K	0	3
2	D	0	2
2	F	0	3
2	H	0	1
2	J	0	3
2	L	0	2
All	All	0	30

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	42	ALA	CA-C	-5.04	1.50	1.53

All (394) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	85	THR	N-CA-C	-10.58	98.61	112.68
2	D	268	ALA	N-CA-C	-9.76	99.39	108.07
2	J	85	THR	N-CA-C	-8.79	102.72	113.97
2	B	104	PRO	N-CA-C	8.64	121.24	110.70
2	L	131	ARG	N-CA-C	-8.50	98.39	108.25
1	K	203	ASP	CA-CB-CG	8.43	121.03	112.60
2	B	141	PRO	N-CA-C	8.12	120.61	110.70
2	D	87	ALA	N-CA-C	-8.10	100.93	108.22
2	H	133	VAL	N-CA-C	-8.09	103.96	113.42
2	H	94	HIS	CA-CB-CG	8.06	121.86	113.80
1	E	215	TYR	N-CA-C	-7.96	95.93	108.90
2	J	80	ASN	N-CA-C	-7.88	102.58	112.90
1	I	84	VAL	N-CA-C	7.82	118.60	110.62
1	C	258	PHE	N-CA-C	-7.68	102.11	112.94
2	D	104	PRO	N-CA-C	7.60	119.97	110.70
1	G	11	VAL	N-CA-C	-7.60	105.14	113.43
1	K	292	SER	N-CA-C	-7.55	104.09	113.38
2	B	85	THR	N-CA-C	-7.53	102.66	112.68
2	B	51	ALA	N-CA-C	-7.49	94.85	110.80
1	C	28	HIS	CA-CB-CG	7.43	121.23	113.80
2	D	339	GLU	N-CA-C	-7.41	101.42	111.87
1	E	359	THR	N-CA-C	-7.41	97.92	108.96
2	J	107	ASP	N-CA-C	-7.37	105.20	114.56
1	A	186	TYR	N-CA-C	-7.37	96.31	108.76
1	A	156	LYS	N-CA-C	-7.32	104.20	113.72
2	D	141	PRO	N-CA-C	7.26	119.56	110.70
2	H	92	VAL	N-CA-C	-7.24	106.03	112.12
2	B	103	CYS	N-CA-C	-7.24	98.34	108.76
1	E	149	VAL	N-CA-C	-7.22	104.81	111.67
2	J	104	PRO	N-CA-C	7.21	119.50	110.70
1	C	337	VAL	N-CA-C	-7.20	105.99	112.90
1	I	203	ASP	CA-CB-CG	7.17	119.77	112.60
1	I	345	VAL	N-CA-C	-7.14	97.13	107.78
2	B	325	TYR	N-CA-C	-7.12	96.72	108.76
1	C	202	GLY	N-CA-C	-7.09	105.02	115.72
1	G	163	ILE	N-CA-C	-7.03	98.26	108.11
1	E	19	VAL	N-CA-C	-7.00	97.09	107.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	320	GLY	N-CA-C	-6.99	104.54	116.01
1	G	276	SER	N-CA-C	-6.98	98.47	109.50
1	K	174	PHE	CA-CB-CG	-6.89	106.91	113.80
2	F	119	ARG	N-CA-C	-6.85	93.91	107.69
2	L	59	GLY	N-CA-C	-6.85	103.03	111.45
2	J	316	PHE	CA-CB-CG	-6.85	106.95	113.80
1	G	202	GLY	N-CA-C	-6.84	104.79	116.01
1	C	181	TYR	N-CA-C	-6.83	105.47	113.88
1	A	28	HIS	CA-CB-CG	6.83	120.63	113.80
2	L	151	ASN	CA-CB-CG	-6.81	105.79	112.60
1	I	258	PHE	CA-CB-CG	-6.78	107.03	113.80
2	B	320	GLY	N-CA-C	-6.77	105.76	115.64
2	B	53	PHE	N-CA-C	-6.75	99.30	110.17
1	I	360	ALA	N-CA-C	-6.75	102.44	110.41
1	I	97	ASP	N-CA-C	-6.74	106.25	114.75
1	E	293	GLU	N-CA-C	-6.72	99.26	109.95
2	L	80	ASN	N-CA-C	-6.68	105.13	113.28
1	C	356	HIS	CA-CB-CG	-6.68	107.12	113.80
2	L	94	HIS	CA-CB-CG	-6.66	107.14	113.80
1	K	204	LEU	N-CA-C	-6.65	98.56	109.40
1	I	206	SER	N-CA-C	-6.64	100.86	108.49
1	E	296	THR	N-CA-C	-6.62	96.43	108.02
2	H	51	ALA	N-CA-C	-6.61	96.72	110.80
1	I	114	CYS	N-CA-C	-6.57	103.42	112.03
1	A	280	SER	N-CA-C	-6.55	98.05	108.73
1	C	276	SER	N-CA-C	-6.53	99.18	109.50
1	E	163	ILE	N-CA-C	-6.52	98.98	108.11
2	J	133	VAL	N-CA-C	-6.52	105.20	113.22
1	I	356	HIS	CA-CB-CG	-6.52	107.28	113.80
1	I	343	ASN	N-CA-C	-6.51	102.98	111.71
2	D	276	LYS	N-CA-C	-6.50	99.67	108.24
1	A	180	VAL	CA-C-N	6.49	128.98	120.28
1	A	180	VAL	C-N-CA	6.49	128.98	120.28
1	I	163	ILE	N-CA-C	-6.48	99.04	108.11
1	G	218	THR	N-CA-C	-6.46	105.44	113.38
1	E	345	VAL	N-CA-C	-6.43	98.78	108.17
1	G	360	ALA	N-CA-C	-6.43	103.61	112.03
1	E	337	VAL	N-CA-C	-6.39	106.51	112.83
2	J	300	ASP	CA-CB-CG	6.37	118.97	112.60
1	G	328	ASN	N-CA-C	-6.35	97.93	108.34
1	I	52	LYS	N-CA-C	-6.33	98.58	108.90
1	C	202	GLY	CA-C-N	6.32	128.75	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	202	GLY	C-N-CA	6.32	128.75	120.28
1	C	214	LEU	N-CA-C	-6.32	99.81	109.41
2	B	319	THR	N-CA-C	-6.29	105.09	112.89
1	G	33	LEU	N-CA-CB	6.29	120.00	109.94
2	H	99	ILE	N-CA-C	-6.28	99.18	108.85
2	D	80	ASN	N-CA-C	-6.28	103.73	112.45
1	E	218	THR	N-CA-C	-6.27	105.10	114.64
1	G	111	SER	N-CA-C	-6.26	100.72	110.42
2	D	111	VAL	N-CA-C	-6.23	99.44	108.17
2	B	140	HIS	CA-C-N	6.22	126.79	120.38
2	B	140	HIS	C-N-CA	6.22	126.79	120.38
2	B	94	HIS	CA-CB-CG	6.22	120.02	113.80
1	A	143	ARG	N-CA-C	-6.18	104.22	112.94
1	G	210	THR	N-CA-C	-6.17	105.69	112.72
1	A	347	LEU	N-CA-CB	6.16	119.02	109.85
1	E	169	SER	N-CA-C	-6.14	97.71	110.80
2	D	140	HIS	CA-C-N	6.14	126.71	120.38
2	D	140	HIS	C-N-CA	6.14	126.71	120.38
2	D	85	THR	N-CA-C	-6.12	101.72	111.02
2	H	294	THR	N-CA-C	-6.12	100.01	109.24
1	I	137	TYR	N-CA-C	-6.09	98.15	108.26
1	G	143	ARG	N-CA-C	-6.09	103.19	112.99
2	F	34	GLU	N-CA-C	-6.08	104.84	112.93
1	G	28	HIS	CA-CB-CG	6.07	119.87	113.80
1	C	273	ALA	N-CA-C	-6.06	105.06	112.88
1	I	353	PHE	N-CA-C	-6.06	97.96	108.69
2	L	107	ASP	N-CA-C	-6.06	107.12	114.75
1	E	297	VAL	N-CA-C	-6.04	99.71	108.17
2	F	54	GLY	N-CA-C	-6.04	106.38	115.32
1	K	28	HIS	CA-CB-CG	6.03	119.83	113.80
2	D	316	PHE	CA-CB-CG	-6.02	107.78	113.80
2	B	67	PHE	CA-CB-CG	6.01	119.81	113.80
1	A	25	ALA	CA-C-N	6.01	127.35	119.84
1	A	25	ALA	C-N-CA	6.01	127.35	119.84
2	L	83	VAL	N-CA-C	-6.01	99.63	109.12
2	H	276	LYS	N-CA-C	-6.01	100.27	108.38
2	L	145	GLY	CA-C-N	5.99	128.67	120.35
2	L	145	GLY	C-N-CA	5.99	128.67	120.35
1	G	145	ALA	CA-C-N	5.97	129.96	121.42
1	G	145	ALA	C-N-CA	5.97	129.96	121.42
2	B	54	GLY	N-CA-C	-5.96	106.50	115.32
2	L	288	HIS	N-CA-C	-5.95	102.86	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	55	LEU	N-CA-C	-5.92	97.94	108.13
2	L	82	HIS	N-CA-C	-5.91	99.37	109.24
2	D	113	PHE	N-CA-C	-5.91	99.56	109.07
1	E	288	PHE	N-CA-C	-5.91	100.52	109.85
1	I	344	ASP	CA-CB-CG	5.90	118.50	112.60
2	D	295	ARG	N-CA-C	-5.89	99.46	108.76
