



Full wwPDB EM Validation Report ⓘ

May 18, 2026 – 02:17 PM JST

PDB ID : 25HN / pdb_000025hn
EMDB ID : EMD-80105
Title : Cryo-EM structure of native Rubisco from Nitrosospira multiformis
Authors : Tanaka, Y.; Nishigaya, Y.
Deposited on : 2026-04-03
Resolution : 2.26 Å(reported)
Based on initial model : 4F0H

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:

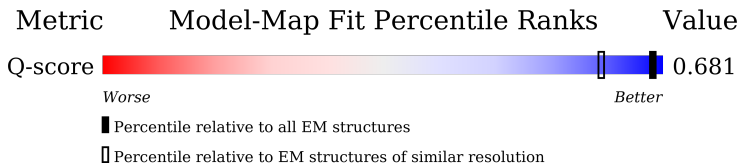
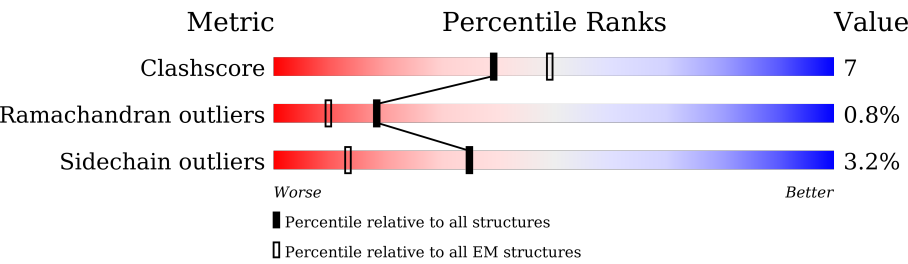
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.26 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	3535 (1.76 - 2.76)

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	489	 19% 74% 16% • 7%
1	C	489	 19% 76% 15% • 7%
1	E	489	 19% 76% 15% • 7%
1	F	489	 19% 75% 16% • 7%

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Mol	Chain	Length	Quality of chain
1	I	489	
1	J	489	
1	M	489	
1	N	489	
2	B	144	
2	D	144	
2	G	144	
2	H	144	
2	K	144	
2	L	144	
2	O	144	
2	P	144	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 38393 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 Ribulose biphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	454	Total	C	N	O	S	0	0
			3552	2264	614	651	23		
1	C	454	Total	C	N	O	S	0	0
			3552	2264	614	651	23		
1	E	454	Total	C	N	O	S	0	0
			3552	2264	614	651	23		
1	F	454	Total	C	N	O	S	0	0
			3552	2264	614	651	23		
1	I	454	Total	C	N	O	S	0	0
			3552	2264	614	651	23		
1	J	454	Total	C	N	O	S	0	0
			3552	2264	614	651	23		
1	M	454	Total	C	N	O	S	0	0
			3552	2264	614	651	23		
1	N	454	Total	C	N	O	S	0	0
			3552	2264	614	651	23		

- Molecule 2 is a protein called Ribulose biphosphate carboxylase small subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	144	Total	C	N	O	S	1	0
			1192	754	209	223	6		
2	D	144	Total	C	N	O	S	1	0
			1192	754	209	223	6		
2	G	144	Total	C	N	O	S	1	0
			1192	754	209	223	6		
2	H	144	Total	C	N	O	S	1	0
			1192	754	209	223	6		
2	K	144	Total	C	N	O	S	1	0
			1192	754	209	223	6		
2	L	144	Total	C	N	O	S	1	0
			1192	754	209	223	6		
2	O	144	Total	C	N	O	S	1	0
			1192	754	209	223	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	144	Total	C	N	O	S	1	0
			1192	754	209	223	6		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	F	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	J	1	Total	Zn	0
			1	1	
3	M	1	Total	Zn	0
			1	1	
3	N	1	Total	Zn	0
			1	1	

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	34	Total	O	0
			34	34	
4	C	37	Total	O	0
			37	37	
4	E	32	Total	O	0
			32	32	
4	F	33	Total	O	0
			33	33	
4	I	36	Total	O	0
			36	36	
4	J	26	Total	O	0
			26	26	
4	M	37	Total	O	0
			37	37	
4	N	32	Total	O	0
			32	32	

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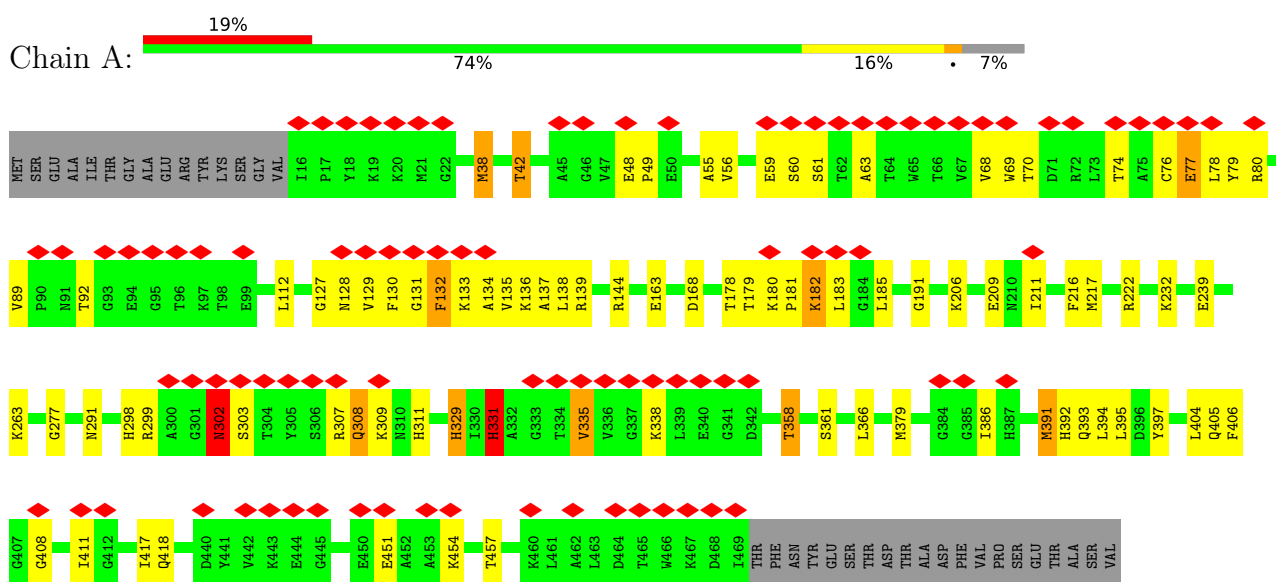
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Mol	Chain	Residues	Atoms		AltConf
4	B	22	Total 22	O 22	0
4	D	19	Total 19	O 19	0
4	G	25	Total 25	O 25	0
4	H	20	Total 20	O 20	0
4	K	19	Total 19	O 19	0
4	L	20	Total 20	O 20	0
4	O	20	Total 20	O 20	0
4	P	21	Total 21	O 21	0

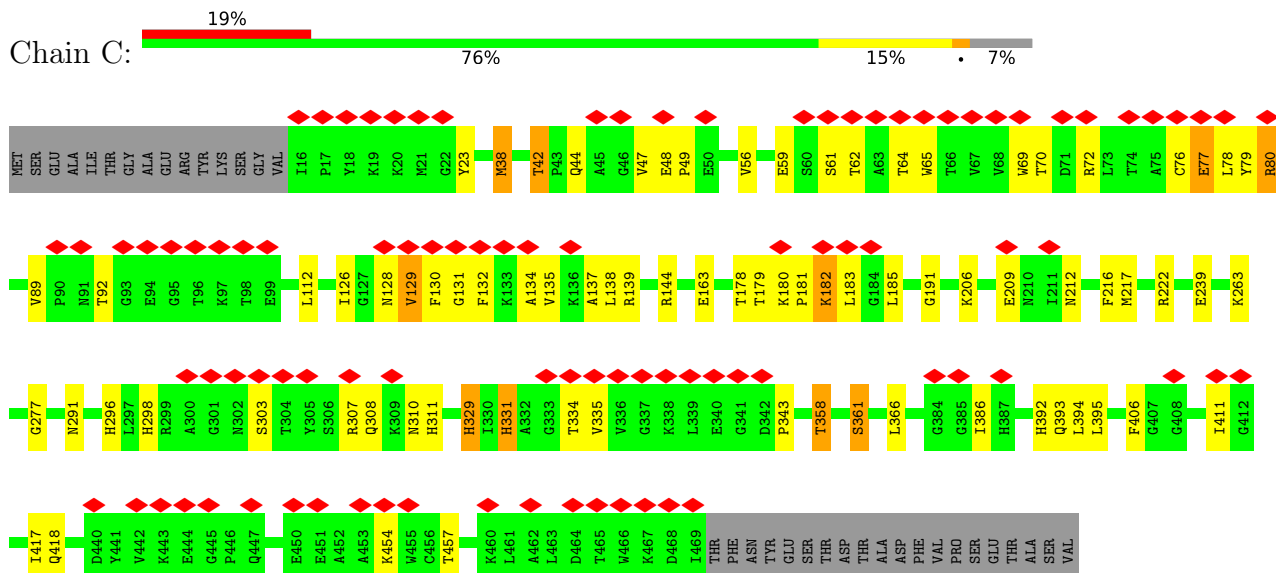
3 Residue-property plots

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

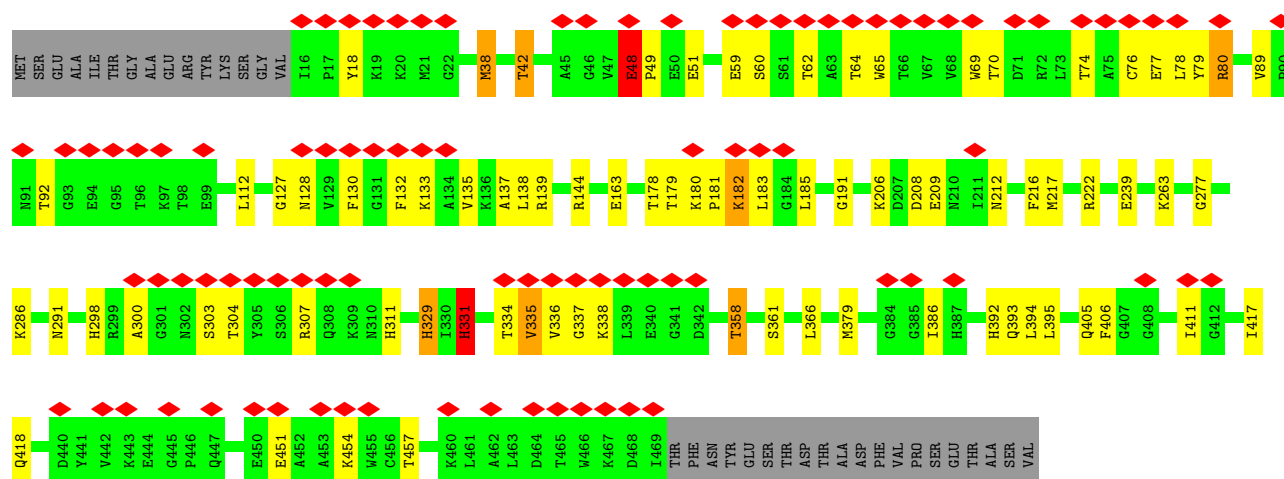
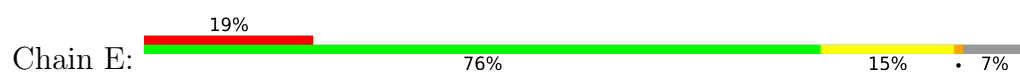
- Molecule 1: Ribulose biphosphate carboxylase large chain



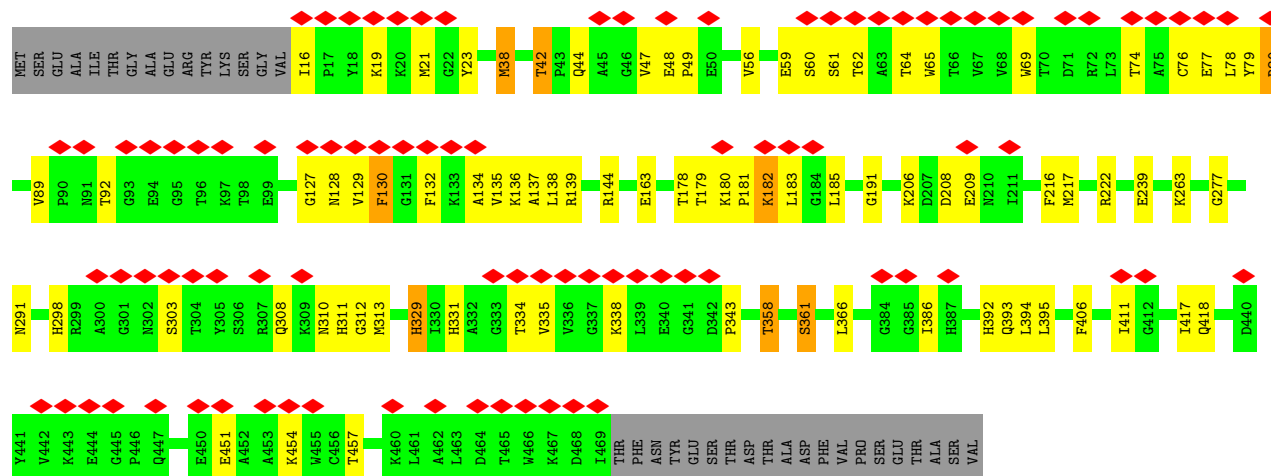
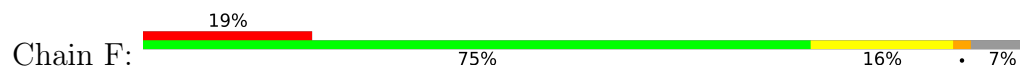
- Molecule 1: Ribulose biphosphate carboxylase large chain



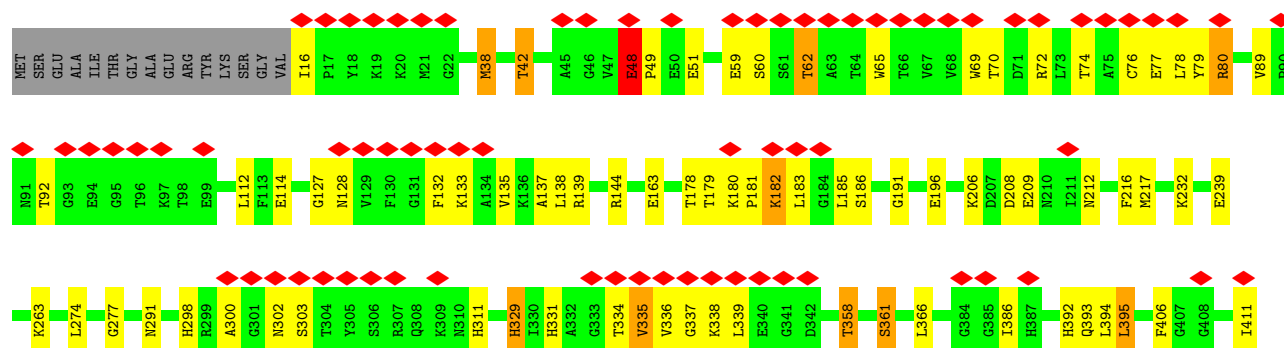
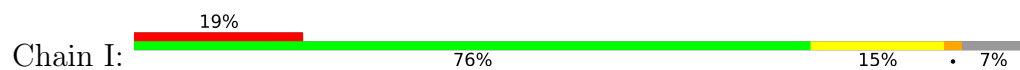
- Molecule 1: Ribulose biphosphate carboxylase large chain

