



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 04:36 AM UTC

PDB ID : 7N6A / pdb_00007n6a
EMDB ID : EMD-24205
Title : Pre-fusion state 1 of EEEV with localized reconstruction
Authors : Chen, C.-L.; Kuhn, R.J.; Klose, T.
Deposited on : 2021-06-07
Resolution : 14.30 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:

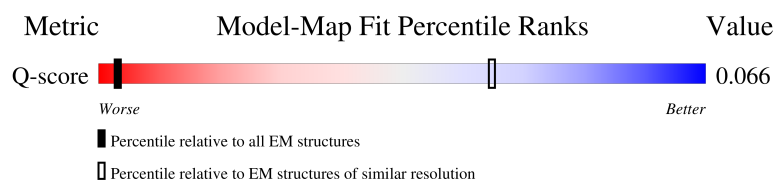
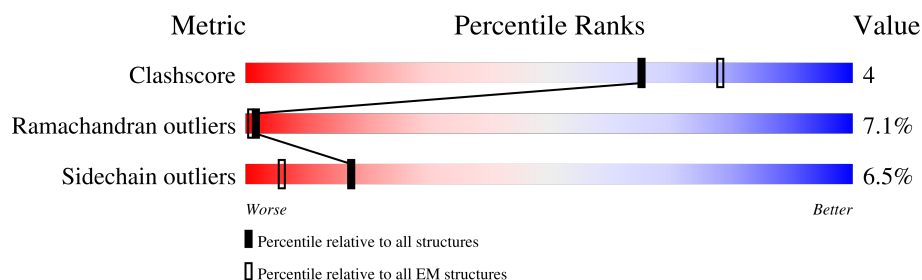
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 14.30 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	48 (13.80 - 14.73)

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	 64%22%••9%
1	K	441	 63%22%5%9%
2	B	420	 65%17%•16%
2	D	420	 62%18%•16%
2	F	420	 58%22%•16%
2	H	420	 62%19%•16%
2	J	420	 59%20%•16%
2	L	420	 62%20%•16%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 34962 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.

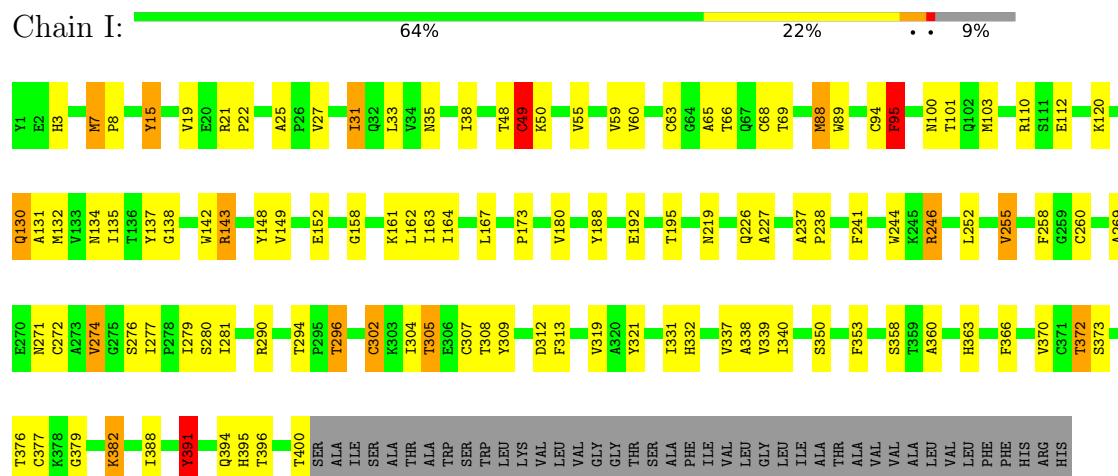
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	400	Total	C	N	O	S	0	0
			3063	1940	511	592	20		
1	C	400	Total	C	N	O	S	0	0
			3063	1940	511	592	20		
1	E	400	Total	C	N	O	S	0	0
			3063	1940	511	592	20		
1	G	400	Total	C	N	O	S	0	0
			3063	1940	511	592	20		
1	I	400	Total	C	N	O	S	0	0
			3063	1940	511	592	20		
1	K	400	Total	C	N	O	S	0	0
			3063	1940	511	592	20		

- Molecule 2 is a protein called Spike glycoprotein E2.

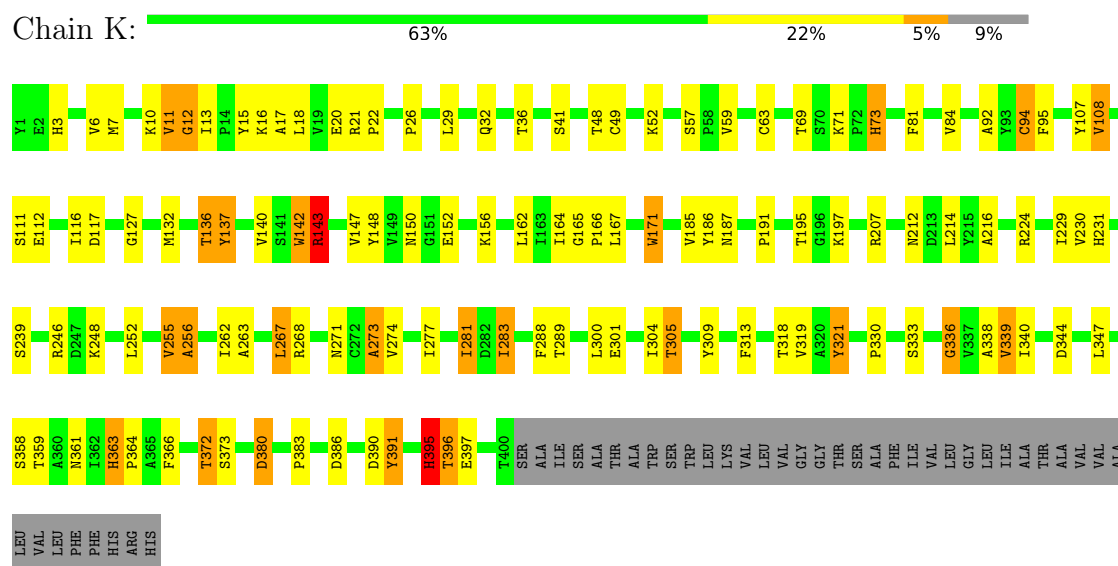
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	351	Total	C	N	O	S	0	0
			2764	1734	510	504	16		
2	D	351	Total	C	N	O	S	0	0
			2764	1734	510	504	16		
2	F	351	Total	C	N	O	S	0	0
			2764	1734	510	504	16		
2	H	351	Total	C	N	O	S	0	0
			2764	1734	510	504	16		
2	J	351	Total	C	N	O	S	0	0
			2764	1734	510	504	16		
2	L	351	Total	C	N	O	S	0	0
			2764	1734	510	504	16		

- Molecule 1: Spike glycoprotein E1

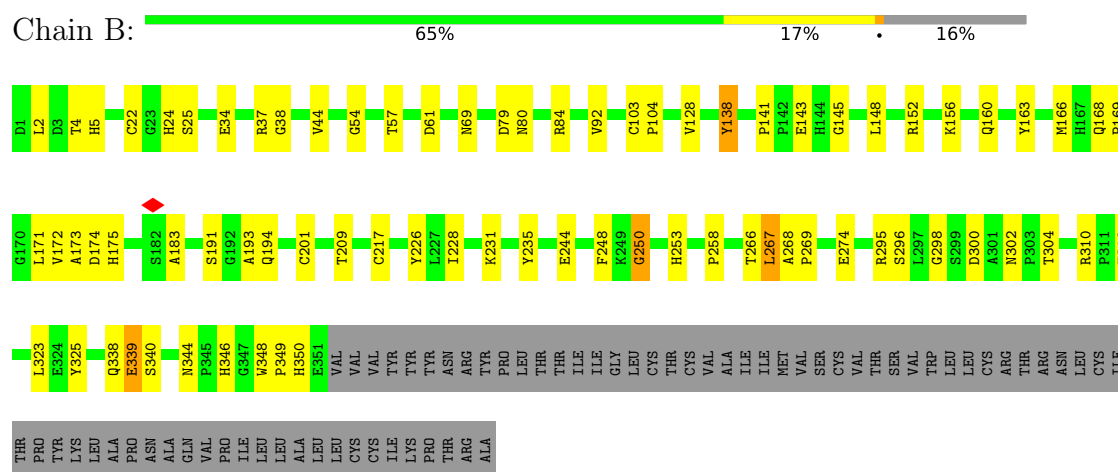
- Molecule 1: Spike glycoprotein E1



- Molecule 1: Spike glycoprotein E1

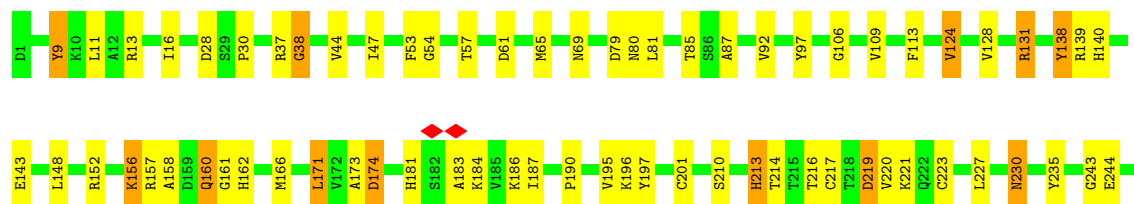


- Molecule 2: Spike glycoprotein E2

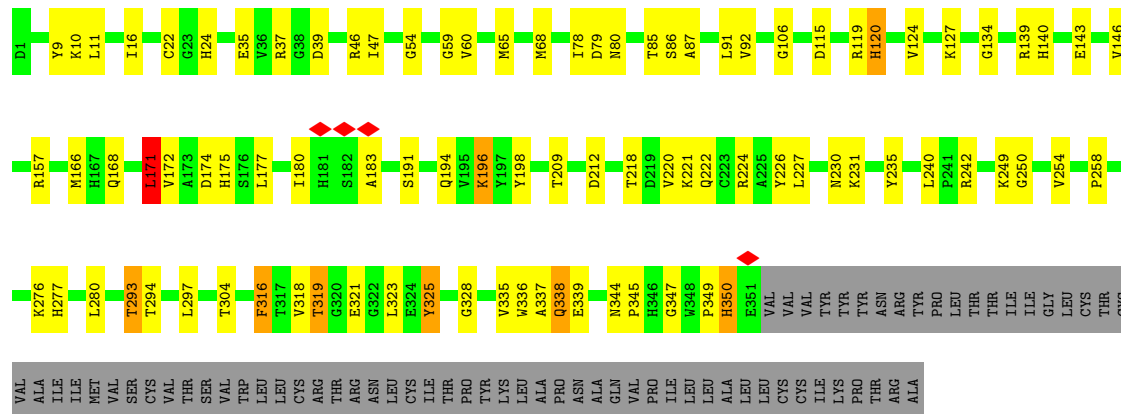


- Molecule 2: Spike glycoprotein E2





- Molecule 2: Spike glycoprotein E2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	135660	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	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.254	Depositor
Minimum map value	-5.570	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size (Å)	573.696, 573.696, 573.696	wwPDB
Map dimensions	108, 108, 108	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	5.312, 5.312, 5.312	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	1.28	0/3147	1.69	68/4294 (1.6%)
1	C	1.27	1/3147 (0.0%)	1.63	59/4294 (1.4%)
1	E	1.29	2/3147 (0.1%)	1.63	59/4294 (1.4%)
1	G	1.29	0/3147	1.63	48/4294 (1.1%)
1	I	1.28	2/3147 (0.1%)	1.62	46/4294 (1.1%)
1	K	1.29	1/3147 (0.0%)	1.66	54/4294 (1.3%)
2	B	1.29	0/2847	1.62	40/3876 (1.0%)
2	D	1.30	1/2847 (0.0%)	1.65	40/3876 (1.0%)
2	F	1.29	0/2847	1.68	46/3876 (1.2%)
2	H	1.29	0/2847	1.64	45/3876 (1.2%)
2	J	1.28	0/2847	1.66	48/3876 (1.2%)
2	L	1.30	0/2847	1.65	49/3876 (1.3%)
All	All	1.29	7/35964 (0.0%)	1.65	602/49020 (1.2%)

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	5
1	E	0	5
1	G	0	4
1	I	0	2
1	K	0	5
2	B	0	3
2	D	0	5
2	F	0	9
2	H	0	5
2	J	0	4
2	L	0	6
All	All	0	55

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	273	ALA	N-CA	-5.60	1.42	1.47
2	D	295	ARG	CA-C	-5.60	1.47	1.53
1	E	29	LEU	CA-C	-5.48	1.47	1.53
1	I	277	ILE	N-CA	-5.11	1.42	1.46
1	C	30	GLN	CA-C	-5.10	1.46	1.52
1	E	271	ASN	CA-C	-5.02	1.48	1.53
1	I	280	SER	CA-C	-5.02	1.46	1.52

