



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:06 AM UTC

PDB ID : 8IO2 / pdb_00008io2
EMDB ID : EMD-35605
Title : The Rubisco assembly intermidate of Arabidopsis thaliana Rubisco accumulation factor 1 (AtRaf1) and Rubisco large subunit (RbcL)
Authors : Wang, R.; Song, H.; Zhang, W.; Wang, N.; Zhang, S.; Shao, R.
Deposited on : 2023-03-10
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

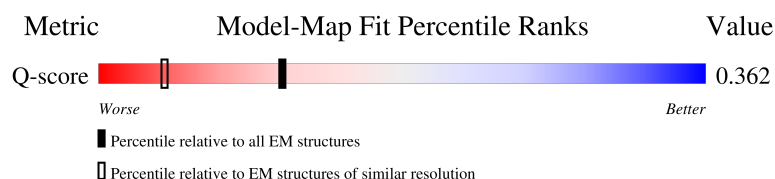
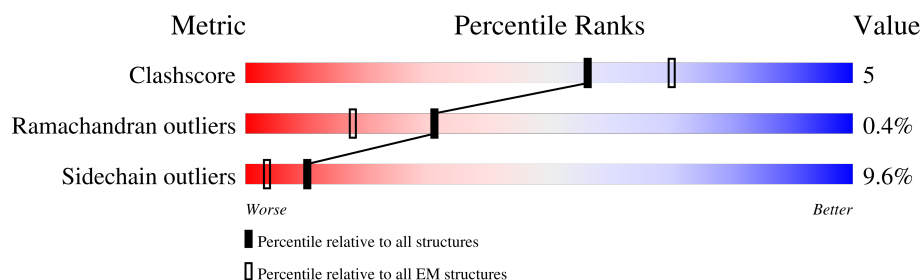
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



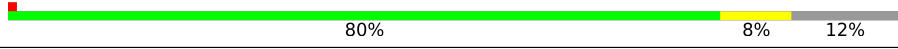
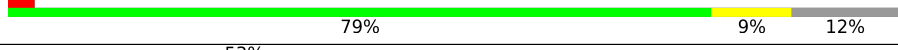
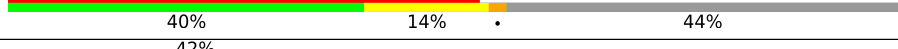
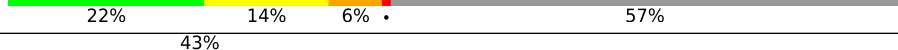
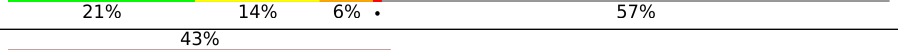
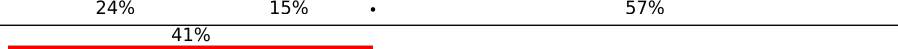
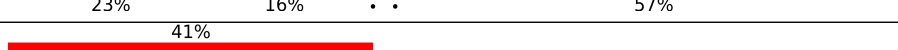
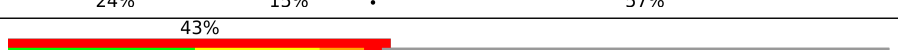
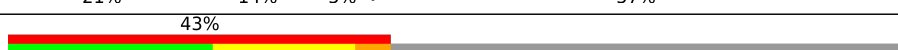
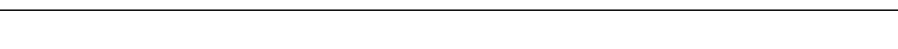
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	A	471	
1	B	471	
1	C	471	
1	D	471	

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Mol	Chain	Length	Quality of chain
1	E	471	
1	F	471	
1	G	471	
1	H	471	
2	I	346	
2	J	346	
2	K	346	
2	L	346	
2	M	346	
2	N	346	
2	O	346	
2	P	346	
2	Q	346	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 36624 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	415	Total	C	N	O	S	0	0
			3250	2065	574	594	17		
1	B	418	Total	C	N	O	S	0	0
			3265	2071	580	598	16		
1	C	416	Total	C	N	O	S	0	0
			3253	2063	578	596	16		
1	D	416	Total	C	N	O	S	0	0
			3262	2070	579	596	17		
1	E	415	Total	C	N	O	S	0	0
			3250	2065	574	594	17		
1	F	418	Total	C	N	O	S	0	0
			3265	2071	580	598	16		
1	G	416	Total	C	N	O	S	0	0
			3253	2063	578	596	16		
1	H	416	Total	C	N	O	S	0	0
			3262	2070	579	596	17		

- Molecule 2 is a protein called Rubisco accumulation factor 1.2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	195	Total	C	N	O	S	0	0
			1536	967	264	302	3		
2	J	149	Total	C	N	O	S	0	0
			1133	730	192	208	3		
2	K	149	Total	C	N	O	S	0	0
			1133	730	192	208	3		
2	L	149	Total	C	N	O	S	0	0
			1133	730	192	208	3		
2	M	150	Total	C	N	O	S	0	0
			1124	723	193	205	3		
2	N	150	Total	C	N	O	S	0	0
			1124	723	193	205	3		
2	O	150	Total	C	N	O	S	0	0
			1124	723	193	205	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	149	Total	C	N	O	S	0	0
			1133	730	192	208	3		
2	Q	150	Total	C	N	O	S	0	0
			1124	723	193	205	3		

There are 171 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	?	-	LYS	deletion	UNP Q9SR19
I	?	-	GLU	deletion	UNP Q9SR19
I	?	-	ALA	deletion	UNP Q9SR19
I	?	-	GLU	deletion	UNP Q9SR19
I	?	-	LYS	deletion	UNP Q9SR19
I	?	-	GLU	deletion	UNP Q9SR19
I	?	-	LYS	deletion	UNP Q9SR19
I	?	-	GLU	deletion	UNP Q9SR19
I	?	-	LYS	deletion	UNP Q9SR19
I	?	-	LYS	deletion	UNP Q9SR19
I	?	-	LYS	deletion	UNP Q9SR19
I	?	-	LYS	deletion	UNP Q9SR19
I	?	-	GLU	deletion	UNP Q9SR19
I	?	-	GLU	deletion	UNP Q9SR19
I	?	-	GLU	deletion	UNP Q9SR19
I	?	-	VAL	deletion	UNP Q9SR19
I	?	-	LYS	deletion	UNP Q9SR19
I	?	-	ALA	deletion	UNP Q9SR19
I	?	-	ILE	deletion	UNP Q9SR19
J	?	-	LYS	deletion	UNP Q9SR19
J	?	-	GLU	deletion	UNP Q9SR19
J	?	-	ALA	deletion	UNP Q9SR19
J	?	-	GLU	deletion	UNP Q9SR19
J	?	-	LYS	deletion	UNP Q9SR19
J	?	-	GLU	deletion	UNP Q9SR19
J	?	-	LYS	deletion	UNP Q9SR19
J	?	-	GLU	deletion	UNP Q9SR19
J	?	-	LYS	deletion	UNP Q9SR19
J	?	-	LYS	deletion	UNP Q9SR19
J	?	-	LYS	deletion	UNP Q9SR19
J	?	-	GLU	deletion	UNP Q9SR19
J	?	-	GLU	deletion	UNP Q9SR19
J	?	-	GLU	deletion	UNP Q9SR19