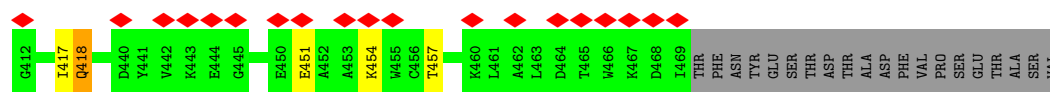


• Molecule 1: Ribulose biphosphate carboxylase large chain

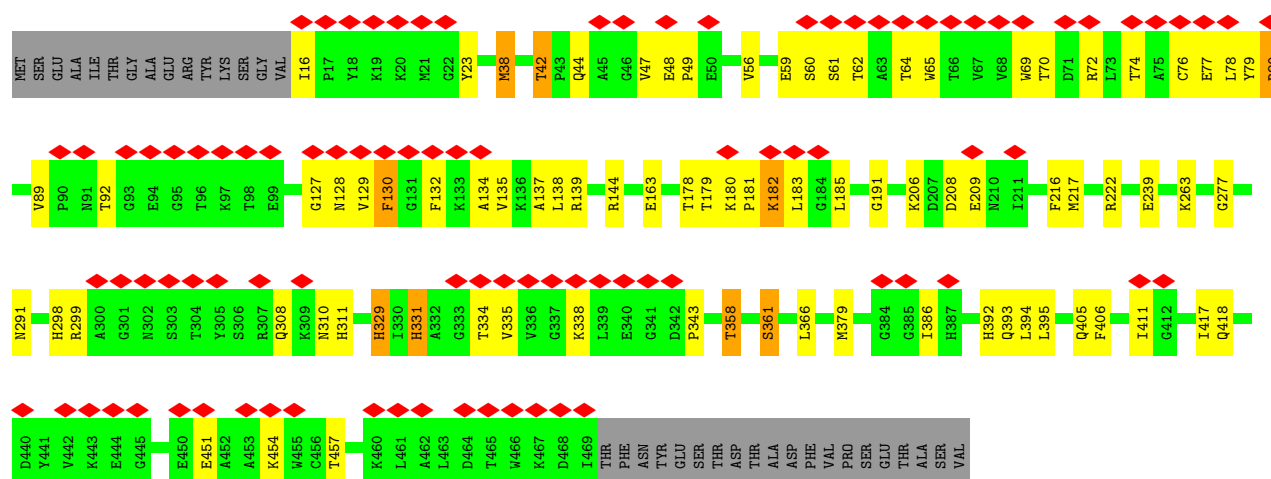
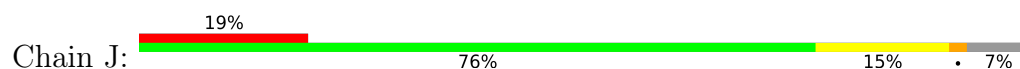


• Molecule 1: Ribulose biphosphate carboxylase large chain

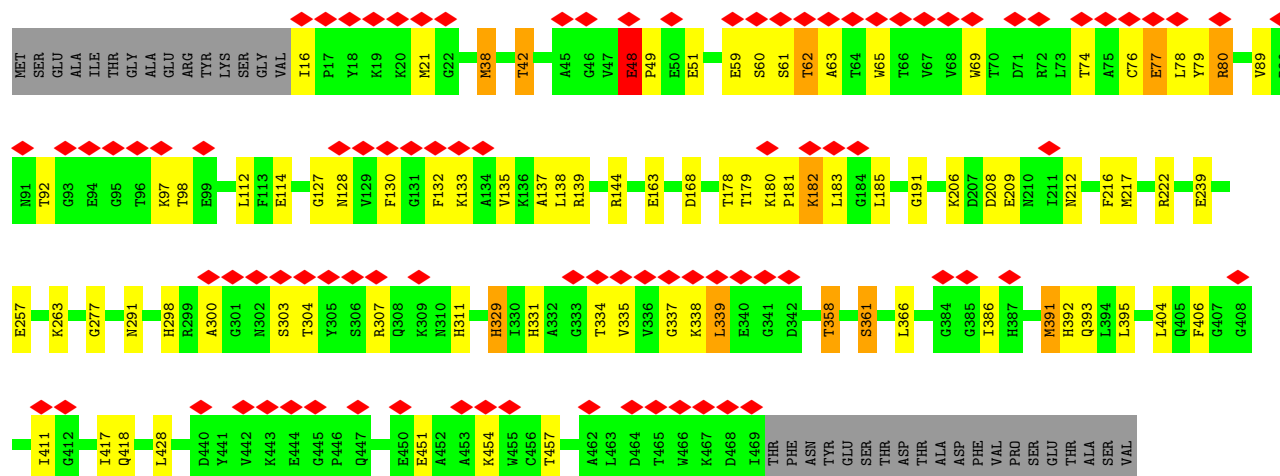
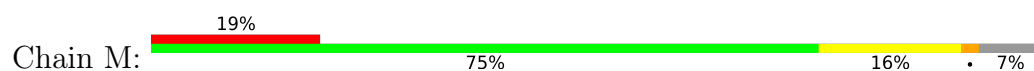




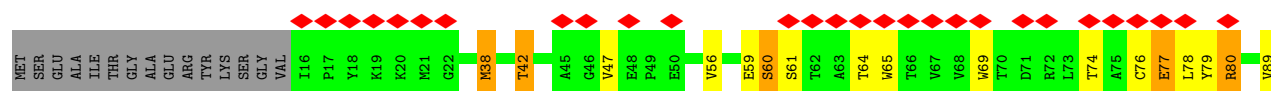
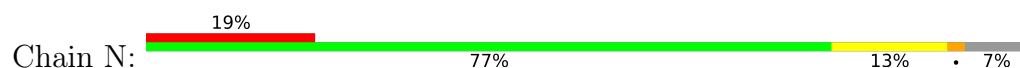
• Molecule 1: Ribulose biphosphate carboxylase large chain

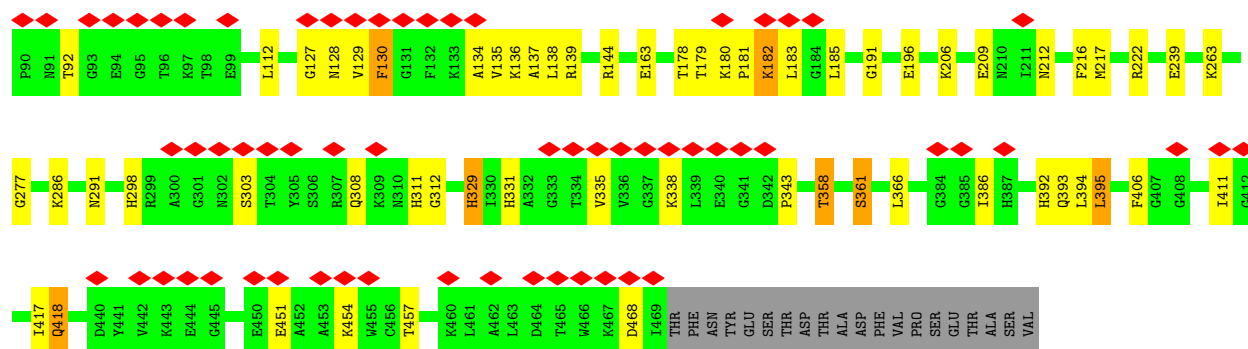


• Molecule 1: Ribulose biphosphate carboxylase large chain

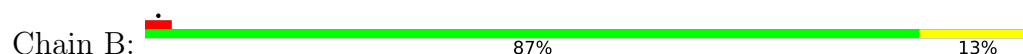


• Molecule 1: Ribulose biphosphate carboxylase large chain

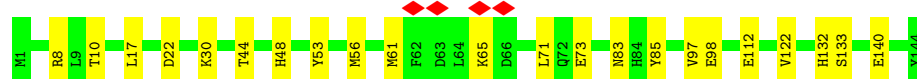
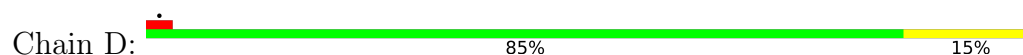




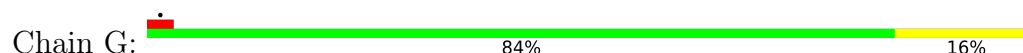
- Molecule 2: Ribulose biphosphate carboxylase small subunit



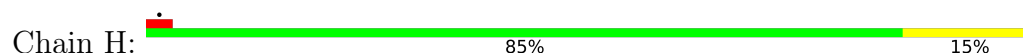
- Molecule 2: Ribulose biphosphate carboxylase small subunit



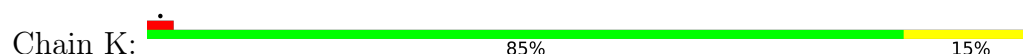
- Molecule 2: Ribulose biphosphate carboxylase small subunit




- Molecule 2: Ribulose biphosphate carboxylase small subunit

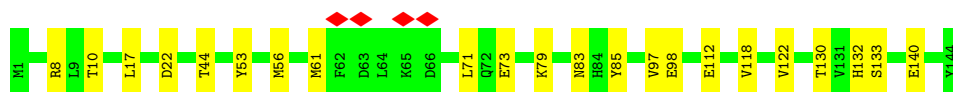


- Molecule 2: Ribulose biphosphate carboxylase small subunit




- Molecule 2: Ribulose biphosphate carboxylase small subunit

Chain L:  85% 15%




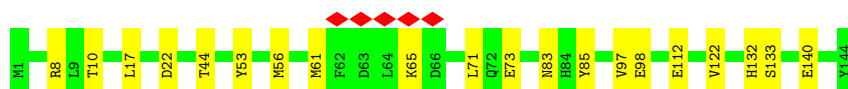
- Molecule 2: Ribulose biphosphate carboxylase small subunit

Chain O:  84% 16%



- Molecule 2: Ribulose biphosphate carboxylase small subunit

Chain P:  86% 14%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D4	Depositor
Number of particles used	64288	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	57000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.143	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	138.7872, 138.7872, 138.7872	wwPDB
Map dimensions	158, 158, 158	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8784, 0.8784, 0.8784	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.78	0/3635	1.16	9/4919 (0.2%)
1	C	0.77	0/3635	1.15	7/4919 (0.1%)
1	E	0.77	0/3635	1.14	8/4919 (0.2%)
1	F	0.76	0/3635	1.13	6/4919 (0.1%)
1	I	0.77	0/3635	1.14	6/4919 (0.1%)
1	J	0.77	0/3635	1.13	7/4919 (0.1%)
1	M	0.77	0/3635	1.14	9/4919 (0.2%)
1	N	0.76	0/3635	1.13	6/4919 (0.1%)
2	B	0.77	0/1225	1.09	1/1661 (0.1%)
2	D	0.78	1/1225 (0.1%)	1.10	1/1661 (0.1%)
2	G	0.77	0/1225	1.09	1/1661 (0.1%)
2	H	0.78	0/1225	1.10	1/1661 (0.1%)
2	K	0.77	0/1225	1.09	1/1661 (0.1%)
2	L	0.77	0/1225	1.09	1/1661 (0.1%)
2	O	0.78	1/1225 (0.1%)	1.10	1/1661 (0.1%)
2	P	0.77	0/1225	1.09	1/1661 (0.1%)
All	All	0.77	2/38880 (0.0%)	1.13	66/52640 (0.1%)

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	3
1	C	0	2
1	E	0	2
1	F	0	2
1	I	0	2
1	J	0	2
1	M	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	3
All	All	0	18

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	48	HIS	CE1-NE2	5.50	1.38	1.32
2	D	48	HIS	CE1-NE2	5.04	1.37	1.32

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	178	THR	CA-CB-OG1	-8.45	96.93	109.60
1	F	178	THR	CA-CB-OG1	-8.43	96.95	109.60
1	C	178	THR	CA-CB-OG1	-8.39	97.01	109.60
1	M	178	THR	CA-CB-OG1	-8.37	97.05	109.60
1	J	178	THR	CA-CB-OG1	-8.34	97.09	109.60
1	A	178	THR	CA-CB-OG1	-8.33	97.11	109.60
1	I	178	THR	CA-CB-OG1	-8.31	97.14	109.60
1	N	178	THR	CA-CB-OG1	-8.29	97.17	109.60
1	C	331	HIS	CB-CG-CD2	8.25	141.92	131.20
1	C	331	HIS	CB-CG-ND1	-7.39	111.61	122.70
1	M	391	MET	CG-SD-CE	-7.29	84.87	100.90
1	I	329	HIS	CA-CB-CG	6.81	120.61	113.80
1	J	329	HIS	CA-CB-CG	6.81	120.61	113.80
1	A	329	HIS	CA-CB-CG	6.80	120.60	113.80
1	C	329	HIS	CA-CB-CG	6.79	120.59	113.80
1	N	329	HIS	CA-CB-CG	6.77	120.57	113.80
1	F	329	HIS	CA-CB-CG	6.74	120.54	113.80
1	M	329	HIS	CA-CB-CG	6.70	120.50	113.80
1	E	329	HIS	CA-CB-CG	6.69	120.49	113.80
1	E	206	LYS	O-C-N	6.48	130.79	123.27
1	M	206	LYS	O-C-N	6.47	130.78	123.27
1	C	206	LYS	O-C-N	6.47	130.77	123.27
1	I	206	LYS	O-C-N	6.45	130.75	123.27
1	N	206	LYS	O-C-N	6.40	130.70	123.27
1	J	206	LYS	O-C-N	6.38	130.67	123.27
1	A	206	LYS	O-C-N	6.37	130.66	123.27
2	P	44	THR	OG1-CB-CG2	-6.30	96.70	109.30
1	F	206	LYS	O-C-N	6.29	130.57	123.27
2	B	44	THR	OG1-CB-CG2	-6.24	96.82	109.30
2	L	44	THR	OG1-CB-CG2	-6.21	96.87	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	44	THR	OG1-CB-CG2	-6.21	96.88	109.30
2	H	44	THR	OG1-CB-CG2	-6.18	96.94	109.30
2	G	44	THR	OG1-CB-CG2	-6.18	96.94	109.30
1	A	302	ASN	CA-CB-CG	6.15	118.75	112.60
1	I	48	GLU	N-CA-CB	6.13	116.85	109.74
2	O	44	THR	OG1-CB-CG2	-6.12	97.07	109.30
1	M	48	GLU	N-CA-CB	6.08	116.80	109.74
1	M	38	MET	CG-SD-CE	-6.08	87.52	100.90
1	E	48	GLU	N-CA-CB	6.07	116.78	109.74
2	D	44	THR	OG1-CB-CG2	-6.05	97.19	109.30
1	E	38	MET	CG-SD-CE	-6.05	87.59	100.90
1	I	38	MET	CG-SD-CE	-6.05	87.59	100.90
1	N	38	MET	CG-SD-CE	-6.04	87.62	100.90
1	J	38	MET	CG-SD-CE	-6.04	87.62	100.90
1	F	38	MET	CG-SD-CE	-6.03	87.63	100.90
1	A	38	MET	CG-SD-CE	-6.02	87.66	100.90
1	C	38	MET	CG-SD-CE	-6.01	87.68	100.90
1	A	133	LYS	N-CA-CB	-5.64	101.83	110.12
1	J	130	PHE	N-CA-C	-5.48	106.79	112.93
1	F	130	PHE	N-CA-C	-5.47	106.81	112.93
1	E	286	LYS	CA-CB-CG	5.39	124.87	114.10
1	N	130	PHE	N-CA-C	-5.34	106.95	112.93
1	N	286	LYS	CA-CB-CG	5.25	124.59	114.10
1	C	334	THR	CA-CB-OG1	-5.22	101.76	109.60
1	F	334	THR	CA-CB-OG1	-5.18	101.83	109.60
1	A	391	MET	CG-SD-CE	-5.16	89.54	100.90
1	A	379	MET	O-C-N	-5.16	116.93	121.31
1	I	114	GLU	CB-CG-CD	5.16	121.36	112.60
1	J	334	THR	CA-CB-OG1	-5.14	101.88	109.60
1	M	48	GLU	CB-CA-C	5.06	117.42	109.37
1	A	168	ASP	CA-CB-CG	5.04	117.64	112.60
1	M	168	ASP	CA-CB-CG	5.04	117.64	112.60
1	E	48	GLU	CB-CA-C	5.02	117.36	109.37
1	J	379	MET	O-C-N	-5.02	117.04	121.31
1	M	114	GLU	CB-CG-CD	5.00	121.11	112.60
1	E	379	MET	O-C-N	-5.00	117.06	121.31

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	179	THR	Peptide
1	A	307	ARG	Sidechain
1	C	139	ARG	Sidechain
1	C	179	THR	Peptide
1	E	139	ARG	Sidechain
1	E	179	THR	Peptide
1	F	139	ARG	Sidechain
1	F	179	THR	Peptide
1	I	139	ARG	Sidechain
1	I	179	THR	Peptide
1	J	139	ARG	Sidechain
1	J	179	THR	Peptide
1	M	139	ARG	Sidechain
1	M	179	THR	Peptide
1	N	139	ARG	Sidechain
1	N	179	THR	Peptide
1	N	60	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3552	0	3514	79	0
1	C	3552	0	3514	78	0
1	E	3552	0	3514	72	0
1	F	3552	0	3514	67	0
1	I	3552	0	3514	70	0
1	J	3552	0	3514	65	0
1	M	3552	0	3514	69	0
1	N	3552	0	3514	63	0
2	B	1192	0	1144	8	0
2	D	1192	0	1144	9	0
2	G	1192	0	1144	11	0
2	H	1192	0	1144	10	0
2	K	1192	0	1144	9	0
2	L	1192	0	1144	9	0
2	O	1192	0	1144	9	0
2	P	1192	0	1144	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	34	0	0	3	0
4	B	22	0	0	0	0
4	C	37	0	0	3	0
4	D	19	0	0	0	0
4	E	32	0	0	4	0
4	F	33	0	0	0	0
4	G	25	0	0	1	0
4	H	20	0	0	0	0
4	I	36	0	0	2	0
4	J	26	0	0	0	0
4	K	19	0	0	0	0
4	L	20	0	0	0	0
4	M	37	0	0	2	0
4	N	32	0	0	1	0
4	O	20	0	0	0	0
4	P	21	0	0	0	0
All	All	38393	0	37264	540	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 7.