All (602) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	305	THR	N-CA-C	-10.48	100.34	113.55
1	K	380	ASP	N-CA-C	-9.43	100.15	112.41
1	G	212	ASN	N-CA-C	-9.35	103.96	114.62
2	B	92	VAL	N-CA-C	-8.57	104.19	111.56
1	I	63	CYS	N-CA-C	-8.28	105.18	114.62
1	E	161	LYS	N-CA-C	-8.27	95.75	109.07
1	E	288	PHE	CA-CB-CG	-8.24	105.56	113.80
1	K	340	ILE	N-CA-C	-8.16	96.69	108.53
2	H	92	VAL	N-CA-C	-8.12	104.57	111.56
2	F	210	SER	N-CA-C	-8.02	100.82	110.44
1	E	163	ILE	N-CA-C	-7.90	97.05	108.11
1	A	393	ALA	N-CA-C	-7.89	100.74	110.61
1	A	305	THR	N-CA-C	-7.89	102.44	112.93
2	F	316	PHE	CA-CB-CG	-7.88	105.92	113.80
2	B	172	VAL	N-CA-C	-7.79	95.97	108.90
2	J	79	ASP	N-CA-C	-7.78	102.88	113.30
2	L	92	VAL	N-CA-C	-7.78	104.87	111.56
2	H	298	GLY	N-CA-C	-7.67	99.40	110.60
2	J	80	ASN	N-CA-C	-7.67	104.16	113.97
2	J	309	GLU	N-CA-C	-7.64	105.13	114.75
1	K	305	THR	N-CA-C	-7.59	102.58	112.68
2	D	104	PRO	CA-C-O	-7.54	115.47	120.90
2	B	104	PRO	CA-C-O	-7.53	115.47	120.90
1	A	7	MET	N-CA-C	-7.53	99.48	108.14
1	A	190	PHE	N-CA-C	-7.52	101.45	108.22
2	J	140	HIS	N-CA-C	-7.47	101.50	108.22
2	J	330	HIS	CA-C-N	7.44	125.09	119.66
2	J	330	HIS	C-N-CA	7.44	125.09	119.66
2	L	304	THR	N-CA-C	-7.39	97.78	109.23
1	G	396	THR	CA-C-N	7.32	131.59	120.82
1	G	396	THR	C-N-CA	7.32	131.59	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	309	GLU	N-CA-C	-7.29	106.31	114.62
2	J	148	LEU	N-CA-C	-7.26	101.68	108.22
2	J	323	LEU	N-CA-C	-7.24	98.31	109.24
2	D	56	LYS	N-CA-C	-7.23	100.49	111.56
1	C	36	THR	N-CA-C	-7.22	103.03	112.41
1	E	311	SER	N-CA-C	-7.21	104.08	113.17
2	H	44	VAL	N-CA-C	-7.20	97.94	108.89
2	L	347	GLY	N-CA-C	-7.20	105.56	114.92
2	L	80	ASN	N-CA-C	-7.16	104.69	113.50
1	K	7	MET	N-CA-C	-7.14	94.03	109.81
1	K	255	VAL	N-CA-C	-7.09	106.09	112.90
2	L	328	GLY	CA-C-N	7.07	129.76	120.28
2	L	328	GLY	C-N-CA	7.07	129.76	120.28
1	G	338	ALA	N-CA-C	-7.06	97.39	108.90
1	A	31	ILE	N-CA-C	-7.04	96.86	106.85
1	I	280	SER	N-CA-C	-7.03	96.25	108.69
2	F	92	VAL	N-CA-C	-7.01	105.53	111.56
1	K	339	VAL	N-CA-C	-7.01	98.30	108.11
1	C	369	GLN	CA-C-N	7.01	130.28	122.22
1	C	369	GLN	C-N-CA	7.01	130.28	122.22
2	D	9	TYR	N-CA-C	7.01	118.61	110.97
2	F	69	ASN	N-CA-C	-7.00	96.87	108.34
1	G	358	SER	N-CA-C	-6.99	98.02	108.99
2	B	174	ASP	N-CA-C	-6.98	95.93	110.80
1	I	258	PHE	CA-CB-CG	-6.98	106.82	113.80
1	G	369	GLN	CA-C-N	6.97	128.21	121.65
1	G	369	GLN	C-N-CA	6.97	128.21	121.65
2	B	80	ASN	N-CA-C	-6.97	104.81	113.38
2	D	168	GLN	N-CA-C	-6.96	101.95	108.22
1	K	81	PHE	CA-CB-CG	-6.96	106.84	113.80
1	A	372	THR	N-CA-CB	6.95	122.23	110.49
1	I	148	TYR	CA-C-N	6.94	129.97	120.46
1	I	148	TYR	C-N-CA	6.94	129.97	120.46
2	F	152	ARG	N-CA-C	-6.94	97.98	108.52
2	D	316	PHE	CA-CB-CG	-6.92	106.88	113.80
2	F	80	ASN	N-CA-C	-6.87	105.18	113.97
1	A	157	ILE	N-CA-C	-6.83	99.33	108.35
1	A	85	TYR	N-CA-C	-6.82	98.94	108.76
1	I	277	ILE	N-CA-C	-6.79	100.33	107.60
1	C	338	ALA	N-CA-C	-6.78	97.53	109.06
1	A	364	PRO	CA-C-O	-6.78	116.30	121.31
1	C	277	ILE	N-CA-C	-6.76	102.82	108.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	124	VAL	CA-C-N	6.76	132.09	122.09
2	J	124	VAL	C-N-CA	6.76	132.09	122.09
1	E	395	HIS	CA-CB-CG	-6.73	107.07	113.80
2	L	316	PHE	CA-CB-CG	-6.70	107.10	113.80
1	E	126	THR	CA-C-N	6.70	126.46	120.10
1	E	126	THR	C-N-CA	6.70	126.46	120.10
2	J	219	ASP	CA-C-N	6.67	129.21	120.60
2	J	219	ASP	C-N-CA	6.67	129.21	120.60
1	K	358	SER	N-CA-C	-6.65	98.55	108.99
2	B	152	ARG	N-CA-C	-6.63	98.44	108.52
2	D	92	VAL	N-CA-C	-6.63	105.86	111.56
2	L	85	THR	N-CA-C	-6.62	105.33	113.41
1	I	294	THR	N-CA-C	-6.62	98.10	109.15
2	F	211	SER	N-CA-C	-6.61	104.93	114.12
2	J	319	THR	CA-C-N	6.61	127.43	120.03
2	J	319	THR	C-N-CA	6.61	127.43	120.03
1	E	19	VAL	N-CA-CB	6.59	119.04	111.39
2	J	13	ARG	N-CA-C	-6.58	102.30	108.22
2	J	298	GLY	N-CA-C	-6.57	101.00	110.60
2	D	206	GLU	N-CA-C	-6.57	105.28	113.55
1	A	343	ASN	N-CA-C	-6.56	102.71	111.96
1	E	129	VAL	CA-C-N	6.55	134.05	121.54
1	E	129	VAL	C-N-CA	6.55	134.05	121.54
2	D	80	ASN	N-CA-C	-6.54	105.45	113.50
1	A	163	ILE	N-CA-C	-6.54	98.96	108.11
2	B	2	LEU	N-CA-C	-6.53	105.94	114.04
2	H	140	HIS	CA-C-N	6.53	124.43	119.66
2	H	140	HIS	C-N-CA	6.53	124.43	119.66
2	D	103	CYS	CA-C-N	6.53	124.42	119.66
2	D	103	CYS	C-N-CA	6.53	124.42	119.66
2	B	160	GLN	N-CA-C	-6.51	104.65	112.59
2	H	80	ASN	N-CA-C	-6.51	105.64	113.97
2	F	140	HIS	CA-C-N	6.49	124.40	119.66
2	F	140	HIS	C-N-CA	6.49	124.40	119.66
1	E	109	GLU	N-CA-C	-6.49	98.81	108.99
1	K	380	ASP	CA-C-N	6.48	130.04	120.90
1	K	380	ASP	C-N-CA	6.48	130.04	120.90
1	C	212	ASN	N-CA-C	-6.44	105.05	114.39
2	H	304	THR	N-CA-C	-6.40	98.95	108.99
2	L	196	LYS	N-CA-C	-6.40	99.29	109.59
1	E	274	VAL	N-CA-C	-6.39	99.90	107.70
1	K	361	ASN	N-CA-C	-6.39	101.06	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	386	ASP	CA-CB-CG	6.38	118.98	112.60
1	C	128	THR	CA-C-N	6.38	129.21	120.35
1	C	128	THR	C-N-CA	6.38	129.21	120.35
2	L	78	ILE	N-CA-C	-6.37	106.48	113.43
1	G	387	HIS	CA-CB-CG	-6.37	107.43	113.80
1	K	395	HIS	CA-CB-CG	6.36	120.16	113.80
2	H	141	PRO	CA-C-O	-6.35	116.33	120.90
2	F	58	ASP	CA-CB-CG	6.35	118.95	112.60
2	H	84	ARG	N-CA-C	-6.34	99.34	108.60
2	F	39	ASP	N-CA-C	-6.33	105.21	114.39
2	F	331	PRO	N-CA-C	6.32	118.41	110.70
2	J	79	ASP	CA-CB-CG	6.31	118.91	112.60
2	J	216	THR	N-CA-C	-6.30	105.72	113.41
1	A	29	LEU	N-CA-C	-6.28	100.00	108.86
1	I	163	ILE	N-CA-C	-6.28	99.31	108.11
2	D	124	VAL	CA-C-N	6.28	131.39	122.09
2	D	124	VAL	C-N-CA	6.28	131.39	122.09
1	C	102	GLN	N-CA-C	-6.27	97.86	108.26
1	A	344	ASP	CA-CB-CG	6.26	118.86	112.60
1	G	190	PHE	N-CA-C	-6.26	102.58	108.22
1	E	89	TRP	N-CA-C	-6.26	104.45	113.21
2	D	330	HIS	CA-CB-CG	6.25	120.05	113.80
1	I	35	ASN	N-CA-C	-6.25	99.54	109.23
1	I	68	CYS	N-CA-C	-6.25	106.62	114.56
1	C	285	ASP	CA-C-N	6.25	128.65	120.28
1	C	285	ASP	C-N-CA	6.25	128.65	120.28
1	E	283	ILE	N-CA-C	-6.24	100.69	108.05
1	G	309	TYR	N-CA-C	-6.23	104.03	112.26
2	L	194	GLN	N-CA-C	-6.23	97.55	108.20
2	H	249	LYS	N-CA-C	-6.23	104.16	112.94
2	J	331	PRO	CA-C-O	-6.21	116.43	120.90
2	L	166	MET	N-CA-C	-6.21	105.19	114.64
1	G	305	THR	N-CA-C	-6.20	103.40	111.71
1	A	102	GLN	N-CA-C	-6.19	98.19	108.34
1	A	340	ILE	N-CA-C	-6.19	99.55	108.53
1	A	149	VAL	N-CA-C	-6.18	107.83	113.71
1	G	31	ILE	N-CA-C	-6.18	98.30	107.51
1	E	174	PHE	CA-CB-CG	-6.18	107.62	113.80
2	H	295	ARG	N-CA-CB	6.16	120.83	110.79
1	C	247	ASP	N-CA-C	-6.15	104.14	112.26
2	B	228	ILE	N-CA-CB	6.15	118.54	111.90
1	I	25	ALA	CA-C-N	6.14	126.15	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	25	ALA	C-N-CA	6.14	126.15	119.89
2	B	103	CYS	CA-C-N	6.13	124.14	119.66
2	B	103	CYS	C-N-CA	6.13	124.14	119.66
1	E	201	PHE	CA-CB-CG	-6.13	107.67	113.80
1	K	267	LEU	N-CA-CB	6.13	120.85	110.49
1	I	358	SER	N-CA-C	-6.10	99.41	108.99
2	D	152	ARG	N-CA-C	-6.09	99.26	108.52
2	L	212	ASP	N-CA-C	-6.09	104.69	113.21
1	E	149	VAL	N-CA-C	-6.08	105.44	111.88
1	A	335	SER	CA-C-N	6.07	129.27	120.11
1	A	335	SER	C-N-CA	6.07	129.27	120.11
2	F	141	PRO	N-CA-C	6.06	116.29	110.47
2	D	11	LEU	N-CA-C	-6.06	103.25	111.55
2	H	9	TYR	N-CA-C	6.05	117.56	110.97
1	E	382	LYS	CA-C-N	6.04	126.60	120.38
1	E	382	LYS	C-N-CA	6.04	126.60	120.38
2	F	130	PHE	N-CA-C	-6.04	98.79	109.06
1	C	164	ILE	N-CA-C	-6.03	99.80	108.48
1	E	274	VAL	N-CA-CB	6.02	117.79	109.84
2	L	134	GLY	CA-C-N	6.02	130.76	121.19
2	L	134	GLY	C-N-CA	6.02	130.76	121.19
2	F	126	HIS	CA-C-N	6.02	129.90	121.24
2	F	126	HIS	C-N-CA	6.02	129.90	121.24
1	C	274	VAL	N-CA-C	-6.02	99.21	107.75
1	K	372	THR	N-CA-CB	6.01	120.65	110.49
2	D	338	GLN	N-CA-C	-6.01	106.92	114.56
1	C	25	ALA	CA-C-N	6.01	125.97	119.78
1	C	25	ALA	C-N-CA	6.01	125.97	119.78
1	A	394	GLN	N-CA-C	-6.01	104.16	112.03
2	J	87	ALA	N-CA-C	-6.01	102.81	108.22
1	E	395	HIS	CA-C-N	6.00	133.00	121.54
1	E	395	HIS	C-N-CA	6.00	133.00	121.54
1	E	25	ALA	CA-C-N	6.00	126.02	119.90
1	E	25	ALA	C-N-CA	6.00	126.02	119.90
1	K	268	ARG	N-CA-C	-6.00	99.42	107.88
2	L	293	THR	N-CA-C	-6.00	99.61	108.79
2	D	298	GLY	N-CA-C	-5.98	102.00	112.53
2	L	79	ASP	CA-CB-CG	5.98	118.58	112.60
2	B	22	CYS	N-CA-C	-5.97	107.82	114.62
2	D	217	CYS	N-CA-C	-5.96	99.28	109.24
1	C	333	SER	CA-C-N	5.95	127.28	119.84
1	C	333	SER	C-N-CA	5.95	127.28	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	5	ALA	N-CA-C	-5.95	98.12	110.80
1	I	279	ILE	N-CA-C	-5.95	99.84	108.71
2	H	194	GLN	N-CA-C	-5.95	98.02	108.20
1	I	302	CYS	N-CA-C	-5.95	99.30	109.24
2	H	103	CYS	CA-C-N	5.95	126.51	120.38
2	H	103	CYS	C-N-CA	5.95	126.51	120.38
1	I	340	ILE	N-CA-C	-5.95	99.91	108.53
1	A	203	ASP	CA-CB-CG	5.94	118.54	112.60
1	E	19	VAL	CB-CA-C	-5.93	104.83	111.23
1	C	311	SER	N-CA-C	-5.92	101.37	109.71
1	I	158	GLY	CA-C-N	5.90	128.19	120.28
1	I	158	GLY	C-N-CA	5.90	128.19	120.28
1	C	97	ASP	N-CA-C	-5.88	105.42	113.30
2	L	124	VAL	CA-C-N	5.88	130.79	122.09
2	L	124	VAL	C-N-CA	5.88	130.79	122.09
2	L	338	GLN	N-CA-CB	5.87	120.42	110.49
2	J	348	TRP	CA-C-N	5.87	127.18	119.84
2	J	348	TRP	C-N-CA	5.87	127.18	119.84
1	A	247	ASP	N-CA-C	-5.87	103.28	110.61
1	I	101	THR	N-CA-C	-5.87	99.84	109.40
1	K	164	ILE	N-CA-C	-5.86	100.04	108.48
1	A	109	GLU	N-CA-C	-5.86	99.79	108.99
1	G	247	ASP	N-CA-C	-5.86	105.79	113.17
2	B	209	THR	N-CA-C	-5.85	104.37	112.03
2	H	331	PRO	CA-C-N	5.85	125.86	119.90
2	H	331	PRO	C-N-CA	5.85	125.86	119.90
1	K	143	ARG	N-CA-C	-5.85	98.73	108.32
1	E	394	GLN	N-CA-C	-5.84	101.71	110.06
1	C	399	PHE	CA-CB-CG	-5.83	107.97	113.80
1	E	180	VAL	N-CA-C	-5.83	99.78	108.46
1	C	7	MET	CA-C-N	5.83	125.84	119.90
1	C	7	MET	C-N-CA	5.83	125.84	119.90
2	L	140	HIS	CA-CB-CG	5.82	119.62	113.80
2	H	321	GLU	N-CA-C	-5.82	105.06	113.21
1	G	3	HIS	CA-CB-CG	5.82	119.62	113.80
2	F	141	PRO	CA-C-O	-5.81	116.72	120.90
2	D	148	LEU	N-CA-C	-5.81	102.99	108.22
2	D	274	GLU	N-CA-C	-5.80	100.53	109.52
1	E	294	THR	N-CA-C	-5.80	101.39	110.14
2	F	346	HIS	N-CA-C	-5.80	105.53	113.30
1	E	358	SER	N-CA-C	-5.79	98.84	108.75
1	I	15	TYR	N-CA-C	-5.78	99.91	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	175	HIS	CA-CB-CG	-5.78	108.02	113.80
1	E	340	ILE	N-CA-C	-5.78	100.15	108.53
2	D	348	TRP	N-CA-C	-5.78	98.87	108.23
2	H	145	GLY	CA-C-N	5.78	129.18	120.75
2	H	145	GLY	C-N-CA	5.78	129.18	120.75
2	H	305	ARG	N-CA-C	-5.78	98.47	108.69
1	K	140	VAL	N-CA-C	-5.78	99.22	107.77
1	K	336	GLY	CA-C-N	5.77	127.83	120.56
1	K	336	GLY	C-N-CA	5.77	127.83	120.56
2	J	11	LEU	N-CA-C	-5.76	106.06	112.57
1	G	141	SER	CA-C-N	5.76	129.45	120.75
1	G	141	SER	C-N-CA	5.76	129.45	120.75
1	K	136	THR	N-CA-C	-5.76	101.67	110.14
1	A	19	VAL	N-CA-CB	5.76	118.07	111.39
2	J	166	MET	N-CA-C	-5.76	104.09	113.19
1	E	97	ASP	N-CA-C	-5.75	104.98	113.61
1	A	15	TYR	N-CA-CB	5.74	119.63	110.16
2	F	330	HIS	CA-C-N	5.74	126.29	120.38
2	F	330	HIS	C-N-CA	5.74	126.29	120.38
1	C	139	SER	N-CA-C	-5.73	105.68	114.16
2	B	304	THR	N-CA-C	-5.72	100.36	109.23
1	G	30	GLN	N-CA-C	-5.72	99.09	108.41
2	H	86	SER	N-CA-C	-5.71	104.08	113.50
2	B	156	LYS	N-CA-C	-5.71	100.41	109.59
1	I	88	MET	N-CA-C	-5.71	107.56	114.75
2	J	106	GLY	CA-C-N	5.70	128.49	120.28
2	J	106	GLY	C-N-CA	5.70	128.49	120.28
1	C	275	GLY	CA-C-N	5.70	132.43	121.54
1	C	275	GLY	C-N-CA	5.70	132.43	121.54
1	I	33	LEU	N-CA-C	-5.70	99.90	108.96
1	C	319	VAL	N-CA-C	-5.70	99.29	107.78
2	B	84	ARG	N-CA-C	-5.69	100.29	108.60
1	K	21	ARG	N-CA-C	-5.69	97.24	109.81
1	I	95	PHE	CA-CB-CG	5.68	119.48	113.80
2	J	69	ASN	N-CA-C	-5.68	99.16	108.41
2	D	106	GLY	CA-C-N	5.67	128.45	120.28
2	D	106	GLY	C-N-CA	5.67	128.45	120.28
2	L	172	VAL	N-CA-C	-5.67	99.48	108.90
2	L	180	ILE	N-CA-C	-5.67	100.17	108.11
2	L	319	THR	CA-C-N	5.67	127.28	120.13
2	L	319	THR	C-N-CA	5.67	127.28	120.13
1	C	340	ILE	N-CA-C	-5.67	100.31	108.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	296	THR	N-CA-C	-5.67	99.94	108.96
2	H	201	CYS	CA-C-N	5.67	126.93	119.84
2	H	201	CYS	C-N-CA	5.67	126.93	119.84
1	A	231	HIS	N-CA-C	-5.66	100.92	108.34
1	A	371	CYS	CA-C-N	5.66	132.34	121.54
1	A	371	CYS	C-N-CA	5.66	132.34	121.54
1	K	212	ASN	N-CA-C	-5.65	105.06	112.41
2	L	221	LYS	N-CA-C	-5.65	104.80	112.26
1	G	224	ARG	CA-C-N	5.65	125.66	119.90
1	G	224	ARG	C-N-CA	5.65	125.66	119.90
1	I	372	THR	N-CA-CB	5.64	120.03	110.49
2	B	145	GLY	CA-C-N	5.63	128.98	120.75
2	B	145	GLY	C-N-CA	5.63	128.98	120.75
2	D	141	PRO	CA-C-N	5.63	125.63	119.89
2	D	141	PRO	C-N-CA	5.63	125.63	119.89
2	D	174	ASP	N-CA-CB	5.63	120.00	110.49
1	E	369	GLN	CA-C-N	5.63	126.94	121.65