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Chain	Residue	Modelled	Actual	Comment	Reference
J	?	-	VAL	deletion	UNP Q9SR19
J	?	-	LYS	deletion	UNP Q9SR19
J	?	-	ALA	deletion	UNP Q9SR19
J	?	-	ILE	deletion	UNP Q9SR19
K	?	-	LYS	deletion	UNP Q9SR19
K	?	-	GLU	deletion	UNP Q9SR19
K	?	-	ALA	deletion	UNP Q9SR19
K	?	-	GLU	deletion	UNP Q9SR19
K	?	-	LYS	deletion	UNP Q9SR19
K	?	-	GLU	deletion	UNP Q9SR19
K	?	-	LYS	deletion	UNP Q9SR19
K	?	-	GLU	deletion	UNP Q9SR19
K	?	-	LYS	deletion	UNP Q9SR19
K	?	-	LYS	deletion	UNP Q9SR19
K	?	-	LYS	deletion	UNP Q9SR19
K	?	-	LYS	deletion	UNP Q9SR19
K	?	-	GLU	deletion	UNP Q9SR19
K	?	-	GLU	deletion	UNP Q9SR19
K	?	-	GLU	deletion	UNP Q9SR19
K	?	-	VAL	deletion	UNP Q9SR19
K	?	-	LYS	deletion	UNP Q9SR19
K	?	-	ALA	deletion	UNP Q9SR19
K	?	-	ILE	deletion	UNP Q9SR19
L	?	-	LYS	deletion	UNP Q9SR19
L	?	-	GLU	deletion	UNP Q9SR19
L	?	-	ALA	deletion	UNP Q9SR19
L	?	-	GLU	deletion	UNP Q9SR19
L	?	-	LYS	deletion	UNP Q9SR19
L	?	-	GLU	deletion	UNP Q9SR19
L	?	-	LYS	deletion	UNP Q9SR19
L	?	-	GLU	deletion	UNP Q9SR19
L	?	-	LYS	deletion	UNP Q9SR19
L	?	-	LYS	deletion	UNP Q9SR19
L	?	-	LYS	deletion	UNP Q9SR19
L	?	-	GLU	deletion	UNP Q9SR19
L	?	-	GLU	deletion	UNP Q9SR19
L	?	-	GLU	deletion	UNP Q9SR19
L	?	-	VAL	deletion	UNP Q9SR19
L	?	-	LYS	deletion	UNP Q9SR19
L	?	-	ALA	deletion	UNP Q9SR19
L	?	-	ILE	deletion	UNP Q9SR19

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Chain	Residue	Modelled	Actual	Comment	Reference
M	?	-	LYS	deletion	UNP Q9SR19
M	?	-	GLU	deletion	UNP Q9SR19
M	?	-	ALA	deletion	UNP Q9SR19
M	?	-	GLU	deletion	UNP Q9SR19
M	?	-	LYS	deletion	UNP Q9SR19
M	?	-	GLU	deletion	UNP Q9SR19
M	?	-	LYS	deletion	UNP Q9SR19
M	?	-	GLU	deletion	UNP Q9SR19
M	?	-	LYS	deletion	UNP Q9SR19
M	?	-	LYS	deletion	UNP Q9SR19
M	?	-	LYS	deletion	UNP Q9SR19
M	?	-	LYS	deletion	UNP Q9SR19
M	?	-	GLU	deletion	UNP Q9SR19
M	?	-	GLU	deletion	UNP Q9SR19
M	?	-	GLU	deletion	UNP Q9SR19
M	?	-	VAL	deletion	UNP Q9SR19
M	?	-	LYS	deletion	UNP Q9SR19
M	?	-	ALA	deletion	UNP Q9SR19
M	?	-	ILE	deletion	UNP Q9SR19
N	?	-	LYS	deletion	UNP Q9SR19
N	?	-	GLU	deletion	UNP Q9SR19
N	?	-	ALA	deletion	UNP Q9SR19
N	?	-	GLU	deletion	UNP Q9SR19
N	?	-	LYS	deletion	UNP Q9SR19
N	?	-	GLU	deletion	UNP Q9SR19
N	?	-	LYS	deletion	UNP Q9SR19
N	?	-	GLU	deletion	UNP Q9SR19
N	?	-	LYS	deletion	UNP Q9SR19
N	?	-	LYS	deletion	UNP Q9SR19
N	?	-	LYS	deletion	UNP Q9SR19
N	?	-	LYS	deletion	UNP Q9SR19
N	?	-	GLU	deletion	UNP Q9SR19
N	?	-	GLU	deletion	UNP Q9SR19
N	?	-	GLU	deletion	UNP Q9SR19
N	?	-	VAL	deletion	UNP Q9SR19
N	?	-	LYS	deletion	UNP Q9SR19
N	?	-	ALA	deletion	UNP Q9SR19
N	?	-	ILE	deletion	UNP Q9SR19
O	?	-	LYS	deletion	UNP Q9SR19
O	?	-	GLU	deletion	UNP Q9SR19
O	?	-	ALA	deletion	UNP Q9SR19
O	?	-	GLU	deletion	UNP Q9SR19

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Chain	Residue	Modelled	Actual	Comment	Reference
O	?	-	LYS	deletion	UNP Q9SR19
O	?	-	GLU	deletion	UNP Q9SR19
O	?	-	LYS	deletion	UNP Q9SR19
O	?	-	GLU	deletion	UNP Q9SR19
O	?	-	LYS	deletion	UNP Q9SR19
O	?	-	LYS	deletion	UNP Q9SR19
O	?	-	LYS	deletion	UNP Q9SR19
O	?	-	LYS	deletion	UNP Q9SR19
O	?	-	GLU	deletion	UNP Q9SR19
O	?	-	GLU	deletion	UNP Q9SR19
O	?	-	GLU	deletion	UNP Q9SR19
O	?	-	VAL	deletion	UNP Q9SR19
O	?	-	LYS	deletion	UNP Q9SR19
O	?	-	ALA	deletion	UNP Q9SR19
O	?	-	ILE	deletion	UNP Q9SR19
P	?	-	LYS	deletion	UNP Q9SR19
P	?	-	GLU	deletion	UNP Q9SR19
P	?	-	ALA	deletion	UNP Q9SR19
P	?	-	GLU	deletion	UNP Q9SR19
P	?	-	LYS	deletion	UNP Q9SR19
P	?	-	GLU	deletion	UNP Q9SR19
P	?	-	LYS	deletion	UNP Q9SR19
P	?	-	GLU	deletion	UNP Q9SR19
P	?	-	LYS	deletion	UNP Q9SR19
P	?	-	LYS	deletion	UNP Q9SR19
P	?	-	LYS	deletion	UNP Q9SR19
P	?	-	GLU	deletion	UNP Q9SR19
P	?	-	GLU	deletion	UNP Q9SR19
P	?	-	GLU	deletion	UNP Q9SR19
P	?	-	VAL	deletion	UNP Q9SR19
P	?	-	LYS	deletion	UNP Q9SR19
P	?	-	ALA	deletion	UNP Q9SR19
P	?	-	ILE	deletion	UNP Q9SR19
Q	?	-	LYS	deletion	UNP Q9SR19
Q	?	-	GLU	deletion	UNP Q9SR19
Q	?	-	ALA	deletion	UNP Q9SR19
Q	?	-	GLU	deletion	UNP Q9SR19
Q	?	-	LYS	deletion	UNP Q9SR19
Q	?	-	GLU	deletion	UNP Q9SR19
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Q	?	-	GLU	deletion	UNP Q9SR19