All (540) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:311:HIS:CD2	1:N:311:HIS:HE2	1.74	1.03
1:A:217:MET:HE3	1:A:222:ARG:HD3	1.38	1.03
1:A:185:LEU:HA	4:C:622:HOH:O	1.63	0.97
1:A:217:MET:CE	1:A:222:ARG:HD3	1.94	0.95
1:C:296:HIS:CE1	1:C:331:HIS:HE1	1.83	0.95
1:A:181:PRO:HG2	1:A:185:LEU:HD11	1.48	0.95
1:C:296:HIS:NE2	1:C:331:HIS:HE1	1.65	0.93
1:E:331:HIS:HE1	4:E:627:HOH:O	1.54	0.90
1:A:130:PHE:HB3	1:C:303:SER:HB3	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:VAL:HG13	1:C:129:VAL:HG21	1.55	0.86
2:O:85:TYR:OH	2:O:112:GLU:OE1	1.95	0.85
2:L:85:TYR:OH	2:L:112:GLU:OE1	1.95	0.84
2:G:85:TYR:OH	2:G:112:GLU:OE1	1.95	0.84
2:D:85:TYR:OH	2:D:112:GLU:OE1	1.95	0.84
2:H:85:TYR:OH	2:H:112:GLU:OE1	1.95	0.84
2:B:85:TYR:OH	2:B:112:GLU:OE1	1.95	0.84
2:P:85:TYR:OH	2:P:112:GLU:OE1	1.95	0.84
2:K:85:TYR:OH	2:K:112:GLU:OE1	1.95	0.83
1:M:311:HIS:NE2	1:N:311:HIS:NE2	2.24	0.83
1:A:60:SER:OG	1:A:127:GLY:O	1.96	0.83
1:E:60:SER:OG	1:E:127:GLY:O	1.97	0.82
1:I:60:SER:OG	1:I:127:GLY:O	1.98	0.82
1:F:60:SER:OG	1:F:127:GLY:O	1.98	0.81
1:N:60:SER:OG	1:N:127:GLY:O	1.97	0.81
1:J:60:SER:OG	1:J:127:GLY:O	1.98	0.80
1:I:311:HIS:NE2	1:J:311:HIS:NE2	2.29	0.79
1:E:300:ALA:HB1	1:F:128:ASN:H	1.45	0.79
1:I:300:ALA:HB1	1:J:128:ASN:H	1.46	0.79
1:A:311:HIS:NE2	1:C:311:HIS:NE2	2.30	0.79
1:E:311:HIS:NE2	1:F:311:HIS:NE2	2.30	0.79
1:M:60:SER:OG	1:M:127:GLY:O	2.00	0.78
1:M:300:ALA:HB1	1:N:128:ASN:H	1.48	0.78
2:D:65:LYS:O	2:D:65:LYS:HG3	1.83	0.78
2:D:61:MET:HE1	2:D:73:GLU:HG3	1.66	0.77
2:K:61:MET:HE1	2:K:73:GLU:HG3	1.66	0.77
2:P:61:MET:HE1	2:P:73:GLU:HG3	1.66	0.77
2:G:61:MET:HE1	2:G:73:GLU:HG3	1.66	0.77
2:L:61:MET:HE1	2:L:73:GLU:HG3	1.66	0.77
2:O:61:MET:HE1	2:O:73:GLU:HG3	1.66	0.77
1:C:296:HIS:NE2	1:C:331:HIS:CE1	2.51	0.77
1:C:129:VAL:HG22	1:C:138:LEU:HD22	1.67	0.76
2:B:61:MET:HE1	2:B:73:GLU:HG3	1.66	0.76
2:H:61:MET:HE1	2:H:73:GLU:HG3	1.66	0.75
1:N:180:LYS:HB2	1:N:411:ILE:HG21	1.67	0.75
1:E:180:LYS:HB2	1:E:411:ILE:HG21	1.66	0.75
1:C:180:LYS:HB2	1:C:411:ILE:HG21	1.68	0.75
1:I:180:LYS:HB2	1:I:411:ILE:HG21	1.67	0.75
1:C:59:GLU:HB2	1:C:129:VAL:HB	1.67	0.74
1:M:180:LYS:HB2	1:M:411:ILE:HG21	1.66	0.74
1:A:180:LYS:HB2	1:A:411:ILE:HG21	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:56:VAL:HG13	1:N:129:VAL:HG21	1.68	0.74
1:I:311:HIS:CD2	1:J:311:HIS:NE2	2.57	0.73
1:F:180:LYS:HB2	1:F:411:ILE:HG21	1.71	0.73
1:F:56:VAL:HG13	1:F:129:VAL:HG21	1.69	0.73
1:A:311:HIS:CD2	1:C:311:HIS:NE2	2.57	0.72
1:C:296:HIS:CE1	1:C:331:HIS:CE1	2.73	0.72
1:J:180:LYS:HB2	1:J:411:ILE:HG21	1.71	0.72
1:C:209:GLU:O	4:C:601:HOH:O	2.08	0.72
1:M:307:ARG:NH1	1:N:136:LYS:O	2.23	0.72
1:J:56:VAL:HG13	1:J:129:VAL:HG21	1.69	0.72
1:E:311:HIS:CD2	1:F:311:HIS:NE2	2.58	0.72
1:A:181:PRO:CG	1:A:185:LEU:HD11	2.19	0.71
1:E:307:ARG:NH1	1:F:136:LYS:O	2.23	0.71
1:A:311:HIS:HE2	1:C:311:HIS:CD2	2.09	0.70
1:A:211:ILE:HD11	1:A:217:MET:HE2	1.73	0.70
1:C:47:VAL:HG11	1:C:134:ALA:HB1	1.74	0.70
1:I:311:HIS:HE2	1:J:311:HIS:CD2	2.09	0.69
1:E:311:HIS:HE2	1:F:311:HIS:CD2	2.10	0.69
1:M:311:HIS:HE2	1:N:311:HIS:CD2	2.10	0.69
1:A:180:LYS:N	1:A:181:PRO:HD2	2.08	0.68
1:E:48:GLU:HB2	1:E:49:PRO:HD2	1.75	0.68
1:E:180:LYS:N	1:E:181:PRO:HD2	2.09	0.68
1:M:48:GLU:HB2	1:M:49:PRO:HD2	1.75	0.68
1:M:311:HIS:CD2	1:N:311:HIS:NE2	2.56	0.67
1:F:180:LYS:N	1:F:181:PRO:HD2	2.09	0.67
1:N:180:LYS:N	1:N:181:PRO:HD2	2.08	0.67
1:C:180:LYS:N	1:C:181:PRO:HD2	2.09	0.67
1:J:180:LYS:N	1:J:181:PRO:HD2	2.09	0.67
1:A:211:ILE:HD11	1:A:217:MET:CE	2.24	0.67
1:I:180:LYS:N	1:I:181:PRO:HD2	2.09	0.67
1:M:180:LYS:N	1:M:181:PRO:HD2	2.09	0.67
1:C:44:GLN:HG3	1:C:132:PHE:CE1	2.30	0.67
1:A:56:VAL:HG13	1:A:129:VAL:HG21	1.78	0.66
1:A:308:GLN:HG3	1:C:311:HIS:CG	2.31	0.66
1:E:18:TYR:OH	1:E:64:THR:O	2.11	0.66
1:I:48:GLU:HB2	1:I:49:PRO:HD2	1.76	0.66
1:I:48:GLU:HG2	1:I:51:GLU:OE1	1.97	0.64
1:A:182:LYS:NZ	1:C:64:THR:OG1	2.30	0.64
1:A:136:LYS:O	1:C:307:ARG:NH1	2.30	0.64
1:A:299:ARG:NH1	1:A:302:ASN:OD1	2.30	0.64
1:E:48:GLU:HG2	1:E:51:GLU:OE1	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:48:GLU:HG2	1:M:51:GLU:OE1	1.98	0.64
1:I:180:LYS:O	1:I:182:LYS:HG2	1.98	0.64
1:M:257:GLU:OE2	4:M:601:HOH:O	2.15	0.64
1:E:180:LYS:O	1:E:182:LYS:HG2	1.97	0.63
1:J:180:LYS:O	1:J:182:LYS:HG2	1.99	0.63
1:M:338:LYS:O	1:M:339:LEU:HB2	1.99	0.63
1:N:180:LYS:O	1:N:182:LYS:HG2	1.98	0.63
1:M:180:LYS:O	1:M:182:LYS:HG2	1.98	0.62
1:E:331:HIS:CE1	4:E:627:HOH:O	2.39	0.62
1:F:48:GLU:HG3	1:F:49:PRO:HD2	1.82	0.61
1:F:180:LYS:O	1:F:182:LYS:HG2	2.00	0.61
1:A:132:PHE:HE1	1:A:134:ALA:HB3	1.63	0.60
1:J:48:GLU:HG3	1:J:49:PRO:HD2	1.82	0.60
1:N:47:VAL:HG11	1:N:134:ALA:HB1	1.84	0.60
1:C:48:GLU:HG3	1:C:49:PRO:HD2	1.83	0.60
1:C:129:VAL:HG22	1:C:138:LEU:CD2	2.31	0.60
1:J:47:VAL:HG11	1:J:134:ALA:HB1	1.84	0.59
1:M:133:LYS:HD2	1:N:338:LYS:HD3	1.85	0.59
1:E:60:SER:OG	1:E:128:ASN:OD1	2.20	0.59
1:I:386:ILE:HG22	1:I:406:PHE:CE2	2.38	0.58
1:C:69:TRP:CH2	2:G:56:MET:HE1	2.38	0.58
1:C:310:ASN:HB2	1:C:311:HIS:HD1	1.69	0.58
1:I:60:SER:H	1:I:128:ASN:HD21	1.51	0.58
1:F:182:LYS:HD2	1:F:208:ASP:OD2	2.04	0.57
1:I:69:TRP:CH2	2:H:56:MET:HE1	2.39	0.57
1:A:217:MET:CE	1:A:222:ARG:CD	2.79	0.57
1:E:69:TRP:CH2	2:D:56:MET:HE1	2.38	0.57
1:F:47:VAL:HG11	1:F:134:ALA:HB1	1.85	0.57
1:I:274:LEU:HD23	1:I:302:ASN:HD21	1.67	0.57
1:J:310:ASN:HB2	1:J:311:HIS:HD1	1.70	0.57
1:E:133:LYS:HD2	1:F:338:LYS:HD3	1.86	0.57
1:F:23:TYR:OH	1:F:62:THR:OG1	2.14	0.57
1:F:310:ASN:HB2	1:F:311:HIS:HD1	1.70	0.57
1:I:133:LYS:HD2	1:J:338:LYS:HD3	1.86	0.57
1:J:392:HIS:NE2	1:J:393:GLN:OE1	2.38	0.57
1:M:392:HIS:NE2	1:M:393:GLN:OE1	2.38	0.57
1:I:60:SER:OG	1:I:128:ASN:OD1	2.20	0.56
1:M:217:MET:SD	1:M:222:ARG:HD3	2.45	0.56
1:N:392:HIS:NE2	1:N:393:GLN:OE1	2.38	0.56
1:E:89:VAL:O	1:E:92:THR:OG1	2.23	0.56
1:F:217:MET:SD	1:F:222:ARG:HD3	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:392:HIS:NE2	1:I:393:GLN:OE1	2.38	0.56
1:M:89:VAL:O	1:M:92:THR:OG1	2.23	0.56
1:A:181:PRO:HG3	1:C:70:THR:HB	1.87	0.56
1:C:89:VAL:O	1:C:92:THR:OG1	2.23	0.56
1:E:60:SER:H	1:E:128:ASN:HD21	1.51	0.56
1:I:89:VAL:O	1:I:92:THR:OG1	2.23	0.56
1:I:180:LYS:HD2	1:J:64:THR:HG21	1.88	0.56
1:N:89:VAL:O	1:N:92:THR:OG1	2.23	0.56
1:C:217:MET:SD	1:C:222:ARG:HD3	2.45	0.56
1:E:163:GLU:CD	1:E:329:HIS:HE2	2.13	0.56
1:E:217:MET:SD	1:E:222:ARG:HD3	2.45	0.56
1:F:89:VAL:O	1:F:92:THR:OG1	2.23	0.56
1:J:89:VAL:O	1:J:92:THR:OG1	2.23	0.56
1:A:89:VAL:O	1:A:92:THR:OG1	2.23	0.56
1:C:163:GLU:CD	1:C:329:HIS:HE2	2.13	0.56
1:J:23:TYR:OH	1:J:62:THR:OG1	2.14	0.56
1:J:217:MET:SD	1:J:222:ARG:HD3	2.45	0.56
1:N:217:MET:SD	1:N:222:ARG:HD3	2.45	0.56
1:I:163:GLU:CD	1:I:329:HIS:HE2	2.13	0.56
1:N:163:GLU:CD	1:N:329:HIS:HE2	2.13	0.56
1:C:386:ILE:HG22	1:C:406:PHE:CE1	2.41	0.56
1:C:392:HIS:NE2	1:C:393:GLN:OE1	2.38	0.56
1:E:392:HIS:NE2	1:E:393:GLN:OE1	2.38	0.56
1:F:69:TRP:CH2	2:K:56:MET:HE1	2.41	0.56
1:J:358:THR:CG2	1:J:366:LEU:HD13	2.36	0.56
1:A:386:ILE:HG22	1:A:406:PHE:CE1	2.40	0.55
1:N:69:TRP:CH2	2:B:56:MET:HE1	2.40	0.55
1:E:277:GLY:HA3	1:F:277:GLY:HA3	1.87	0.55
1:A:308:GLN:OE1	1:C:311:HIS:ND1	2.39	0.55
1:M:358:THR:CG2	1:M:366:LEU:HD13	2.36	0.55
1:A:277:GLY:HA3	1:C:277:GLY:HA3	1.87	0.55
1:F:392:HIS:NE2	1:F:393:GLN:OE1	2.38	0.55
1:A:76:CYS:O	1:A:77:GLU:HG3	2.07	0.55
1:A:392:HIS:NE2	1:A:393:GLN:OE1	2.39	0.55
1:E:386:ILE:HG22	1:E:406:PHE:CE1	2.42	0.55
1:N:358:THR:CG2	1:N:366:LEU:HD13	2.36	0.55
1:C:23:TYR:OH	1:C:62:THR:OG1	2.14	0.55
1:C:76:CYS:O	1:C:77:GLU:HG3	2.07	0.55
1:J:335:VAL:HG13	1:J:343:PRO:HB3	1.88	0.55
1:F:163:GLU:CD	1:F:329:HIS:HE2	2.13	0.55
1:F:358:THR:CG2	1:F:366:LEU:HD13	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:358:THR:CG2	1:I:366:LEU:HD13	2.36	0.55
1:M:76:CYS:O	1:M:77:GLU:HG3	2.07	0.55
1:A:163:GLU:CD	1:A:329:HIS:HE2	2.13	0.55
1:A:358:THR:CG2	1:A:366:LEU:HD13	2.36	0.55
1:C:180:LYS:HB3	1:C:411:ILE:HD13	1.89	0.55
1:J:69:TRP:CH2	2:O:56:MET:HE1	2.41	0.55
1:N:335:VAL:HG13	1:N:343:PRO:HB3	1.89	0.55
1:I:277:GLY:HA3	1:J:277:GLY:HA3	1.87	0.55
1:J:386:ILE:HG22	1:J:406:PHE:CE1	2.42	0.55
1:N:386:ILE:HG22	1:N:406:PHE:CE1	2.42	0.55
1:C:358:THR:CG2	1:C:366:LEU:HD13	2.36	0.55
1:F:386:ILE:HG22	1:F:406:PHE:CE1	2.41	0.55
1:J:163:GLU:CD	1:J:329:HIS:HE2	2.13	0.55
1:M:277:GLY:HA3	1:N:277:GLY:HA3	1.87	0.54
1:E:358:THR:CG2	1:E:366:LEU:HD13	2.37	0.54
1:M:163:GLU:CD	1:M:329:HIS:HE2	2.13	0.54
1:E:405:GLN:HG3	4:E:627:HOH:O	2.07	0.54
1:M:180:LYS:HD2	1:N:64:THR:HG21	1.90	0.54
1:M:386:ILE:HG22	1:M:406:PHE:CE1	2.42	0.54
1:I:62:THR:OG1	1:I:79:TYR:O	2.25	0.54
1:A:308:GLN:HG3	1:C:311:HIS:CD2	2.43	0.54
1:N:76:CYS:O	1:N:77:GLU:HG3	2.07	0.54
1:E:62:THR:C	1:F:182:LYS:HG3	2.33	0.53
1:C:180:LYS:CB	1:C:411:ILE:HG21	2.38	0.53
1:E:392:HIS:CE1	1:E:393:GLN:OE1	2.62	0.53
1:C:392:HIS:CE1	1:C:393:GLN:OE1	2.62	0.53
1:N:209:GLU:HB3	1:N:298:HIS:CD2	2.44	0.53
1:A:392:HIS:CE1	1:A:393:GLN:OE1	2.62	0.53
1:F:335:VAL:HG13	1:F:343:PRO:HB3	1.88	0.53
1:F:392:HIS:CE1	1:F:393:GLN:OE1	2.62	0.53
1:C:335:VAL:HG13	1:C:343:PRO:HB3	1.89	0.53
1:J:392:HIS:CE1	1:J:393:GLN:OE1	2.62	0.53
1:M:392:HIS:CE1	1:M:393:GLN:OE1	2.62	0.53
1:E:180:LYS:HD2	1:F:64:THR:HG21	1.91	0.53
1:I:209:GLU:HB3	1:I:298:HIS:CD2	2.44	0.53
1:N:392:HIS:CE1	1:N:393:GLN:OE1	2.62	0.53
1:E:334:THR:CG2	1:E:337:GLY:HA3	2.39	0.52
1:C:209:GLU:HB3	1:C:298:HIS:CD2	2.44	0.52
1:I:392:HIS:CE1	1:I:393:GLN:OE1	2.62	0.52
1:J:209:GLU:HB3	1:J:298:HIS:CD2	2.44	0.52
1:A:132:PHE:CE1	1:A:134:ALA:HB3	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:209:GLU:HB3	1:M:298:HIS:CD2	2.44	0.52
1:A:180:LYS:CB	1:A:411:ILE:HG21	2.38	0.52
1:E:311:HIS:HB3	1:F:308:GLN:OE1	2.09	0.52
1:I:303:SER:HB3	1:J:130:PHE:HB3	1.91	0.52
1:N:56:VAL:HG13	1:N:129:VAL:CG2	2.38	0.52
1:E:209:GLU:HB3	1:E:298:HIS:CD2	2.44	0.52
1:C:180:LYS:HD3	1:C:182:LYS:HD3	1.92	0.52
1:F:209:GLU:HB3	1:F:298:HIS:CD2	2.44	0.52
1:C:59:GLU:HB3	1:C:128:ASN:C	2.35	0.52
1:F:42:THR:HG23	1:F:137:ALA:H	1.75	0.52
1:F:180:LYS:CB	1:F:411:ILE:HG21	2.39	0.52
1:I:361:SER:O	1:I:361:SER:OG	2.28	0.52
1:N:361:SER:O	1:N:361:SER:OG	2.28	0.51
1:A:42:THR:HG23	1:A:137:ALA:H	1.75	0.51
1:A:209:GLU:HB3	1:A:298:HIS:CD2	2.45	0.51
1:J:42:THR:HG23	1:J:137:ALA:H	1.75	0.51
1:A:182:LYS:HE2	1:C:62:THR:HA	1.92	0.51
1:I:311:HIS:HB3	1:J:308:GLN:OE1	2.10	0.51
1:J:56:VAL:HG13	1:J:129:VAL:CG2	2.39	0.51
1:M:311:HIS:HB3	1:N:308:GLN:NE2	2.26	0.51
1:I:180:LYS:CB	1:I:411:ILE:HG21	2.39	0.51
1:N:42:THR:HG23	1:N:137:ALA:H	1.75	0.51
1:A:69:TRP:CH2	2:P:56:MET:HE1	2.46	0.51
1:I:386:ILE:HG22	1:I:406:PHE:HE2	1.76	0.51
1:J:180:LYS:CB	1:J:411:ILE:HG21	2.39	0.51
1:E:180:LYS:CB	1:E:411:ILE:HG21	2.40	0.51
1:N:59:GLU:HB3	1:N:128:ASN:O	2.11	0.51
1:F:59:GLU:HB2	1:F:129:VAL:HG23	1.93	0.50
1:J:59:GLU:HB3	1:J:128:ASN:O	2.11	0.50
1:J:76:CYS:O	1:J:77:GLU:HG2	2.12	0.50
1:N:180:LYS:CB	1:N:411:ILE:HG21	2.40	0.50
1:F:76:CYS:O	1:F:77:GLU:HG2	2.11	0.50
1:I:42:THR:HG23	1:I:137:ALA:H	1.76	0.50
1:A:311:HIS:HB3	1:C:308:GLN:OE1	2.10	0.50
1:A:405:GLN:HG3	4:A:601:HOH:O	2.10	0.50
1:F:180:LYS:HB3	1:F:411:ILE:HD13	1.93	0.50
1:E:76:CYS:O	1:E:77:GLU:HG2	2.12	0.50
1:E:338:LYS:O	1:F:132:PHE:HB3	2.12	0.50
1:M:180:LYS:CB	1:M:411:ILE:HG21	2.41	0.50
1:M:303:SER:HB3	1:N:130:PHE:HB3	1.94	0.50
1:C:361:SER:O	1:C:361:SER:OG	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:THR:HG23	1:E:137:ALA:H	1.77	0.49
1:J:16:ILE:HG13	1:J:65:TRP:HB2	1.94	0.49
1:N:59:GLU:HB2	1:N:129:VAL:HG23	1.94	0.49
1:F:59:GLU:HB3	1:F:128:ASN:O	2.11	0.49
1:J:163:GLU:OE2	1:J:329:HIS:NE2	2.42	0.49
1:M:163:GLU:OE2	1:M:329:HIS:NE2	2.42	0.49
1:A:59:GLU:HB3	1:A:128:ASN:O	2.13	0.49
2:B:22:ASP:OD2	2:B:71:LEU:HD11	2.13	0.49
1:J:180:LYS:HB3	1:J:411:ILE:HD13	1.94	0.49
2:D:22:ASP:OD2	2:D:71:LEU:HD11	2.13	0.49
2:O:22:ASP:OD2	2:O:71:LEU:HD11	2.13	0.49
1:E:334:THR:HG22	1:E:337:GLY:HA3	1.95	0.49
1:I:76:CYS:O	1:I:77:GLU:HG2	2.12	0.49
1:M:42:THR:HG23	1:M:137:ALA:H	1.77	0.49
1:M:69:TRP:CH2	2:L:56:MET:HE1	2.48	0.49
2:G:22:ASP:OD2	2:G:71:LEU:HD11	2.13	0.49
2:H:22:ASP:OD2	2:H:71:LEU:HD11	2.13	0.49
2:L:22:ASP:OD2	2:L:71:LEU:HD11	2.13	0.49
1:J:59:GLU:HB2	1:J:129:VAL:HG23	1.93	0.49
1:M:130:PHE:CG	1:N:303:SER:HB3	2.48	0.49
1:E:183:LEU:HB3	1:E:216:PHE:CZ	2.48	0.49
1:F:42:THR:CG2	1:F:137:ALA:HB3	2.43	0.49
1:M:391:MET:HE1	1:M:404:LEU:CD1	2.43	0.49