1	E	369	GLN	C-N-CA	5.63	126.94	121.65
1	K	108	VAL	N-CA-C	-5.62	100.32	108.87
2	B	171	LEU	N-CA-C	5.62	117.55	110.24
1	I	180	VAL	N-CA-C	-5.62	100.13	108.45
1	A	15	TYR	N-CA-C	-5.62	100.13	109.46
2	D	194	GLN	N-CA-C	-5.62	98.59	108.20
1	I	274	VAL	N-CA-CB	5.62	120.51	111.23
1	G	290	ARG	N-CA-C	5.62	117.95	110.53
2	L	276	LYS	N-CA-C	-5.62	100.98	108.34
1	K	185	VAL	N-CA-C	-5.62	100.33	108.36
1	I	161	LYS	N-CA-C	-5.61	100.03	109.07
2	D	346	HIS	CA-CB-CG	5.61	119.41	113.80
1	A	366	PHE	N-CA-C	-5.60	100.57	109.59
1	I	31	ILE	N-CA-CB	5.60	118.41	111.41
2	L	212	ASP	CA-CB-CG	5.60	118.20	112.60
1	G	383	PRO	N-CA-C	5.59	117.53	110.70
1	E	279	ILE	N-CA-C	-5.58	100.40	108.71
2	L	344	ASN	CA-C-N	5.57	126.81	119.84
2	L	344	ASN	C-N-CA	5.57	126.81	119.84
2	D	159	ASP	CA-CB-CG	5.57	118.17	112.60
1	C	157	ILE	N-CA-C	-5.57	100.32	108.11
2	F	191	SER	N-CA-C	-5.57	105.42	113.21
1	G	395	HIS	CA-C-N	5.56	132.16	121.54
1	G	395	HIS	C-N-CA	5.56	132.16	121.54
2	J	9	TYR	N-CA-C	5.56	117.03	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	391	TYR	CA-C-N	5.56	125.88	119.93
1	G	391	TYR	C-N-CA	5.56	125.88	119.93
1	C	332	HIS	N-CA-CB	5.55	120.07	111.24
1	G	237	ALA	CA-C-N	5.55	126.78	119.84
1	G	237	ALA	C-N-CA	5.55	126.78	119.84
2	H	336	TRP	N-CA-CB	5.53	119.19	110.23
1	K	13	ILE	CA-C-N	5.53	125.53	119.89
1	K	13	ILE	C-N-CA	5.53	125.53	119.89
1	C	166	PRO	CA-C-N	5.52	132.09	121.54
1	C	166	PRO	C-N-CA	5.52	132.09	121.54
1	I	49	CYS	N-CA-C	-5.52	99.04	110.80
2	H	11	LEU	N-CA-C	-5.52	104.75	112.25
1	I	59	VAL	N-CA-C	-5.52	100.44	108.17
1	C	377	CYS	CA-C-N	5.51	129.08	120.75
1	C	377	CYS	C-N-CA	5.51	129.08	120.75
1	C	339	VAL	N-CA-C	-5.51	100.45	108.17
1	A	268	ARG	N-CA-C	-5.51	100.34	108.99
2	F	305	ARG	N-CA-C	-5.51	98.94	108.69
1	G	215	TYR	N-CA-C	-5.51	99.31	108.34
2	L	39	ASP	N-CA-C	-5.51	106.61	113.38
1	A	391	TYR	CA-C-N	5.50	125.50	119.89
1	A	391	TYR	C-N-CA	5.50	125.50	119.89
2	B	69	ASN	N-CA-C	-5.50	99.45	108.41
1	I	290	ARG	N-CA-CB	5.50	118.22	110.36
2	J	219	ASP	N-CA-CB	5.48	119.75	110.49
1	K	36	THR	N-CA-C	-5.48	99.48	109.56
1	A	169	SER	N-CA-C	-5.47	103.77	110.61
1	E	164	ILE	N-CA-C	-5.47	100.60	108.48
1	E	251	PRO	CA-C-N	5.47	128.15	120.28
1	E	251	PRO	C-N-CA	5.47	128.15	120.28
2	J	54	GLY	N-CA-C	-5.47	100.22	113.18
1	K	283	ILE	N-CA-C	-5.46	101.94	107.89
1	A	215	TYR	N-CA-C	-5.46	99.38	108.34
2	L	9	TYR	N-CA-C	5.46	116.92	110.97
1	C	293	GLU	N-CA-C	-5.46	106.21	112.92
2	J	160	GLN	N-CA-C	-5.45	99.18	110.80
1	A	108	VAL	N-CA-C	-5.45	100.58	108.87
1	C	19	VAL	CB-CA-C	-5.45	105.34	111.23
1	A	369	GLN	CA-C-N	5.45	126.77	121.65
1	A	369	GLN	C-N-CA	5.45	126.77	121.65
2	J	28	ASP	CA-CB-CG	5.44	118.04	112.60
1	I	173	PRO	CA-C-N	5.44	128.57	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	173	PRO	C-N-CA	5.44	128.57	120.90
2	F	309	GLU	N-CA-C	-5.43	105.67	114.09
1	I	296	THR	N-CA-C	-5.43	100.94	109.25
2	F	215	THR	N-CA-C	-5.43	106.51	114.39
1	I	339	VAL	N-CA-C	-5.43	100.51	108.11
2	B	141	PRO	CA-C-N	5.43	125.44	119.90
2	B	141	PRO	C-N-CA	5.43	125.44	119.90
2	D	143	GLU	N-CA-C	-5.42	105.30	112.94
2	D	130	PHE	N-CA-C	-5.41	103.84	110.61
2	L	218	THR	N-CA-C	5.41	116.86	111.07
1	A	16	LYS	CA-C-N	5.41	131.88	121.54
1	A	16	LYS	C-N-CA	5.41	131.88	121.54
1	K	73	HIS	CA-C-N	5.41	126.60	119.84
1	K	73	HIS	C-N-CA	5.41	126.60	119.84
2	J	138	TYR	CA-C-N	5.40	131.85	121.54
2	J	138	TYR	C-N-CA	5.40	131.85	121.54
1	A	48	THR	N-CA-C	-5.40	101.21	109.41
1	A	19	VAL	CB-CA-C	-5.39	105.41	111.23
1	K	171	TRP	N-CA-C	-5.39	101.33	109.85
1	E	334	PRO	CA-C-N	5.39	129.78	122.07
1	E	334	PRO	C-N-CA	5.39	129.78	122.07
2	B	166	MET	N-CA-C	-5.39	106.45	114.64
1	C	237	ALA	CA-C-N	5.39	126.57	119.84
1	C	237	ALA	C-N-CA	5.39	126.57	119.84
2	J	201	CYS	CA-C-N	5.39	126.57	119.84
2	J	201	CYS	C-N-CA	5.39	126.57	119.84
2	L	54	GLY	N-CA-C	-5.39	100.42	113.18
1	C	387	HIS	N-CA-C	-5.38	100.40	109.07
2	H	28	ASP	CA-CB-CG	-5.38	107.22	112.60
1	E	338	ALA	N-CA-C	-5.38	99.34	110.80
2	B	24	HIS	N-CA-C	-5.38	106.03	112.59
1	G	231	HIS	N-CA-CB	5.38	119.57	110.49
1	A	335	SER	N-CA-C	5.37	117.20	110.91
2	D	69	ASN	N-CA-C	-5.37	99.65	108.41
2	L	59	GLY	CA-C-N	5.37	131.64	121.97
2	L	59	GLY	C-N-CA	5.37	131.64	121.97
1	K	12	GLY	CA-C-N	5.37	130.51	119.72
1	K	12	GLY	C-N-CA	5.37	130.51	119.72
1	A	29	LEU	N-CA-CB	5.36	120.26	111.31
1	K	301	GLU	N-CA-C	-5.36	100.58	108.99
2	D	113	PHE	N-CA-C	-5.35	100.18	108.90
2	J	217	CYS	N-CA-C	-5.35	99.69	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	11	LEU	N-CA-C	-5.35	106.53	112.57
1	I	376	THR	CA-C-N	5.34	130.04	122.24
1	I	376	THR	C-N-CA	5.34	130.04	122.24
1	E	136	THR	N-CA-C	-5.34	101.46	109.95
1	G	245	LYS	N-CA-C	-5.34	105.82	114.09
2	J	174	ASP	N-CA-CB	5.34	119.51	110.49
2	H	79	ASP	N-CA-C	-5.33	106.45	113.17
1	G	147	VAL	N-CA-C	-5.33	100.64	108.85
1	A	285	ASP	CA-CB-CG	5.32	117.92	112.60
2	F	3	ASP	N-CA-C	-5.32	104.22	111.56
2	F	262	LYS	CA-C-N	5.32	128.27	120.71
2	F	262	LYS	C-N-CA	5.32	128.27	120.71
2	D	293	THR	N-CA-C	-5.32	100.66	108.79
1	G	166	PRO	CA-C-N	5.31	128.63	120.82
1	G	166	PRO	C-N-CA	5.31	128.63	120.82
1	K	59	VAL	N-CA-C	-5.31	98.29	109.34
1	A	171	TRP	N-CA-C	-5.31	101.11	109.50
2	J	267	LEU	N-CA-C	-5.31	99.64	108.34
1	C	41	SER	N-CA-C	-5.30	100.09	108.73
2	H	174	ASP	CA-CB-CG	5.30	117.90	112.60
1	C	215	TYR	N-CA-C	-5.30	99.65	108.34
1	E	385	LYS	N-CA-C	-5.30	106.49	113.17
2	H	90	SER	N-CA-C	-5.30	99.78	108.41
1	K	92	ALA	CA-C-N	5.30	127.38	120.28
1	K	92	ALA	C-N-CA	5.30	127.38	120.28
2	B	267	LEU	N-CA-C	-5.29	98.96	108.48
1	I	363	HIS	N-CA-C	-5.29	101.00	109.04
1	I	377	CYS	CA-C-N	5.29	128.73	120.75
1	I	377	CYS	C-N-CA	5.29	128.73	120.75
1	E	280	SER	N-CA-C	-5.29	99.33	108.69
2	J	324	GLU	N-CA-C	-5.28	101.34	109.52
1	G	229	ILE	CA-C-N	5.28	131.47	121.97
1	G	229	ILE	C-N-CA	5.28	131.47	121.97
1	C	266	PRO	CA-C-N	5.28	131.62	121.54
1	C	266	PRO	C-N-CA	5.28	131.62	121.54
1	K	148	TYR	N-CA-C	-5.28	105.91	114.09
2	J	344	ASN	CA-CB-CG	5.27	117.87	112.60
1	C	38	ILE	N-CA-C	-5.27	100.15	108.90
2	F	79	ASP	N-CA-C	-5.26	106.91	113.38
2	D	325	TYR	N-CA-C	-5.26	99.01	108.48
2	L	220	VAL	N-CA-C	-5.26	106.75	112.80
1	I	379	GLY	N-CA-C	-5.26	103.08	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	268	ARG	N-CA-C	-5.25	101.32	109.14
2	J	304	THR	N-CA-C	-5.24	100.76	108.99
2	B	79	ASP	N-CA-C	-5.24	106.48	112.92
1	K	281	ILE	N-CA-C	-5.24	100.66	108.46
1	K	156	LYS	N-CA-C	-5.23	105.56	112.94
2	B	248	PHE	CA-CB-CG	-5.23	108.57	113.80
2	F	53	PHE	N-CA-C	-5.23	103.78	110.53
1	E	301	GLU	N-CA-C	-5.23	100.78	108.99
2	F	334	ARG	N-CA-C	-5.23	100.78	108.99
2	L	115	ASP	N-CA-C	-5.23	106.92	113.72
1	A	385	LYS	N-CA-C	-5.23	105.77	113.61
1	A	256	ALA	CA-C-O	-5.22	115.90	119.29
2	B	34	GLU	N-CA-C	-5.22	101.82	109.81
2	H	317	THR	CA-C-N	5.22	127.61	120.35
2	H	317	THR	C-N-CA	5.22	127.61	120.35
2	F	34	GLU	N-CA-C	-5.22	101.83	109.81
1	A	168	SER	N-CA-C	-5.21	106.51	112.92
2	L	240	LEU	CA-C-N	5.21	125.95	120.11
2	L	240	LEU	C-N-CA	5.21	125.95	120.11
1	E	368	LEU	N-CA-C	-5.21	99.79	108.34
1	I	308	THR	N-CA-C	-5.21	99.46	108.69
2	H	13	ARG	N-CA-C	-5.21	99.79	108.23
1	C	185	VAL	N-CA-CB	5.21	117.24	110.99
1	E	377	CYS	CA-C-N	5.21	128.62	120.75
1	E	377	CYS	C-N-CA	5.21	128.62	120.75
2	H	124	VAL	CA-C-N	5.21	129.80	122.09
2	H	124	VAL	C-N-CA	5.21	129.80	122.09
1	G	392	PRO	N-CA-C	5.21	119.75	111.26
1	K	95	PHE	N-CA-C	-5.21	105.69	111.36
1	G	203	ASP	CA-CB-CG	5.20	117.80	112.60
1	C	341	LYS	N-CA-C	-5.20	105.06	111.40
2	B	54	GLY	N-CA-C	-5.19	100.87	113.18
2	F	168	GLN	CA-C-N	5.19	125.13	119.78
2	F	168	GLN	C-N-CA	5.19	125.13	119.78
1	K	214	LEU	CA-C-N	5.19	130.09	122.77
1	K	214	LEU	C-N-CA	5.19	130.09	122.77
1	C	294	THR	N-CA-C	-5.19	99.83	109.06
2	D	248	PHE	CA-CB-CG	-5.19	108.61	113.80
2	L	47	ILE	N-CA-C	-5.19	100.41	108.86
2	L	106	GLY	CA-C-N	5.19	127.75	120.28
2	L	106	GLY	C-N-CA	5.19	127.75	120.28
1	K	289	THR	N-CA-C	-5.19	100.79	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	GLY	N-CA-C	-5.18	106.33	111.56
2	B	325	TYR	N-CA-C	-5.18	99.15	108.48
2	H	288	HIS	CA-C-N	5.18	126.32	119.84
2	H	288	HIS	C-N-CA	5.18	126.32	119.84
2	F	248	PHE	N-CA-C	-5.18	98.82	107.99
1	K	212	ASN	CA-C-N	5.18	128.13	120.82
1	K	212	ASN	C-N-CA	5.18	128.13	120.82
2	H	118	ASN	CA-CB-CG	5.18	117.78	112.60
2	J	38	GLY	CA-C-N	5.18	127.22	120.28
2	J	38	GLY	C-N-CA	5.18	127.22	120.28
2	B	250	GLY	CA-C-N	5.17	128.12	120.82
2	B	250	GLY	C-N-CA	5.17	128.12	120.82
1	I	241	PHE	N-CA-C	-5.17	105.97	113.21
1	A	280	SER	N-CA-C	-5.17	99.54	108.69
2	B	268	ALA	CA-C-N	5.17	126.30	119.84
2	B	268	ALA	C-N-CA	5.17	126.30	119.84
2	D	295	ARG	N-CA-C	-5.16	98.61	107.23
2	F	317	THR	CA-C-N	5.16	127.50	120.63
2	F	317	THR	C-N-CA	5.16	127.50	120.63
2	L	250	GLY	N-CA-C	-5.16	106.82	115.80
2	F	106	GLY	CA-C-N	5.16	127.71	120.28
2	F	106	GLY	C-N-CA	5.16	127.71	120.28
1	I	237	ALA	CA-C-N	5.15	126.28	119.84
1	I	237	ALA	C-N-CA	5.15	126.28	119.84
1	E	31	ILE	N-CA-CB	5.15	118.16	111.67
2	H	200	LYS	CA-C-N	5.15	127.55	120.39
2	H	200	LYS	C-N-CA	5.15	127.55	120.39
2	J	316	PHE	CA-CB-CG	-5.15	108.65	113.80
1	A	75	ASP	N-CA-CB	5.14	119.19	110.49
2	B	148	LEU	N-CA-C	-5.14	103.59	108.22
2	H	252	LEU	N-CA-C	-5.14	100.32	109.06
2	H	172	VAL	N-CA-C	-5.14	100.37	108.90
1	E	173	PRO	N-CA-C	-5.13	109.34	114.68
2	D	201	CYS	CA-C-N	5.13	126.26	119.84
2	D	201	CYS	C-N-CA	5.13	126.26	119.84
2	B	194	GLN	N-CA-C	-5.13	99.43	108.20
1	E	389	VAL	CA-C-N	5.13	131.34	121.54
1	E	389	VAL	C-N-CA	5.13	131.34	121.54
1	A	293	GLU	N-CA-C	-5.13	106.33	112.59
1	G	187	ASN	CA-CB-CG	5.13	117.73	112.60
2	J	92	VAL	N-CA-C	-5.13	107.15	111.56
2	B	348	TRP	CA-C-N	5.13	126.25	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	348	TRP	C-N-CA	5.13	126.25	119.84
1	E	311	SER	CA-C-N	5.13	128.05	120.82
1	E	311	SER	C-N-CA	5.13	128.05	120.82
1	A	208	THR	CA-C-N	5.12	127.65	120.28
1	A	208	THR	C-N-CA	5.12	127.65	120.28
2	F	215	THR	CA-C-N	5.12	127.14	120.28
2	F	215	THR	C-N-CA	5.12	127.14	120.28
2	H	323	LEU	N-CA-C	-5.12	101.51	109.24
2	J	53	PHE	N-CA-C	-5.12	103.93	110.53
1	C	322	LYS	N-CA-C	-5.11	99.91	110.80
1	I	382	LYS	N-CA-C	-5.11	102.21	109.62
1	G	266	PRO	CA-C-N	5.11	131.30	121.54
1	G	266	PRO	C-N-CA	5.11	131.30	121.54
2	L	336	TRP	N-CA-CB	5.10	117.52	110.17
1	A	244	TRP	CB-CG-CD2	5.10	133.94	126.80
1	C	33	LEU	CA-C-N	5.09	127.44	120.46
1	C	33	LEU	C-N-CA	5.09	127.44	120.46
2	L	87	ALA	CA-C-N	5.09	126.21	119.84
2	L	87	ALA	C-N-CA	5.09	126.21	119.84
1	K	256	ALA	CA-C-N	5.09	125.02	119.78
1	K	256	ALA	C-N-CA	5.09	125.02	119.78
2	F	131	ARG	CA-C-N	5.08	126.20	119.84
2	F	131	ARG	C-N-CA	5.08	126.20	119.84
2	B	201	CYS	CA-C-N	5.08	126.19	119.84
2	B	201	CYS	C-N-CA	5.08	126.19	119.84
1	E	72	PRO	CA-N-CD	-5.08	104.89	112.00
1	G	153	THR	CA-C-N	5.08	126.19	119.84
1	G	153	THR	C-N-CA	5.08	126.19	119.84
1	A	275	GLY	CA-C-N	5.07	131.22	121.54
1	A	275	GLY	C-N-CA	5.07	131.22	121.54
1	A	389	VAL	CA-C-N	5.06	131.21	121.54
1	A	389	VAL	C-N-CA	5.06	131.21	121.54
1	A	251	PRO	CA-C-N	5.06	128.70	120.60
1	A	251	PRO	C-N-CA	5.06	128.70	120.60
1	G	247	ASP	CA-C-N	5.05	131.19	121.54
1	G	247	ASP	C-N-CA	5.05	131.19	121.54
2	J	152	ARG	N-CA-C	-5.05	100.84	108.52
1	A	267	LEU	N-CA-C	-5.05	100.04	110.80
1	A	388	ILE	CA-C-N	5.05	128.32	120.34
1	A	388	ILE	C-N-CA	5.05	128.32	120.34
1	K	229	ILE	CA-C-N	5.05	131.06	121.97
1	K	229	ILE	C-N-CA	5.05	131.06	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	232	THR	CA-C-N	5.05	124.98	119.78
1	E	232	THR	C-N-CA	5.05	124.98	119.78
1	E	237	ALA	CA-C-N	5.05	126.15	119.84
1	E	237	ALA	C-N-CA	5.05	126.15	119.84
1	A	38	ILE	CA-C-N	5.05	131.47	122.13
1	A	38	ILE	C-N-CA	5.05	131.47	122.13
2	F	41	HIS	N-CA-C	-5.04	106.97	112.72
1	K	111	SER	CA-C-N	5.04	127.97	120.31
1	K	111	SER	C-N-CA	5.04	127.97	120.31
2	F	151	ASN	N-CA-C	-5.03	102.32	110.32
1	A	289	THR	N-CA-C	-5.03	101.51	109.76
1	K	277	ILE	N-CA-C	-5.03	98.02	108.88
1	A	143	ARG	N-CA-C	-5.03	100.08	108.32
1	G	73	HIS	CA-C-N	5.02	124.95	119.78
1	G	73	HIS	C-N-CA	5.02	124.95	119.78
2	F	9	TYR	N-CA-C	5.01	116.44	110.97
1	C	109	GLU	N-CA-C	-5.01	101.12	108.99
2	F	254	VAL	N-CA-C	-5.01	102.43	107.89
1	C	266	PRO	N-CA-C	-5.01	108.09	114.35
1	C	394	GLN	CA-C-N	5.01	131.10	121.54
1	C	394	GLN	C-N-CA	5.01	131.10	121.54
1	C	180	VAL	N-CA-C	-5.01	101.00	108.46
1	G	279	ILE	N-CA-C	-5.00	101.25	108.71
2	H	240	LEU	CA-C-N	5.00	126.09	119.84
2	H	240	LEU	C-N-CA	5.00	126.09	119.84