1	I	151	GLY	CA-C-N	5.88	128.16	120.28
1	I	151	GLY	C-N-CA	5.88	128.16	120.28
2	H	293	THR	N-CA-C	-5.87	99.83	109.40
1	G	48	THR	N-CA-C	-5.87	100.13	109.23
2	H	58	ASP	CA-C-N	5.87	126.85	121.86
2	H	58	ASP	C-N-CA	5.87	126.85	121.86
2	J	267	LEU	N-CA-C	-5.87	98.84	108.76
1	E	138	GLY	N-CA-C	-5.84	105.74	112.29
1	C	211	SER	N-CA-CB	5.84	120.36	110.49
2	F	10	LYS	N-CA-C	-5.83	103.90	111.71
2	D	86	SER	N-CA-C	-5.82	104.40	112.03
2	B	48	GLN	N-CA-C	-5.81	97.70	107.99
1	G	348	ALA	N-CA-C	-5.81	105.07	113.21
1	G	345	VAL	N-CA-C	-5.81	99.69	108.17
2	H	87	ALA	N-CA-C	-5.81	102.99	108.22
1	I	186	TYR	N-CA-C	-5.80	98.95	108.76
1	C	359	THR	N-CA-C	-5.80	100.32	108.96
2	J	55	LEU	N-CA-C	-5.79	98.06	108.48
1	K	103	MET	N-CA-C	-5.79	99.29	108.73
1	K	357	PHE	CA-C-N	5.77	131.63	122.62
1	K	357	PHE	C-N-CA	5.77	131.63	122.62
2	F	104	PRO	N-CA-C	5.77	117.74	110.70
1	E	376	THR	N-CA-C	-5.77	99.61	109.24
1	I	10	LYS	N-CA-C	-5.76	98.22	108.13
2	H	80	ASN	N-CA-C	-5.75	105.46	112.88
1	G	202	GLY	CA-C-N	5.75	127.98	120.28
1	G	202	GLY	C-N-CA	5.75	127.98	120.28
1	K	334	PRO	N-CA-C	-5.74	107.17	114.35
2	D	81	LEU	N-CA-C	-5.73	97.84	107.99
1	A	293	GLU	N-CA-C	-5.73	106.33	113.38
2	D	83	VAL	N-CA-C	-5.73	101.48	109.45
1	A	353	PHE	N-CA-C	-5.73	98.55	108.69
1	E	340	ILE	N-CA-C	-5.73	100.17	108.87
2	B	103	CYS	CA-C-N	5.72	126.28	120.38
2	B	103	CYS	C-N-CA	5.72	126.28	120.38
2	D	327	TRP	N-CA-C	-5.72	96.19	107.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	326	THR	N-CA-C	-5.72	99.92	109.24
1	E	170	ALA	N-CA-C	-5.70	105.99	113.17
2	F	336	TRP	N-CA-C	-5.70	104.08	111.71
2	F	69	ASN	N-CA-C	-5.68	106.39	113.38
2	J	82	HIS	N-CA-C	-5.68	100.15	109.40
2	J	33	ILE	CA-C-N	5.66	127.79	120.44
2	J	33	ILE	C-N-CA	5.66	127.79	120.44
2	F	58	ASP	CA-C-N	5.65	126.66	121.86
2	F	58	ASP	C-N-CA	5.65	126.66	121.86
1	K	165	GLY	CA-C-N	5.65	125.66	119.90
1	K	165	GLY	C-N-CA	5.65	125.66	119.90
1	K	343	ASN	N-CA-C	-5.64	104.99	112.94
1	C	184	GLU	N-CA-C	-5.62	98.82	110.80
2	B	92	VAL	N-CA-C	-5.62	107.40	112.12
2	L	331	PRO	N-CA-C	-5.62	103.84	110.70
2	H	53	PHE	N-CA-C	-5.62	101.12	110.17
1	E	347	LEU	N-CA-CB	5.62	118.22	109.85
2	B	127	LYS	CA-C-N	5.61	128.01	120.50
2	B	127	LYS	C-N-CA	5.61	128.01	120.50
2	B	263	CYS	CA-C-N	5.61	132.06	121.97
2	B	263	CYS	C-N-CA	5.61	132.06	121.97
2	F	116	GLY	CA-C-N	5.60	126.84	119.84
2	F	116	GLY	C-N-CA	5.60	126.84	119.84
2	D	68	MET	N-CA-C	-5.60	101.91	110.14
1	I	21	ARG	N-CA-C	-5.59	101.70	110.14
2	B	39	ASP	CA-C-N	5.59	129.19	120.75
2	B	39	ASP	C-N-CA	5.59	129.19	120.75
2	H	90	SER	N-CA-C	-5.59	99.42	108.52
2	L	335	VAL	N-CA-C	-5.59	100.25	108.85
2	F	100	LEU	N-CA-C	-5.58	98.82	108.69
2	H	69	ASN	N-CA-C	-5.58	106.47	113.28
2	D	293	THR	CA-CB-OG1	5.58	117.96	109.60
1	K	7	MET	CA-C-N	5.57	125.50	119.76
1	K	7	MET	C-N-CA	5.57	125.50	119.76
2	H	26	ARG	N-CA-C	-5.54	100.36	109.40
1	E	241	PHE	CA-CB-CG	-5.54	108.26	113.80
2	L	79	ASP	CA-CB-CG	5.54	118.14	112.60
2	L	320	GLY	N-CA-C	-5.54	107.38	115.63
2	H	297	LEU	N-CA-C	-5.54	106.41	112.72
2	F	338	GLN	N-CA-C	-5.53	106.38	113.02
1	E	261	SER	CA-C-N	5.53	127.98	120.63
1	E	261	SER	C-N-CA	5.53	127.98	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	329	ASN	N-CA-CB	5.53	119.83	110.49
2	J	54	GLY	N-CA-C	-5.52	107.16	115.32
1	A	156	LYS	CA-C-N	5.51	128.01	120.35
1	A	156	LYS	C-N-CA	5.51	128.01	120.35
1	K	208	THR	N-CA-C	-5.50	101.06	109.41
1	A	174	PHE	N-CA-C	-5.49	98.97	108.69
1	E	98	THR	N-CA-C	-5.49	107.58	114.56
2	L	75	SER	N-CA-C	-5.49	101.00	109.52
2	F	122	CYS	N-CA-C	-5.48	100.77	109.59
1	I	304	ILE	N-CA-C	-5.46	100.02	107.99
2	L	276	LYS	N-CA-C	-5.46	101.04	108.24
2	F	276	LYS	N-CA-C	-5.45	101.04	108.24
1	A	165	GLY	CA-C-N	5.43	126.63	119.84
1	A	165	GLY	C-N-CA	5.43	126.63	119.84
1	C	273	ALA	CA-C-N	5.43	127.77	120.50
1	C	273	ALA	C-N-CA	5.43	127.77	120.50
2	D	19	CYS	CA-C-N	5.43	125.51	119.32
2	D	19	CYS	C-N-CA	5.43	125.51	119.32
1	I	340	ILE	N-CA-C	-5.42	100.63	108.71
2	F	293	THR	N-CA-C	-5.42	100.57	109.40
1	E	378	LYS	N-CA-C	-5.42	100.49	108.99
1	E	72	PRO	N-CA-C	-5.41	107.08	114.98
1	G	174	PHE	N-CA-C	-5.41	102.14	109.54
1	K	55	VAL	N-CA-C	-5.40	99.17	107.71
1	E	343	ASN	N-CA-C	-5.40	105.65	113.21
2	D	128	VAL	N-CA-C	-5.40	100.55	108.11
2	J	333	LYS	N-CA-C	-5.40	100.38	109.07
1	A	360	ALA	N-CA-C	-5.40	105.65	113.21
2	J	83	VAL	N-CA-C	-5.40	100.59	109.12
2	J	46	ARG	N-CA-C	-5.40	100.38	109.07
1	A	48	THR	N-CA-C	-5.39	100.88	109.23
2	H	51	ALA	N-CA-CB	5.38	119.59	110.49
2	B	68	MET	N-CA-C	-5.38	98.46	107.99
1	I	25	ALA	CA-C-N	5.38	126.56	119.84
1	I	25	ALA	C-N-CA	5.38	126.56	119.84
2	J	331	PRO	CA-C-N	5.37	126.55	119.84
2	J	331	PRO	C-N-CA	5.37	126.55	119.84
1	G	73	HIS	N-CA-C	-5.37	103.29	108.07
2	B	337	ALA	CA-C-N	5.36	127.46	120.28
2	B	337	ALA	C-N-CA	5.36	127.46	120.28
2	H	330	HIS	CA-C-N	5.35	125.89	120.38
2	H	330	HIS	C-N-CA	5.35	125.89	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	104	PRO	CA-C-O	-5.34	112.81	120.56
2	L	74	LYS	N-CA-CB	5.34	119.51	110.49
1	C	348	ALA	CA-C-N	5.34	127.97	120.28
1	C	348	ALA	C-N-CA	5.34	127.97	120.28
1	K	242	GLU	CA-C-N	5.33	127.43	120.28
1	K	242	GLU	C-N-CA	5.33	127.43	120.28
1	C	7	MET	CA-C-N	5.33	125.25	119.76
1	C	7	MET	C-N-CA	5.33	125.25	119.76
1	C	340	ILE	N-CA-C	-5.33	100.77	108.71
2	L	99	ILE	N-CA-C	-5.33	100.64	108.85
2	F	32	ALA	CA-C-N	5.33	127.64	120.50
2	F	32	ALA	C-N-CA	5.33	127.64	120.50
2	B	22	CYS	N-CA-C	-5.32	101.21	109.14
2	F	145	GLY	CA-C-N	5.32	127.74	120.35