1:A:42:THR:CG2	1:A:137:ALA:HB3	2.43	0.48
1:J:358:THR:HG21	1:J:366:LEU:HD13	1.95	0.48
1:C:126:ILE:HG13	1:C:126:ILE:O	2.13	0.48
1:M:183:LEU:HB3	1:M:216:PHE:CZ	2.47	0.48
1:M:311:HIS:HB3	1:N:308:GLN:HE21	1.78	0.48
1:N:42:THR:CG2	1:N:137:ALA:HB3	2.42	0.48
1:A:217:MET:HE1	1:A:222:ARG:HD3	1.90	0.48
1:A:391:MET:HE1	1:A:404:LEU:HD13	1.93	0.48
1:F:56:VAL:HG13	1:F:129:VAL:CG2	2.39	0.48
1:A:68:VAL:HG11	1:C:411:ILE:HG12	1.95	0.48
1:C:183:LEU:HB3	1:C:216:PHE:CZ	2.48	0.48
1:E:42:THR:CG2	1:E:137:ALA:HB3	2.43	0.48
1:E:303:SER:HB3	1:F:130:PHE:HB3	1.96	0.48
2:P:22:ASP:OD2	2:P:71:LEU:HD11	2.13	0.48
1:C:42:THR:HG23	1:C:137:ALA:H	1.78	0.48
1:E:358:THR:HG21	1:E:366:LEU:HD13	1.95	0.48
1:I:183:LEU:HB3	1:I:216:PHE:CZ	2.48	0.48
2:K:22:ASP:OD2	2:K:71:LEU:HD11	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LEU:HB3	1:A:216:PHE:CZ	2.48	0.48
1:A:131:GLY:O	1:A:132:PHE:HB3	2.14	0.48
1:J:42:THR:CG2	1:J:137:ALA:HB3	2.43	0.48
1:A:163:GLU:OE2	1:A:329:HIS:NE2	2.42	0.48
1:F:163:GLU:OE2	1:F:329:HIS:NE2	2.42	0.48
1:F:183:LEU:HB3	1:F:216:PHE:CZ	2.49	0.47
1:F:358:THR:HG21	1:F:366:LEU:HD13	1.95	0.47
1:I:42:THR:CG2	1:I:137:ALA:HB3	2.43	0.47
1:M:74:THR:HG22	1:N:185:LEU:HD23	1.96	0.47
1:N:183:LEU:HB3	1:N:216:PHE:CZ	2.48	0.47
1:A:211:ILE:CD1	1:A:217:MET:HE2	2.44	0.47
1:N:239:GLU:OE2	2:P:10:THR:OG1	2.31	0.47
1:A:180:LYS:O	1:A:182:LYS:HG3	2.14	0.47
1:E:70:THR:HB	1:F:181:PRO:HG3	1.96	0.47
1:E:60:SER:H	1:E:128:ASN:ND2	2.13	0.47
1:J:183:LEU:HB3	1:J:216:PHE:CZ	2.49	0.47
1:M:42:THR:CG2	1:M:137:ALA:HB3	2.44	0.47
1:M:77:GLU:HA	1:M:80:ARG:HG2	1.95	0.47
1:M:334:THR:CG2	1:M:337:GLY:HA3	2.44	0.47
1:A:180:LYS:HG3	1:A:408:GLY:HA2	1.97	0.47
1:I:358:THR:HG21	1:I:366:LEU:HD13	1.95	0.47
1:M:62:THR:OG1	1:M:79:TYR:O	2.32	0.47
1:A:358:THR:HG21	1:A:366:LEU:HD13	1.95	0.47
1:C:42:THR:CG2	1:C:137:ALA:HB3	2.45	0.47
1:M:182:LYS:HD2	1:M:208:ASP:OD2	2.15	0.47
1:N:358:THR:HG21	1:N:366:LEU:HD13	1.95	0.47
1:C:358:THR:HG21	1:C:366:LEU:HD13	1.96	0.47
1:I:59:GLU:HB3	1:I:128:ASN:O	2.15	0.47
1:I:182:LYS:HD2	1:I:208:ASP:OD2	2.15	0.47
1:N:163:GLU:OE2	1:N:329:HIS:NE2	2.42	0.47
1:C:386:ILE:HG23	1:C:394:LEU:HD11	1.97	0.47
1:E:59:GLU:HB3	1:E:128:ASN:O	2.15	0.47
1:F:361:SER:O	1:F:361:SER:OG	2.28	0.47
1:I:163:GLU:OE2	1:I:329:HIS:NE2	2.42	0.47
1:E:304:THR:HG23	1:F:312:GLY:HA2	1.96	0.46
1:F:386:ILE:HG23	1:F:394:LEU:HD11	1.97	0.46
1:J:182:LYS:HD2	1:J:208:ASP:OD2	2.15	0.46
1:N:212:ASN:ND2	4:N:603:HOH:O	2.47	0.46
1:A:338:LYS:NZ	1:C:131:GLY:HA3	2.30	0.46
1:F:16:ILE:HG12	1:F:21:MET:HE1	1.97	0.46
1:C:77:GLU:HA	1:C:80:ARG:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:THR:HG22	1:F:185:LEU:HD23	1.98	0.46
1:E:386:ILE:HG23	1:E:394:LEU:HD11	1.98	0.46
1:I:185:LEU:HD23	1:J:74:THR:HG22	1.97	0.46
1:M:59:GLU:HB3	1:M:128:ASN:O	2.15	0.46
1:M:358:THR:HG21	1:M:366:LEU:HD13	1.95	0.46
1:J:386:ILE:HG23	1:J:394:LEU:HD11	1.97	0.46
1:N:77:GLU:HA	1:N:80:ARG:HG2	1.97	0.46
1:C:239:GLU:OE2	2:D:10:THR:OG1	2.31	0.46
1:C:78:LEU:HD23	1:C:79:TYR:CZ	2.51	0.46
1:I:386:ILE:HG23	1:I:394:LEU:HD11	1.97	0.46
1:A:181:PRO:CB	1:A:185:LEU:HD11	2.46	0.46
1:M:361:SER:O	1:M:361:SER:OG	2.28	0.46
1:A:77:GLU:HA	1:A:80:ARG:HD2	1.98	0.45
1:E:78:LEU:HD23	1:E:79:TYR:CZ	2.52	0.45
1:J:144:ARG:C	1:J:144:ARG:HD2	2.42	0.45
1:J:361:SER:O	1:J:361:SER:OG	2.28	0.45
1:M:144:ARG:HD2	1:M:144:ARG:C	2.41	0.45
1:N:144:ARG:HD2	1:N:144:ARG:C	2.42	0.45
1:A:144:ARG:HD2	1:A:144:ARG:C	2.42	0.45
1:A:180:LYS:N	1:A:181:PRO:CD	2.78	0.45
1:F:144:ARG:HD2	1:F:144:ARG:C	2.41	0.45
1:I:144:ARG:HD2	1:I:144:ARG:C	2.42	0.45
1:A:335:VAL:HG21	1:A:397:TYR:HB3	1.96	0.45
1:I:232:LYS:HD3	4:I:607:HOH:O	2.17	0.45
1:N:386:ILE:HG23	1:N:394:LEU:HD11	1.97	0.45
1:F:78:LEU:HD23	1:F:79:TYR:CZ	2.51	0.45
1:I:74:THR:HG22	1:J:185:LEU:HD23	1.99	0.45
1:A:78:LEU:HD23	1:A:79:TYR:CZ	2.52	0.45
1:I:138:LEU:O	1:I:311:HIS:HA	2.17	0.45
1:A:48:GLU:HB3	1:A:49:PRO:HD2	1.99	0.45
1:A:138:LEU:O	1:A:311:HIS:HA	2.17	0.45
1:E:144:ARG:C	1:E:144:ARG:HD2	2.42	0.45
1:J:78:LEU:HD23	1:J:79:TYR:CZ	2.51	0.45
1:M:185:LEU:HD23	1:N:74:THR:HG22	1.99	0.45
1:E:239:GLU:OE2	2:G:10:THR:OG1	2.32	0.45
1:A:217:MET:HE1	1:A:222:ARG:CD	2.46	0.45
1:N:78:LEU:HD23	1:N:79:TYR:CZ	2.51	0.45
1:C:56:VAL:HG22	1:C:129:VAL:CG2	2.47	0.45
1:C:144:ARG:HD2	1:C:144:ARG:C	2.42	0.45
1:F:138:LEU:O	1:F:311:HIS:HA	2.17	0.45
1:N:138:LEU:O	1:N:311:HIS:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:GLU:OE2	1:E:329:HIS:NE2	2.41	0.44
1:I:60:SER:H	1:I:128:ASN:ND2	2.15	0.44
1:I:78:LEU:HD23	1:I:79:TYR:CZ	2.52	0.44
1:M:78:LEU:HD23	1:M:79:TYR:CZ	2.51	0.44
1:C:163:GLU:OE2	1:C:329:HIS:NE2	2.42	0.44
1:E:335:VAL:HG12	1:E:336:VAL:HG13	1.99	0.44
1:A:181:PRO:HB2	1:A:185:LEU:HD11	2.00	0.44
1:A:59:GLU:HB2	1:A:129:VAL:HG23	1.98	0.44
1:A:331:HIS:NE2	4:A:601:HOH:O	2.27	0.44
1:J:138:LEU:O	1:J:311:HIS:HA	2.17	0.44
1:A:232:LYS:HD3	4:A:610:HOH:O	2.17	0.44
1:A:239:GLU:OE2	2:B:10:THR:OG1	2.32	0.44
1:E:138:LEU:O	1:E:311:HIS:HA	2.17	0.44
1:A:303:SER:HB2	1:C:130:PHE:HB3	2.00	0.43
1:F:239:GLU:OE2	2:H:10:THR:OG1	2.32	0.43
1:M:16:ILE:HD11	1:M:21:MET:HE3	2.00	0.43
1:M:180:LYS:HB3	1:M:411:ILE:HD13	2.00	0.43
1:M:391:MET:HE1	1:M:404:LEU:HD13	2.00	0.43
1:I:191:GLY:HA3	2:O:53:TYR:OH	2.19	0.43
1:M:304:THR:HG23	1:N:312:GLY:HA2	2.00	0.43
1:E:79:TYR:HA	1:E:112:LEU:HD21	2.01	0.43
1:F:180:LYS:N	1:F:181:PRO:CD	2.79	0.43
1:I:77:GLU:HA	1:I:80:ARG:HG2	2.00	0.43
1:I:181:PRO:HG3	1:J:70:THR:HB	2.01	0.43
1:M:191:GLY:HA3	2:B:53:TYR:OH	2.19	0.43
1:E:180:LYS:N	1:E:181:PRO:CD	2.80	0.43
1:E:182:LYS:HD2	1:E:208:ASP:OD2	2.18	0.43
1:J:191:GLY:HA3	2:H:53:TYR:OH	2.19	0.43
1:M:97:LYS:HG3	1:M:98:THR:HG23	2.00	0.43
1:N:191:GLY:HA3	2:L:53:TYR:OH	2.19	0.43
2:H:97:VAL:O	2:H:98:GLU:C	2.62	0.43
1:C:138:LEU:O	1:C:311:HIS:HA	2.17	0.43
1:E:77:GLU:HA	1:E:80:ARG:HG2	2.01	0.43
1:J:77:GLU:HA	1:J:80:ARG:HG2	2.01	0.43
1:A:55:ALA:HB1	1:A:132:PHE:CE1	2.53	0.43
1:A:191:GLY:HA3	2:G:53:TYR:OH	2.18	0.43
1:J:38:MET:HE2	1:J:38:MET:C	2.44	0.43
2:B:97:VAL:O	2:B:98:GLU:C	2.62	0.43
1:C:132:PHE:CD1	1:C:132:PHE:C	2.97	0.43
1:I:70:THR:HB	1:J:181:PRO:HG3	2.01	0.43
1:I:79:TYR:HA	1:I:112:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:38:MET:HE2	1:M:38:MET:C	2.44	0.43
2:P:8:ARG:NH2	2:P:17:LEU:O	2.52	0.43
1:E:180:LYS:HB3	1:E:411:ILE:HD13	2.00	0.43
1:I:38:MET:C	1:I:38:MET:HE2	2.44	0.43
1:I:334:THR:CG2	1:I:337:GLY:HA3	2.48	0.43
1:M:138:LEU:O	1:M:311:HIS:HA	2.18	0.43
1:M:358:THR:HG23	1:M:366:LEU:HD13	2.01	0.43
1:M:391:MET:HE2	1:M:428:LEU:HD13	2.01	0.43
1:N:38:MET:C	1:N:38:MET:HE2	2.44	0.43
2:K:8:ARG:NH2	2:K:17:LEU:O	2.52	0.43
1:A:74:THR:HG22	1:C:185:LEU:HD23	2.01	0.42
1:E:62:THR:HA	1:F:182:LYS:CB	2.48	0.42
1:E:191:GLY:HA3	2:K:53:TYR:OH	2.19	0.42
1:F:77:GLU:HA	1:F:80:ARG:HG2	2.01	0.42
1:M:303:SER:OG	1:M:307:ARG:HD2	2.19	0.42
2:L:8:ARG:NH2	2:L:17:LEU:O	2.52	0.42
1:A:263:LYS:HE2	1:A:291:ASN:OD1	2.20	0.42
1:A:386:ILE:HG22	1:A:406:PHE:HE1	1.82	0.42
1:C:56:VAL:CG1	1:C:129:VAL:HG21	2.39	0.42
1:C:454:LYS:HE3	1:C:454:LYS:HB3	1.88	0.42
1:E:303:SER:OG	1:E:307:ARG:HD2	2.19	0.42
1:F:38:MET:C	1:F:38:MET:HE2	2.44	0.42
1:I:338:LYS:O	1:J:132:PHE:HB3	2.19	0.42
1:M:263:LYS:HE2	1:M:291:ASN:OD1	2.19	0.42
2:B:8:ARG:NH2	2:B:17:LEU:O	2.52	0.42
2:H:8:ARG:NH2	2:H:17:LEU:O	2.52	0.42
2:O:8:ARG:NH2	2:O:17:LEU:O	2.52	0.42
1:C:38:MET:HE2	1:C:38:MET:C	2.44	0.42
1:I:16:ILE:HG21	1:I:65:TRP:HB2	2.00	0.42
1:A:38:MET:C	1:A:38:MET:HE2	2.44	0.42
1:C:180:LYS:N	1:C:181:PRO:CD	2.80	0.42
1:E:38:MET:HE2	1:E:38:MET:C	2.44	0.42
1:E:300:ALA:HB1	1:F:128:ASN:N	2.24	0.42
1:F:64:THR:HG22	1:F:65:TRP:O	2.20	0.42
1:F:263:LYS:HE2	1:F:291:ASN:OD1	2.20	0.42
1:J:263:LYS:HE2	1:J:291:ASN:OD1	2.20	0.42
1:J:358:THR:HG23	1:J:366:LEU:HD13	2.02	0.42
1:M:74:THR:HG22	1:N:185:LEU:CD2	2.50	0.42
1:F:191:GLY:HA3	2:D:53:TYR:OH	2.19	0.42
1:I:212:ASN:ND2	4:I:602:HOH:O	2.51	0.42
1:N:180:LYS:N	1:N:181:PRO:CD	2.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:72:ARG:O	2:H:93:SER:OG	2.33	0.42
1:M:132:PHE:H	1:M:133:LYS:HD3	1.84	0.42
2:D:8:ARG:NH2	2:D:17:LEU:O	2.52	0.42
2:L:97:VAL:O	2:L:98:GLU:C	2.62	0.42
1:C:191:GLY:HA3	2:P:53:TYR:OH	2.19	0.42
1:E:185:LEU:HD23	1:F:74:THR:HG22	2.01	0.42
1:I:263:LYS:HE2	1:I:291:ASN:OD1	2.20	0.42
1:M:79:TYR:HA	1:M:112:LEU:HD21	2.01	0.42
1:N:358:THR:HG23	1:N:366:LEU:HD13	2.02	0.42
1:N:386:ILE:HG22	1:N:406:PHE:HE1	1.85	0.42
2:G:8:ARG:NH2	2:G:17:LEU:O	2.52	0.42
1:C:358:THR:HG23	1:C:366:LEU:HD13	2.01	0.42
1:I:180:LYS:N	1:I:181:PRO:CD	2.80	0.42
1:N:64:THR:HG22	1:N:65:TRP:O	2.19	0.42
1:N:263:LYS:HE2	1:N:291:ASN:OD1	2.20	0.42
1:N:451:GLU:O	1:N:454:LYS:HG3	2.20	0.42
2:O:97:VAL:O	2:O:98:GLU:C	2.62	0.42
1:A:451:GLU:O	1:A:454:LYS:HG3	2.20	0.42
1:C:263:LYS:HE2	1:C:291:ASN:OD1	2.20	0.42
1:E:263:LYS:HE2	1:E:291:ASN:OD1	2.20	0.42
1:I:48:GLU:CB	1:I:49:PRO:HD2	2.47	0.42
1:I:335:VAL:HG12	1:I:336:VAL:HG13	2.02	0.42
1:I:358:THR:HG23	1:I:366:LEU:HD13	2.02	0.42
1:J:180:LYS:N	1:J:181:PRO:CD	2.79	0.42
1:N:79:TYR:HA	1:N:112:LEU:HD21	2.02	0.42
1:E:212:ASN:ND2	4:E:602:HOH:O	2.51	0.42
2:G:97:VAL:O	2:G:98:GLU:C	2.62	0.42
1:A:70:THR:OG1	1:C:181:PRO:HD3	2.20	0.41
1:C:180:LYS:O	1:C:182:LYS:HG2	2.19	0.41
1:I:451:GLU:O	1:I:454:LYS:HG3	2.20	0.41
1:M:16:ILE:HG21	1:M:65:TRP:HB2	2.02	0.41
1:I:132:PHE:H	1:I:133:LYS:HD3	1.85	0.41
1:J:72:ARG:O	2:O:93:SER:OG	2.35	0.41
1:J:239:GLU:OE2	2:L:10:THR:OG1	2.31	0.41
1:M:180:LYS:N	1:M:181:PRO:CD	2.80	0.41
1:E:130:PHE:CG	1:F:303:SER:HB3	2.56	0.41
2:D:97:VAL:O	2:D:98:GLU:C	2.62	0.41
1:C:386:ILE:HG22	1:C:406:PHE:HE1	1.84	0.41
1:I:180:LYS:HB3	1:I:411:ILE:HD13	2.00	0.41
1:E:64:THR:HG23	1:E:65:TRP:CD1	2.56	0.41
1:I:186:SER:HA	1:I:217:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:386:ILE:CG2	1:I:406:PHE:CE2	3.03	0.41
1:M:451:GLU:O	1:M:454:LYS:HG3	2.20	0.41
1:A:79:TYR:HA	1:A:112:LEU:HD21	2.02	0.41
1:A:386:ILE:HG23	1:A:394:LEU:HD11	2.01	0.41
1:C:72:ARG:O	2:G:93:SER:OG	2.36	0.41
1:E:132:PHE:H	1:E:133:LYS:HD3	1.85	0.41
1:E:451:GLU:O	1:E:454:LYS:HG3	2.21	0.41
1:M:61:SER:O	1:M:63:ALA:N	2.54	0.41
1:E:48:GLU:CB	1:E:49:PRO:HD2	2.47	0.41
1:F:44:GLN:HG3	1:F:132:PHE:HE1	1.86	0.41
1:F:313:MET:HE3	1:F:313:MET:HB2	1.70	0.41
1:F:386:ILE:HG22	1:F:406:PHE:HE1	1.84	0.41
1:I:196:GLU:OE1	1:I:418:GLN:NE2	2.53	0.41
1:J:44:GLN:HG3	1:J:132:PHE:HE1	1.86	0.41
1:J:299:ARG:NE	1:J:331:HIS:O	2.45	0.41
1:J:386:ILE:HG22	1:J:406:PHE:HE1	1.84	0.41
1:J:451:GLU:O	1:J:454:LYS:HG3	2.20	0.41
1:M:239:GLU:OE2	2:O:10:THR:OG1	2.31	0.41
1:N:196:GLU:OE1	1:N:418:GLN:NE2	2.53	0.41
2:K:97:VAL:O	2:K:98:GLU:C	2.62	0.41
1:C:64:THR:HG22	1:C:65:TRP:O	2.20	0.41
1:C:79:TYR:HA	1:C:112:LEU:HD21	2.03	0.41
1:I:239:GLU:OE2	2:K:10:THR:OG1	2.32	0.41
1:M:212:ASN:ND2	4:M:603:HOH:O	2.51	0.41
1:F:451:GLU:O	1:F:454:LYS:HG3	2.21	0.40
2:G:118:VAL:HB	2:G:130:THR:HB	2.03	0.40
1:I:395:LEU:HD23	1:I:395:LEU:HA	1.88	0.40
1:J:16:ILE:HG13	1:J:65:TRP:CB	2.52	0.40
1:J:64:THR:HG22	1:J:65:TRP:O	2.21	0.40
1:N:468:ASP:OD1	1:N:468:ASP:N	2.54	0.40
2:G:50:ARG:NH2	4:G:202:HOH:O	2.50	0.40
2:K:118:VAL:HB	2:K:130:THR:HB	2.03	0.40
2:H:81:TYR:HB3	2:H:84:HIS:CD2	2.57	0.40
2:P:97:VAL:O	2:P:98:GLU:C	2.62	0.40
1:C:212:ASN:ND2	4:C:604:HOH:O	2.53	0.40
1:N:395:LEU:HD23	1:N:395:LEU:HA	1.88	0.40
2:L:118:VAL:HB	2:L:130:THR:HB	2.04	0.40
1:A:74:THR:HG22	1:C:185:LEU:CD2	2.52	0.40
1:E:386:ILE:HG22	1:E:406:PHE:HE1	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	452/489 (92%)	423 (94%)	22 (5%)	7 (2%)	8	4
1	C	452/489 (92%)	427 (94%)	23 (5%)	2 (0%)	30	31
1	E	452/489 (92%)	423 (94%)	26 (6%)	3 (1%)	18	17
1	F	452/489 (92%)	424 (94%)	25 (6%)	3 (1%)	18	17
1	I	452/489 (92%)	422 (93%)	27 (6%)	3 (1%)	18	17
1	J	452/489 (92%)	425 (94%)	24 (5%)	3 (1%)	18	17
1	M	452/489 (92%)	422 (93%)	26 (6%)	4 (1%)	14	12
1	N	452/489 (92%)	425 (94%)	24 (5%)	3 (1%)	18	17
2	B	143/144 (99%)	137 (96%)	5 (4%)	1 (1%)	18	17
2	D	143/144 (99%)	137 (96%)	5 (4%)	1 (1%)	18	17
2	G	143/144 (99%)	137 (96%)	5 (4%)	1 (1%)	18	17
2	H	143/144 (99%)	137 (96%)	5 (4%)	1 (1%)	18	17
2	K	143/144 (99%)	137 (96%)	5 (4%)	1 (1%)	18	17
2	L	143/144 (99%)	137 (96%)	5 (4%)	1 (1%)	18	17
2	O	143/144 (99%)	137 (96%)	5 (4%)	1 (1%)	18	17
2	P	143/144 (99%)	137 (96%)	5 (4%)	1 (1%)	18	17
All	All	4760/5064 (94%)	4487 (94%)	237 (5%)	36 (1%)	18	14