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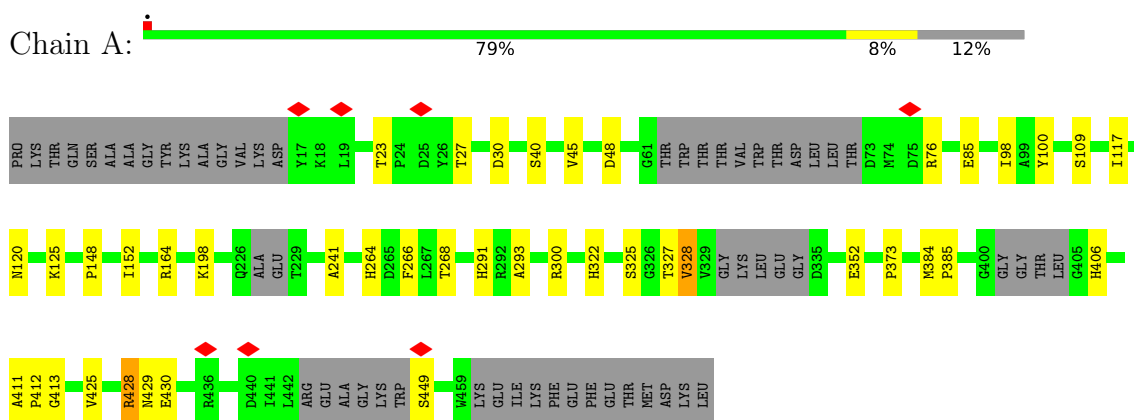
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Chain	Residue	Modelled	Actual	Comment	Reference
Q	?	-	LYS	deletion	UNP Q9SR19
Q	?	-	LYS	deletion	UNP Q9SR19
Q	?	-	LYS	deletion	UNP Q9SR19
Q	?	-	LYS	deletion	UNP Q9SR19
Q	?	-	GLU	deletion	UNP Q9SR19
Q	?	-	GLU	deletion	UNP Q9SR19
Q	?	-	GLU	deletion	UNP Q9SR19
Q	?	-	VAL	deletion	UNP Q9SR19
Q	?	-	LYS	deletion	UNP Q9SR19
Q	?	-	ALA	deletion	UNP Q9SR19
Q	?	-	ILE	deletion	UNP Q9SR19

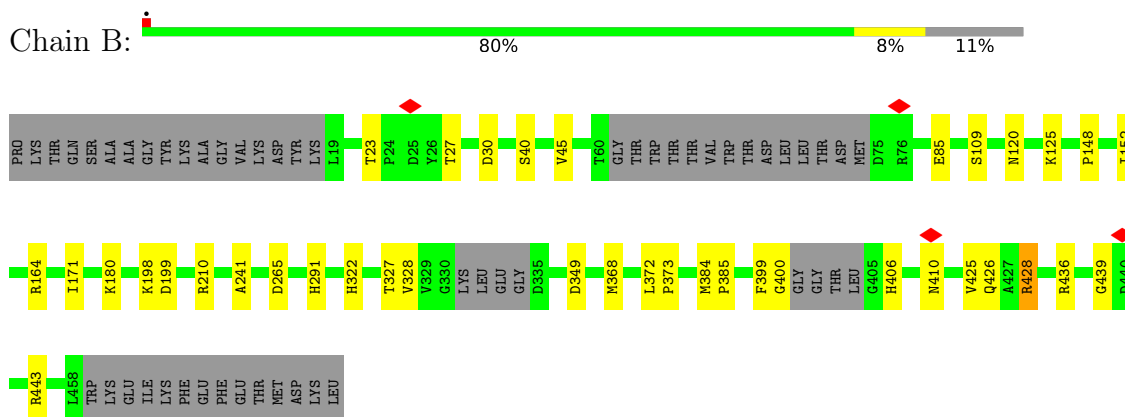
3 Residue-property plots

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.

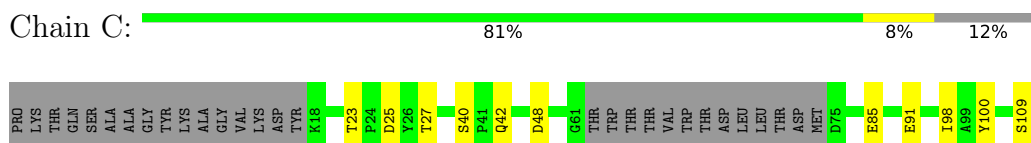
- Molecule 1: Ribulose biphosphate carboxylase large chain

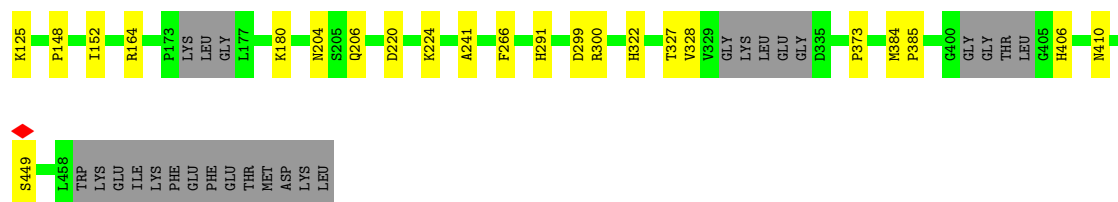


- Molecule 1: Ribulose biphosphate carboxylase large chain



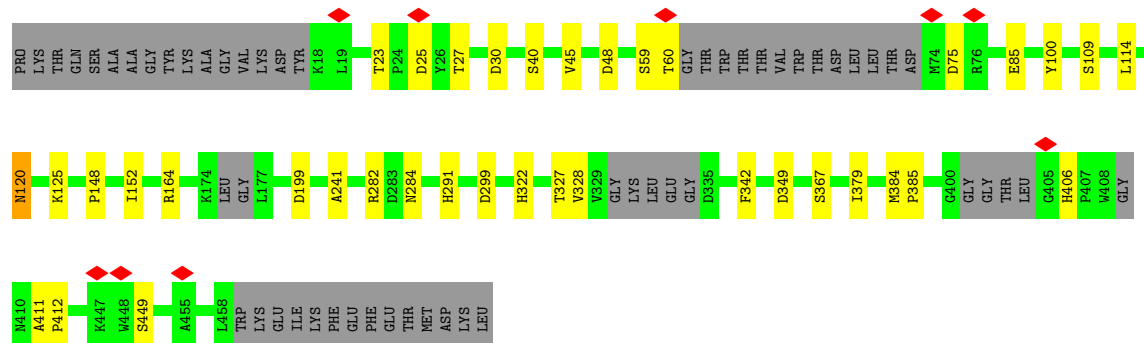
- Molecule 1: Ribulose biphosphate carboxylase large chain





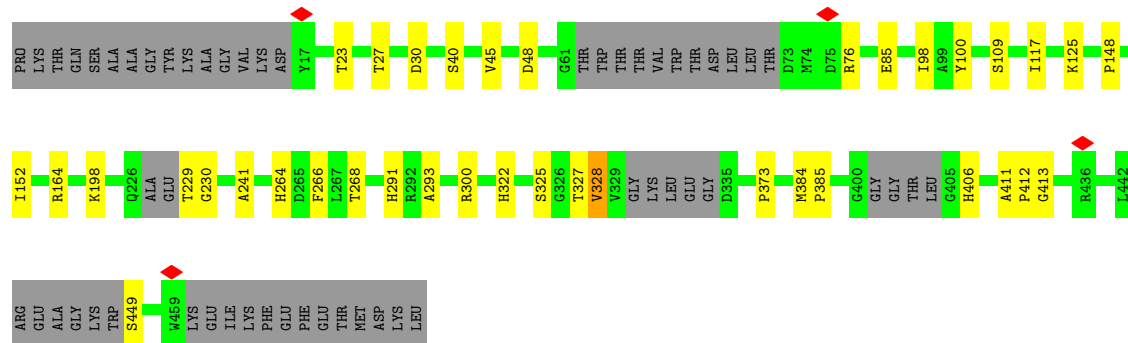
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain D: 80% 8% 12%