2	F	145	GLY	C-N-CA	5.32	127.74	120.35
2	H	339	GLU	N-CA-C	-5.32	106.75	113.18
1	G	322	LYS	N-CA-C	-5.31	100.24	108.90
1	K	276	SER	N-CA-C	-5.31	101.11	109.50
1	A	273	ALA	N-CA-C	-5.30	105.51	112.41
2	J	331	PRO	N-CA-C	-5.29	104.24	110.70
2	D	298	GLY	N-CA-C	-5.29	104.47	112.41
2	L	10	LYS	N-CA-C	-5.29	104.00	110.61
2	D	22	CYS	N-CA-C	-5.29	101.26	109.14
2	L	104	PRO	CA-C-O	-5.29	112.89	120.56
1	C	291	ILE	N-CA-CB	5.29	118.02	111.41
1	E	206	SER	N-CA-C	-5.28	99.55	110.80
1	I	301	GLU	N-CA-C	-5.28	100.69	108.99
2	H	54	GLY	N-CA-C	-5.28	107.75	115.72
2	L	46	ARG	N-CA-C	-5.28	100.57	109.07
2	H	9	TYR	CA-C-N	5.28	127.35	120.28
2	H	9	TYR	C-N-CA	5.28	127.35	120.28
2	B	60	VAL	N-CA-C	5.27	116.34	108.54
2	J	116	GLY	CA-C-N	5.27	125.57	119.93
2	J	116	GLY	C-N-CA	5.27	125.57	119.93
2	F	106	GLY	CA-C-N	5.26	127.33	120.28
2	F	106	GLY	C-N-CA	5.26	127.33	120.28
2	B	142	PRO	N-CA-C	-5.26	101.64	112.47
2	D	331	PRO	CA-C-N	5.25	126.40	119.84
2	D	331	PRO	C-N-CA	5.25	126.40	119.84
2	F	36	VAL	N-CA-C	-5.24	100.32	108.81
2	F	102	GLN	N-CA-C	-5.24	99.98	108.52
1	G	343	ASN	CA-CB-CG	-5.24	107.36	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	TYR	N-CA-C	-5.24	100.37	108.90
2	L	287	ASP	N-CA-C	-5.24	106.94	113.38
1	G	280	SER	N-CA-C	-5.22	100.22	108.73
2	F	292	LEU	N-CA-C	-5.21	100.02	108.52
2	D	134	GLY	N-CA-C	-5.21	100.83	113.18
1	K	151	GLY	CA-C-N	5.21	127.26	120.28
1	K	151	GLY	C-N-CA	5.21	127.26	120.28
1	C	185	VAL	N-CA-C	-5.20	100.99	108.53
1	I	231	HIS	N-CA-CB	5.20	114.81	109.51
2	B	329	ASN	CA-CB-CG	-5.19	107.41	112.60
1	A	137	TYR	N-CA-CB	5.19	119.22	110.77
2	D	329	ASN	CA-CB-CG	5.18	117.78	112.60
2	F	327	TRP	CA-C-N	5.18	131.57	121.41
2	F	327	TRP	C-N-CA	5.18	131.57	121.41
1	G	7	MET	CA-C-N	5.18	125.10	119.76
1	G	7	MET	C-N-CA	5.18	125.10	119.76
1	E	274	VAL	N-CA-C	-5.18	101.01	108.42
1	G	311	SER	CA-C-N	5.18	127.17	120.44
1	G	311	SER	C-N-CA	5.18	127.17	120.44
2	H	39	ASP	N-CA-C	-5.18	103.83	111.81
2	D	92	VAL	N-CA-C	-5.18	107.77	112.12
1	C	99	GLU	N-CA-C	-5.18	106.74	113.16
2	B	70	GLY	N-CA-C	-5.17	106.60	115.08
2	H	288	HIS	N-CA-C	-5.17	103.57	108.22
2	B	114	HIS	CA-CB-CG	-5.16	108.64	113.80
1	E	23	GLY	N-CA-C	-5.16	108.10	115.64
1	A	203	ASP	CA-CB-CG	5.16	117.76	112.60
2	H	148	LEU	CA-C-N	5.16	126.29	119.84
2	H	148	LEU	C-N-CA	5.16	126.29	119.84
1	C	291	ILE	N-CA-C	-5.15	99.83	107.51
2	B	296	SER	N-CA-CB	5.14	118.27	110.45
1	I	280	SER	N-CA-C	-5.14	100.14	108.52
1	K	235	THR	N-CA-C	-5.14	102.17	110.14
1	C	280	SER	N-CA-C	-5.13	100.15	108.52
1	K	206	SER	N-CA-C	-5.13	99.87	110.80
1	I	170	ALA	N-CA-C	-5.13	99.88	110.80
2	D	329	ASN	N-CA-CB	5.12	119.15	110.49
1	I	204	LEU	N-CA-C	-5.12	101.05	109.40
2	F	126	HIS	CA-C-N	5.12	127.98	120.71
2	F	126	HIS	C-N-CA	5.12	127.98	120.71
2	L	51	ALA	N-CA-C	-5.12	102.91	110.48
2	B	138	TYR	CA-C-N	5.11	128.47	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	138	TYR	C-N-CA	5.11	128.47	120.75
2	B	327	TRP	CA-C-N	5.11	131.42	121.41
2	B	327	TRP	C-N-CA	5.11	131.42	121.41
2	L	331	PRO	CA-C-N	5.10	126.22	119.84
2	L	331	PRO	C-N-CA	5.10	126.22	119.84
2	F	121	THR	N-CA-C	-5.10	99.30	108.48
2	B	80	ASN	N-CA-C	-5.09	107.74	114.31
2	F	295	ARG	N-CA-C	-5.09	100.72	108.76
2	J	136	GLU	CA-C-N	5.09	131.26	121.54
2	J	136	GLU	C-N-CA	5.09	131.26	121.54
1	E	289	THR	N-CA-C	-5.08	101.02	109.46
1	K	351	GLY	N-CA-C	-5.08	108.10	115.27
2	H	295	ARG	N-CA-C	-5.08	100.73	108.76
2	D	138	TYR	CA-C-N	5.08	131.25	121.54
2	D	138	TYR	C-N-CA	5.08	131.25	121.54
2	L	257	VAL	CA-C-N	5.08	125.08	119.90
2	L	257	VAL	C-N-CA	5.08	125.08	119.90
1	A	237	ALA	N-CA-C	-5.08	103.28	110.29
2	B	300	ASP	CA-CB-CG	5.08	117.68	112.60
1	E	52	LYS	N-CA-C	-5.07	100.63	108.90
1	G	247	ASP	N-CA-C	-5.07	106.94	112.72
1	G	165	GLY	N-CA-C	-5.07	105.86	112.10
2	B	96	GLY	CA-C-N	5.07	127.58	120.28
2	B	96	GLY	C-N-CA	5.07	127.58	120.28
1	I	291	ILE	N-CA-CB	5.07	119.59	111.23
1	I	296	THR	N-CA-C	-5.07	100.91	108.96
1	A	276	SER	N-CA-C	-5.06	101.50	109.50
1	E	211	SER	N-CA-CB	5.06	119.05	110.49
1	A	224	ARG	CA-C-N	5.06	126.16	119.84
1	A	224	ARG	C-N-CA	5.06	126.16	119.84
1	K	169	SER	N-CA-C	-5.06	107.06	113.18
2	B	107	ASP	N-CA-C	-5.05	107.28	113.50
1	A	143	ARG	CA-C-N	5.05	131.18	121.54
1	A	143	ARG	C-N-CA	5.05	131.18	121.54
1	E	333	SER	N-CA-C	-5.05	98.65	109.81
2	F	310	ARG	N-CA-CB	5.05	119.36	110.37
2	H	338	GLN	N-CA-C	-5.05	106.81	113.17
2	J	146	VAL	CA-C-N	5.05	131.18	121.54
2	J	146	VAL	C-N-CA	5.05	131.18	121.54
2	J	336	TRP	CA-C-N	5.05	129.53	122.36
2	J	336	TRP	C-N-CA	5.05	129.53	122.36
1	I	98	THR	N-CA-C	-5.04	107.51	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	ASP	CA-CB-CG	5.03	117.63	112.60
2	L	141	PRO	N-CA-C	5.03	116.84	110.70
2	J	138	TYR	CA-C-N	5.03	131.15	121.54
2	J	138	TYR	C-N-CA	5.03	131.15	121.54
1	K	371	CYS	N-CA-C	5.03	118.19	111.75
1	A	348	ALA	N-CA-C	-5.03	100.09	110.80
2	H	41	HIS	N-CA-C	-5.03	105.88	112.41
2	B	316	PHE	CA-CB-CG	-5.02	108.78	113.80
1	E	82	THR	CA-C-N	5.02	127.69	120.11
1	E	82	THR	C-N-CA	5.02	127.69	120.11
2	J	75	SER	N-CA-C	-5.02	101.74	109.52
2	F	131	ARG	CA-C-N	5.02	124.95	119.78
2	F	131	ARG	C-N-CA	5.02	124.95	119.78
2	B	111	VAL	N-CA-C	-5.01	101.15	108.17
2	L	77	LYS	N-CA-C	-5.01	103.06	110.48
1	K	161	LYS	N-CA-C	-5.01	100.90	108.67
2	B	331	PRO	CA-C-N	5.01	126.10	119.84
2	B	331	PRO	C-N-CA	5.01	126.10	119.84
1	K	338	ALA	N-CA-C	-5.01	101.13	108.99
2	L	140	HIS	N-CA-C	-5.00	98.75	109.81
1	G	14	PRO	N-CA-C	-5.00	102.77	111.32