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	SER
1	C	61	SER
1	F	61	SER
1	J	61	SER
1	M	339	LEU
1	N	61	SER

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Mol	Chain	Res	Type
1	A	132	PHE
1	A	182	LYS
1	C	182	LYS
1	E	182	LYS
1	I	182	LYS
1	M	182	LYS
1	A	63	ALA
1	A	302	ASN
1	A	331	HIS
1	J	182	LYS
1	J	331	HIS
1	N	182	LYS
1	E	331	HIS
1	F	182	LYS
1	F	331	HIS
1	I	331	HIS
1	M	331	HIS
1	N	331	HIS
2	B	122	VAL
2	D	122	VAL
2	G	122	VAL
2	H	122	VAL
2	K	122	VAL
2	L	122	VAL
2	O	122	VAL
2	P	122	VAL
1	A	335	VAL
1	E	335	VAL
1	I	335	VAL
1	M	335	VAL

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	365/395 (92%)	352 (96%)	13 (4%)	31 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	365/395 (92%)	354 (97%)	11 (3%)	36	45
1	E	365/395 (92%)	354 (97%)	11 (3%)	36	45
1	F	365/395 (92%)	355 (97%)	10 (3%)	39	49
1	I	365/395 (92%)	353 (97%)	12 (3%)	33	42
1	J	365/395 (92%)	355 (97%)	10 (3%)	39	49
1	M	365/395 (92%)	353 (97%)	12 (3%)	33	42
1	N	365/395 (92%)	355 (97%)	10 (3%)	39	49
2	B	129/128 (101%)	125 (97%)	4 (3%)	35	44
2	D	129/128 (101%)	124 (96%)	5 (4%)	28	35
2	G	129/128 (101%)	125 (97%)	4 (3%)	35	44
2	H	129/128 (101%)	125 (97%)	4 (3%)	35	44
2	K	129/128 (101%)	124 (96%)	5 (4%)	28	35
2	L	129/128 (101%)	124 (96%)	5 (4%)	28	35
2	O	129/128 (101%)	123 (95%)	6 (5%)	23	26
2	P	129/128 (101%)	124 (96%)	5 (4%)	28	35
All	All	3952/4184 (94%)	3825 (97%)	127 (3%)	35	43