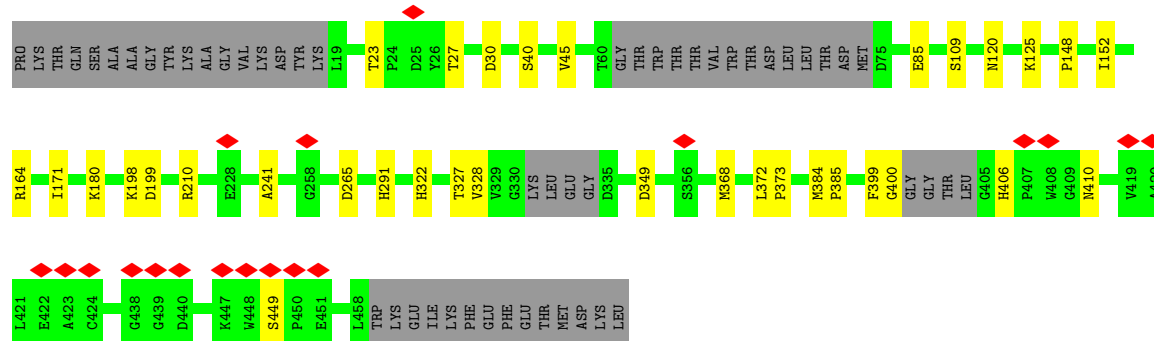
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain E: 80% 8% 12%

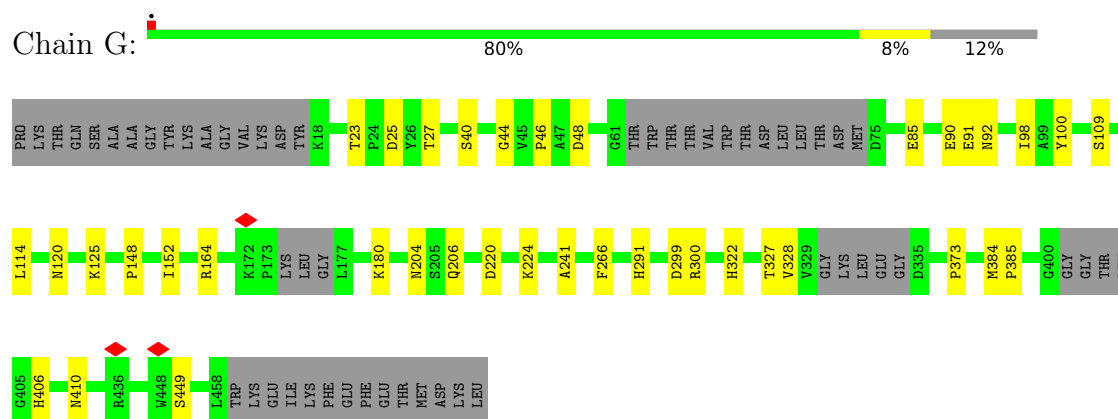


- Molecule 1: Ribulose biphosphate carboxylase large chain

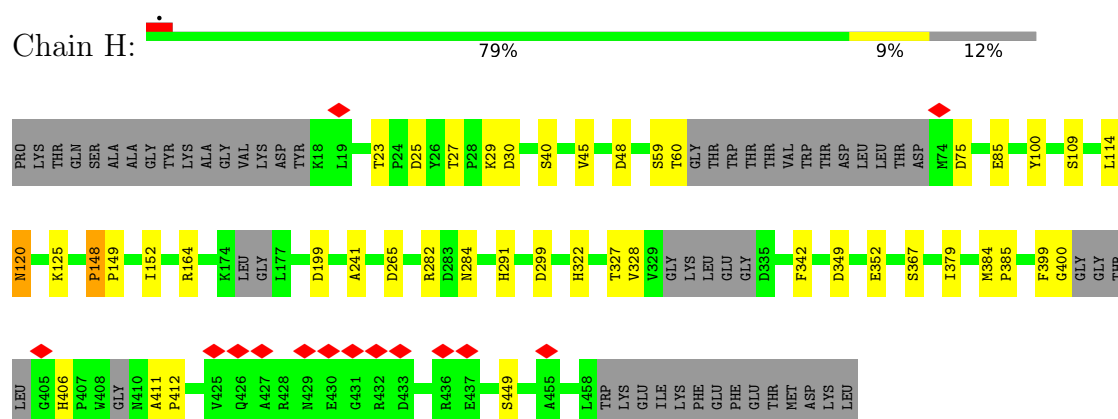
Chain F: 82% 7% 11%



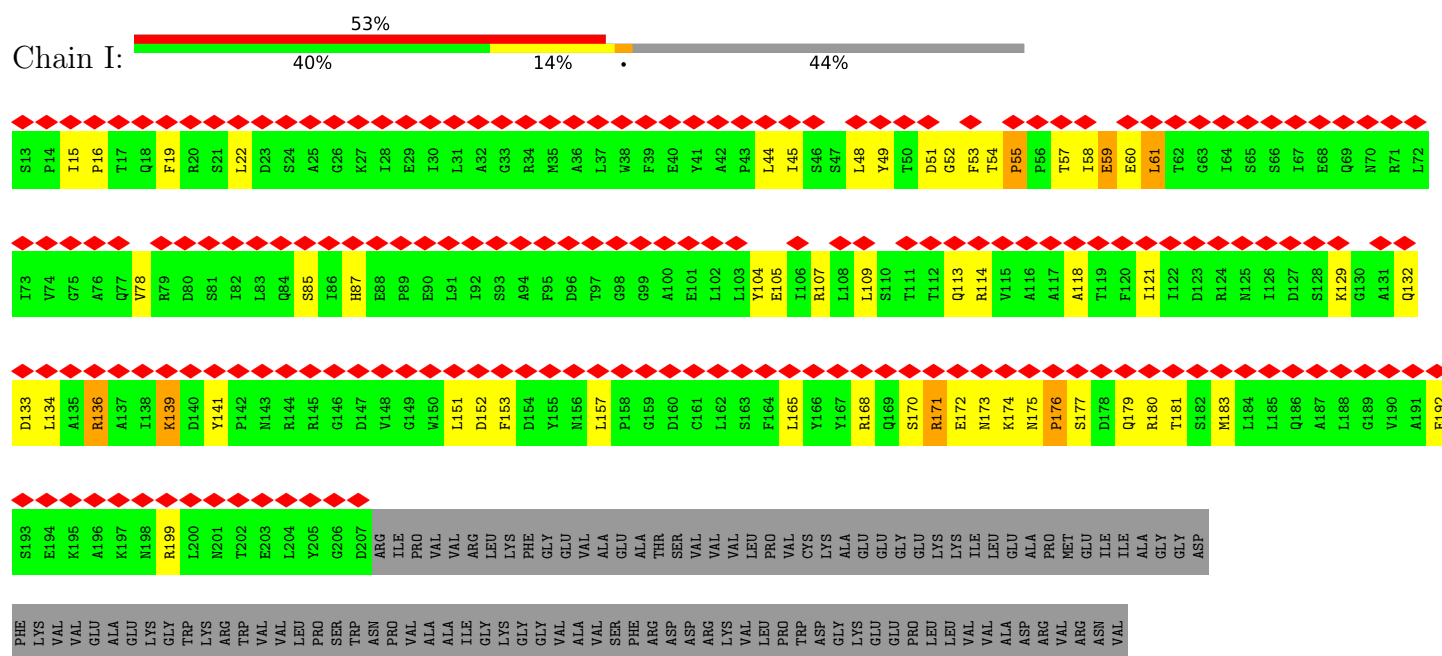
- Molecule 1: Ribulose biphosphate carboxylase large chain