There are no chirality outliers.

All (55) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	TYR	Sidechain
1	A	309	TYR	Sidechain
2	B	138	TYR	Sidechain
2	B	235	TYR	Sidechain
2	B	295	ARG	Sidechain
1	C	110	ARG	Sidechain
1	C	137	TYR	Sidechain
1	C	24	TYR	Sidechain
1	C	270	GLU	Peptide
1	C	76	TYR	Sidechain
2	D	197	TYR	Sidechain
2	D	295	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	D	9	TYR	Sidechain
2	D	97	TYR	Sidechain
2	D	98	TYR	Sidechain
1	E	355	PHE	Sidechain
1	E	385	LYS	Peptide
1	E	391	TYR	Sidechain
1	E	46	TYR	Sidechain
1	E	93	TYR	Sidechain
2	F	138	TYR	Sidechain
2	F	15	TYR	Sidechain
2	F	168	GLN	Peptide
2	F	226	TYR	Sidechain
2	F	263	CYS	Peptide
2	F	278	ARG	Sidechain
2	F	295	ARG	Sidechain
2	F	97	TYR	Sidechain
2	F	98	TYR	Sidechain
1	G	186	TYR	Sidechain
1	G	3	HIS	Sidechain
1	G	46	TYR	Sidechain
1	G	93	TYR	Sidechain
2	H	135	ARG	Sidechain
2	H	138	TYR	Sidechain
2	H	226	TYR	Sidechain
2	H	235	TYR	Sidechain
2	H	97	TYR	Sidechain
1	I	137	TYR	Sidechain
1	I	309	TYR	Sidechain
2	J	131	ARG	Sidechain
2	J	138	TYR	Sidechain
2	J	235	TYR	Sidechain
2	J	37	ARG	Sidechain
1	K	186	TYR	Sidechain
1	K	26	PRO	Mainchain
1	K	309	TYR	Sidechain
1	K	321	TYR	Sidechain
1	K	391	TYR	Sidechain
2	L	139	ARG	Sidechain
2	L	226	TYR	Sidechain
2	L	235	TYR	Sidechain
2	L	325	TYR	Sidechain
2	L	37	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	L	46	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	3063	0	2950	39	0
1	C	3063	0	2950	29	0
1	E	3063	0	2950	32	0
1	G	3063	0	2950	37	0
1	I	3063	0	2950	27	0
1	K	3063	0	2950	34	0
2	B	2764	0	2679	10	0
2	D	2764	0	2679	23	0
2	F	2764	0	2679	21	0
2	H	2764	0	2679	19	0
2	J	2764	0	2679	22	0
2	L	2764	0	2679	17	0
All	All	34962	0	33774	277	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 4.