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	264	LEU	Peptide
1	A	265	GLU	Peptide
1	C	256	ALA	Peptide
1	C	265	GLU	Peptide
1	C	321	TYR	Sidechain
1	C	46	TYR	Sidechain
2	D	138	TYR	Sidechain
2	D	139	ARG	Sidechain
1	E	15	TYR	Sidechain
1	E	264	LEU	Peptide
1	E	265	GLU	Peptide
1	E	321	TYR	Sidechain
2	F	138	TYR	Sidechain
2	F	256	PHE	Sidechain
2	F	46	ARG	Sidechain
1	G	122	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	G	264	LEU	Peptide
1	G	265	GLU	Peptide
1	G	321	TYR	Sidechain
2	H	305	ARG	Sidechain
1	I	137	TYR	Sidechain
1	I	265	GLU	Peptide
2	J	153	TYR	Sidechain
2	J	256	PHE	Sidechain
2	J	325	TYR	Sidechain
1	K	193	TYR	Sidechain
1	K	264	LEU	Peptide
1	K	265	GLU	Peptide
2	L	278	ARG	Sidechain
2	L	295	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2907	0	2805	24	0
1	C	2907	0	2805	18	0
1	E	2907	0	2805	16	0
1	G	2907	0	2805	22	0
1	I	2907	0	2805	18	0
1	K	2907	0	2805	15	0
2	B	1874	0	1831	14	0
2	D	1874	0	1831	7	0
2	F	1874	0	1831	10	0
2	H	1874	0	1831	8	0
2	J	1874	0	1831	9	0
2	L	1874	0	1831	16	0
All	All	28686	0	27816	169	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 (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ALA:HB3	1:A:355:PHE:CZ	2.33	0.63
1:C:360:ALA:HA	2:D:278:ARG:HE	1.68	0.57
1:A:28:HIS:CD2	1:A:343:ASN:HB2	2.40	0.56
1:K:180:VAL:HG13	1:K:264:LEU:HD21	1.86	0.56
1:I:38:ILE:HD11	1:I:170:ALA:HB1	1.88	0.56
1:A:110:ARG:H	1:A:211:SER:HB3	1.70	0.56
1:I:137:TYR:H	1:I:143:ARG:HH22	1.54	0.56
2:L:268:ALA:HB3	2:L:327:TRP:CH2	2.41	0.55
1:C:46:TYR:HB2	1:C:206:SER:H	1.71	0.55
1:A:136:THR:HG23	1:A:141:SER:HA	1.87	0.55
1:K:18:LEU:HG	1:K:332:HIS:CG	2.42	0.54
2:L:278:ARG:HA	2:L:278:ARG:HE	1.73	0.54
2:L:24:HIS:CG	2:L:25:SER:H	2.26	0.53
2:B:267:LEU:HA	2:B:288:HIS:CE1	2.43	0.53
2:B:139:ARG:HE	2:B:139:ARG:H	1.57	0.53
2:L:268:ALA:HB1	2:L:286:PRO:HA	1.91	0.53
1:C:331:ILE:HG12	1:C:368:LEU:HD11	1.91	0.52
1:I:28:HIS:CE1	1:I:328:ASN:HB3	2.45	0.52
1:K:317:ALA:HB3	1:K:355:PHE:CZ	2.46	0.51
2:L:135:ARG:HE	2:L:291:LEU:HD23	1.76	0.51
2:B:127:LYS:H	2:B:127:LYS:HD2	1.75	0.51
1:E:273:ALA:HB1	2:F:298:GLY:H	1.74	0.51
1:G:317:ALA:HB3	1:G:355:PHE:CZ	2.46	0.51
2:F:81:LEU:HD11	2:F:111:VAL:HG12	1.93	0.50
1:K:185:VAL:HB	1:K:264:LEU:HD22	1.92	0.50
1:A:28:HIS:CE1	1:A:136:THR:HG21	2.46	0.50
1:A:329:CYS:HB3	1:A:371:CYS:H	1.76	0.50
1:E:317:ALA:HB3	1:E:355:PHE:CZ	2.46	0.50
2:H:320:GLY:HA2	2:H:338:GLN:HB3	1.93	0.50
1:E:134:ASN:HA	1:E:144:SER:HA	1.94	0.50
1:I:155:ALA:HB3	1:I:162:LEU:HB2	1.94	0.50
2:H:297:LEU:H	2:H:323:LEU:HA	1.77	0.49
1:A:330:PRO:HA	1:A:343:ASN:O	2.12	0.49
1:C:40:PRO:HA	1:C:127:GLY:HA3	1.94	0.49
1:C:272:CYS:HB3	1:C:274:VAL:HG12	1.94	0.49
2:B:267:LEU:HD22	2:B:330:HIS:CE1	2.48	0.49
2:H:54:GLY:CA	2:H:94:HIS:HB3	2.43	0.49
2:B:278:ARG:HH21	2:B:320:GLY:HA3	1.78	0.48
1:G:48:THR:HG23	1:G:204:LEU:H	1.76	0.48
1:G:294:THR:H	1:G:295:PRO:HD2	1.78	0.48
2:J:157:ARG:HD2	2:J:157:ARG:H	1.79	0.48
1:G:317:ALA:HB3	1:G:355:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:24:HIS:CG	2:H:25:SER:H	2.31	0.48
1:E:38:ILE:HG23	1:E:129:VAL:HG22	1.95	0.48
2:H:56:LYS:HG3	2:H:58:ASP:H	1.79	0.48
1:E:29:LEU:C	1:E:343:ASN:HD21	2.21	0.48
2:J:95:HIS:CE1	2:J:158:ALA:H	2.32	0.47
2:H:119:ARG:HH22	2:J:63:ALA:HB1	1.79	0.47
1:C:317:ALA:HB3	1:C:355:PHE:CZ	2.48	0.47
2:B:320:GLY:HA2	2:B:340:SER:H	1.80	0.47
1:A:27:VAL:HG11	1:A:283:ILE:HG21	1.97	0.47
2:B:54:GLY:CA	2:B:94:HIS:HB3	2.44	0.47
2:L:54:GLY:HA3	2:L:94:HIS:CG	2.50	0.47
2:B:98:TYR:C	2:B:99:ILE:HD12	2.40	0.47
1:C:48:THR:HG21	1:C:201:PHE:CE1	2.49	0.47
2:F:267:LEU:HD22	2:F:330:HIS:CE1	2.50	0.47
1:C:329:CYS:HB3	1:C:371:CYS:H	1.80	0.46
1:G:16:LYS:HB2	1:G:332:HIS:CE1	2.50	0.46
2:J:119:ARG:HE	2:L:82:HIS:CD2	2.33	0.46
2:F:295:ARG:HA	2:F:302:ASN:O	2.16	0.46
1:I:317:ALA:HB3	1:I:355:PHE:CZ	2.50	0.46
2:D:56:LYS:HG3	2:D:58:ASP:H	1.81	0.46
1:C:315:GLY:HA3	1:C:357:PHE:CZ	2.51	0.46
1:G:345:VAL:HG23	1:G:353:PHE:CD1	2.51	0.46
1:I:38:ILE:HD12	1:I:38:ILE:N	2.31	0.46
2:D:322:GLY:HA3	2:D:336:TRP:HA	1.98	0.45
1:G:147:VAL:HG11	1:G:164:ILE:H	1.81	0.45
2:L:94:HIS:CE1	2:L:99:ILE:HG23	2.51	0.45
1:A:222:LEU:HD22	1:A:222:LEU:H	1.80	0.45
2:B:91:LEU:HA	2:B:101:ALA:HA	1.98	0.45
1:C:315:GLY:HA3	1:C:357:PHE:CE1	2.52	0.45
1:C:331:ILE:CG1	1:C:368:LEU:HD11	2.47	0.45
1:E:38:ILE:HG21	1:E:172:SER:N	2.30	0.45
2:F:273:VAL:HG13	2:F:280:LEU:HD21	1.98	0.45
1:A:179:VAL:HG13	1:A:201:PHE:CZ	2.51	0.45
1:G:25:ALA:H	1:G:289:THR:HG23	1.82	0.45
1:G:347:LEU:HD13	1:G:349:GLU:H	1.80	0.45
1:I:27:VAL:HA	1:I:287:ALA:HB3	1.98	0.45
1:E:329:CYS:HB3	1:E:371:CYS:H	1.81	0.45
1:G:323:SER:HB3	1:G:347:LEU:HD11	1.99	0.45
1:I:38:ILE:HD11	1:I:170:ALA:CB	2.47	0.45
1:I:222:LEU:HD22	1:I:222:LEU:H	1.81	0.45
2:J:38:GLY:H	2:J:128:VAL:HG21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:259:GLY:HA3	2:L:297:LEU:HA	1.98	0.45
1:K:40:PRO:HA	1:K:127:GLY:HA3	1.98	0.45
1:G:258:PHE:HB3	1:G:273:ALA:H	1.81	0.45
1:A:76:TYR:HA	1:A:107:TYR:HB3	1.99	0.45
1:G:28:HIS:CE1	1:G:342:GLU:HA	2.51	0.45
1:K:323:SER:H	1:K:349:GLU:HG2	1.82	0.45
1:A:40:PRO:HA	1:A:127:GLY:HA3	1.98	0.44
1:A:121:ALA:HB1	1:A:190:PHE:CE1	2.52	0.44
1:A:28:HIS:CE1	1:A:342:GLU:HA	2.52	0.44
1:A:172:SER:C	1:A:174:PHE:H	2.25	0.44
1:C:28:HIS:CD2	1:C:343:ASN:HB3	2.51	0.44
2:F:31:ILE:HD13	2:F:111:VAL:HB	1.99	0.44
1:I:136:THR:HG21	1:I:343:ASN:HB3	1.98	0.44
2:B:56:LYS:HG3	2:B:58:ASP:H	1.82	0.44
1:I:304:ILE:H	1:I:379:GLY:HA3	1.81	0.44
1:E:264:LEU:H	1:E:264:LEU:HD22	1.82	0.44
2:J:56:LYS:HG3	2:J:58:ASP:H	1.82	0.44
1:K:28:HIS:NE2	1:K:136:THR:HG21	2.33	0.44
1:A:345:VAL:HG23	1:A:353:PHE:CG	2.52	0.44
1:C:161:LYS:H	1:C:282:ASP:HB3	1.82	0.44
2:J:81:LEU:HD12	2:J:113:PHE:CE1	2.52	0.44
1:K:121:ALA:HB1	1:K:190:PHE:CE1	2.52	0.44
2:H:65:MET:HE1	2:H:67:PHE:HB3	1.99	0.44
1:A:323:SER:H	1:A:349:GLU:HG2	1.82	0.44
2:F:114:HIS:CE1	2:F:119:ARG:HE	2.36	0.44
1:G:309:TYR:HA	1:G:381:CYS:HB3	2.00	0.44
1:G:40:PRO:HA	1:G:127:GLY:HA3	1.98	0.43
1:G:370:VAL:HG12	1:G:371:CYS:H	1.83	0.43
1:I:3:HIS:HB2	1:I:19:VAL:HG13	1.99	0.43
1:A:150:ASN:HA	1:A:167:LEU:H	1.84	0.43
2:F:81:LEU:HD13	2:F:113:PHE:CE2	2.53	0.43
1:C:171:TRP:H	1:C:274:VAL:HG11	1.83	0.43
2:B:143:GLU:O	2:B:144:HIS:CG	2.71	0.43
1:G:330:PRO:HG2	1:G:369:GLN:HE22	1.84	0.43
1:A:7:MET:HE3	1:A:33:LEU:HD22	2.00	0.43
2:B:54:GLY:HA3	2:B:94:HIS:HB3	2.00	0.43
1:I:259:GLY:HA2	2:J:297:LEU:HD23	2.00	0.43
1:K:331:ILE:HD12	1:K:368:LEU:HD12	2.00	0.43
1:C:137:TYR:H	1:C:143:ARG:HH22	1.67	0.42
1:K:329:CYS:SG	1:K:347:LEU:HD11	2.59	0.42
1:C:184:GLU:HB3	1:C:186:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:MET:HE2	1:E:279:ILE:HD11	2.01	0.42
1:G:28:HIS:CE1	1:G:136:THR:HG22	2.54	0.42
1:G:338:ALA:HB2	1:G:359:THR:HG22	2.02	0.42
2:F:56:LYS:HG3	2:F:58:ASP:H	1.83	0.42
2:F:95:HIS:HB2	2:F:256:PHE:CE1	2.55	0.42
2:H:95:HIS:O	2:H:95:HIS:CG	2.72	0.42
1:I:7:MET:SD	1:I:133:VAL:HG13	2.59	0.42
2:B:60:VAL:HG21	2:B:159:ASP:HB2	2.01	0.42
1:C:10:LYS:HA	2:D:336:TRP:CH2	2.55	0.42
1:E:368:LEU:HD23	1:E:377:CYS:SG	2.60	0.42
2:L:65:MET:HE3	2:L:81:LEU:HD13	2.01	0.42
1:A:16:LYS:HB2	1:A:332:HIS:CE1	2.55	0.42
1:E:40:PRO:HA	1:E:127:GLY:HA3	2.02	0.42
1:I:300:LEU:HD21	1:I:370:VAL:HG21	2.01	0.42
1:E:31:ILE:HA	1:E:134:ASN:O	2.20	0.42
1:G:28:HIS:HA	1:G:343:ASN:HB2	2.02	0.42
1:I:133:VAL:HG12	1:I:135:ILE:HG13	2.02	0.42
2:D:10:LYS:HB2	2:D:96:GLY:HA3	2.02	0.42
2:D:135:ARG:HE	2:D:332:PRO:HD3	1.84	0.42
1:K:27:VAL:HG22	1:K:289:THR:H	1.85	0.42
2:L:65:MET:HE2	2:L:65:MET:HB2	1.95	0.41
1:E:46:TYR:HB2	1:E:206:SER:H	1.85	0.41
1:K:341:LYS:H	1:K:357:PHE:HA	1.85	0.41
2:L:268:ALA:HB1	2:L:269:PRO:HD2	2.02	0.41
1:I:315:GLY:HA3	1:I:357:PHE:CZ	2.55	0.41
1:A:121:ALA:HB1	1:A:190:PHE:CZ	2.55	0.41
2:L:54:GLY:HA3	2:L:94:HIS:CD2	2.56	0.41
2:L:268:ALA:HB3	2:L:327:TRP:CZ2	2.55	0.41
1:A:46:TYR:CB	1:A:206:SER:H	2.33	0.41
1:G:76:TYR:HA	1:G:107:TYR:HB3	2.02	0.41
2:D:295:ARG:HA	2:D:302:ASN:H	1.85	0.41
2:J:83:VAL:HG21	2:J:91:LEU:HD21	2.02	0.41
1:A:46:TYR:CE1	1:A:121:ALA:HB2	2.55	0.41
2:B:318:VAL:HG11	2:B:340:SER:HB2	2.03	0.41
1:E:135:ILE:HD12	1:E:135:ILE:H	1.85	0.41
1:G:294:THR:H	1:G:295:PRO:CD	2.34	0.41
1:E:38:ILE:HD12	1:E:38:ILE:N	2.35	0.40
1:G:28:HIS:HB2	1:G:344:ASP:CB	2.51	0.40
1:I:84:VAL:HA	1:I:224:ARG:HH22	1.86	0.40
2:L:24:HIS:CG	2:L:25:SER:N	2.89	0.40
1:K:167:LEU:HG	1:K:169:SER:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:TYR:HB2	1:A:206:SER:H	1.87	0.40
1:C:25:ALA:H	1:C:291:ILE:H	1.70	0.40
1:E:315:GLY:HA3	1:E:357:PHE:CE1	2.57	0.40
1:K:273:ALA:HB2	2:L:336:TRP:CZ3	2.56	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	379/441 (86%)	325 (86%)	38 (10%)	16 (4%)	2	17
1	C	379/441 (86%)	324 (86%)	36 (10%)	19 (5%)	1	16
1	E	379/441 (86%)	333 (88%)	33 (9%)	13 (3%)	3	21
1	G	379/441 (86%)	332 (88%)	29 (8%)	18 (5%)	2	16
1	I	379/441 (86%)	320 (84%)	44 (12%)	15 (4%)	2	18
1	K	379/441 (86%)	332 (88%)	35 (9%)	12 (3%)	3	21
2	B	234/420 (56%)	193 (82%)	27 (12%)	14 (6%)	1	13
2	D	234/420 (56%)	195 (83%)	29 (12%)	10 (4%)	2	17
2	F	234/420 (56%)	197 (84%)	27 (12%)	10 (4%)	2	17
2	H	234/420 (56%)	197 (84%)	21 (9%)	16 (7%)	1	11
2	J	234/420 (56%)	195 (83%)	27 (12%)	12 (5%)	1	15
2	L	234/420 (56%)	193 (82%)	30 (13%)	11 (5%)	2	16
All	All	3678/5166 (71%)	3136 (85%)	376 (10%)	166 (4%)	3	17