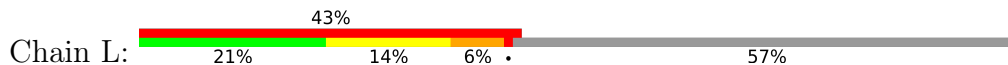


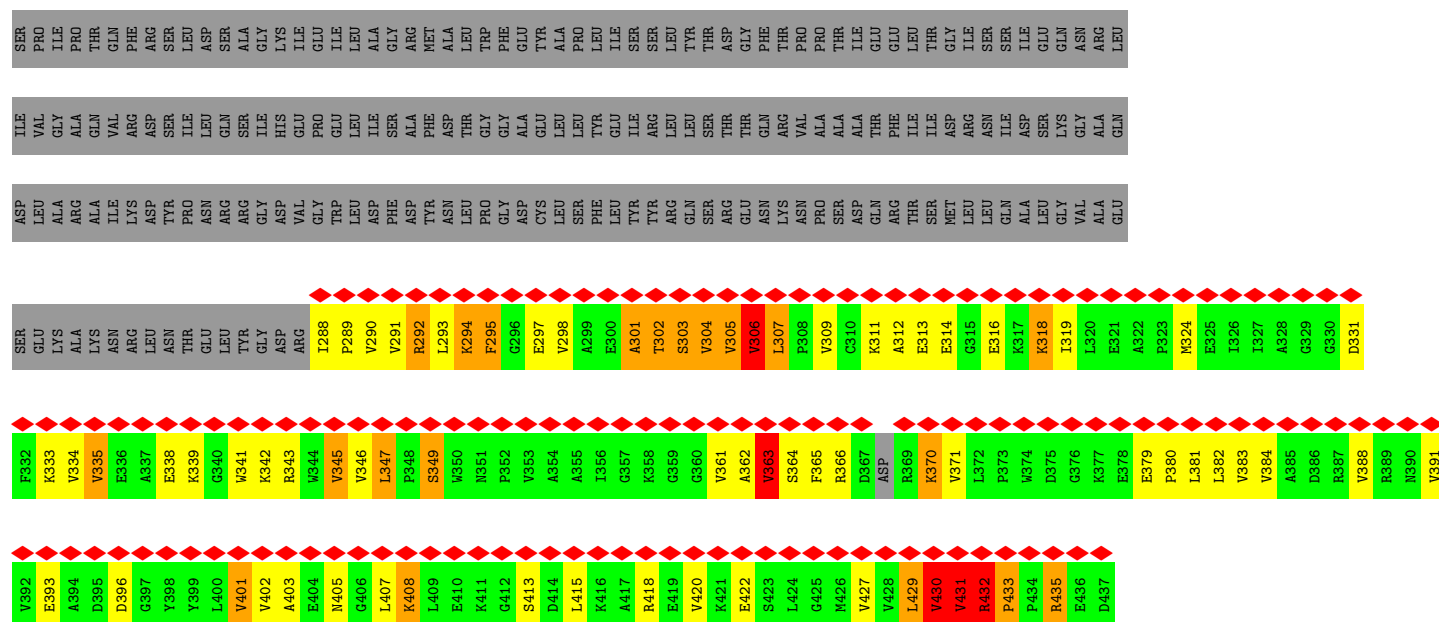
- Molecule 1: Ribulose biphosphate carboxylase large chain



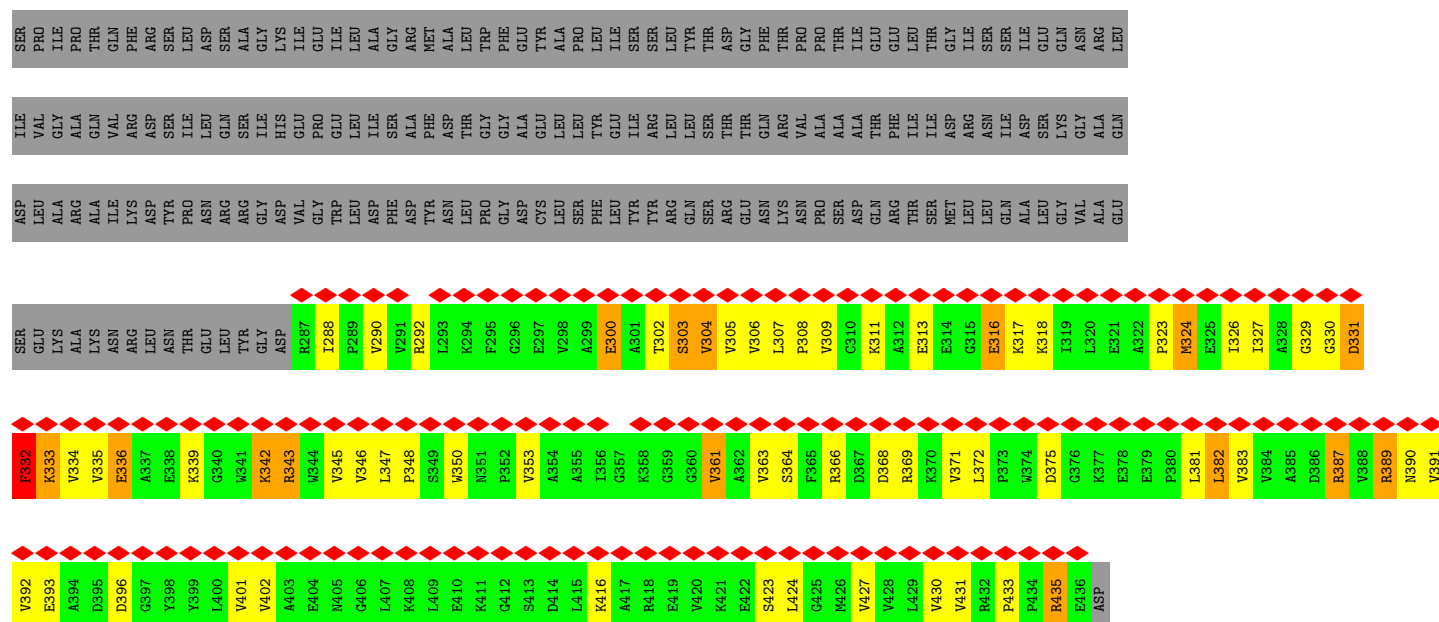
- Molecule 2: Rubisco accumulation factor 1.2, chloroplastic



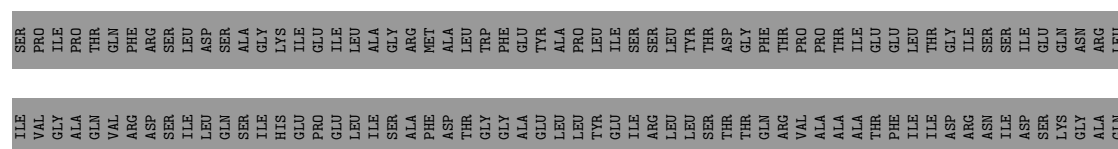
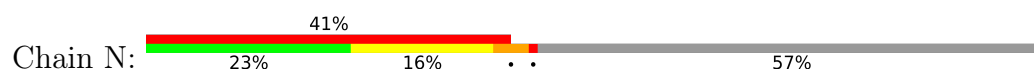