All (277) 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:136:THR:HG23	1:A:142:TRP:H	1.51	0.75
1:A:136:THR:HG22	1:A:137:TYR:H	1.56	0.71
1:I:38:ILE:HD13	1:I:269:ALA:H	1.58	0.68
2:F:280:LEU:HD11	2:F:335:VAL:HG11	1.77	0.65
2:D:167:HIS:CG	2:D:168:GLN:H	2.15	0.64
1:E:33:LEU:HD22	1:E:277:ILE:HD12	1.80	0.62
1:G:110:ARG:HD3	1:G:110:ARG:H	1.65	0.62
1:G:337:VAL:HG12	2:H:346:HIS:CE1	2.35	0.61
1:A:17:ALA:HA	1:A:332:HIS:CD2	2.36	0.60
1:C:304:ILE:HG12	1:C:380:ASP:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:38:GLY:H	2:J:128:VAL:HG12	1.67	0.60
1:I:7:MET:HA	1:I:7:MET:HE3	1.85	0.59
1:K:321:TYR:CD2	1:K:347:LEU:HD22	2.38	0.58
1:I:400:THR:HG23	2:J:345:PRO:HG2	1.86	0.57
1:A:11:VAL:HA	1:A:35:ASN:H	1.69	0.57
1:A:3:HIS:CE1	1:A:17:ALA:HB1	2.40	0.56
1:E:57:SER:H	2:F:236:ASN:HB3	1.70	0.56
1:A:274:VAL:HG22	1:A:275:GLY:H	1.70	0.55
1:A:17:ALA:HA	1:A:336:GLY:H	1.72	0.55
1:A:88:MET:HB2	2:B:173:ALA:H	1.71	0.55
2:H:275:HIS:HE1	2:H:338:GLN:H	1.55	0.54
1:A:331:ILE:HD12	1:A:368:LEU:HD21	1.88	0.54
1:I:400:THR:HG22	2:J:339:GLU:H	1.73	0.54
2:F:135:ARG:HH11	2:F:329:ASN:HA	1.72	0.54
1:K:304:ILE:HG23	1:K:380:ASP:H	1.73	0.54
2:J:65:MET:HE1	2:J:113:PHE:HB3	1.90	0.54
2:J:65:MET:HE3	2:J:81:LEU:HD13	1.90	0.54
1:I:302:CYS:SG	1:I:319:VAL:HG22	2.48	0.53
2:H:294:THR:HG22	2:H:325:TYR:HA	1.89	0.53
1:E:135:ILE:HB	1:E:143:ARG:HH11	1.73	0.53
1:E:48:THR:HG22	1:E:49:CYS:H	1.74	0.53
1:C:39:ILE:H	1:C:129:VAL:HG12	1.72	0.53
1:I:48:THR:HG22	1:I:49:CYS:H	1.74	0.53
1:E:387:HIS:CE1	2:F:278:ARG:HA	2.43	0.52
1:C:28:HIS:CD2	1:C:28:HIS:H	2.26	0.52
1:C:57:SER:H	2:D:242:ARG:HH21	1.56	0.52
1:E:400:THR:HA	2:F:338:GLN:HA	1.92	0.52
1:E:323:SER:H	1:E:349:GLU:HA	1.75	0.52
1:I:27:VAL:CG1	1:I:138:GLY:H	2.23	0.52
2:J:294:THR:HG21	2:J:316:PHE:CD2	2.45	0.52
1:I:394:GLN:HE22	1:I:400:THR:HG21	1.74	0.52
2:H:294:THR:HG21	2:H:316:PHE:CD2	2.44	0.52
1:I:112:GLU:HA	2:J:162:HIS:CD2	2.46	0.51
1:A:3:HIS:CE1	1:A:5:ALA:HB2	2.46	0.51
1:G:16:LYS:HB2	1:G:332:HIS:CE1	2.46	0.51
1:I:15:TYR:CD1	1:I:395:HIS:HB2	2.46	0.51
2:H:53:PHE:O	2:H:94:HIS:CD2	2.64	0.51
1:I:8:PRO:HA	1:I:276:SER:HA	1.93	0.51
1:K:16:LYS:H	1:K:339:VAL:HG22	1.75	0.51
1:C:180:VAL:HG13	1:C:185:VAL:HG22	1.93	0.51
1:K:17:ALA:HA	1:K:336:GLY:HA2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:HIS:CD2	1:A:333:SER:O	2.64	0.51
1:E:332:HIS:CD2	1:E:333:SER:O	2.63	0.51
1:C:27:VAL:CG1	1:C:138:GLY:H	2.23	0.51
1:G:298:SER:H	1:G:323:SER:HA	1.76	0.51
1:E:15:TYR:CG	1:E:395:HIS:CD2	2.99	0.50
2:F:44:VAL:HG21	2:F:153:TYR:H	1.76	0.50
1:G:391:TYR:CZ	2:H:297:LEU:HD11	2.46	0.50
1:G:8:PRO:HA	1:G:276:SER:HA	1.94	0.50
1:I:319:VAL:HG11	1:I:321:TYR:CE1	2.46	0.50
1:G:302:CYS:SG	1:G:319:VAL:HG22	2.52	0.50
2:D:40:ALA:HB2	2:D:153:TYR:CE2	2.45	0.50
1:G:231:HIS:CD2	2:H:26:ARG:HH12	2.29	0.50
1:K:10:LYS:HD2	1:K:12:GLY:H	1.75	0.50
1:G:355:PHE:CZ	1:G:368:LEU:HD22	2.47	0.50
1:G:357:PHE:CD2	1:G:359:THR:HG23	2.46	0.50
1:G:17:ALA:HB3	1:G:29:LEU:HD23	1.94	0.50
1:K:136:THR:HA	1:K:142:TRP:H	1.77	0.50
2:F:298:GLY:H	2:F:319:THR:HG21	1.77	0.49
2:L:171:LEU:H	2:L:227:LEU:H	1.59	0.49
1:C:362:ILE:HD12	1:C:362:ILE:H	1.77	0.49
1:G:265:GLU:C	1:G:267:LEU:H	2.21	0.49
1:I:388:ILE:HA	2:J:335:VAL:HG23	1.95	0.49
1:I:332:HIS:CE1	1:I:338:ALA:O	2.66	0.49
1:A:110:ARG:H	1:A:110:ARG:HD3	1.78	0.48
1:G:16:LYS:HG3	1:G:28:HIS:CE1	2.48	0.48
1:A:16:LYS:HG3	1:A:340:ILE:H	1.79	0.48
2:F:187:ILE:HD11	2:F:226:TYR:H	1.78	0.48
1:K:333:SER:CB	1:K:338:ALA:H	2.26	0.48
2:L:198:TYR:HB3	2:L:224:ARG:HH21	1.77	0.48
2:H:282:LEU:HD13	2:H:325:TYR:CE1	2.48	0.48
1:C:185:VAL:HG11	1:C:267:LEU:HD11	1.95	0.48
2:H:316:PHE:HB3	2:H:323:LEU:HD11	1.96	0.48
1:K:15:TYR:HA	1:K:339:VAL:HG11	1.95	0.48
1:A:33:LEU:HD13	1:A:277:ILE:H	1.79	0.48
1:A:332:HIS:CE1	1:A:338:ALA:HB3	2.49	0.48
1:G:110:ARG:H	1:G:110:ARG:CD	2.27	0.48
1:C:321:TYR:CE1	1:C:370:VAL:HG11	2.48	0.48
1:E:15:TYR:CE2	1:E:395:HIS:CE1	3.02	0.47
2:H:171:LEU:HB3	2:H:226:TYR:CD1	2.48	0.47
1:I:260:CYS:HA	1:I:272:CYS:HA	1.96	0.47
2:D:22:CYS:HB3	2:D:27:CYS:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:15:TYR:CE2	2:H:234:VAL:HG21	2.50	0.47
1:I:7:MET:HE3	1:I:7:MET:CA	2.44	0.47
2:B:296:SER:HA	2:B:323:LEU:HA	1.95	0.47
1:K:338:ALA:HB2	1:K:366:PHE:CD2	2.49	0.47
2:D:294:THR:HG21	2:D:316:PHE:CG	2.49	0.47
2:D:327:TRP:H	2:D:330:HIS:CE1	2.33	0.47
1:I:130:GLN:HA	1:I:149:VAL:H	1.78	0.47
1:A:180:VAL:HG13	1:A:185:VAL:HG22	1.97	0.47
1:A:345:VAL:HG11	1:A:355:PHE:HB3	1.96	0.47
2:D:167:HIS:CG	2:D:168:GLN:N	2.83	0.47
2:F:171:LEU:H	2:F:171:LEU:HD23	1.80	0.47
2:H:167:HIS:CE1	2:H:236:ASN:HA	2.50	0.47
2:J:196:LYS:HZ2	2:J:243:GLY:HA2	1.80	0.47
1:C:183:HIS:H	1:C:183:HIS:CD2	2.32	0.46
1:C:332:HIS:CD2	1:C:340:ILE:HB	2.50	0.46
1:C:360:ALA:HB2	1:C:394:GLN:HG3	1.98	0.46
1:G:21:ARG:HG3	1:G:24:TYR:H	1.80	0.46
1:I:31:ILE:HA	1:I:134:ASN:O	2.15	0.46
1:C:33:LEU:HD13	1:C:277:ILE:H	1.80	0.46
1:A:273:ALA:HB3	2:B:298:GLY:H	1.80	0.46
2:D:297:LEU:H	2:D:323:LEU:HA	1.81	0.46
1:E:302:CYS:SG	1:E:319:VAL:HG22	2.55	0.46
2:D:347:GLY:HA2	1:G:23:GLY:HA2	1.96	0.46
1:G:3:HIS:HA	1:G:19:VAL:HG13	1.98	0.46
1:K:167:LEU:H	1:K:167:LEU:HD22	1.80	0.46
1:I:88:MET:HB2	2:J:173:ALA:HB2	1.97	0.46
2:J:190:PRO:HD3	2:J:227:LEU:HD22	1.98	0.46
1:K:252:LEU:HA	1:K:255:VAL:HG22	1.97	0.46
2:J:47:ILE:HG23	2:J:109:VAL:HG21	1.98	0.46
1:E:321:TYR:CE1	1:E:370:VAL:HG11	2.51	0.46
2:F:5:HIS:CD2	2:F:253:HIS:CE1	3.03	0.46
2:F:323:LEU:O	2:F:335:VAL:HG22	2.16	0.46
1:A:91:GLY:H	2:B:175:HIS:CD2	2.33	0.46
1:C:16:LYS:H	1:C:339:VAL:HG22	1.80	0.46
1:G:342:GLU:HG2	1:G:356:HIS:H	1.80	0.46
1:A:21:ARG:HH21	1:I:382:LYS:CG	2.29	0.46
1:C:156:LYS:HA	1:C:161:LYS:HA	1.97	0.46
1:E:15:TYR:CE2	1:E:32:GLN:HA	2.51	0.46
1:K:330:PRO:HA	1:K:344:ASP:HA	1.97	0.46
1:C:16:LYS:CG	1:C:332:HIS:CE1	3.00	0.45
1:C:394:GLN:O	1:C:395:HIS:CG	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:337:VAL:HG13	1:G:399:PHE:CZ	2.51	0.45
1:I:3:HIS:CG	1:I:19:VAL:HG13	2.51	0.45
2:F:296:SER:H	2:F:302:ASN:HB3	1.80	0.45
2:L:294:THR:HG21	2:L:316:PHE:CG	2.51	0.45
2:H:171:LEU:HA	2:H:227:LEU:H	1.82	0.45
1:A:13:ILE:HD11	1:A:395:HIS:HA	1.98	0.45
1:E:329:CYS:HB2	1:E:347:LEU:HD11	1.99	0.45
1:K:3:HIS:CD2	1:K:20:GLU:H	2.34	0.45
1:K:363:HIS:CG	1:K:364:PRO:HD2	2.51	0.45
1:E:110:ARG:H	1:E:110:ARG:CD	2.30	0.45
1:A:16:LYS:HA	1:A:30:GLN:HA	1.98	0.45
1:A:143:ARG:HH22	1:A:162:LEU:HD13	1.82	0.45
2:H:346:HIS:CG	2:H:347:GLY:N	2.85	0.45
2:J:16:ILE:HB	2:J:173:ALA:H	1.82	0.45
1:K:363:HIS:CG	1:K:364:PRO:CD	3.00	0.45
1:E:3:HIS:HB2	1:E:19:VAL:HG22	1.99	0.45
1:C:16:LYS:HG2	1:C:332:HIS:CE1	2.52	0.45
1:E:16:LYS:HB2	1:E:332:HIS:CE1	2.52	0.44
1:A:366:PHE:CE2	1:A:368:LEU:HD13	2.52	0.44
1:C:183:HIS:CD2	2:D:135:ARG:HH22	2.35	0.44
1:K:333:SER:HB2	1:K:338:ALA:H	1.82	0.44
2:J:16:ILE:HG23	2:J:30:PRO:HA	1.99	0.44
2:B:37:ARG:HH12	2:B:258:PRO:HD3	1.83	0.44
2:F:95:HIS:CD2	2:F:255:PRO:HG3	2.52	0.44
2:B:38:GLY:HA3	2:B:128:VAL:HG13	1.99	0.44
2:J:187:ILE:HG13	2:J:227:LEU:HD21	1.98	0.44
1:A:19:VAL:CG2	1:A:29:LEU:HD21	2.48	0.44
2:D:171:LEU:HA	2:D:227:LEU:H	1.81	0.44
1:E:136:THR:HA	1:E:142:TRP:H	1.82	0.44
1:G:331:ILE:HG22	1:G:370:VAL:HA	1.98	0.44
1:K:165:GLY:HA3	1:K:166:PRO:C	2.43	0.44
1:A:91:GLY:H	2:B:175:HIS:CG	2.36	0.44
1:A:366:PHE:CZ	1:A:368:LEU:HD13	2.53	0.44
2:D:171:LEU:HD22	2:D:226:TYR:CE1	2.52	0.44
1:K:41:SER:H	1:K:127:GLY:HA3	1.82	0.44
2:B:138:TYR:CG	2:B:266:THR:HG21	2.53	0.44
2:F:292:LEU:HD21	2:F:316:PHE:CE2	2.53	0.44
1:A:294:THR:HA	1:A:328:ASN:O	2.18	0.43
1:A:332:HIS:HE1	1:A:338:ALA:O	2.01	0.43
2:L:171:LEU:H	2:L:227:LEU:N	2.14	0.43
2:B:163:TYR:HA	2:B:253:HIS:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:10:LYS:HA	2:F:55:LEU:HD21	2.00	0.43
2:F:135:ARG:HH22	2:F:332:PRO:HG3	1.82	0.43
1:I:60:VAL:HG13	1:I:103:MET:H	1.83	0.43
1:I:331:ILE:HG22	1:I:370:VAL:HA	2.00	0.43
2:F:277:HIS:HA	2:F:340:SER:H	1.83	0.43
1:K:363:HIS:CD2	1:K:364:PRO:HD3	2.54	0.43
1:C:362:ILE:HG21	2:D:350:HIS:H	1.84	0.43
1:E:360:ALA:HB1	1:E:396:THR:HG22	2.01	0.43
1:G:28:HIS:O	1:G:29:LEU:HD13	2.18	0.43
1:K:108:VAL:H	1:K:216:ALA:HB1	1.84	0.43
2:D:100:LEU:HD11	2:D:153:TYR:HB2	2.01	0.43
1:G:88:MET:HB2	2:H:173:ALA:H	1.84	0.43
1:G:108:VAL:H	1:G:216:ALA:HB1	1.82	0.43
2:J:181:HIS:CG	2:J:181:HIS:O	2.72	0.43
1:K:11:VAL:HG23	1:K:271:ASN:HA	2.00	0.43
2:L:319:THR:O	2:L:337:ALA:HB2	2.18	0.43
1:A:309:TYR:CE1	1:A:315:GLY:HA3	2.54	0.43
1:K:112:GLU:CG	2:L:254:VAL:HG21	2.49	0.43
1:K:143:ARG:HH12	1:K:147:VAL:HG12	1.84	0.43
2:F:97:TYR:CD1	2:F:234:VAL:HA	2.53	0.43
1:G:332:HIS:CE1	1:G:339:VAL:HA	2.54	0.43
2:H:163:TYR:HA	2:H:253:HIS:HA	2.01	0.42
2:L:198:TYR:CB	2:L:224:ARG:HH21	2.32	0.42
1:E:304:ILE:HA	1:E:317:ALA:HA	2.01	0.42
2:F:116:GLY:HA3	2:F:120:HIS:CD2	2.54	0.42
2:F:348:TRP:H	2:F:349:PRO:CD	2.32	0.42
1:A:302:CYS:SG	1:A:317:ALA:HB1	2.59	0.42
1:E:156:LYS:HA	1:E:161:LYS:HA	2.01	0.42
2:D:95:HIS:CD2	2:D:157:ARG:HE	2.37	0.42
2:D:297:LEU:HD13	2:D:298:GLY:H	1.84	0.42
1:E:180:VAL:HG12	1:E:264:LEU:HA	2.02	0.42
1:E:332:HIS:HE1	1:E:339:VAL:HA	1.83	0.42
1:K:17:ALA:H	1:K:29:LEU:HB2	1.85	0.42
1:A:362:ILE:HG21	2:B:344:ASN:H	1.83	0.42
1:G:253:ASN:HA	1:G:261:SER:HA	2.02	0.42
1:K:71:LYS:HG3	2:L:168:GLN:HE22	1.84	0.42
2:L:294:THR:HG22	2:L:325:TYR:HA	2.01	0.42
1:A:16:LYS:O	1:A:332:HIS:CG	2.72	0.42
1:C:27:VAL:HG11	1:C:138:GLY:H	1.83	0.42
1:C:255:VAL:HA	2:D:301:ALA:HB1	2.02	0.42
1:A:357:PHE:CG	1:A:366:PHE:CZ	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:363:HIS:CD2	2:L:349:PRO:HA	2.54	0.42
2:L:277:HIS:HB2	2:L:350:HIS:CG	2.55	0.42
2:D:46:ARG:HH22	2:D:254:VAL:HB	1.85	0.42
1:G:29:LEU:HG	1:G:135:ILE:HG21	2.02	0.42
2:L:318:VAL:HA	2:L:323:LEU:HB2	2.02	0.42
1:E:29:LEU:CD1	1:E:135:ILE:HG23	2.50	0.41
1:G:9:ASN:HD22	1:G:274:VAL:HG12	1.85	0.41
1:K:112:GLU:HB2	2:L:258:PRO:HD2	2.02	0.41
1:K:112:GLU:CB	2:L:258:PRO:HD2	2.50	0.41
1:A:3:HIS:CE1	1:A:29:LEU:HD23	2.56	0.41
1:C:302:CYS:SG	1:C:319:VAL:HG22	2.60	0.41
1:C:331:ILE:O	1:C:332:HIS:CD2	2.72	0.41
1:E:9:ASN:HB2	1:E:277:ILE:HD11	2.02	0.41
1:E:295:PRO:HB3	1:E:325:LYS:H	1.85	0.41
2:J:195:VAL:H	2:J:210:SER:HA	1.85	0.41
1:K:15:TYR:CE1	1:K:32:GLN:HA	2.54	0.41
2:D:150:CYS:SG	2:D:265:ALA:HB2	2.60	0.41
1:E:33:LEU:HD21	1:E:279:ILE:HG12	2.02	0.41
1:G:28:HIS:CD2	1:G:343:ASN:HA	2.55	0.41
2:H:318:VAL:HA	2:H:323:LEU:HB2	2.03	0.41
1:E:319:VAL:HG11	1:E:321:TYR:CE1	2.55	0.41
1:G:15:TYR:HB2	1:G:395:HIS:CE1	2.55	0.41
1:G:332:HIS:CD2	1:G:333:SER:O	2.73	0.41
2:J:263:CYS:SG	2:J:265:ALA:HB2	2.61	0.41
2:F:293:THR:HA	2:F:304:THR:HB	2.03	0.41
1:G:19:VAL:HG23	1:G:29:LEU:HD21	2.02	0.41
2:H:5:HIS:CD2	2:H:95:HIS:HE1	2.39	0.41
2:J:184:LYS:HB3	2:J:213:HIS:CE1	2.56	0.41
1:K:319:VAL:HB	1:K:321:TYR:CD2	2.56	0.41
1:K:395:HIS:CD2	1:K:396:THR:HG22	2.56	0.41
1:G:52:LYS:HA	1:G:52:LYS:HE2	2.02	0.41
1:C:259:GLY:HA2	2:D:298:GLY:O	2.21	0.41
2:D:170:GLY:HA3	2:D:242:ARG:HA	2.02	0.41
2:D:275:HIS:CE1	2:D:335:VAL:HG22	2.55	0.41
2:D:296:SER:HB2	2:D:302:ASN:HD22	1.86	0.41
1:E:15:TYR:CD2	1:E:395:HIS:CG	3.08	0.41
1:G:7:MET:SD	1:G:17:ALA:HA	2.61	0.41
1:I:8:PRO:HB2	1:I:396:THR:HA	2.03	0.41
1:E:143:ARG:HH21	1:E:145:ALA:HB3	1.86	0.41
1:K:11:VAL:HG11	2:L:297:LEU:HD12	2.03	0.41
1:A:48:THR:HG22	1:A:49:CYS:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:VAL:HG11	1:A:264:LEU:HA	2.03	0.40
1:C:9:ASN:HD22	1:C:272:CYS:HB3	1.86	0.40
1:C:297:VAL:HG21	1:C:370:VAL:HG12	2.03	0.40
2:L:297:LEU:H	2:L:323:LEU:HA	1.86	0.40
1:A:244:TRP:H	1:A:248:LYS:HA	1.87	0.40
1:E:290:ARG:HH11	1:E:290:ARG:HA	1.86	0.40
1:G:332:HIS:HE1	1:G:339:VAL:HA	1.87	0.40
1:G:337:VAL:HG13	1:G:399:PHE:CE1	2.56	0.40
2:H:118:ASN:H	2:H:118:ASN:HD22	1.69	0.40
1:K:273:ALA:HB1	2:L:321:GLU:CB	2.51	0.40
1:A:60:VAL:HG23	1:A:103:MET:H	1.86	0.40
1:E:18:LEU:HB3	1:E:335:SER:H	1.86	0.40
1:G:171:TRP:CZ2	1:G:258:PHE:HB3	2.56	0.40
1:I:391:TYR:CE1	2:J:297:LEU:CD1	3.04	0.40
1:C:143:ARG:HH12	1:C:145:ALA:H	1.70	0.40
1:C:243:ARG:HB2	1:C:244:TRP:H	1.75	0.40
1:I:135:ILE:HB	1:I:143:ARG:HE	1.87	0.40
2:J:230:ASN:H	2:J:230:ASN:HD22	1.68	0.40
1:K:29:LEU:HD13	1:K:137:TYR:HA	2.04	0.40
1:G:359:THR:HG21	1:G:364:PRO:HB2	2.04	0.40
1:I:95:PHE:HB3	2:J:223:CYS:HA	2.04	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	398/441 (90%)	313 (79%)	47 (12%)	38 (10%)	0	8
1	C	398/441 (90%)	322 (81%)	47 (12%)	29 (7%)	1	10
1	E	398/441 (90%)	315 (79%)	48 (12%)	35 (9%)	0	8
1	G	398/441 (90%)	299 (75%)	63 (16%)	36 (9%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	398/441 (90%)	310 (78%)	55 (14%)	33 (8%)	0	9
1	K	398/441 (90%)	308 (77%)	56 (14%)	34 (8%)	0	9
2	B	349/420 (83%)	280 (80%)	50 (14%)	19 (5%)	1	15
2	D	349/420 (83%)	291 (83%)	46 (13%)	12 (3%)	3	21
2	F	349/420 (83%)	276 (79%)	50 (14%)	23 (7%)	1	12
2	H	349/420 (83%)	277 (79%)	51 (15%)	21 (6%)	1	13
2	J	349/420 (83%)	284 (81%)	45 (13%)	20 (6%)	1	14
2	L	349/420 (83%)	291 (83%)	40 (12%)	18 (5%)	1	15
All	All	4482/5166 (87%)	3566 (80%)	598 (13%)	318 (7%)	2	11

All (318) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ALA
1	A	22	PRO
1	A	100	ASN
1	A	142	TRP
1	A	227	ALA
1	A	244	TRP
1	A	258	PHE
1	A	267	LEU
1	A	390	ASP
2	B	57	THR
2	B	183	ALA
2	B	191	SER
2	B	300	ASP
2	B	339	GLU
2	B	346	HIS
1	C	73	HIS
1	C	150	ASN
1	C	168	SER
1	C	169	SER
1	C	267	LEU
1	C	310	ALA
1	C	395	HIS
2	D	135	ARG
2	D	174	ASP
2	D	219	ASP
2	D	321	GLU

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Mol	Chain	Res	Type
1	E	57	SER
1	E	72	PRO
1	E	130	GLN
1	E	152	GLU
1	E	244	TRP
1	E	250	ALA
1	E	306	GLU
1	E	310	ALA
1	E	326	ALA
1	E	387	HIS
1	E	390	ASP
1	E	396	THR
1	E	398	SER
2	F	136	GLU
2	F	174	ASP
2	F	219	ASP
2	F	230	ASN
2	F	321	GLU
2	F	339	GLU
2	F	348	TRP
1	G	2	GLU
1	G	11	VAL
1	G	89	TRP
1	G	169	SER
1	G	231	HIS
1	G	386	ASP
1	G	394	GLN
1	G	398	SER
2	H	5	HIS
2	H	25	SER
2	H	40	ALA
2	H	57	THR
2	H	140	HIS
2	H	143	GLU
2	H	168	GLN
2	H	203	ASP
2	H	246	ASP
2	H	267	LEU
2	H	277	HIS
1	I	65	ALA
1	I	100	ASN
1	I	192	GLU