All (166) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	TRP
1	A	206	SER
1	A	291	ILE
1	A	292	SER
1	A	294	THR
2	B	51	ALA
1	C	111	SER
1	C	115	SER
1	C	157	ILE
1	C	207	ARG
1	C	266	PRO
1	C	292	SER
2	D	69	ASN
2	D	142	PRO
1	E	74	PRO
1	E	115	SER
1	E	160	ALA
1	E	211	SER
1	E	265	GLU
1	G	150	ASN
1	G	193	TYR
1	G	206	SER
1	G	265	GLU
2	H	51	ALA
1	I	265	GLU
1	I	333	SER
2	J	147	GLU
1	K	57	SER
2	L	74	LYS
2	L	128	VAL
1	A	348	ALA
2	B	133	VAL
2	B	142	PRO
2	B	144	HIS
2	B	328	GLY
1	C	208	THR
1	C	371	CYS
2	D	139	ARG
2	D	329	ASN
1	E	141	SER
2	F	39	ASP
2	F	86	SER
2	F	328	GLY

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Mol	Chain	Res	Type
1	G	92	ALA
1	G	160	ALA
1	G	291	ILE
1	G	294	THR
1	G	349	GLU
2	H	31	ILE
2	H	71	LYS
1	I	150	ASN
1	I	160	ALA
1	I	170	ALA
1	I	291	ILE
1	I	335	SER
2	J	79	ASP
2	J	86	SER
2	J	139	ARG
2	J	338	GLN
1	K	157	ILE
1	K	171	TRP
1	K	229	ILE
2	L	338	GLN
1	A	90	GLY
1	A	114	CYS
1	A	265	GLU
1	A	350	SER
2	B	26	ARG
2	B	31	ILE
2	B	79	ASP
2	B	86	SER
2	B	299	SER
2	B	337	ALA
1	C	176	ASN
1	C	184	GLU
1	C	206	SER
1	C	211	SER
1	C	267	LEU
2	D	73	GLN
2	D	105	PRO
1	E	140	VAL
1	E	206	SER
2	F	27	CYS
2	F	79	ASP
2	F	115	ASP

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Mol	Chain	Res	Type
1	G	335	SER
2	H	107	ASP
2	H	139	ARG
1	I	89	TRP
1	I	93	TYR
2	J	30	PRO
2	J	72	THR
2	J	158	ALA
1	K	93	TYR
1	K	160	ALA
1	K	207	ARG
1	K	227	ALA
1	K	265	GLU
2	L	79	ASP
2	L	86	SER
2	L	129	GLU
2	L	152	ARG
1	A	86	PRO
1	A	183	HIS
1	A	193	TYR
1	A	380	ASP
1	C	141	SER
1	C	379	GLY
2	D	133	VAL
1	E	371	CYS
2	F	105	PRO
1	G	94	CYS
1	G	213	ASP
2	H	19	CYS
2	H	32	ALA
2	H	33	ILE
2	H	142	PRO
2	H	266	THR
1	I	201	PHE
1	I	290	ARG
2	J	137	LYS
2	J	138	TYR
1	K	203	ASP
2	L	158	ALA
1	A	26	PRO
1	A	167	LEU
2	B	78	ILE

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Mol	Chain	Res	Type
1	C	250	ALA
1	E	86	PRO
1	E	310	ALA
2	F	310	ARG
1	I	87	PHE
1	I	212	ASN
1	I	371	CYS
2	J	329	ASN
2	L	69	ASN
2	L	140	HIS
2	B	264	ILE
2	F	142	PRO
1	G	93	TYR
1	G	181	TYR
1	G	267	LEU
1	K	291	ILE
1	C	26	PRO
1	G	257	PRO
2	H	116	GLY
2	J	142	PRO
2	D	30	PRO
1	E	166	PRO
1	G	173	PRO
2	H	20	PRO
2	B	141	PRO
1	C	251	PRO
1	C	265	GLU
2	D	31	ILE
2	H	30	PRO
1	K	172	SER
2	D	303	PRO
1	E	25	ALA
2	F	103	CYS
1	G	116	ILE
2	H	38	GLY
2	H	140	HIS
2	H	269	PRO
1	I	266	PRO
2	L	310	ARG

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	321/370 (87%)	302 (94%)	19 (6%)	18	39
1	C	321/370 (87%)	302 (94%)	19 (6%)	18	39
1	E	321/370 (87%)	306 (95%)	15 (5%)	23	45
1	G	321/370 (87%)	307 (96%)	14 (4%)	25	47
1	I	321/370 (87%)	310 (97%)	11 (3%)	32	54
1	K	321/370 (87%)	301 (94%)	20 (6%)	16	38
2	B	206/367 (56%)	189 (92%)	17 (8%)	10	30
2	D	206/367 (56%)	188 (91%)	18 (9%)	9	29
2	F	206/367 (56%)	195 (95%)	11 (5%)	20	41
2	H	206/367 (56%)	197 (96%)	9 (4%)	25	47
2	J	206/367 (56%)	198 (96%)	8 (4%)	28	49
2	L	206/367 (56%)	195 (95%)	11 (5%)	20	41
All	All	3162/4422 (72%)	2990 (95%)	172 (5%)	21	41

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	PRO
1	A	31	ILE
1	A	33	LEU
1	A	42	THR
1	A	114	CYS
1	A	150	ASN
1	A	153	THR
1	A	180	VAL
1	A	248	LYS
1	A	279	ILE
1	A	290	ARG
1	A	294	THR
1	A	297	VAL
1	A	303	LYS

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Mol	Chain	Res	Type
1	A	345	VAL
1	A	359	THR
1	A	368	LEU
1	A	369	GLN
1	A	378	LYS
2	B	10	LYS
2	B	26	ARG
2	B	45	ILE
2	B	49	THR
2	B	67	PHE
2	B	74	LYS
2	B	81	LEU
2	B	83	VAL
2	B	127	LYS
2	B	139	ARG
2	B	266	THR
2	B	267	LEU
2	B	308	ILE
2	B	318	VAL
2	B	324	GLU
2	B	332	PRO
2	B	335	VAL
1	C	7	MET
1	C	26	PRO
1	C	28	HIS
1	C	36	THR
1	C	134	ASN
1	C	135	ILE
1	C	136	THR
1	C	147	VAL
1	C	162	LEU
1	C	214	LEU
1	C	218	THR
1	C	267	LEU
1	C	277	ILE
1	C	289	THR
1	C	332	HIS
1	C	345	VAL
1	C	347	LEU
1	C	372	THR
1	C	378	LYS
2	D	10	LYS

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Mol	Chain	Res	Type
2	D	45	ILE
2	D	49	THR
2	D	71	LYS
2	D	99	ILE
2	D	127	LYS
2	D	131	ARG
2	D	137	LYS
2	D	139	ARG
2	D	157	ARG
2	D	254	VAL
2	D	284	LEU
2	D	290	THR
2	D	292	LEU
2	D	293	THR
2	D	309	GLU
2	D	318	VAL
2	D	336	TRP
1	E	26	PRO
1	E	37	ARG
1	E	38	ILE
1	E	74	PRO
1	E	120	LYS
1	E	134	ASN
1	E	135	ILE
1	E	156	LYS
1	E	167	LEU
1	E	185	VAL
1	E	264	LEU
1	E	288	PHE
1	E	319	VAL
1	E	332	HIS
1	E	345	VAL
2	F	36	VAL
2	F	49	THR
2	F	99	ILE
2	F	119	ARG
2	F	127	LYS
2	F	293	THR
2	F	294	THR
2	F	295	ARG
2	F	305	ARG
2	F	319	THR

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Mol	Chain	Res	Type
2	F	324	GLU
1	G	30	GLN
1	G	135	ILE
1	G	157	ILE
1	G	178	VAL
1	G	185	VAL
1	G	277	ILE
1	G	290	ARG
1	G	331	ILE
1	G	347	LEU
1	G	359	THR
1	G	369	GLN
1	G	371	CYS
1	G	375	VAL
1	G	378	LYS
2	H	71	LYS
2	H	78	ILE
2	H	94	HIS
2	H	128	VAL
2	H	139	ARG
2	H	270	GLU
2	H	279	THR
2	H	334	ARG
2	H	338	GLN
1	I	30	GLN
1	I	31	ILE
1	I	120	LYS
1	I	124	VAL
1	I	134	ASN
1	I	290	ARG
1	I	294	THR
1	I	319	VAL
1	I	341	LYS
1	I	345	VAL
1	I	367	LYS
2	J	49	THR
2	J	99	ILE
2	J	131	ARG
2	J	139	ARG
2	J	254	VAL
2	J	324	GLU
2	J	332	PRO

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Mol	Chain	Res	Type
2	J	338	GLN
1	K	30	GLN
1	K	31	ILE
1	K	66	THR
1	K	93	TYR
1	K	135	ILE
1	K	137	TYR
1	K	147	VAL
1	K	185	VAL
1	K	235	THR
1	K	267	LEU
1	K	279	ILE
1	K	289	THR
1	K	297	VAL
1	K	303	LYS
1	K	306	GLU
1	K	319	VAL
1	K	321	TYR
1	K	345	VAL
1	K	359	THR
1	K	378	LYS
2	L	47	ILE
2	L	73	GLN
2	L	77	LYS
2	L	119	ARG
2	L	127	LYS
2	L	278	ARG
2	L	279	THR
2	L	290	THR
2	L	295	ARG
2	L	323	LEU
2	L	332	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	43	ASN
1	A	67	GLN
1	A	134	ASN
1	A	183	HIS
1	A	223	GLN

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Mol	Chain	Res	Type
1	A	253	ASN
2	B	41	HIS
2	B	69	ASN
2	B	94	HIS
2	B	120	HIS
2	B	126	HIS
2	B	140	HIS
2	B	144	HIS
2	B	155	HIS
2	B	275	HIS
2	B	283	HIS
2	B	302	ASN
2	B	306	GLN
2	B	330	HIS
1	C	32	GLN
1	C	77	GLN
1	C	79	GLN
1	C	176	ASN
1	C	217	ASN
1	C	231	HIS
1	C	361	ASN
1	C	363	HIS
1	C	369	GLN
2	D	41	HIS
2	D	48	GLN
2	D	73	GLN
2	D	94	HIS
2	D	95	HIS
2	D	120	HIS
2	D	288	HIS
1	E	28	HIS
1	E	30	GLN
1	E	43	ASN
1	E	67	GLN
1	E	73	HIS
1	E	176	ASN
1	E	217	ASN
1	E	219	ASN
1	E	223	GLN
1	E	236	GLN
1	E	253	ASN
1	E	328	ASN

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Mol	Chain	Res	Type
1	E	343	ASN
2	F	24	HIS
2	F	41	HIS
2	F	95	HIS
2	F	102	GLN
2	F	114	HIS
2	F	126	HIS
2	F	283	HIS
2	F	285	HIS
2	F	288	HIS
2	F	330	HIS
1	G	28	HIS
1	G	30	GLN
1	G	43	ASN
1	G	77	GLN
1	G	130	GLN
1	G	187	ASN
1	G	223	GLN
1	G	231	HIS
1	G	236	GLN
1	G	361	ASN
1	G	363	HIS
1	G	369	GLN
2	H	48	GLN
2	H	82	HIS
2	H	94	HIS
2	H	95	HIS
2	H	102	GLN
2	H	120	HIS
2	H	126	HIS
2	H	140	HIS
2	H	151	ASN
2	H	277	HIS
2	H	283	HIS
2	H	330	HIS
1	I	43	ASN
1	I	67	GLN
1	I	102	GLN
1	I	176	ASN
1	I	217	ASN
1	I	231	HIS
1	I	253	ASN

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Mol	Chain	Res	Type
1	I	271	ASN
1	I	343	ASN
1	I	361	ASN
2	J	41	HIS
2	J	48	GLN
2	J	82	HIS
2	J	94	HIS
2	J	95	HIS
2	J	102	GLN
2	J	114	HIS
2	J	140	HIS
2	J	144	HIS
2	J	155	HIS
2	J	275	HIS
2	J	277	HIS
2	J	285	HIS
2	J	329	ASN
2	J	330	HIS
1	K	28	HIS
1	K	30	GLN
1	K	43	ASN
1	K	79	GLN
1	K	187	ASN
1	K	219	ASN
1	K	223	GLN
1	K	231	HIS
1	K	236	GLN
1	K	369	GLN
2	L	21	ASN
2	L	24	HIS
2	L	41	HIS
2	L	82	HIS
2	L	120	HIS
2	L	126	HIS
2	L	151	ASN
2	L	288	HIS
2	L	330	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

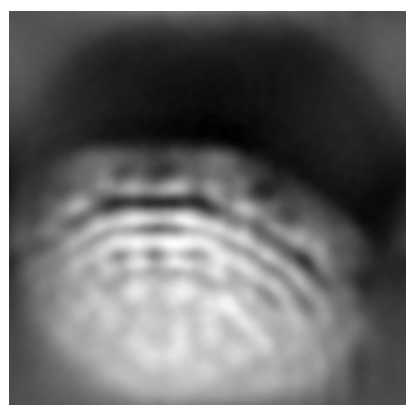
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24201. These allow visual inspection of the internal detail of the map and identification of artifacts.