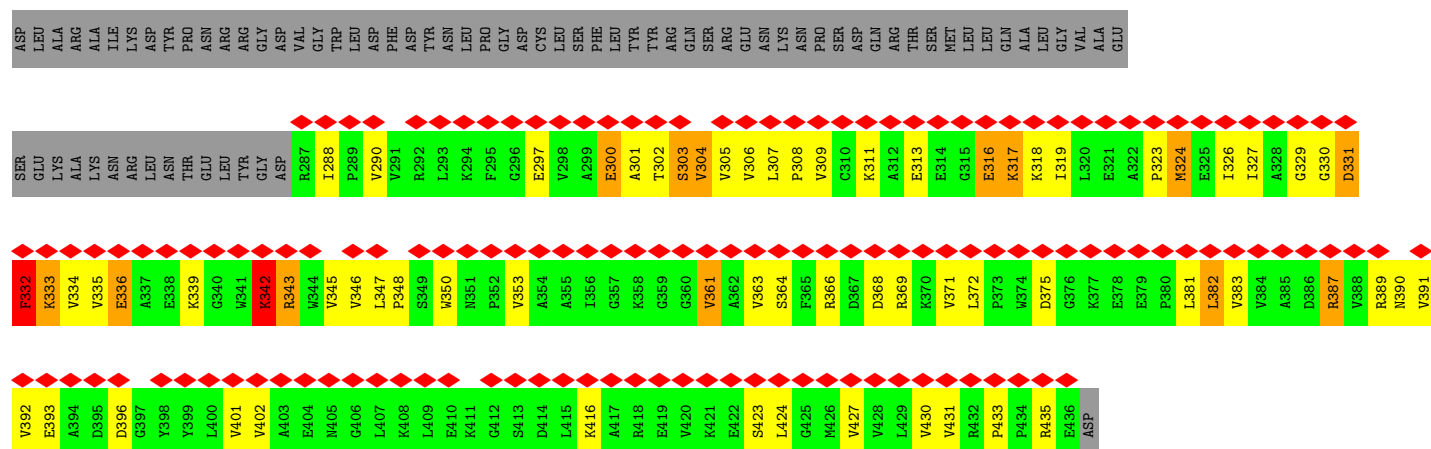


• Molecule 2: Rubisco accumulation factor 1.2, chloroplastic

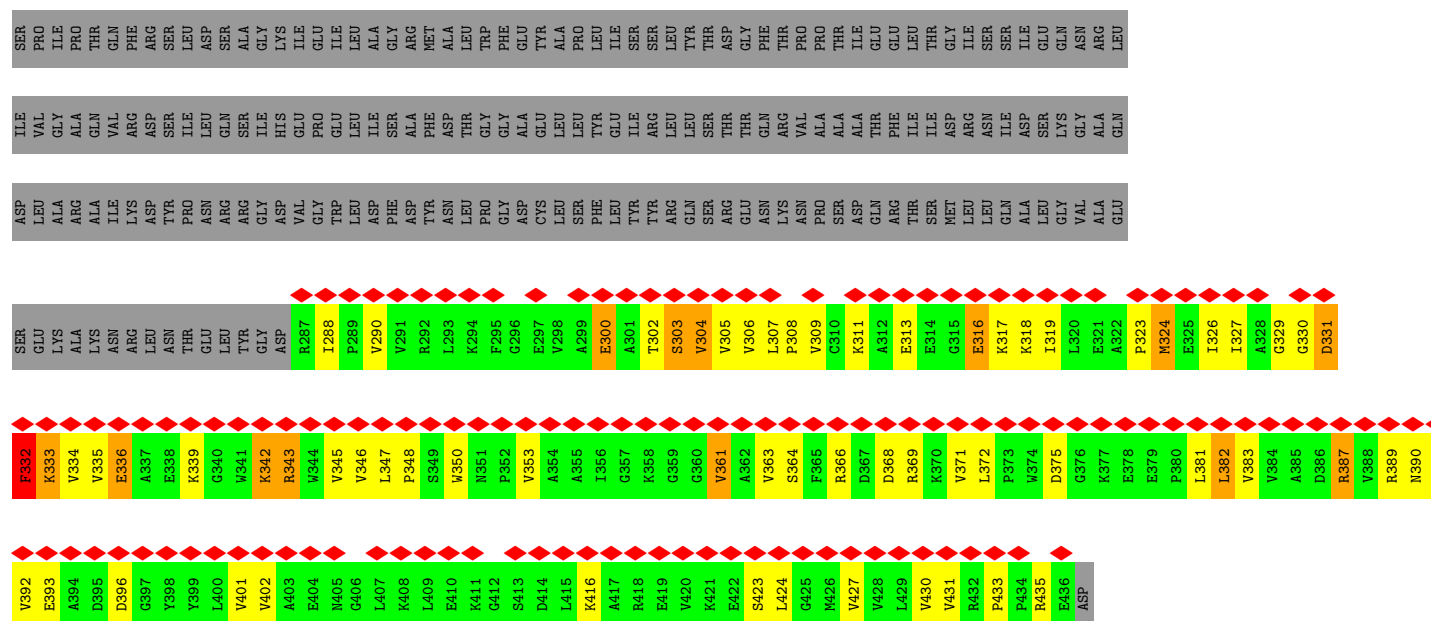
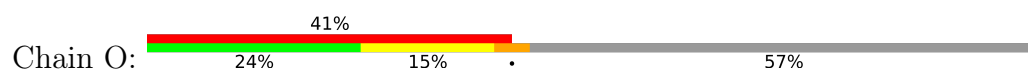


• Molecule 2: Rubisco accumulation factor 1.2, chloroplastic

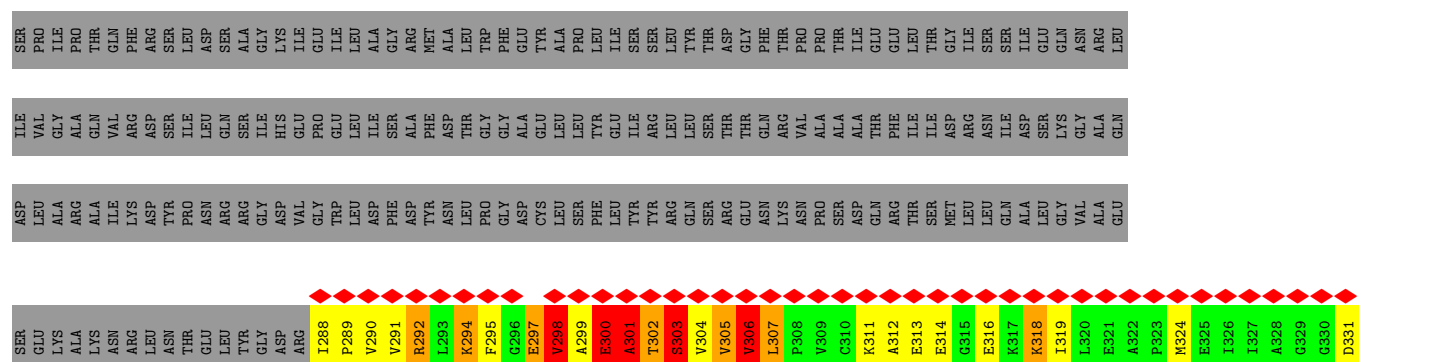
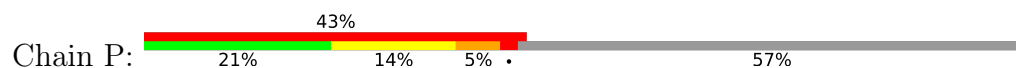