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Mol	Chain	Res	Type
1	I	255	VAL
1	I	274	VAL
1	I	360	ALA
1	I	373	SER
2	J	139	ARG
2	J	158	ALA
2	J	171	LEU
2	J	174	ASP
2	J	219	ASP
1	K	73	HIS
1	K	117	ASP
1	K	263	ALA
1	K	267	LEU
1	K	372	THR
1	K	383	PRO
1	K	386	ASP
1	K	390	ASP
1	K	396	THR
2	L	22	CYS
2	L	60	VAL
2	L	143	GLU
2	L	338	GLN
1	A	89	TRP
1	A	175	ASP
1	A	245	LYS
1	A	372	THR
2	B	193	ALA
2	B	340	SER
2	B	350	HIS
1	C	11	VAL
1	C	49	CYS
1	C	142	TRP
1	C	167	LEU
1	C	227	ALA
1	C	276	SER
1	C	299	ASP
1	C	306	GLU
1	C	372	THR
1	C	386	ASP
1	C	396	THR
2	D	203	ASP
1	E	22	PRO

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Mol	Chain	Res	Type
1	E	49	CYS
1	E	160	ALA
1	E	172	SER
1	E	337	VAL
1	E	338	ALA
1	E	372	THR
2	F	26	ARG
2	F	160	GLN
2	F	168	GLN
2	F	183	ALA
2	F	338	GLN
1	G	34	VAL
1	G	230	VAL
1	G	248	LYS
1	G	267	LEU
1	G	300	LEU
1	G	306	GLU
1	G	360	ALA
1	G	372	THR
1	G	390	ASP
2	H	241	PRO
2	H	338	GLN
1	I	49	CYS
1	I	89	TRP
1	I	142	TRP
1	I	227	ALA
1	I	350	SER
1	I	372	THR
2	J	61	ASP
2	J	156	LYS
2	J	157	ARG
2	J	213	HIS
2	J	346	HIS
1	K	63	CYS
1	K	231	HIS
1	K	373	SER
2	L	174	ASP
2	L	183	ALA
2	L	242	ARG
2	L	339	GLU
2	L	345	PRO
1	A	38	ILE

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Mol	Chain	Res	Type
1	A	49	CYS
1	A	69	THR
1	A	75	ASP
1	A	95	PHE
1	A	191	PRO
1	A	219	ASN
1	A	241	PHE
1	A	276	SER
2	B	25	SER
2	B	143	GLU
2	B	244	GLU
2	B	338	GLN
1	C	152	GLU
1	C	170	ALA
1	C	322	LYS
2	D	154	THR
2	D	159	ASP
2	D	183	ALA
1	E	139	SER
1	E	183	HIS
1	E	373	SER
2	F	43	GLY
2	F	59	GLY
2	F	267	LEU
1	G	22	PRO
1	G	49	CYS
1	G	63	CYS
1	G	100	ASN
1	G	127	GLY
1	G	160	ALA
1	G	195	THR
1	G	219	ASN
1	G	314	GLY
1	G	396	THR
2	H	43	GLY
2	H	170	GLY
2	H	183	ALA
2	H	343	GLY
1	I	22	PRO
1	I	131	ALA
1	I	132	MET
1	I	152	GLU

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Mol	Chain	Res	Type
1	I	246	ARG
1	I	307	CYS
1	I	313	PHE
2	J	161	GLY
2	J	183	ALA
2	J	244	GLU
2	J	250	GLY
2	J	347	GLY
1	K	49	CYS
1	K	94	CYS
1	K	152	GLU
1	K	230	VAL
1	K	246	ARG
1	K	288	PHE
1	K	395	HIS
1	K	397	GLU
2	L	24	HIS
2	L	86	SER
2	L	171	LEU
2	L	231	LYS
2	L	350	HIS
1	A	35	ASN
1	A	57	SER
1	A	246	ARG
1	A	313	PHE
1	A	373	SER
1	A	381	CYS
1	A	387	HIS
1	A	398	SER
1	C	22	PRO
1	C	75	ASP
1	C	117	ASP
1	C	244	TRP
2	D	136	GLU
1	E	193	TYR
1	E	241	PHE
1	E	275	GLY
1	E	299	ASP
1	E	371	CYS
1	E	399	PHE
2	F	32	ALA
2	F	55	LEU

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Mol	Chain	Res	Type
2	F	233	TRP
1	G	238	PRO
1	G	371	CYS
1	G	373	SER
2	H	256	PHE
1	I	66	THR
1	I	69	THR
1	I	195	THR
1	I	271	ASN
1	I	312	ASP
2	J	57	THR
1	K	57	SER
1	K	191	PRO
1	K	239	SER
1	K	391	TYR
2	L	16	ILE
2	L	222	GLN
1	A	73	HIS
1	A	257	PRO
1	A	334	PRO
1	A	397	GLU
2	B	61	ASP
2	B	169	PRO
1	C	88	MET
1	E	30	GLN
1	E	142	TRP
1	E	153	THR
1	E	169	SER
2	F	22	CYS
2	F	61	ASP
2	F	231	LYS
1	G	88	MET
1	G	304	ILE
2	H	61	ASP
1	I	219	ASN
1	I	244	TRP
1	I	305	THR
2	J	143	GLU
2	J	160	GLN
2	J	342	GLU
1	K	142	TRP
1	K	150	ASN

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Mol	Chain	Res	Type
1	K	195	THR
1	K	207	ARG
2	L	120	HIS
2	L	191	SER
1	A	193	TYR
2	B	168	GLN
2	B	250	GLY
1	C	89	TRP
1	C	238	PRO
1	C	324	SER
2	D	345	PRO
1	E	227	ALA
1	E	334	PRO
1	G	75	ASP
1	G	98	THR
2	H	159	ASP
2	H	191	SER
1	I	238	PRO
1	I	304	ILE
2	J	349	PRO
1	K	116	ILE
1	K	137	TYR
1	K	313	PHE
1	I	337	VAL
1	A	154	PRO
2	D	190	PRO
1	G	391	TYR
1	I	21	ARG
1	I	391	TYR
1	K	22	PRO
1	K	84	VAL
2	B	302	ASN
2	F	250	GLY
1	G	284	PRO
1	K	256	ALA
1	A	153	THR
2	B	349	PRO
2	F	270	GLU
1	A	259	GLY
2	D	140	HIS

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	339/370 (92%)	314 (93%)	25 (7%)	13	33
1	C	339/370 (92%)	321 (95%)	18 (5%)	20	41
1	E	339/370 (92%)	316 (93%)	23 (7%)	14	36
1	G	339/370 (92%)	318 (94%)	21 (6%)	16	38
1	I	339/370 (92%)	316 (93%)	23 (7%)	14	36
1	K	339/370 (92%)	313 (92%)	26 (8%)	12	32
2	B	304/367 (83%)	292 (96%)	12 (4%)	28	49
2	D	304/367 (83%)	287 (94%)	17 (6%)	19	40
2	F	304/367 (83%)	281 (92%)	23 (8%)	12	33
2	H	304/367 (83%)	288 (95%)	16 (5%)	20	41
2	J	304/367 (83%)	278 (91%)	26 (9%)	10	29
2	L	304/367 (83%)	284 (93%)	20 (7%)	15	37
All	All	3858/4422 (87%)	3608 (94%)	250 (6%)	17	37

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	13	ILE
1	A	18	LEU
1	A	29	LEU
1	A	34	VAL
1	A	52	LYS
1	A	105	GLU
1	A	107	TYR
1	A	147	VAL
1	A	174	PHE
1	A	197	LYS
1	A	229	ILE
1	A	244	TRP
1	A	262	ILE

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Mol	Chain	Res	Type
1	A	281	ILE
1	A	290	ARG
1	A	316	ILE
1	A	319	VAL
1	A	353	PHE
1	A	355	PHE
1	A	359	THR
1	A	366	PHE
1	A	378	LYS
1	A	392	PRO
1	A	394	GLN
2	B	4	THR
2	B	5	HIS
2	B	44	VAL
2	B	217	CYS
2	B	226	TYR
2	B	231	LYS
2	B	267	LEU
2	B	269	PRO
2	B	274	GLU
2	B	310	ARG
2	B	312	THR
2	B	339	GLU
1	C	16	LYS
1	C	18	LEU
1	C	34	VAL
1	C	52	LYS
1	C	53	THR
1	C	107	TYR
1	C	143	ARG
1	C	214	LEU
1	C	245	LYS
1	C	246	ARG
1	C	248	LYS
1	C	283	ILE
1	C	318	THR
1	C	334	PRO
1	C	339	VAL
1	C	341	LYS
1	C	354	THR
1	C	362	ILE
2	D	16	ILE

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Mol	Chain	Res	Type
2	D	85	THR
2	D	95	HIS
2	D	99	ILE
2	D	127	LYS
2	D	131	ARG
2	D	139	ARG
2	D	217	CYS
2	D	236	ASN
2	D	239	ARG
2	D	251	LYS
2	D	263	CYS
2	D	297	LEU
2	D	306	GLN
2	D	310	ARG
2	D	326	THR
2	D	330	HIS
1	E	9	ASN
1	E	29	LEU
1	E	72	PRO
1	E	80	VAL
1	E	95	PHE
1	E	124	VAL
1	E	128	THR
1	E	135	ILE
1	E	143	ARG
1	E	150	ASN
1	E	179	VAL
1	E	217	ASN
1	E	229	ILE
1	E	244	TRP
1	E	246	ARG
1	E	262	ILE
1	E	291	ILE
1	E	297	VAL
1	E	300	LEU
1	E	331	ILE
1	E	337	VAL
1	E	359	THR
1	E	385	LYS
2	F	15	TYR
2	F	16	ILE
2	F	34	GLU

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Mol	Chain	Res	Type
2	F	46	ARG
2	F	47	ILE
2	F	85	THR
2	F	97	TYR
2	F	118	ASN
2	F	131	ARG
2	F	139	ARG
2	F	146	VAL
2	F	167	HIS
2	F	175	HIS
2	F	186	LYS
2	F	228	ILE
2	F	230	ASN
2	F	267	LEU
2	F	275	HIS
2	F	279	THR
2	F	293	THR
2	F	310	ARG
2	F	321	GLU
2	F	324	GLU
1	G	10	LYS
1	G	16	LYS
1	G	18	LEU
1	G	26	PRO
1	G	29	LEU
1	G	36	THR
1	G	52	LYS
1	G	93	TYR
1	G	162	LEU
1	G	171	TRP
1	G	181	TYR
1	G	212	ASN
1	G	246	ARG
1	G	253	ASN
1	G	267	LEU
1	G	283	ILE
1	G	331	ILE
1	G	359	THR
1	G	392	PRO
1	G	396	THR
1	G	397	GLU
2	H	44	VAL

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Mol	Chain	Res	Type
2	H	46	ARG
2	H	83	VAL
2	H	103	CYS
2	H	118	ASN
2	H	128	VAL
2	H	131	ARG
2	H	139	ARG
2	H	148	LEU
2	H	151	ASN
2	H	168	GLN
2	H	171	LEU
2	H	172	VAL
2	H	293	THR
2	H	310	ARG
2	H	324	GLU
1	I	7	MET
1	I	50	LYS
1	I	55	VAL
1	I	94	CYS
1	I	95	PHE
1	I	110	ARG
1	I	120	LYS
1	I	130	GLN
1	I	143	ARG
1	I	162	LEU
1	I	164	ILE
1	I	167	LEU
1	I	188	TYR
1	I	226	GLN
1	I	246	ARG
1	I	252	LEU
1	I	255	VAL
1	I	281	ILE
1	I	296	THR
1	I	305	THR
1	I	353	PHE
1	I	366	PHE
1	I	391	TYR
2	J	9	TYR
2	J	44	VAL
2	J	85	THR
2	J	97	TYR

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Mol	Chain	Res	Type
2	J	124	VAL
2	J	131	ARG
2	J	156	LYS
2	J	171	LEU
2	J	186	LYS
2	J	197	TYR
2	J	214	THR
2	J	220	VAL
2	J	221	LYS
2	J	230	ASN
2	J	254	VAL
2	J	264	ILE
2	J	266	THR
2	J	267	LEU
2	J	277	HIS
2	J	305	ARG
2	J	306	GLN
2	J	310	ARG
2	J	325	TYR
2	J	329	ASN
2	J	335	VAL
2	J	346	HIS
1	K	6	VAL
1	K	11	VAL
1	K	18	LEU
1	K	48	THR
1	K	52	LYS
1	K	69	THR
1	K	94	CYS
1	K	107	TYR
1	K	132	MET
1	K	143	ARG
1	K	162	LEU
1	K	171	TRP
1	K	187	ASN
1	K	197	LYS
1	K	224	ARG
1	K	248	LYS
1	K	262	ILE
1	K	274	VAL
1	K	281	ILE
1	K	283	ILE

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Mol	Chain	Res	Type
1	K	300	LEU
1	K	305	THR
1	K	318	THR
1	K	359	THR
1	K	363	HIS
1	K	395	HIS
2	L	10	LYS
2	L	35	GLU
2	L	65	MET
2	L	68	MET
2	L	91	LEU
2	L	119	ARG
2	L	120	HIS
2	L	127	LYS
2	L	146	VAL
2	L	157	ARG
2	L	171	LEU
2	L	177	LEU
2	L	196	LYS
2	L	209	THR
2	L	230	ASN
2	L	249	LYS
2	L	272	LEU
2	L	280	LEU
2	L	293	THR
2	L	335	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (146) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	9	ASN
1	A	28	HIS
1	A	43	ASN
1	A	73	HIS
1	A	134	ASN
1	A	176	ASN
1	A	387	HIS
2	B	41	HIS
2	B	73	GLN
2	B	82	HIS
2	B	94	HIS

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Mol	Chain	Res	Type
2	B	102	GLN
2	B	114	HIS
2	B	120	HIS
2	B	140	HIS
2	B	167	HIS
2	B	175	HIS
2	B	230	ASN
2	B	285	HIS
2	B	338	GLN
2	B	344	ASN
1	C	28	HIS
1	C	125	HIS
1	C	183	HIS
1	C	271	ASN
1	C	328	ASN
1	C	332	HIS
2	D	41	HIS
2	D	48	GLN
2	D	82	HIS
2	D	126	HIS
2	D	162	HIS
2	D	167	HIS
2	D	175	HIS
2	D	213	HIS
2	D	230	ASN
2	D	275	HIS
2	D	285	HIS
2	D	288	HIS
2	D	302	ASN
2	D	306	GLN
2	D	330	HIS
1	E	9	ASN
1	E	77	GLN
1	E	130	GLN
1	E	212	ASN
1	E	217	ASN
1	E	253	ASN
1	E	361	ASN
1	E	395	HIS
2	F	5	HIS
2	F	21	ASN
2	F	82	HIS

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Mol	Chain	Res	Type
2	F	95	HIS
2	F	114	HIS
2	F	120	HIS
2	F	144	HIS
2	F	162	HIS
2	F	194	GLN
2	F	275	HIS
2	F	277	HIS
2	F	288	HIS
2	F	302	ASN
2	F	350	HIS
1	G	30	GLN
1	G	183	HIS
1	G	217	ASN
1	G	226	GLN
1	G	236	GLN
1	G	332	HIS
2	H	5	HIS
2	H	21	ASN
2	H	24	HIS
2	H	80	ASN
2	H	82	HIS
2	H	118	ASN
2	H	120	HIS
2	H	126	HIS
2	H	144	HIS
2	H	151	ASN
2	H	155	HIS
2	H	162	HIS
2	H	167	HIS
2	H	175	HIS
2	H	213	HIS
2	H	253	HIS
2	H	275	HIS
2	H	306	GLN
2	H	330	HIS
2	H	350	HIS
1	I	32	GLN
1	I	35	ASN
1	I	43	ASN
1	I	67	GLN
1	I	79	GLN

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Mol	Chain	Res	Type
1	I	118	HIS
1	I	134	ASN
1	I	187	ASN
1	I	223	GLN
1	I	387	HIS
1	I	394	GLN
2	J	82	HIS
2	J	94	HIS
2	J	95	HIS
2	J	144	HIS
2	J	155	HIS
2	J	162	HIS
2	J	213	HIS
2	J	222	GLN
2	J	230	ASN
2	J	253	HIS
2	J	275	HIS
2	J	283	HIS
2	J	288	HIS
2	J	302	ASN
2	J	306	GLN
2	J	346	HIS
1	K	3	HIS
1	K	30	GLN
1	K	77	GLN
1	K	79	GLN
1	K	102	GLN
1	K	118	HIS
1	K	134	ASN
1	K	212	ASN
1	K	356	HIS
1	K	361	ASN
1	K	363	HIS
1	K	395	HIS
2	L	24	HIS
2	L	73	GLN
2	L	82	HIS
2	L	95	HIS
2	L	114	HIS
2	L	126	HIS
2	L	144	HIS
2	L	160	GLN

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Mol	Chain	Res	Type
2	L	162	HIS
2	L	167	HIS
2	L	168	GLN
2	L	253	HIS
2	L	275	HIS
2	L	285	HIS
2	L	346	HIS
2	L	350	HIS

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.