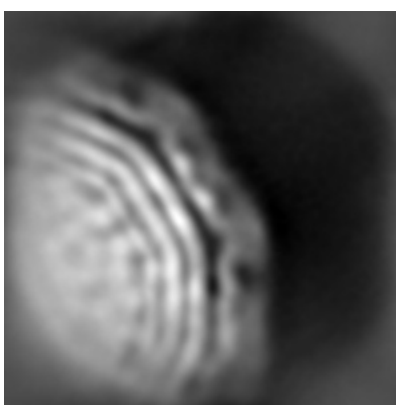
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

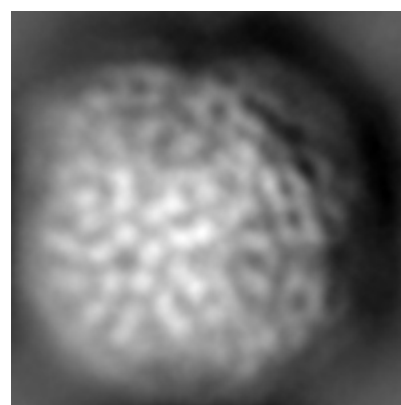
6.1.1 Primary map



X



Y

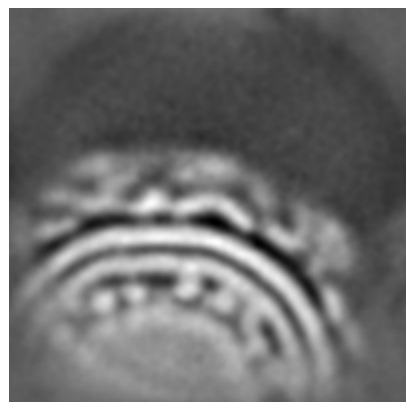


Z

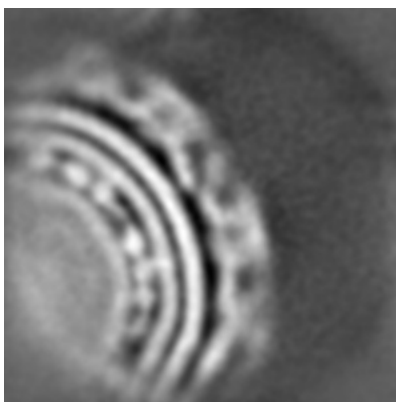
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

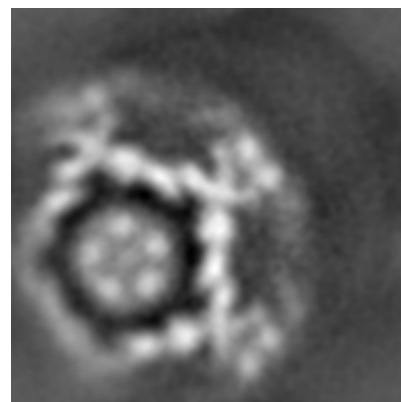
6.2.1 Primary map



X Index: 72



Y Index: 72

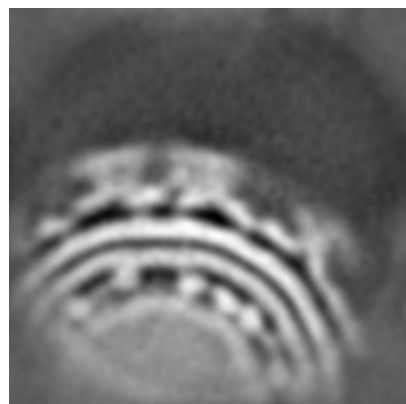


Z Index: 72

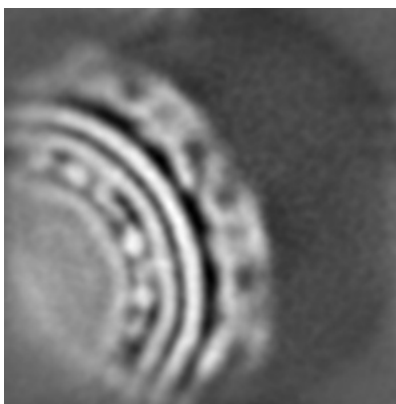
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

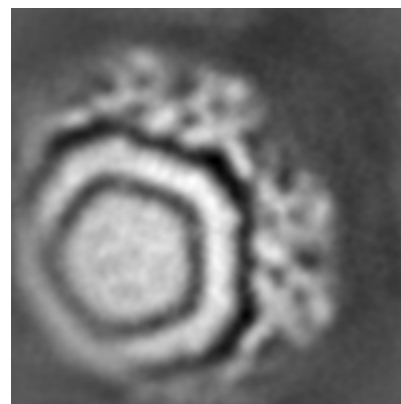
6.3.1 Primary map



X Index: 68



Y Index: 73

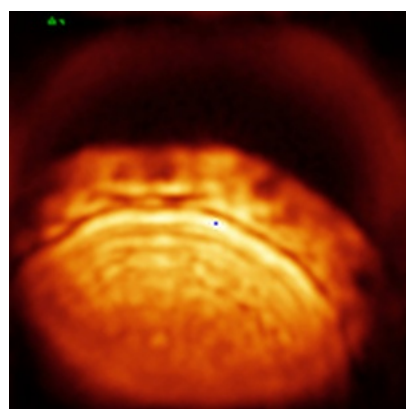


Z Index: 60

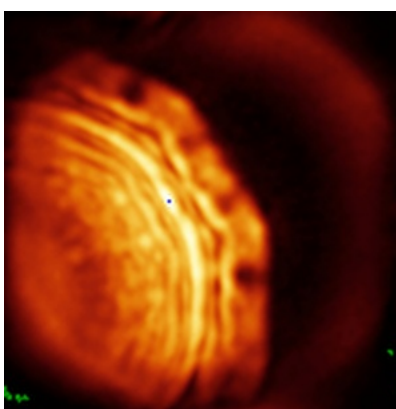
The images above show the largest variance slices of the map in three orthogonal directions.

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

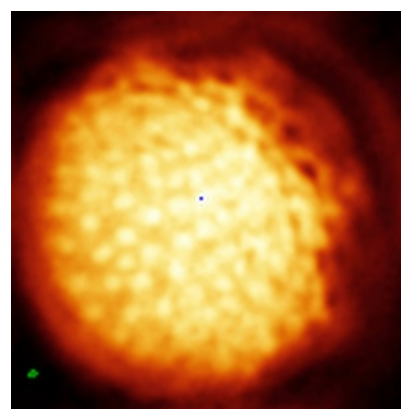
6.4.1 Primary map



X



Y

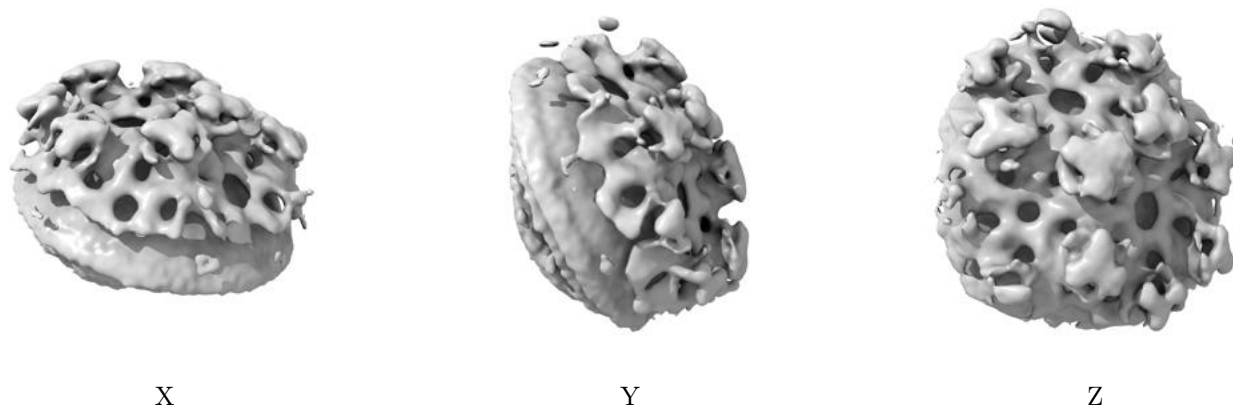


Z

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



The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

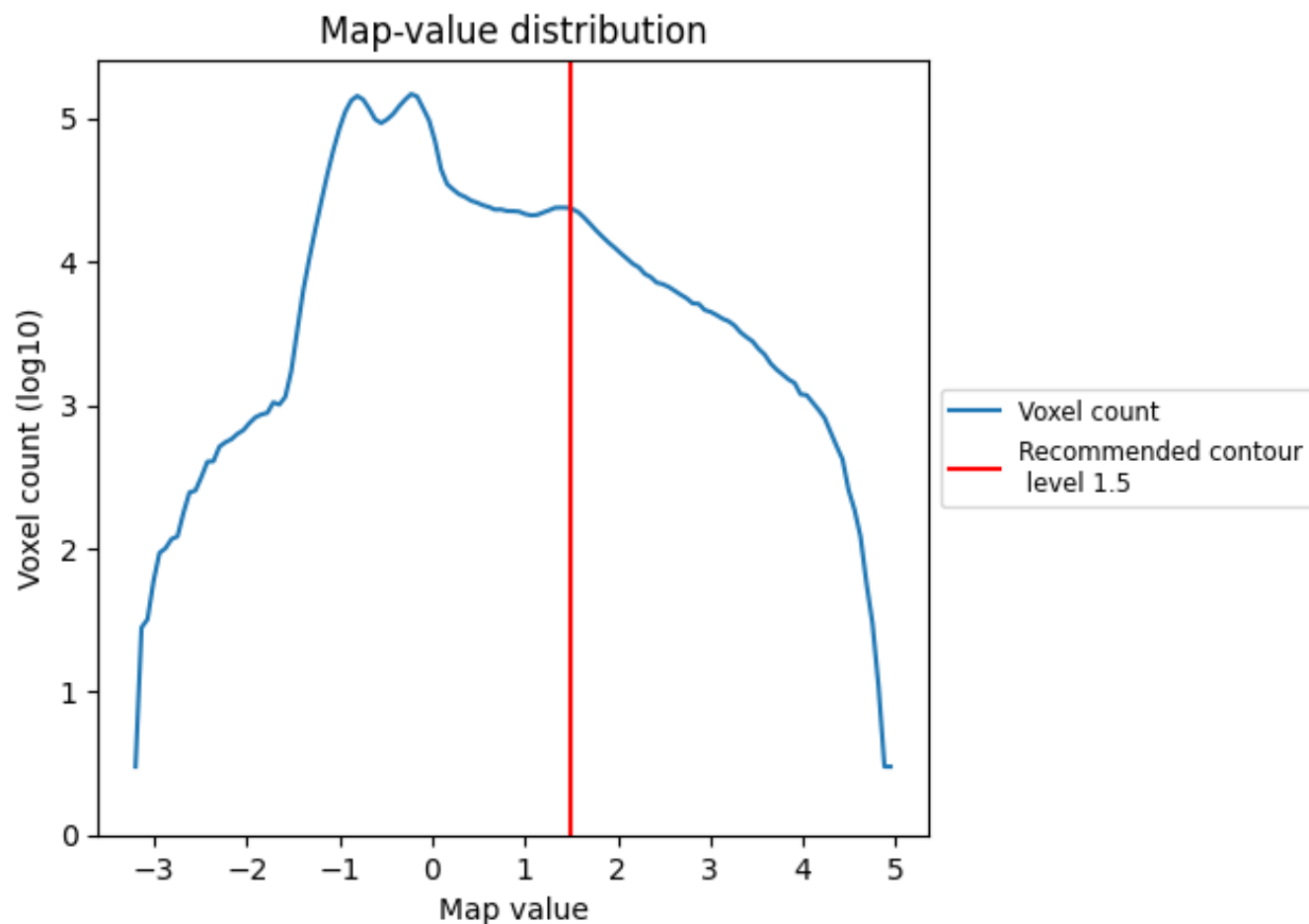
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