• Molecule 2: Rubisco accumulation factor 1.2, chloroplastic



• Molecule 2: Rubisco accumulation factor 1.2, chloroplastic





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	535498	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	216.31999, 216.31999, 216.31999	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.52, 0.52, 0.52	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	1.12	3/3328 (0.1%)	1.22	36/4502 (0.8%)
1	B	1.13	2/3344 (0.1%)	1.23	30/4526 (0.7%)
1	C	1.13	2/3331 (0.1%)	1.21	33/4507 (0.7%)
1	D	1.15	2/3339 (0.1%)	1.23	35/4515 (0.8%)
1	E	1.13	3/3328 (0.1%)	1.22	36/4502 (0.8%)
1	F	1.13	2/3344 (0.1%)	1.24	32/4526 (0.7%)
1	G	1.13	2/3331 (0.1%)	1.21	31/4507 (0.7%)
1	H	1.15	2/3339 (0.1%)	1.23	35/4515 (0.8%)
2	I	0.36	0/1564	0.73	7/2120 (0.3%)
2	J	0.69	2/1153 (0.2%)	1.56	18/1565 (1.2%)
2	K	0.62	0/1153	1.28	14/1565 (0.9%)
2	L	0.68	2/1153 (0.2%)	1.55	18/1565 (1.2%)
2	M	0.54	0/1145	1.17	10/1560 (0.6%)
2	N	0.55	0/1145	1.17	10/1560 (0.6%)
2	O	0.56	0/1145	1.17	10/1560 (0.6%)
2	P	0.72	2/1153 (0.2%)	1.68	20/1565 (1.3%)
2	Q	0.54	0/1145	1.18	10/1560 (0.6%)
All	All	1.01	24/37440 (0.1%)	1.24	385/50720 (0.8%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	342	PHE	CB-CG	-8.57	1.30	1.50
1	H	342	PHE	CB-CG	-8.57	1.30	1.50
1	H	291	HIS	CB-CG	-6.78	1.40	1.50
1	D	291	HIS	CB-CG	-6.75	1.40	1.50
1	B	291	HIS	CB-CG	-6.51	1.41	1.50
1	F	291	HIS	CB-CG	-6.51	1.41	1.50
2	P	433	PRO	CA-C	6.20	1.57	1.52
1	C	291	HIS	CB-CG	-6.18	1.41	1.50
1	G	291	HIS	CB-CG	-6.18	1.41	1.50
2	L	433	PRO	CA-C	6.17	1.57	1.52
2	J	433	PRO	CA-C	6.15	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	HIS	CB-CG	-6.00	1.41	1.50
1	E	291	HIS	CB-CG	-6.00	1.41	1.50
2	P	300	GLU	N-CA	5.95	1.53	1.46
1	C	373	PRO	N-CD	-5.15	1.40	1.47
1	G	373	PRO	N-CD	-5.15	1.40	1.47
1	E	373	PRO	N-CD	-5.14	1.40	1.47
1	A	373	PRO	N-CD	-5.11	1.40	1.47
1	B	373	PRO	N-CD	-5.05	1.40	1.47
1	F	373	PRO	N-CD	-5.05	1.40	1.47
1	A	264	HIS	CB-CG	-5.03	1.43	1.50
2	L	430	VAL	N-CA	5.02	1.51	1.46
1	E	264	HIS	CB-CG	-5.02	1.43	1.50
2	J	430	VAL	N-CA	5.01	1.51	1.46