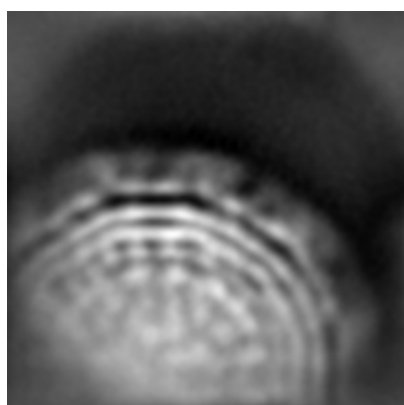
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24205. These allow visual inspection of the internal detail of the map and identification of artifacts.

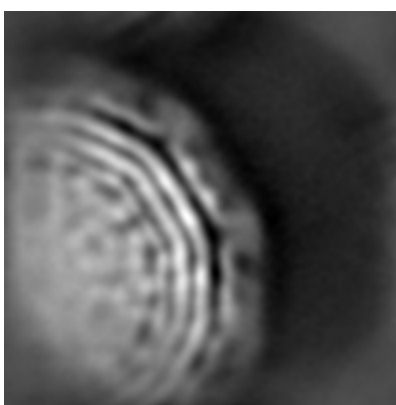
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

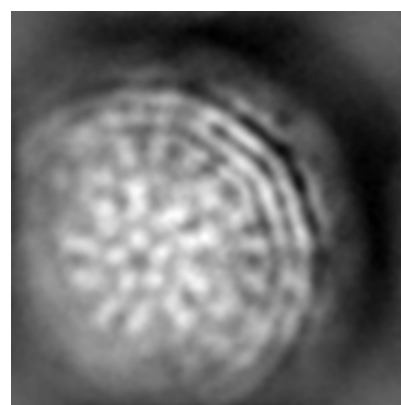
6.1.1 Primary map



X



Y

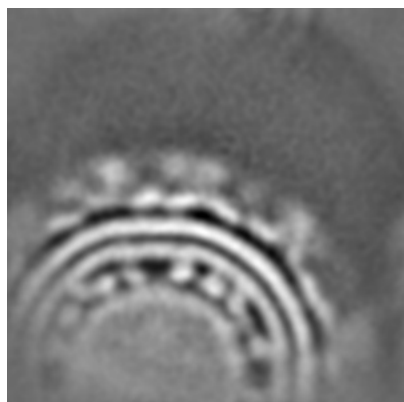


Z

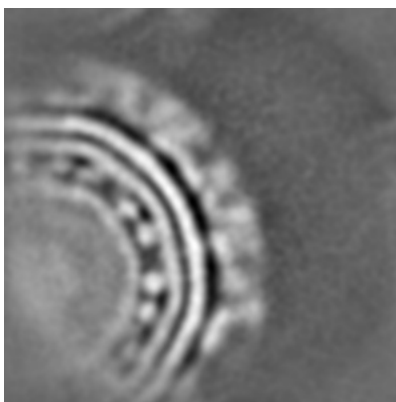
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

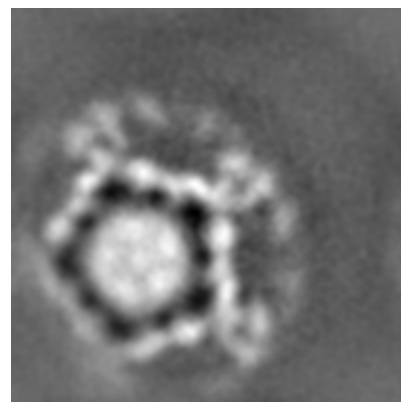
6.2.1 Primary map



X Index: 54



Y Index: 54

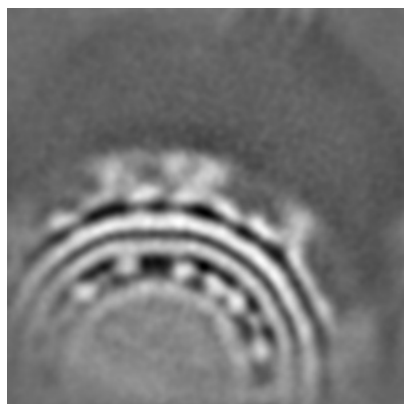


Z Index: 54

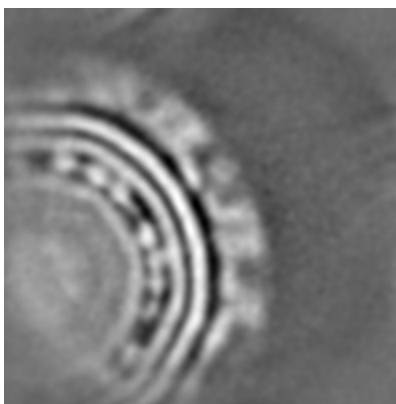
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

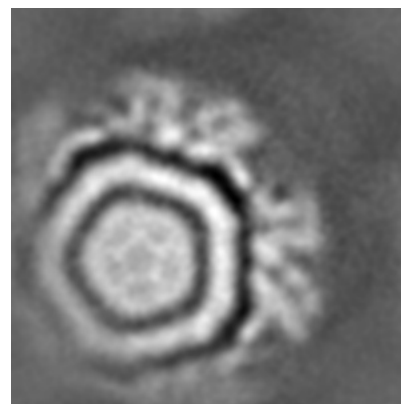
6.3.1 Primary map



X Index: 52



Y Index: 52

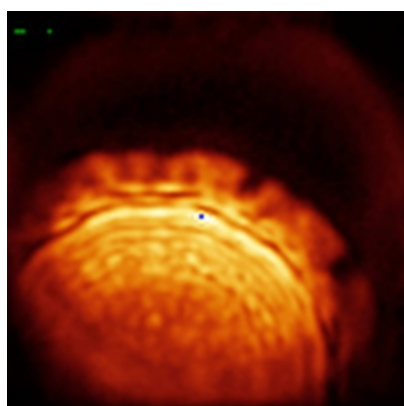


Z Index: 47

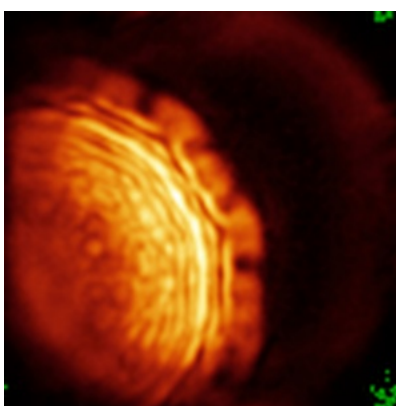
The images above show the largest variance slices of the map in three orthogonal directions.

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

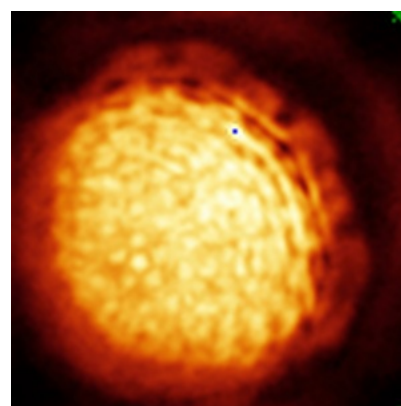
6.4.1 Primary map



X



Y

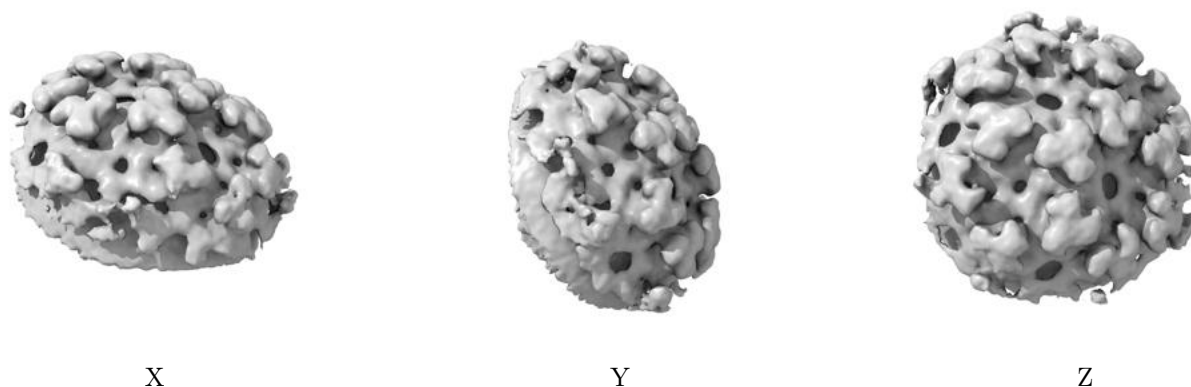


Z

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 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

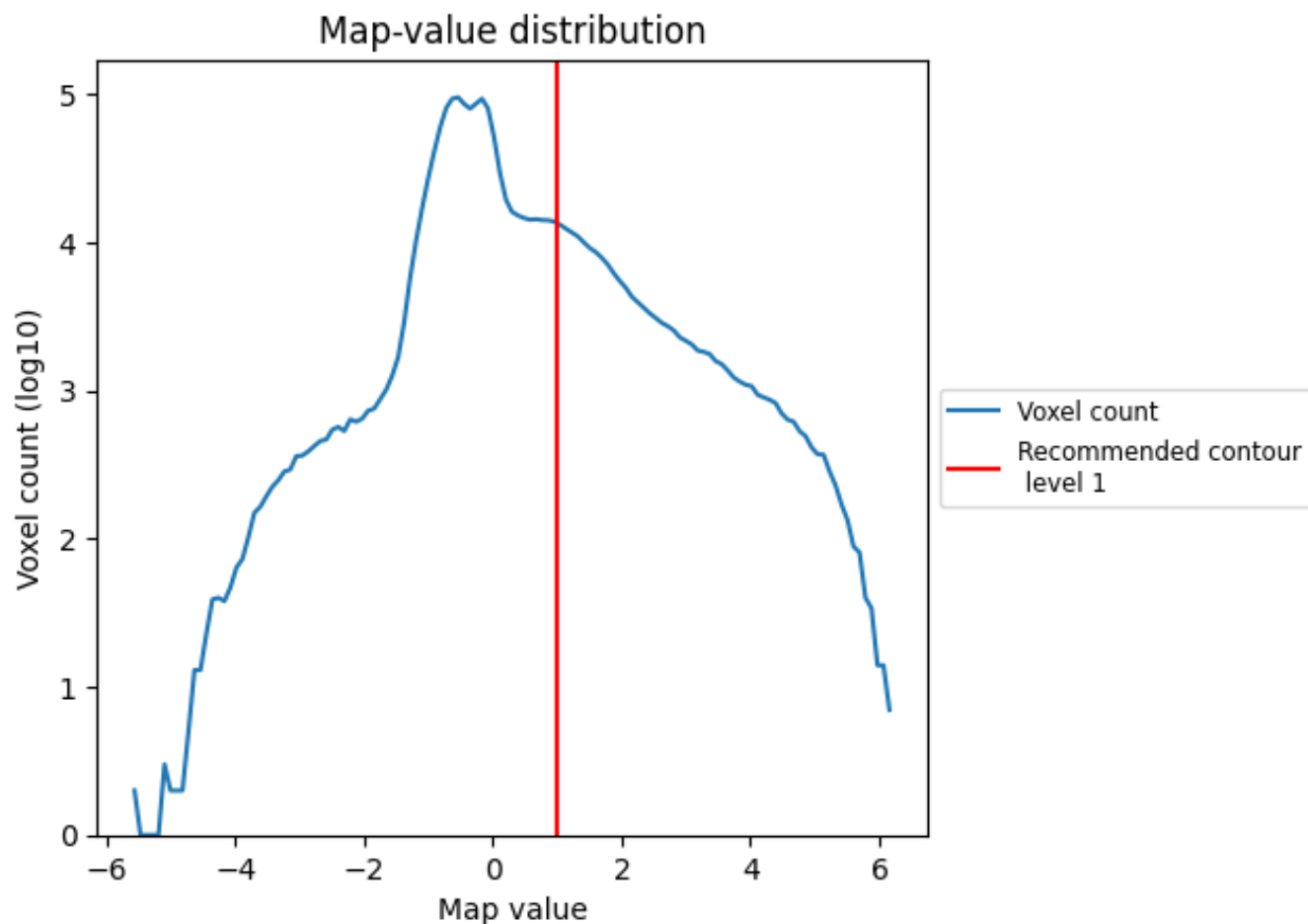
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

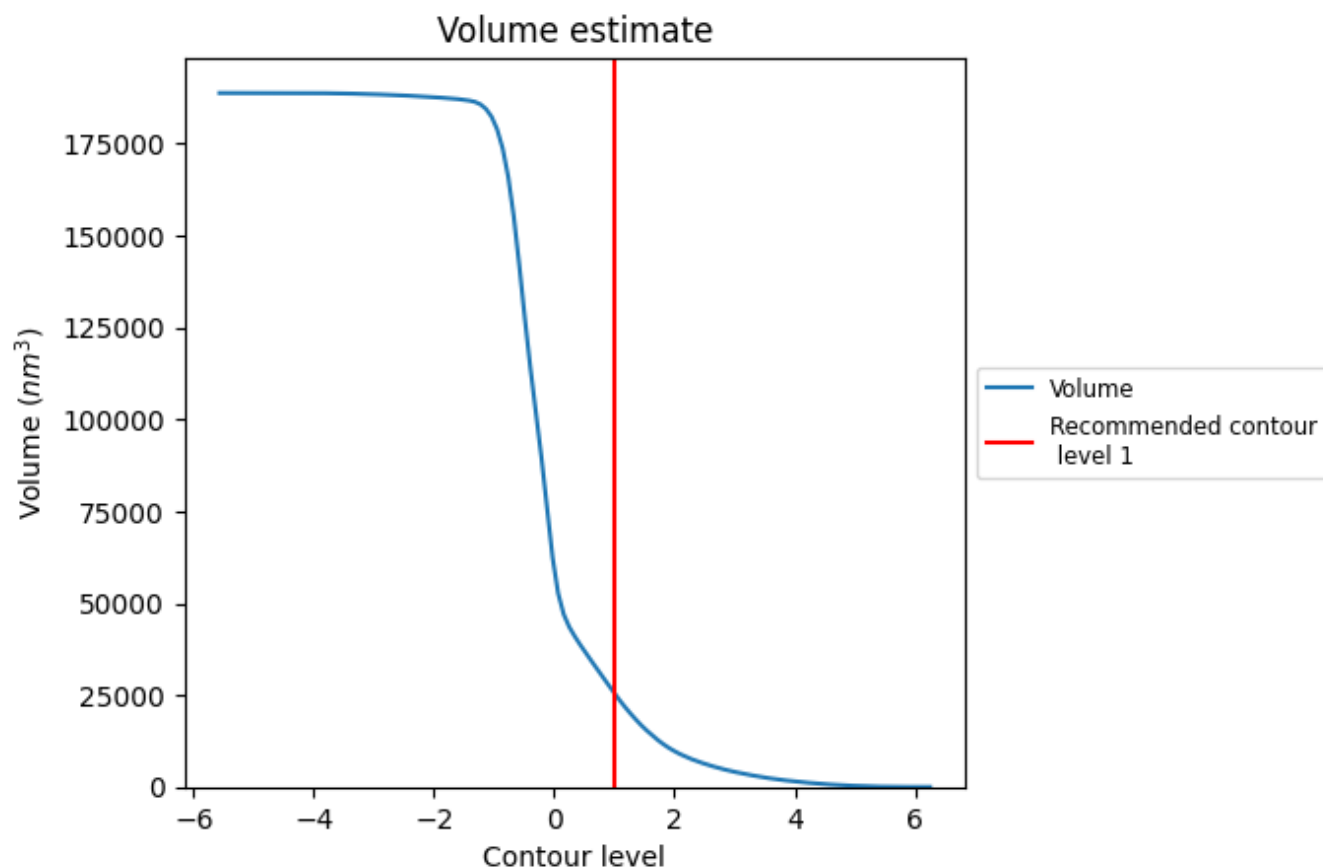
This section contains the results of statistical analysis of the map.

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.