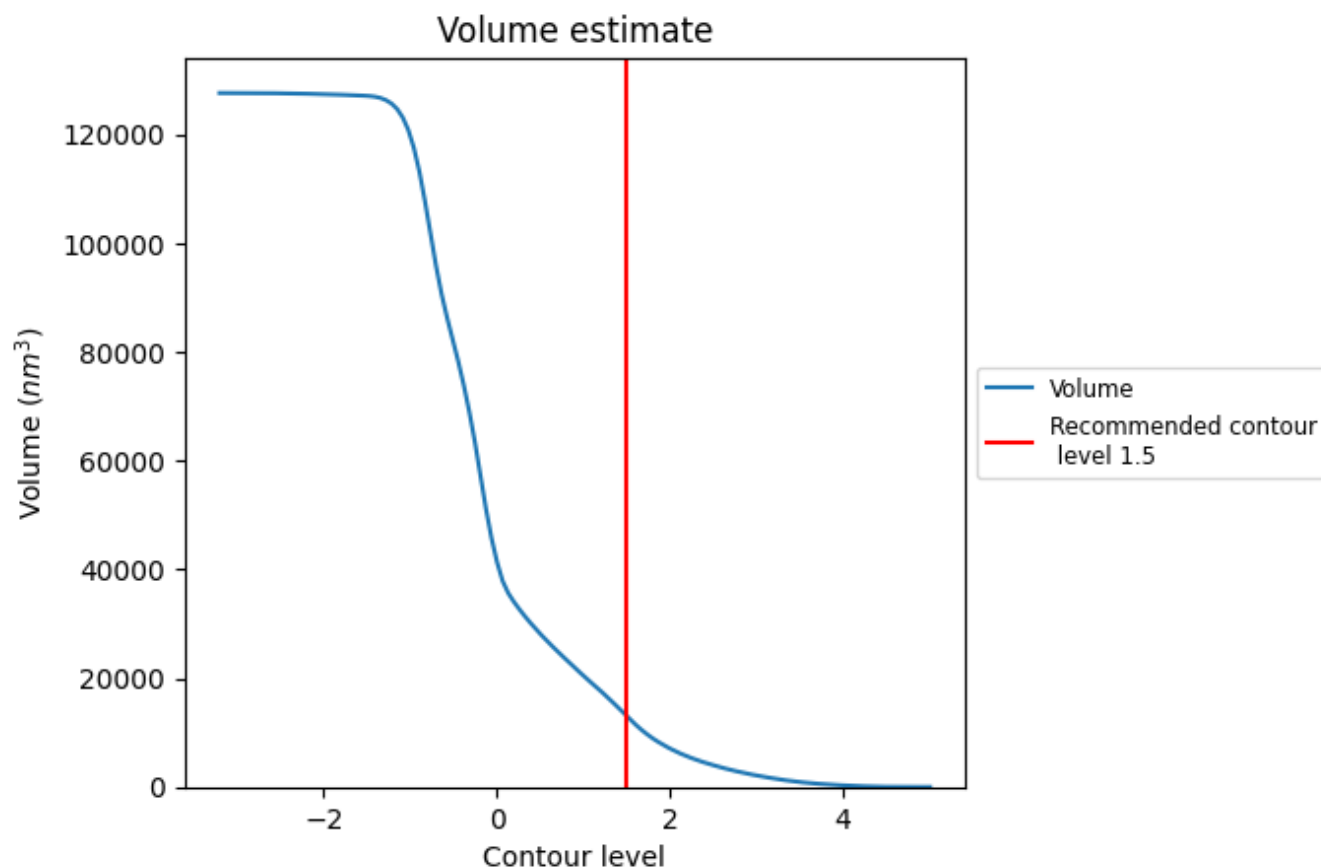
This section contains the results of statistical analysis of the map.

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.

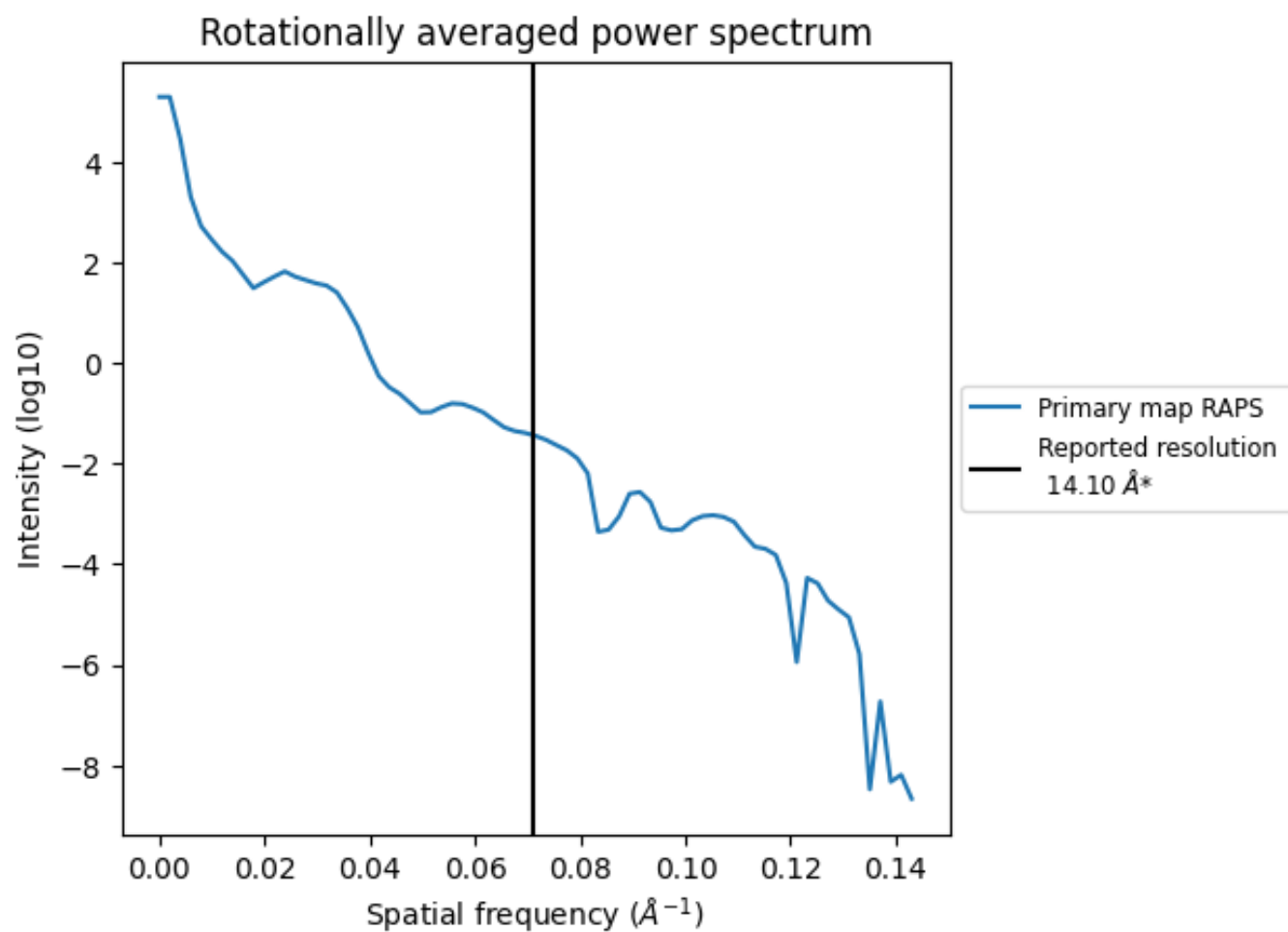
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 13083 nm³; this corresponds to an approximate mass of 11818 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 ⓘ