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	THR
1	A	77	GLU
1	A	135	VAL
1	A	302	ASN
1	A	308	GLN
1	A	309	LYS
1	A	331	HIS
1	A	358	THR
1	A	361	SER
1	A	395	LEU
1	A	417	ILE
1	A	418	GLN
1	A	457	THR
1	C	42	THR
1	C	77	GLU
1	C	80	ARG
1	C	129	VAL

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Mol	Chain	Res	Type
1	C	135	VAL
1	C	358	THR
1	C	361	SER
1	C	395	LEU
1	C	417	ILE
1	C	418	GLN
1	C	457	THR
1	E	42	THR
1	E	48	GLU
1	E	80	ARG
1	E	135	VAL
1	E	331	HIS
1	E	358	THR
1	E	361	SER
1	E	395	LEU
1	E	417	ILE
1	E	418	GLN
1	E	457	THR
1	F	19	LYS
1	F	42	THR
1	F	80	ARG
1	F	135	VAL
1	F	358	THR
1	F	361	SER
1	F	395	LEU
1	F	417	ILE
1	F	418	GLN
1	F	457	THR
1	I	42	THR
1	I	48	GLU
1	I	62	THR
1	I	80	ARG
1	I	135	VAL
1	I	339	LEU
1	I	358	THR
1	I	361	SER
1	I	395	LEU
1	I	417	ILE
1	I	418	GLN
1	I	457	THR
1	J	42	THR
1	J	80	ARG

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Mol	Chain	Res	Type
1	J	135	VAL
1	J	358	THR
1	J	361	SER
1	J	395	LEU
1	J	405	GLN
1	J	417	ILE
1	J	418	GLN
1	J	457	THR
1	M	42	THR
1	M	48	GLU
1	M	62	THR
1	M	77	GLU
1	M	80	ARG
1	M	135	VAL
1	M	358	THR
1	M	361	SER
1	M	395	LEU
1	M	417	ILE
1	M	418	GLN
1	M	457	THR
1	N	42	THR
1	N	77	GLU
1	N	80	ARG
1	N	135	VAL
1	N	358	THR
1	N	361	SER
1	N	395	LEU
1	N	417	ILE
1	N	418	GLN
1	N	457	THR
2	B	83	ASN
2	B	132	HIS
2	B	133	SER
2	B	140	GLU
2	D	30	LYS
2	D	83	ASN
2	D	132	HIS
2	D	133	SER
2	D	140	GLU
2	G	83	ASN
2	G	132	HIS
2	G	133	SER

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Mol	Chain	Res	Type
2	G	140	GLU
2	H	83	ASN
2	H	132	HIS
2	H	133	SER
2	H	140	GLU
2	K	65	LYS
2	K	83	ASN
2	K	132	HIS
2	K	133	SER
2	K	140	GLU
2	L	79	LYS
2	L	83	ASN
2	L	132	HIS
2	L	133	SER
2	L	140	GLU
2	O	30	LYS
2	O	65	LYS
2	O	83	ASN
2	O	132	HIS
2	O	133	SER
2	O	140	GLU
2	P	65	LYS
2	P	83	ASN
2	P	132	HIS
2	P	133	SER
2	P	140	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	128	ASN
1	C	100	GLN
1	C	331	HIS
1	F	128	ASN
1	F	189	ASN
1	I	100	GLN
1	I	302	ASN
1	I	308	GLN
1	J	100	GLN
1	J	128	ASN
1	J	310	ASN

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Mol	Chain	Res	Type
1	M	128	ASN
1	M	212	ASN
1	N	189	ASN
1	N	308	GLN
2	B	72	GLN
2	B	75	ASN
2	D	75	ASN
2	G	72	GLN
2	G	75	ASN
2	G	83	ASN
2	H	75	ASN
2	H	84	HIS
2	K	75	ASN
2	L	75	ASN
2	O	75	ASN
2	P	72	GLN
2	P	75	ASN

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](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

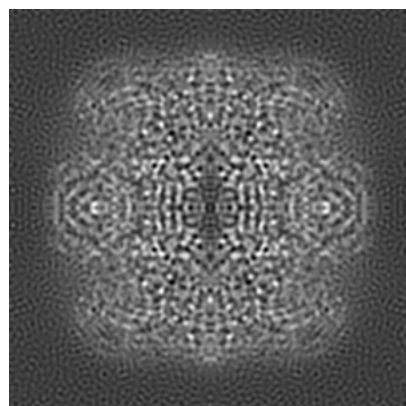
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-80105. These allow visual inspection of the internal detail of the map and identification of artifacts.

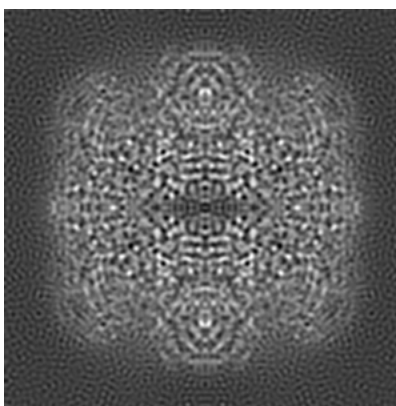
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

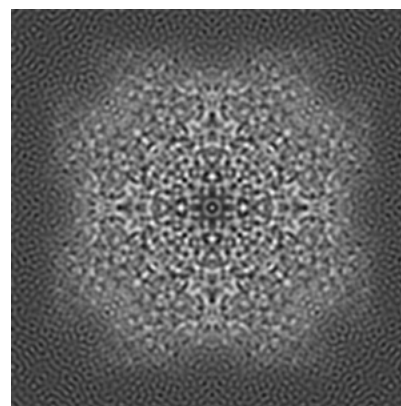
6.1.1 Primary map



X

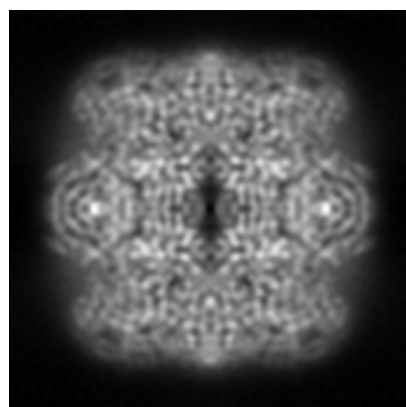


Y

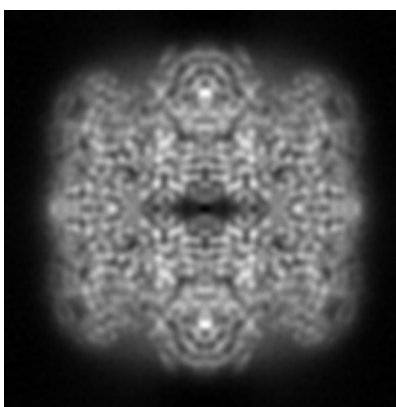


Z

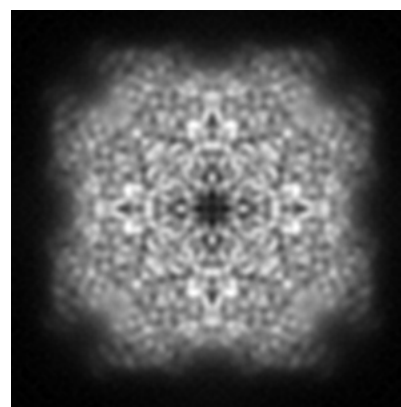
6.1.2 Raw map



X



Y

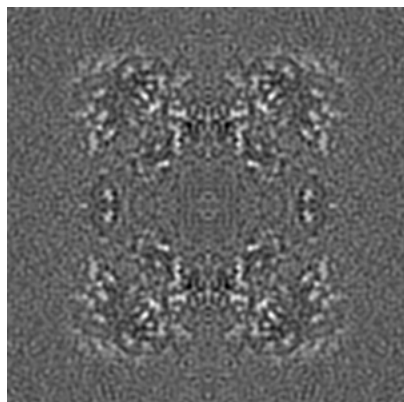


Z

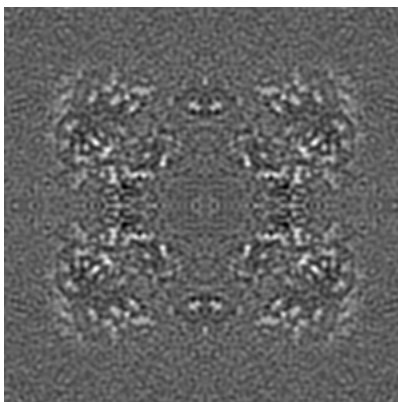
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

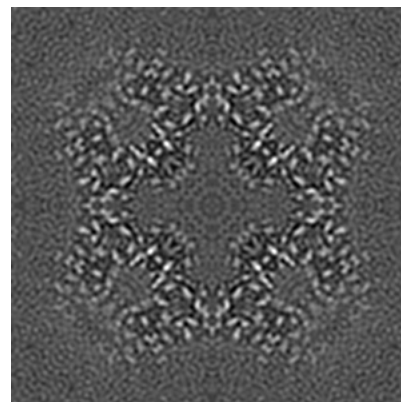
6.2.1 Primary map



X Index: 79

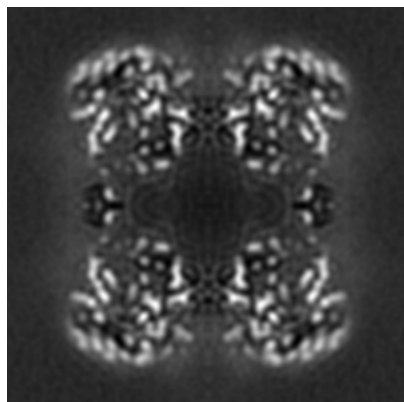


Y Index: 79

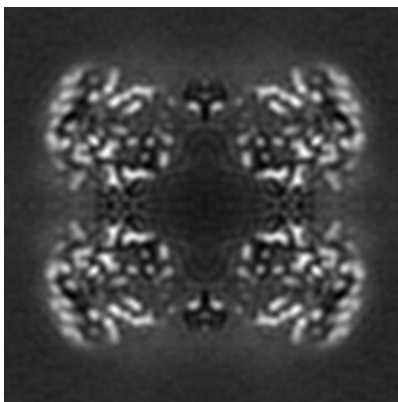


Z Index: 79

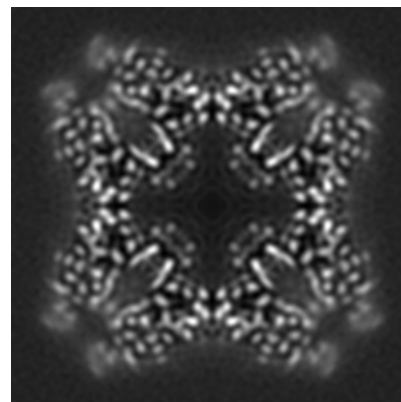
6.2.2 Raw map



X Index: 79



Y Index: 79

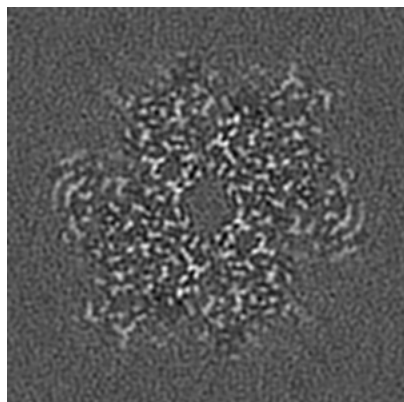


Z Index: 79

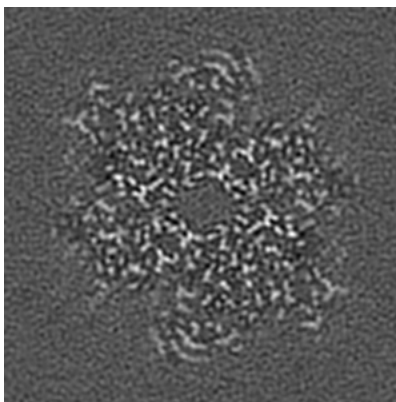
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

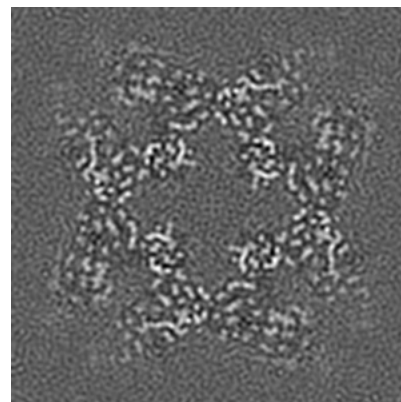
6.3.1 Primary map



X Index: 99

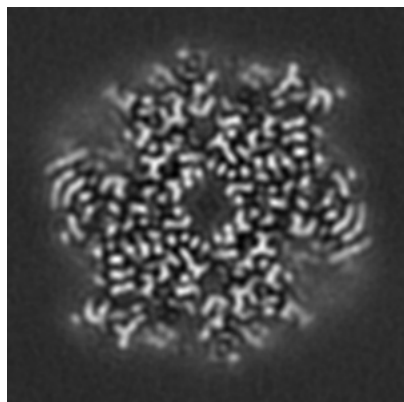


Y Index: 99

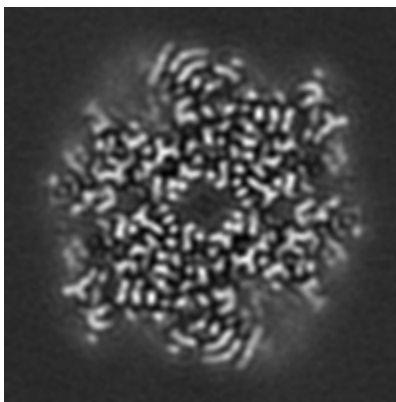


Z Index: 81

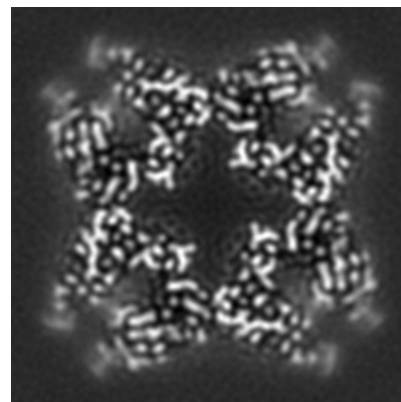
6.3.2 Raw map



X Index: 99



Y Index: 59

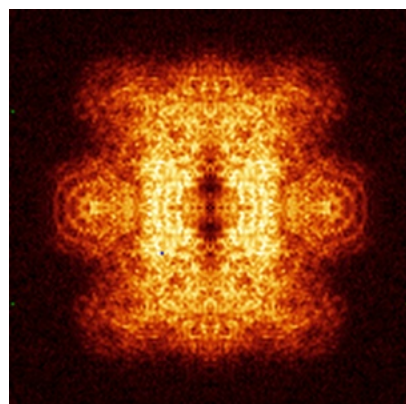


Z Index: 77

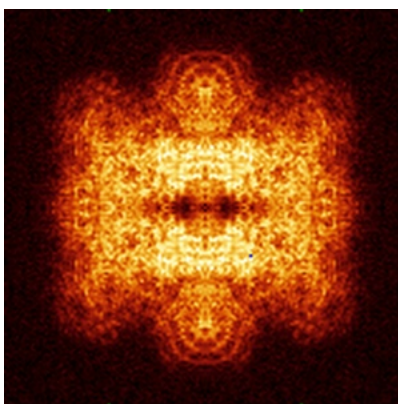
The images above show the largest variance slices of the map in three orthogonal directions.