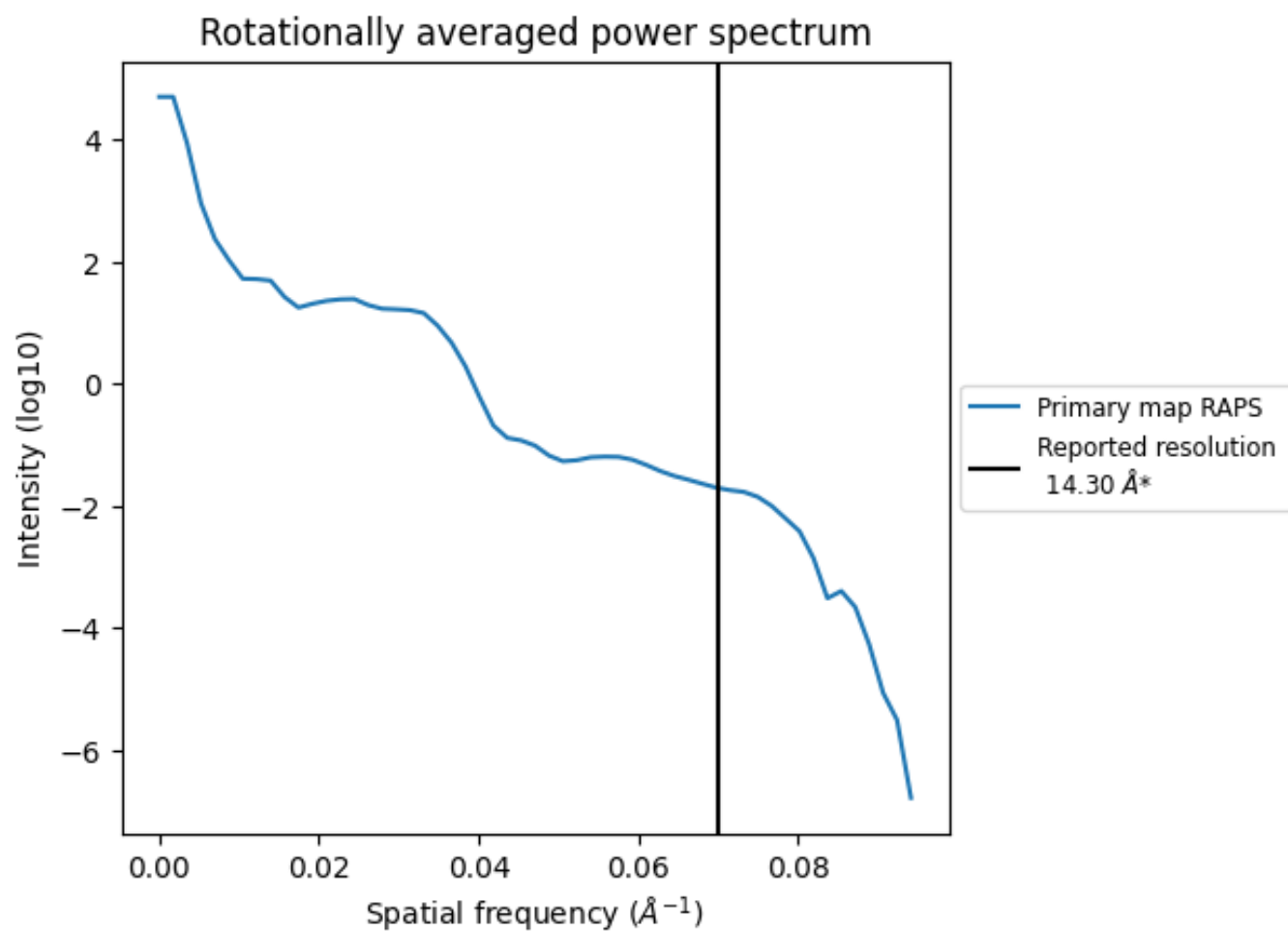
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 25541 nm^3 ; this corresponds to an approximate mass of 23072 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 ⓘ

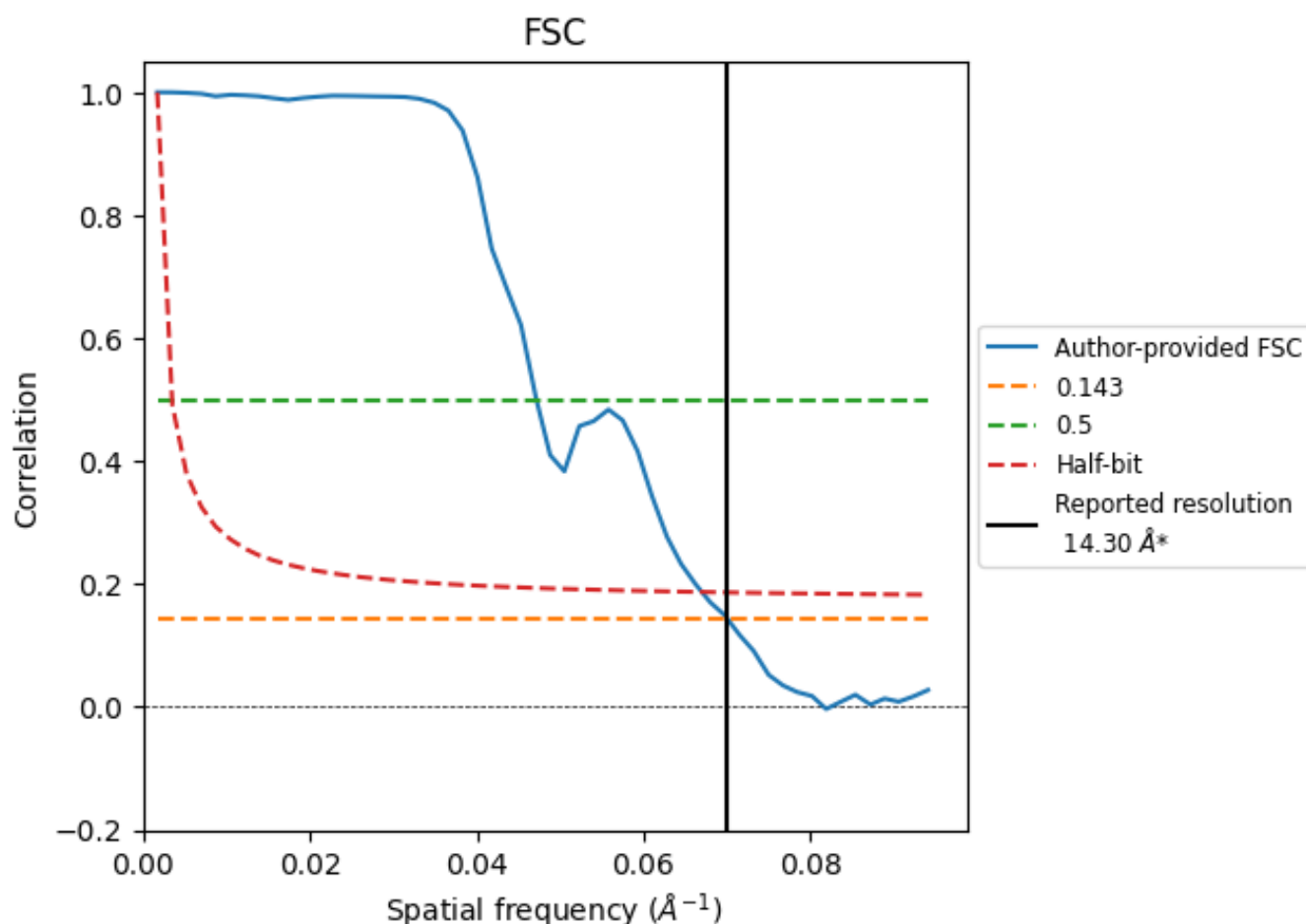


*Reported resolution corresponds to spatial frequency of 0.070 Å⁻¹

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 0.070 Å⁻¹

8.2 Resolution estimates [i](#)

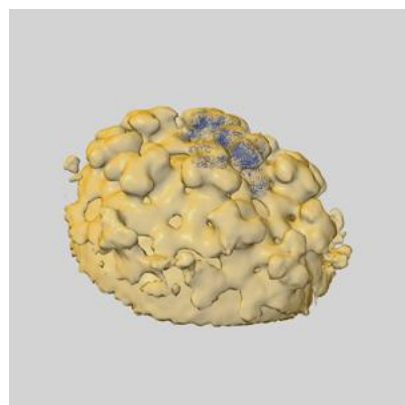
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	14.30	-	-
Author-provided FSC curve	14.27	21.23	14.93
Unmasked-calculated*	-	-	-

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

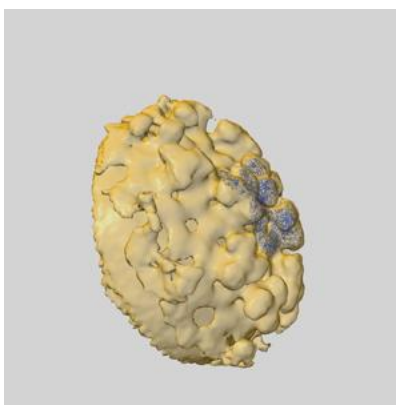
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24205 and PDB model 7N6A. Per-residue inclusion information can be found in section [3](#) on page [5](#).

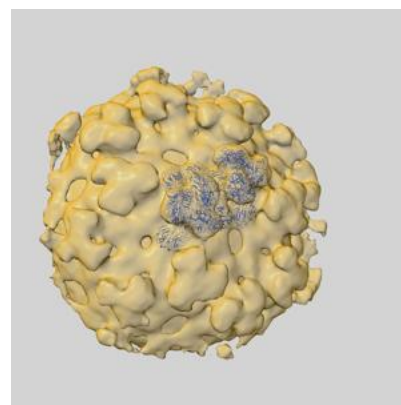
9.1 Map-model overlay [i](#)



X



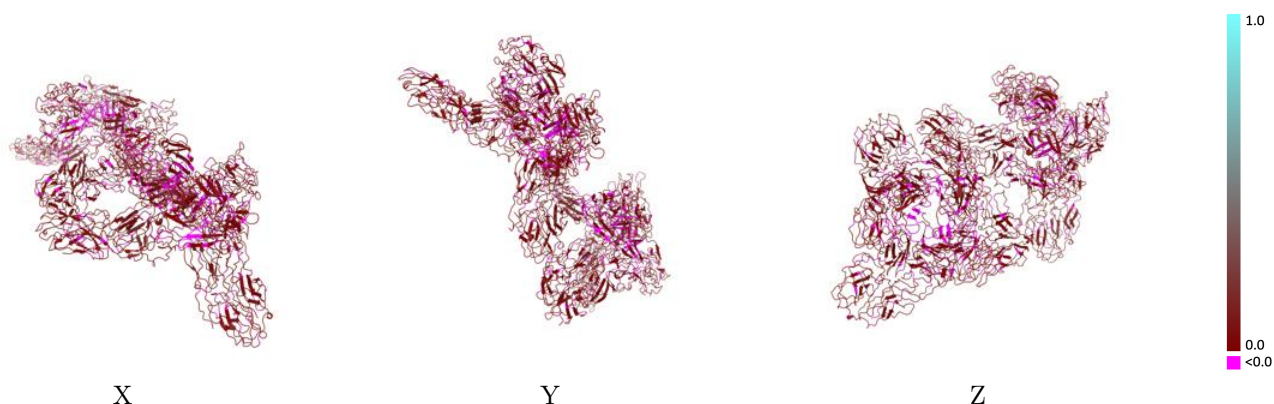
Y



Z

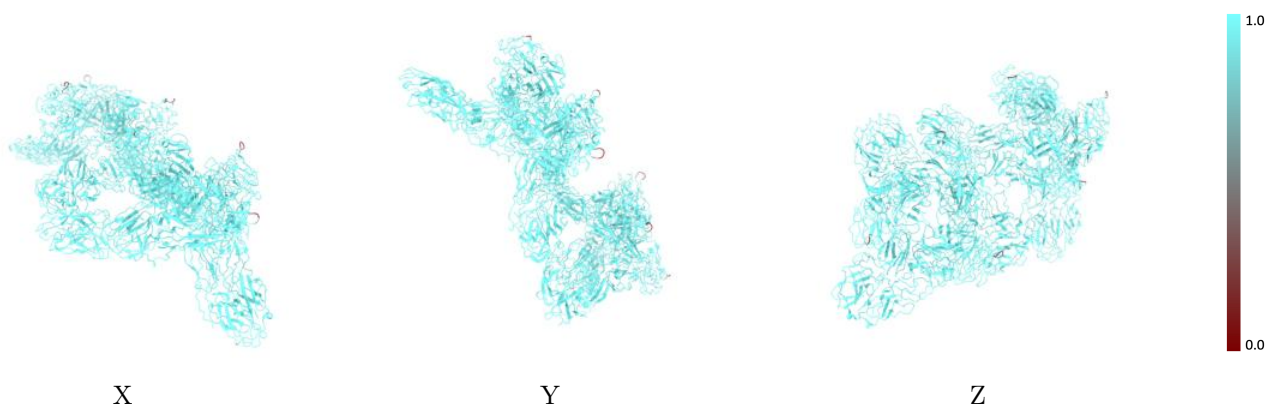
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



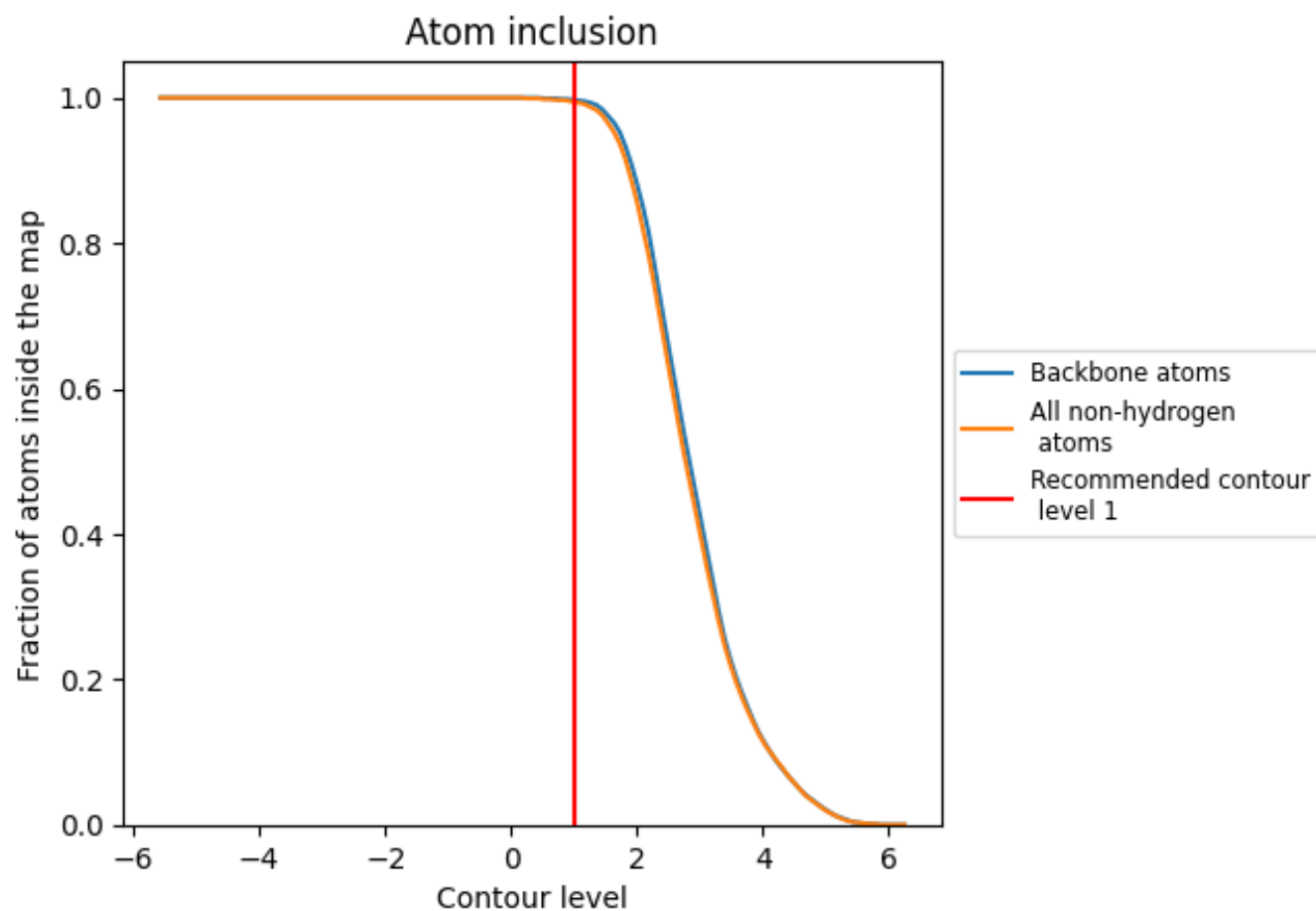
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9940	0.0660
A	1.0000	0.0740
B	0.9950	0.0620
C	0.9980	0.0680
D	0.9910	0.0710
E	0.9990	0.0660
F	0.9900	0.0660
G	0.9990	0.0660
H	0.9900	0.0640
I	0.9990	0.0690
J	0.9860	0.0550
K	0.9990	0.0620
L	0.9840	0.0590

1.0

0.0

<0.0