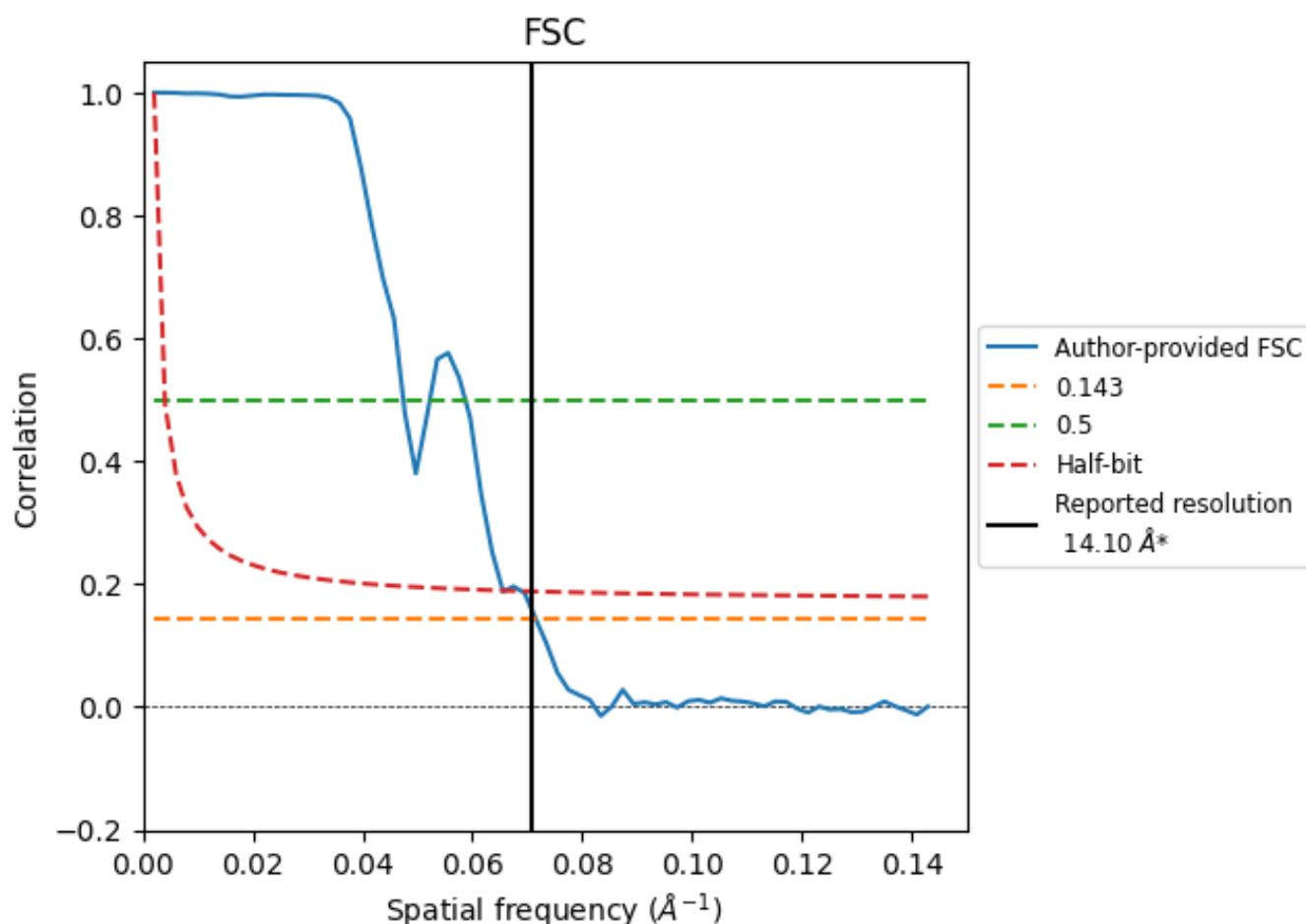


*Reported resolution corresponds to spatial frequency of 0.071 Å⁻¹

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 0.071 Å⁻¹

8.2 Resolution estimates [i](#)

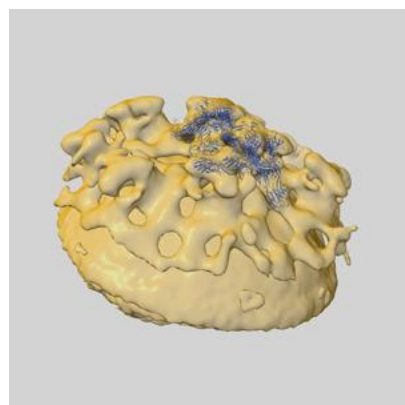
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	14.10	-	-
Author-provided FSC curve	13.97	21.10	15.27
Unmasked-calculated*	-	-	-

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

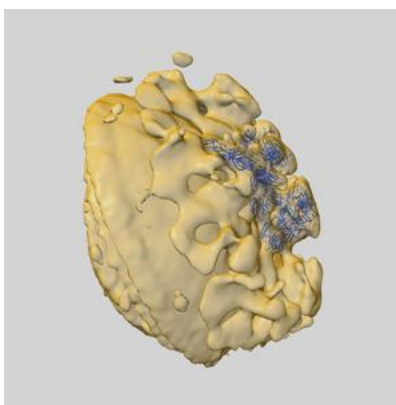
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24201 and PDB model 7N69. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

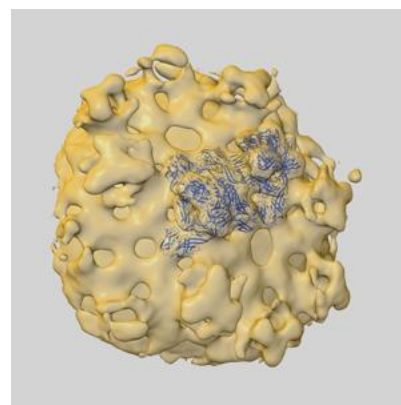
9.1 Map-model overlay [i](#)



X



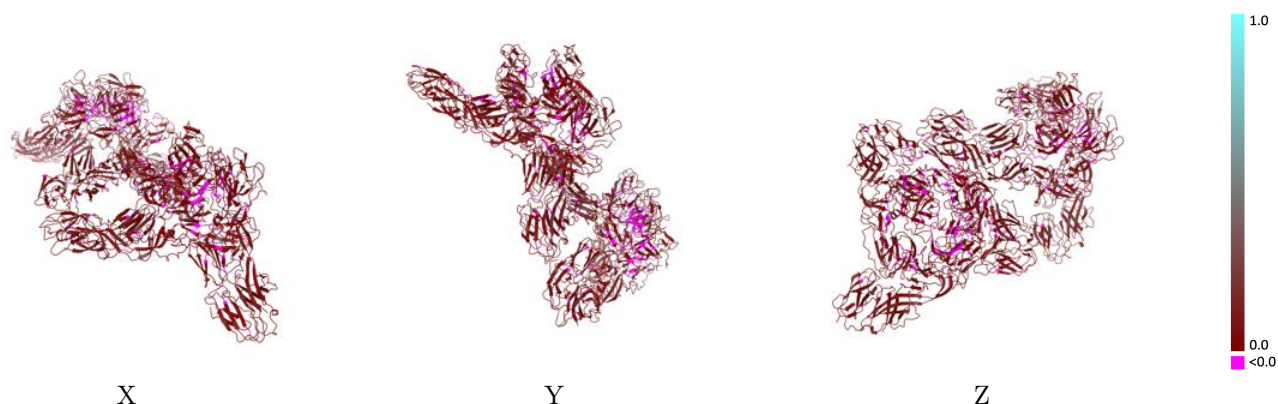
Y



Z

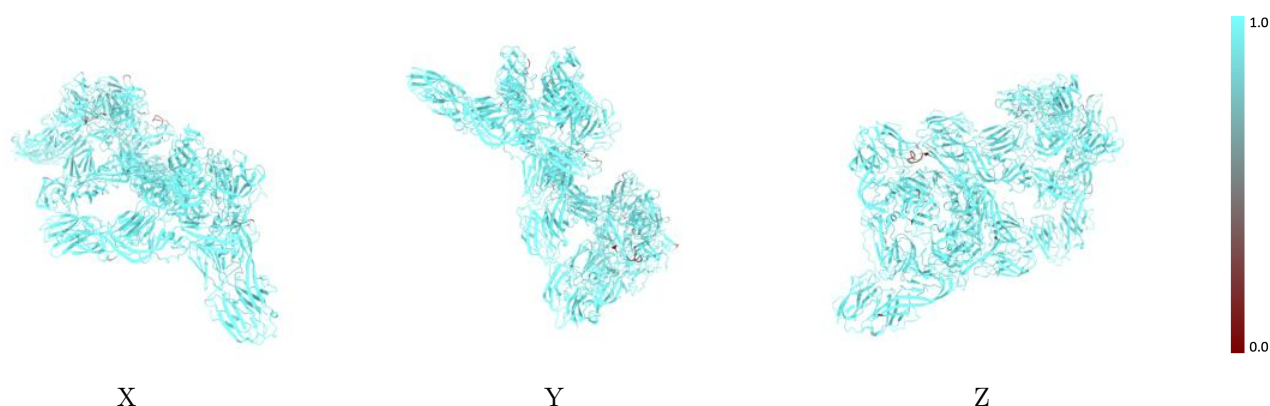
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



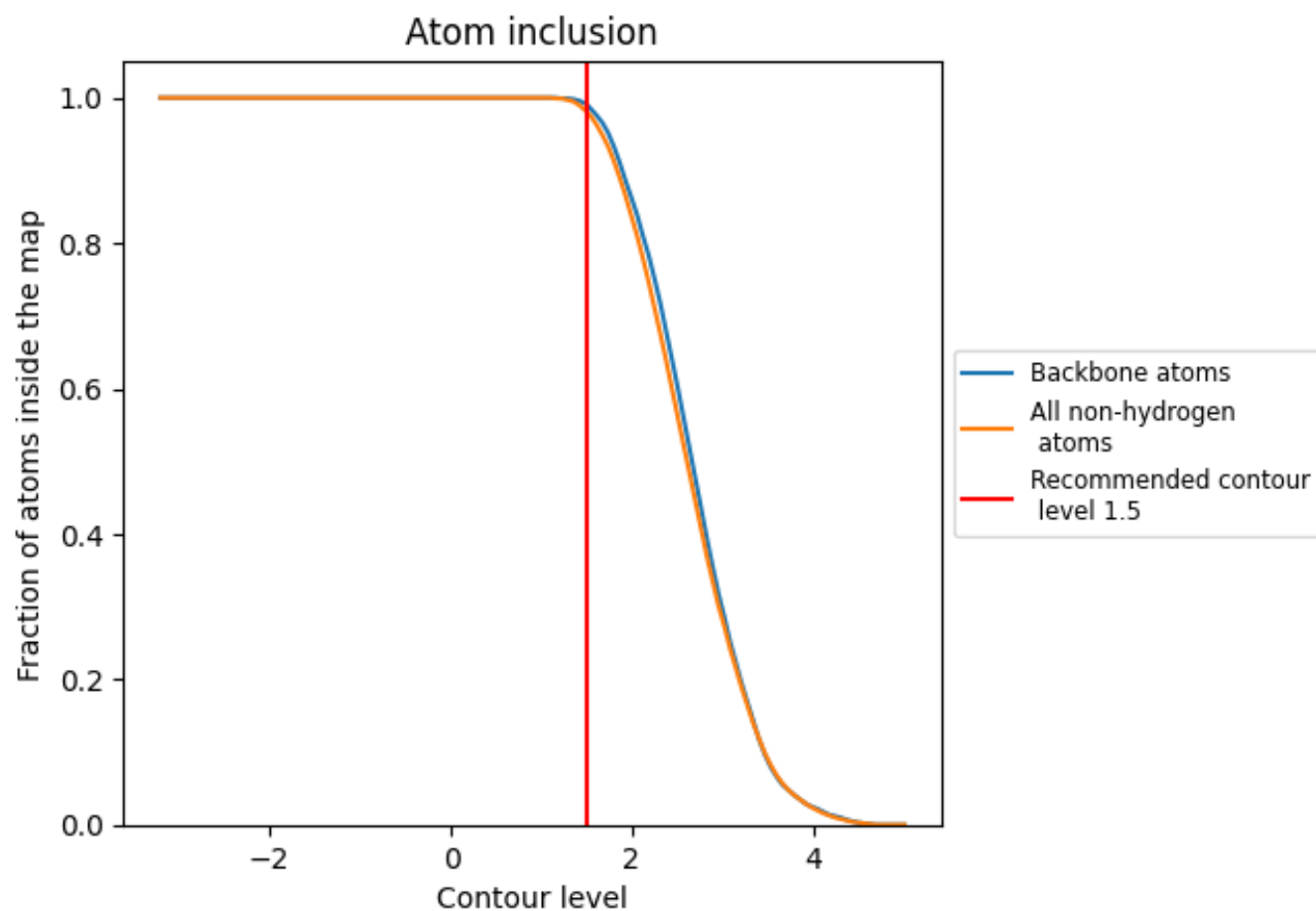
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9810	0.0810
A	0.9880	0.0930
B	0.9950	0.0730
C	0.9790	0.0910
D	0.9910	0.0780
E	0.9730	0.0870
F	0.9910	0.0750
G	0.9590	0.0910
H	0.9830	0.0680
I	0.9830	0.0860
J	0.9790	0.0680
K	0.9850	0.0830
L	0.9780	0.0580