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

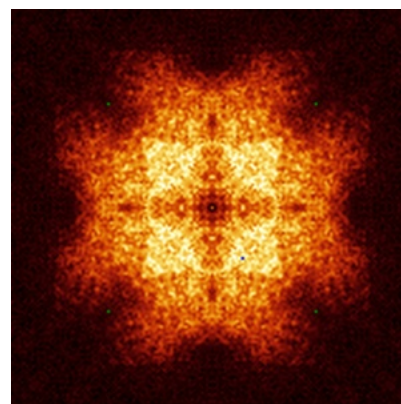
6.4.1 Primary map



X

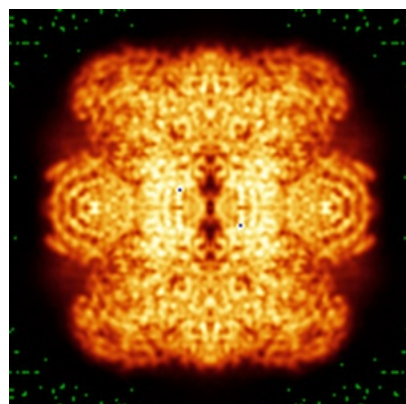


Y

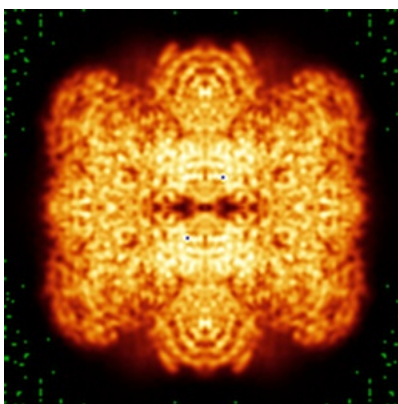


Z

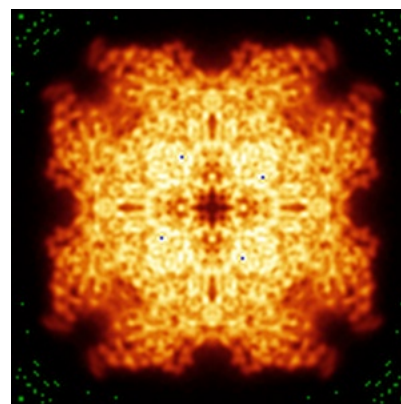
6.4.2 Raw map



X



Y

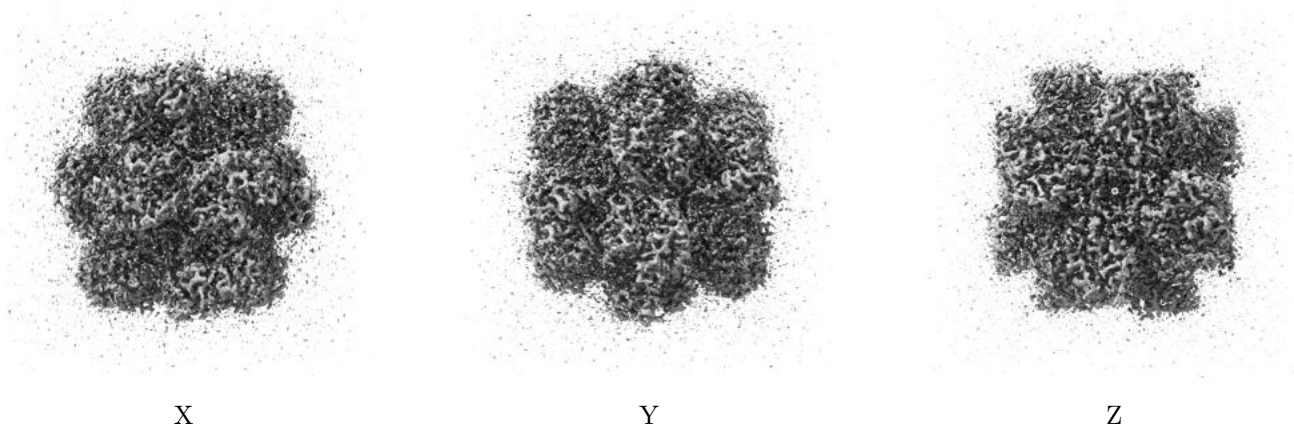


Z

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

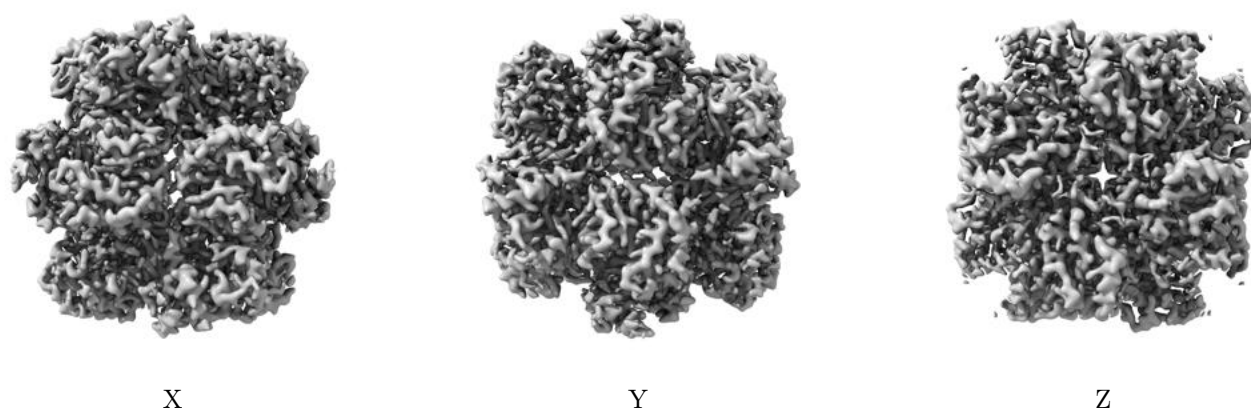
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

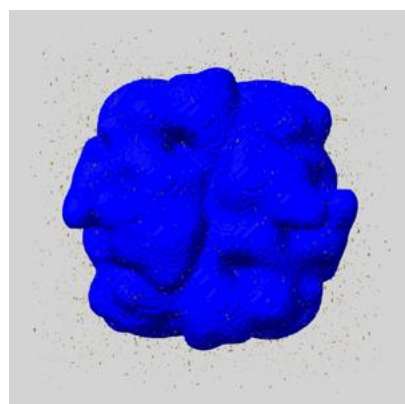
6.6 Mask visualisation [i](#)

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

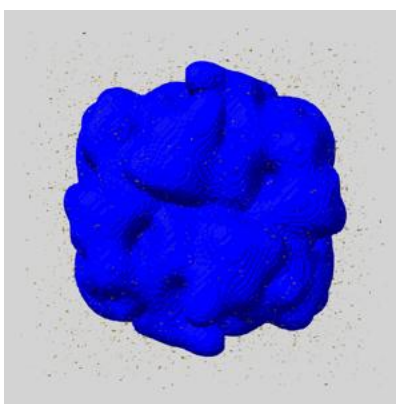
A mask typically either:

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

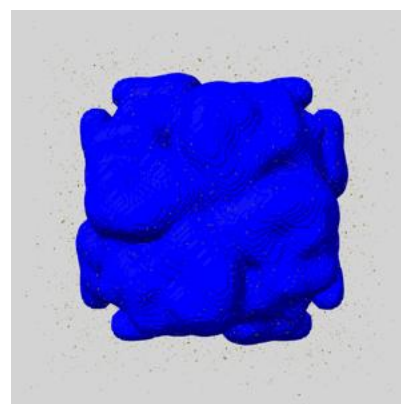
6.6.1 emd_80105_msk_1.map [i](#)



X



Y

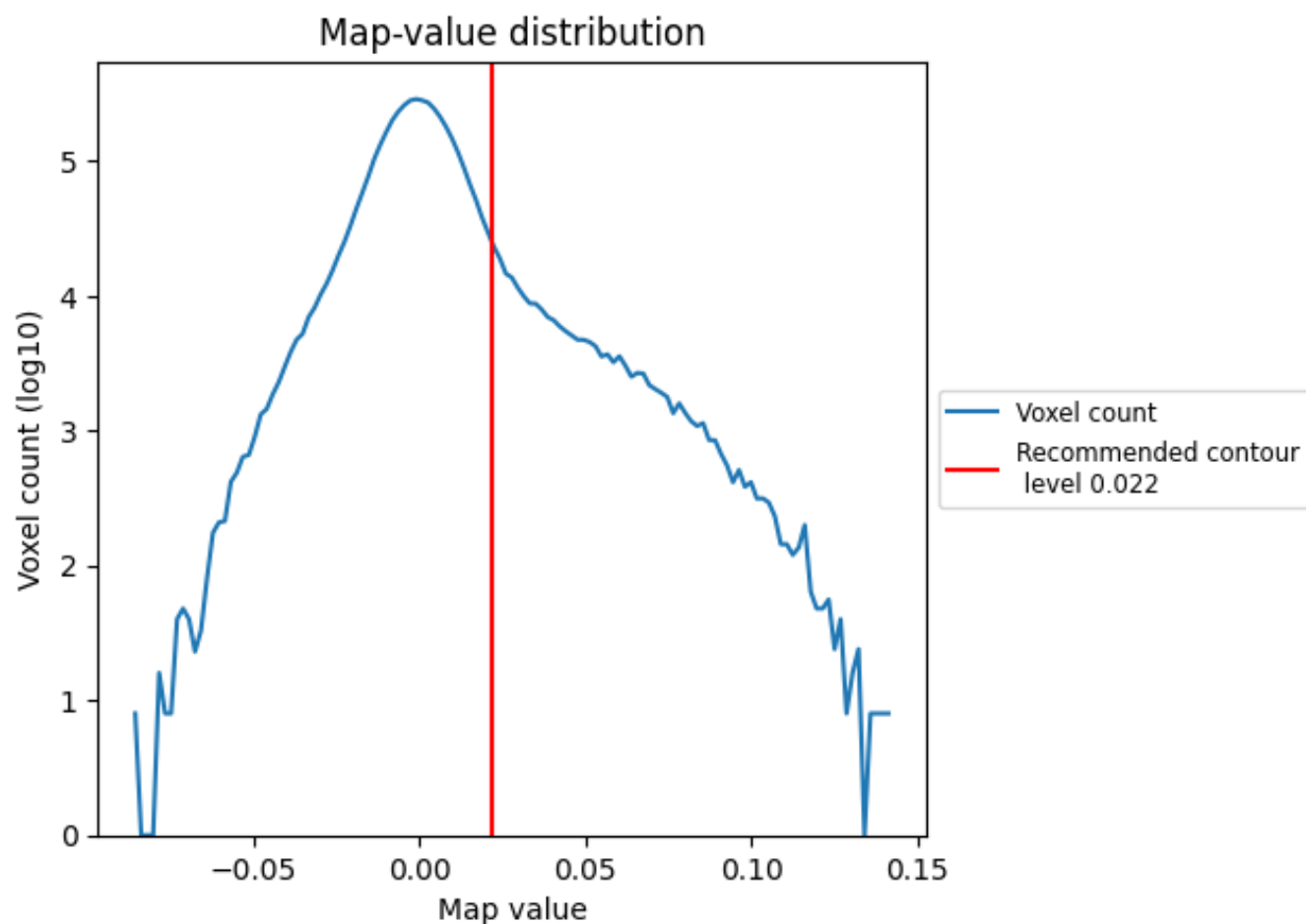


Z

7 Map analysis [i](#)

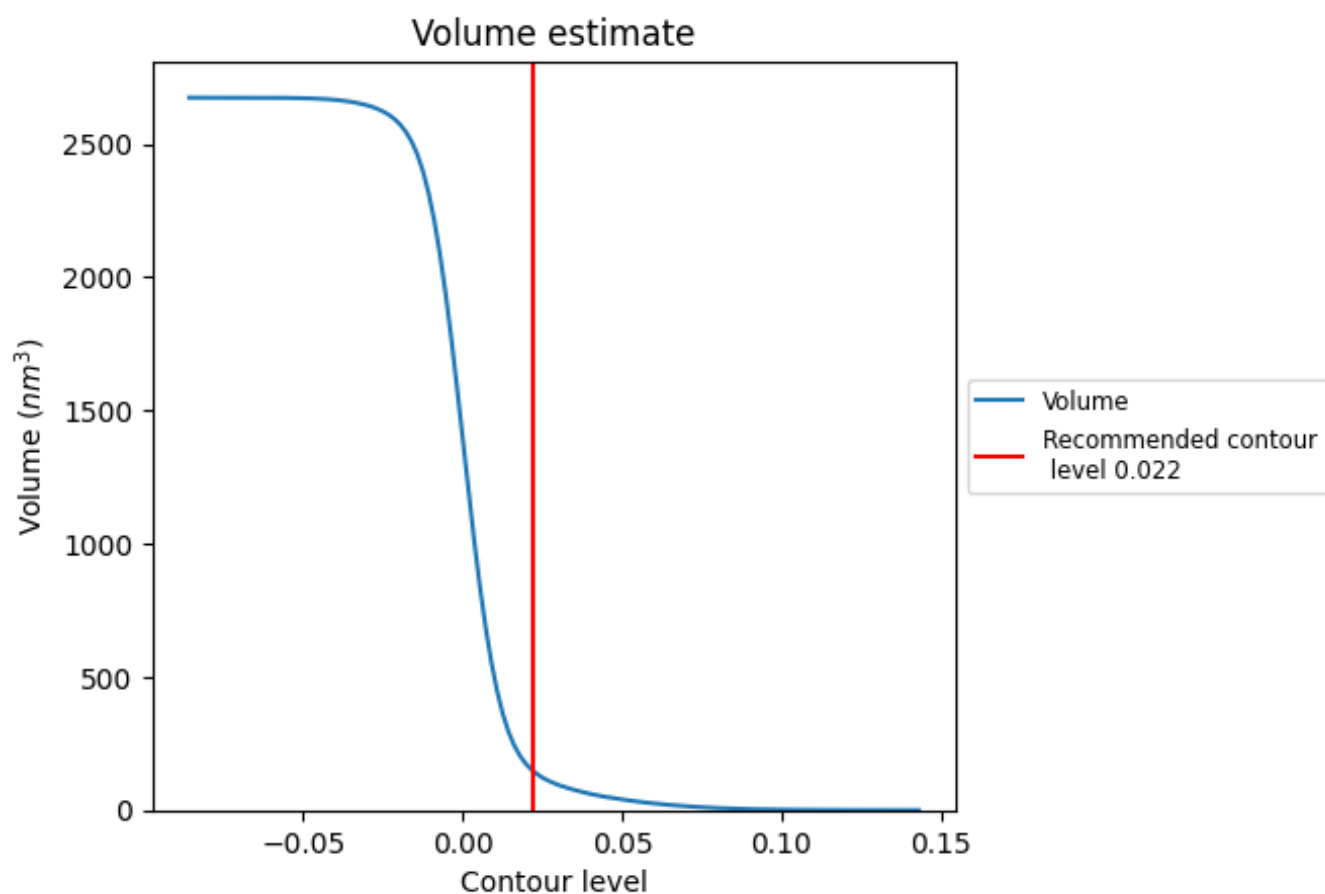
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

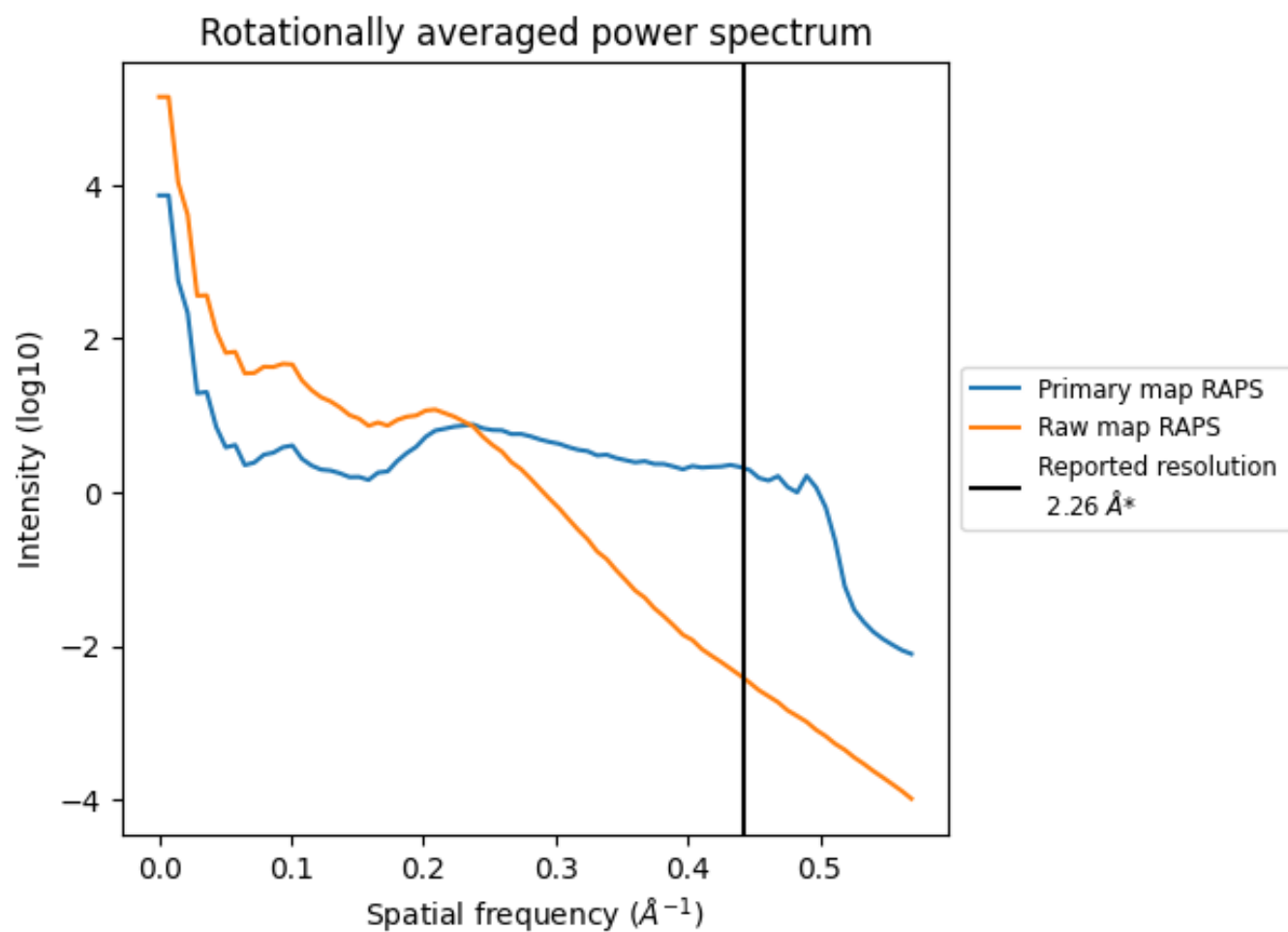
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 148 nm^3 ; this corresponds to an approximate mass of 134 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 ⓘ

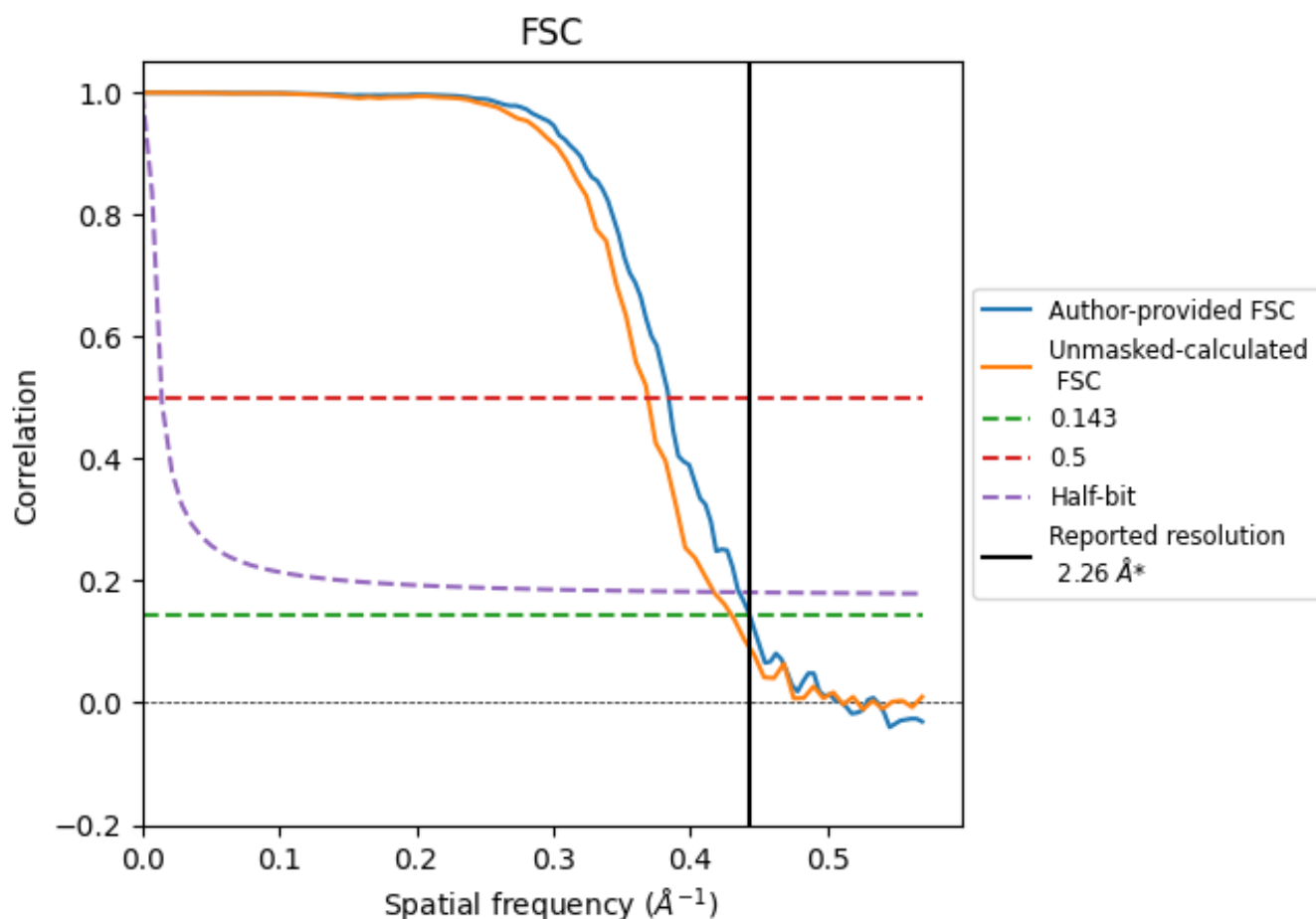


*Reported resolution corresponds to spatial frequency of 0.442 Å⁻¹

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 0.442 \AA^{-1}

8.2 Resolution estimates [i](#)

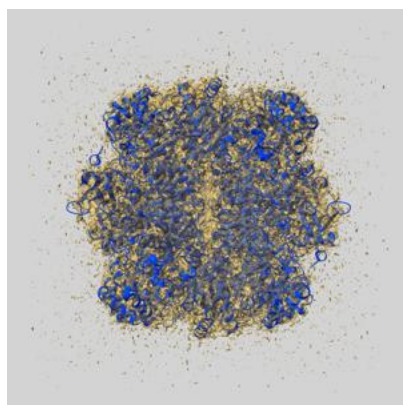
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.26	-	-
Author-provided FSC curve	2.26	2.60	2.29
Unmasked-calculated*	2.32	2.71	2.40

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

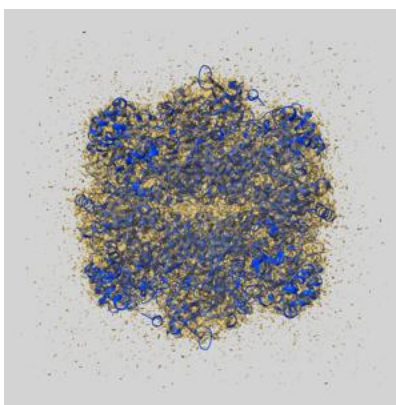
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-80105 and PDB model 25HN. Per-residue inclusion information can be found in section [3](#) on page [7](#).

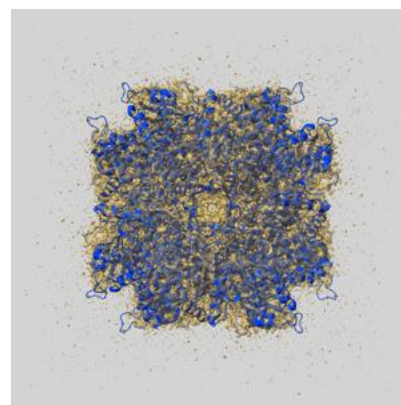
9.1 Map-model overlay [i](#)



X



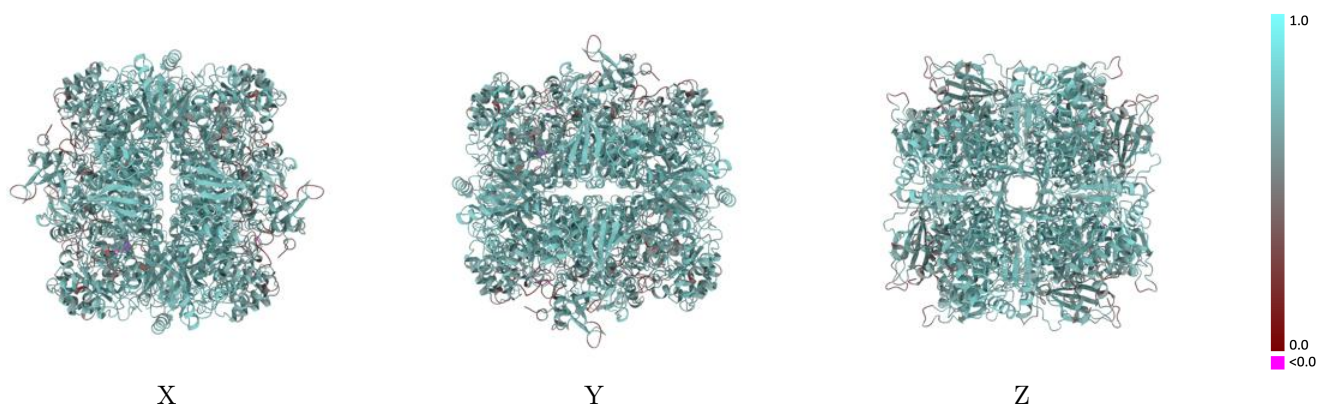
Y



Z

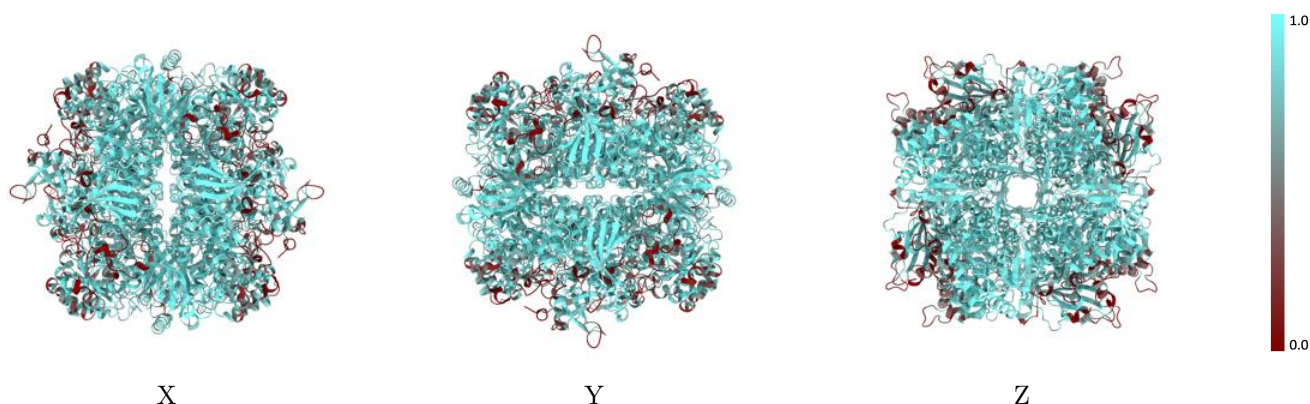
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



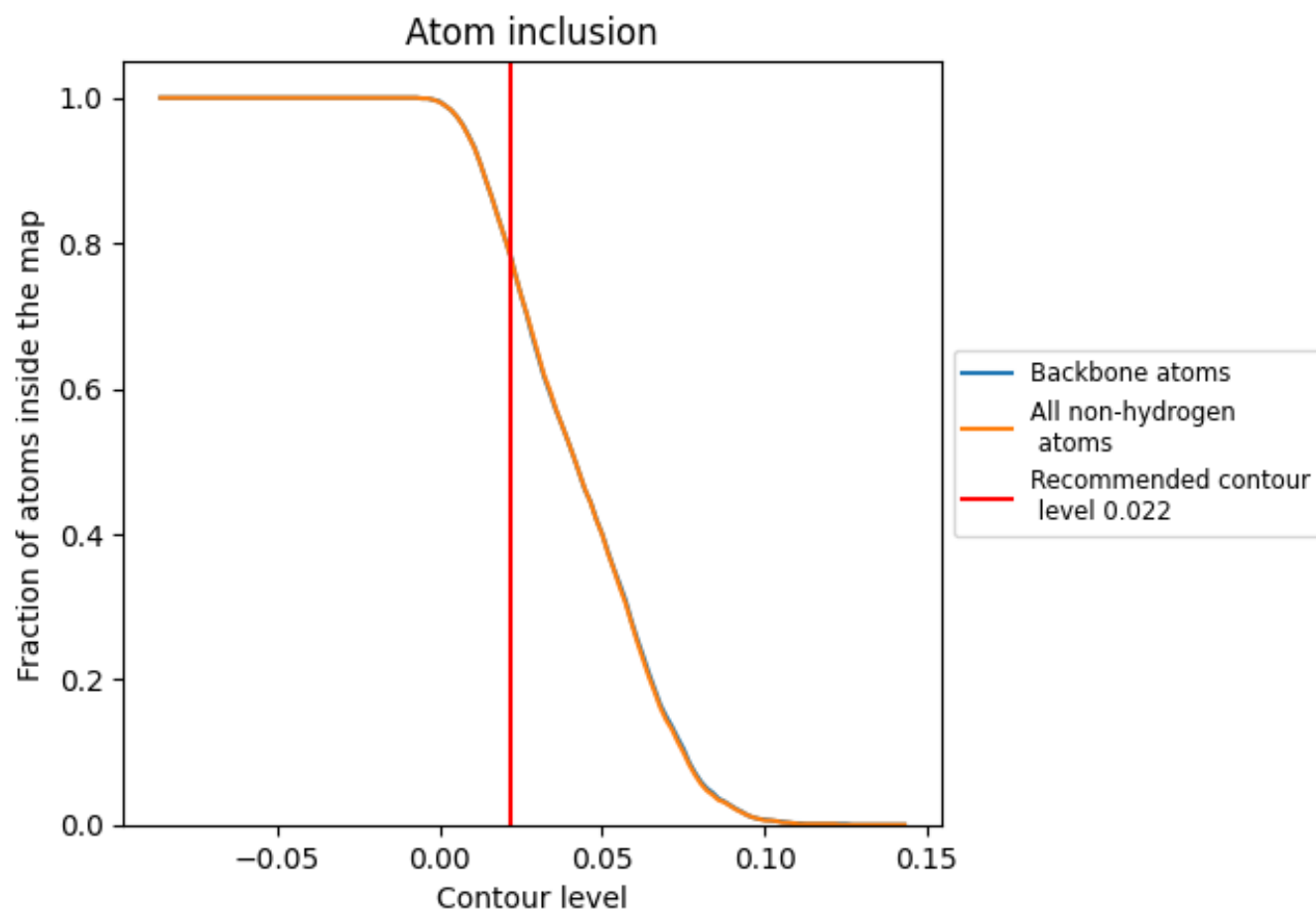
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.7800</div>	<div><div></div>0.6810</div>
A	<div><div></div>0.7510</div>	<div><div></div>0.6700</div>
B	<div><div></div>0.8660</div>	<div><div></div>0.7100</div>
C	<div><div></div>0.7500</div>	<div><div></div>0.6720</div>
D	<div><div></div>0.8660</div>	<div><div></div>0.7110</div>
E	<div><div></div>0.7490</div>	<div><div></div>0.6680</div>
F	<div><div></div>0.7530</div>	<div><div></div>0.6730</div>
G	<div><div></div>0.8660</div>	<div><div></div>0.7090</div>
H	<div><div></div>0.8660</div>	<div><div></div>0.7090</div>
I	<div><div></div>0.7530</div>	<div><div></div>0.6710</div>
J	<div><div></div>0.7520</div>	<div><div></div>0.6730</div>
K	<div><div></div>0.8660</div>	<div><div></div>0.7090</div>
L	<div><div></div>0.8680</div>	<div><div></div>0.7100</div>
M	<div><div></div>0.7510</div>	<div><div></div>0.6690</div>
N	<div><div></div>0.7540</div>	<div><div></div>0.6730</div>
O	<div><div></div>0.8660</div>	<div><div></div>0.7110</div>
P	<div><div></div>0.8660</div>	<div><div></div>0.7100</div>

1.0

0.0

<0.0