All (385) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	431	VAL	N-CA-C	30.86	138.82	110.74
2	L	431	VAL	N-CA-C	30.82	138.79	110.74
2	J	431	VAL	N-CA-C	30.80	138.77	110.74
2	P	298	VAL	N-CA-C	-19.15	80.04	107.99
2	P	302	THR	N-CA-C	14.33	136.36	107.41
2	P	301	ALA	N-CA-C	12.55	137.52	110.80
2	L	433	PRO	N-CA-C	10.70	123.75	110.70
2	J	433	PRO	N-CA-C	10.69	123.74	110.70
2	P	433	PRO	N-CA-C	10.66	123.70	110.70
2	K	304	VAL	N-CA-C	10.47	122.39	109.30
2	P	303	SER	N-CA-C	10.12	124.05	108.96
2	J	303	SER	N-CA-C	10.10	123.35	108.60
2	L	331	ASP	N-CA-C	-9.95	102.22	114.75
2	K	331	ASP	N-CA-C	-9.93	102.23	114.75
2	K	303	SER	N-CA-C	9.93	121.34	108.24
2	P	331	ASP	N-CA-C	-9.92	102.25	114.75
2	J	331	ASP	N-CA-C	-9.89	102.28	114.75
2	J	304	VAL	N-CA-C	9.66	122.41	109.37
2	L	303	SER	N-CA-C	9.59	122.60	108.60
2	I	171	ARG	N-CA-C	9.42	121.15	111.07
2	L	304	VAL	N-CA-C	9.33	121.97	109.37
2	M	330	GLY	N-CA-C	9.30	122.63	111.93
2	N	330	GLY	N-CA-C	9.29	122.62	111.93
2	O	330	GLY	N-CA-C	9.29	122.62	111.93
2	Q	330	GLY	N-CA-C	9.29	122.61	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	431	VAL	CB-CA-C	-8.91	100.18	111.94
2	L	431	VAL	CB-CA-C	-8.91	100.18	111.94
2	J	431	VAL	CB-CA-C	-8.90	100.19	111.94
2	L	301	ALA	N-CA-C	8.54	128.99	110.80
2	J	301	ALA	N-CA-C	8.52	128.95	110.80
1	F	40	SER	CA-C-N	8.29	128.32	119.78
1	F	40	SER	C-N-CA	8.29	128.32	119.78
1	B	40	SER	CA-C-N	8.26	128.29	119.78
1	B	40	SER	C-N-CA	8.26	128.29	119.78
1	C	23	THR	CA-C-N	8.20	127.93	119.56
1	C	23	THR	C-N-CA	8.20	127.93	119.56
1	G	23	THR	CA-C-N	8.20	127.93	119.56
1	G	23	THR	C-N-CA	8.20	127.93	119.56
2	K	431	VAL	N-CA-C	7.98	125.94	109.34
1	D	342	PHE	CB-CA-C	-7.85	98.25	110.81
1	H	342	PHE	CB-CA-C	-7.85	98.25	110.81
1	C	125	LYS	N-CA-C	7.84	120.73	111.71
1	G	125	LYS	N-CA-C	7.84	120.73	111.71
1	D	125	LYS	N-CA-C	7.75	120.62	111.71
1	H	125	LYS	N-CA-C	7.75	120.62	111.71
1	A	328	VAL	N-CA-C	-7.64	106.45	113.71
1	E	328	VAL	N-CA-C	-7.64	106.45	113.71
1	A	125	LYS	N-CA-C	7.54	120.38	111.71
1	E	125	LYS	N-CA-C	7.54	120.38	111.71
2	N	433	PRO	N-CA-C	7.48	118.58	110.58
2	Q	433	PRO	N-CA-C	7.45	118.55	110.58
2	M	433	PRO	N-CA-C	7.31	118.40	110.58
1	C	148	PRO	CA-C-N	7.03	127.34	119.32
1	C	148	PRO	C-N-CA	7.03	127.34	119.32
1	G	148	PRO	CA-C-N	7.03	127.34	119.32
1	G	148	PRO	C-N-CA	7.03	127.34	119.32
1	B	410	ASN	N-CA-C	7.03	118.73	111.14
1	B	148	PRO	CA-C-N	7.02	127.32	119.32
1	B	148	PRO	C-N-CA	7.02	127.32	119.32
1	F	148	PRO	CA-C-N	7.02	127.32	119.32
1	F	148	PRO	C-N-CA	7.02	127.32	119.32
1	B	164	ARG	CA-C-N	7.00	127.00	119.78
1	B	164	ARG	C-N-CA	7.00	127.00	119.78
1	D	23	THR	CA-C-N	7.00	127.16	119.87
1	D	23	THR	C-N-CA	7.00	127.16	119.87
1	F	164	ARG	CA-C-N	7.00	127.00	119.78
1	F	164	ARG	C-N-CA	7.00	127.00	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	23	THR	CA-C-N	7.00	127.16	119.87
1	H	23	THR	C-N-CA	7.00	127.16	119.87
1	F	410	ASN	N-CA-C	6.99	118.69	111.14
1	C	410	ASN	N-CA-C	6.95	118.93	111.36
1	G	410	ASN	N-CA-C	6.95	118.93	111.36
1	A	148	PRO	CA-C-N	6.93	127.22	119.32
1	A	148	PRO	C-N-CA	6.93	127.22	119.32
1	E	148	PRO	CA-C-N	6.93	127.22	119.32
1	E	148	PRO	C-N-CA	6.93	127.22	119.32
1	C	109	SER	N-CA-C	6.93	120.14	108.02
1	G	109	SER	N-CA-C	6.93	120.14	108.02
2	P	300	GLU	CB-CA-C	6.87	124.08	110.42
1	A	23	THR	CA-C-N	6.81	126.51	119.56
1	A	23	THR	C-N-CA	6.81	126.51	119.56
1	E	23	THR	CA-C-N	6.81	126.51	119.56
1	E	23	THR	C-N-CA	6.81	126.51	119.56
2	K	301	ALA	N-CA-C	6.80	125.29	110.80
1	D	109	SER	N-CA-C	6.73	119.79	108.02
2	M	332	PHE	N-CA-CB	6.71	120.36	110.56
2	L	293	LEU	N-CA-C	-6.71	98.27	108.67
1	H	109	SER	N-CA-C	6.71	119.75	108.02
1	B	109	SER	N-CA-C	6.70	119.75	108.02
1	F	109	SER	N-CA-C	6.70	119.75	108.02
2	K	293	LEU	N-CA-C	-6.70	98.28	108.67
2	O	332	PHE	N-CA-CB	6.70	120.35	110.56
2	N	332	PHE	N-CA-CB	6.70	120.34	110.56
1	B	125	LYS	N-CA-C	6.68	119.39	111.71
1	F	125	LYS	N-CA-C	6.68	119.39	111.71
2	J	293	LEU	N-CA-C	-6.68	98.31	108.67
2	Q	332	PHE	N-CA-CB	6.67	120.29	110.56
1	A	45	VAL	CA-C-N	6.62	126.60	119.78
1	A	45	VAL	C-N-CA	6.62	126.60	119.78
1	E	45	VAL	CA-C-N	6.62	126.60	119.78
1	E	45	VAL	C-N-CA	6.62	126.60	119.78
1	C	164	ARG	CA-C-N	6.60	126.58	119.78
1	C	164	ARG	C-N-CA	6.60	126.58	119.78
1	G	164	ARG	CA-C-N	6.60	126.58	119.78
1	G	164	ARG	C-N-CA	6.60	126.58	119.78
2	L	306	VAL	N-CA-C	6.56	118.24	108.46
2	P	298	VAL	CB-CA-C	-6.55	102.01	110.98
1	D	164	ARG	CA-C-N	6.54	126.52	119.78
1	D	164	ARG	C-N-CA	6.54	126.52	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	164	ARG	CA-C-N	6.54	126.52	119.78
1	H	164	ARG	C-N-CA	6.54	126.52	119.78
2	I	180	ARG	N-CA-C	-6.46	104.32	111.36
2	P	302	THR	CB-CA-C	-6.42	100.50	111.41
1	A	109	SER	N-CA-C	6.39	119.20	108.02
1	E	109	SER	N-CA-C	6.39	119.20	108.02
1	F	449	SER	CA-C-N	6.37	126.85	119.47
1	F	449	SER	C-N-CA	6.37	126.85	119.47
1	H	152	ILE	N-CA-C	6.36	116.53	110.42
1	A	406	HIS	CA-C-N	6.35	126.04	119.56
1	A	406	HIS	C-N-CA	6.35	126.04	119.56
2	N	329	GLY	N-CA-C	-6.35	98.12	113.18
2	O	329	GLY	N-CA-C	-6.35	98.14	113.18
1	E	406	HIS	CA-C-N	6.35	126.03	119.56
1	E	406	HIS	C-N-CA	6.35	126.03	119.56
1	D	152	ILE	N-CA-C	6.34	116.51	110.42
2	Q	329	GLY	N-CA-C	-6.34	98.15	113.18
1	E	40	SER	CA-C-N	6.33	126.24	119.85
1	E	40	SER	C-N-CA	6.33	126.24	119.85
2	M	329	GLY	N-CA-C	-6.33	98.19	113.18
1	D	40	SER	CA-C-N	6.32	126.23	119.85
1	D	40	SER	C-N-CA	6.32	126.23	119.85
1	H	40	SER	CA-C-N	6.32	126.23	119.85
1	H	40	SER	C-N-CA	6.32	126.23	119.85
1	A	40	SER	CA-C-N	6.30	126.22	119.85
1	A	40	SER	C-N-CA	6.30	126.22	119.85
1	C	152	ILE	N-CA-C	6.30	116.47	110.42
1	G	152	ILE	N-CA-C	6.30	116.47	110.42
1	B	322	HIS	CA-CB-CG	6.28	120.08	113.80
1	F	322	HIS	CA-CB-CG	6.28	120.08	113.80
1	A	27	THR	CA-C-N	6.27	126.23	119.78
1	A	27	THR	C-N-CA	6.27	126.23	119.78
2	L	380	PRO	CA-C-O	-6.27	114.06	122.08
1	E	27	THR	CA-C-N	6.26	126.23	119.78
1	E	27	THR	C-N-CA	6.26	126.23	119.78
2	P	380	PRO	CA-C-O	-6.25	114.07	122.08
2	J	380	PRO	CA-C-O	-6.23	114.10	122.08
2	K	380	PRO	CA-C-O	-6.23	114.11	122.08
1	D	164	ARG	N-CA-C	6.22	113.82	108.22
1	E	152	ILE	N-CA-C	6.21	116.39	110.42
2	I	53	PHE	N-CA-C	6.21	119.62	109.24
1	A	152	ILE	N-CA-C	6.18	116.36	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	GLU	CA-C-N	6.17	126.14	120.03
1	B	85	GLU	C-N-CA	6.17	126.14	120.03
1	F	85	GLU	CA-C-N	6.17	126.14	120.03
1	F	85	GLU	C-N-CA	6.17	126.14	120.03
1	H	164	ARG	N-CA-C	6.16	113.76	108.22
1	C	40	SER	CA-C-N	6.16	126.07	119.85
1	C	40	SER	C-N-CA	6.16	126.07	119.85
1	G	40	SER	CA-C-N	6.16	126.07	119.85
1	G	40	SER	C-N-CA	6.16	126.07	119.85
1	B	152	ILE	N-CA-C	6.14	116.32	110.42
1	F	152	ILE	N-CA-C	6.14	116.32	110.42
1	A	164	ARG	CA-C-N	6.13	126.09	119.78
1	A	164	ARG	C-N-CA	6.13	126.09	119.78
1	E	164	ARG	CA-C-N	6.13	126.09	119.78
1	E	164	ARG	C-N-CA	6.13	126.09	119.78
1	A	322	HIS	CA-CB-CG	6.13	119.93	113.80
1	E	322	HIS	CA-CB-CG	6.13	119.93	113.80
1	D	449	SER	CA-C-N	6.11	125.79	119.56
1	D	449	SER	C-N-CA	6.11	125.79	119.56
1	C	322	HIS	CA-CB-CG	6.10	119.90	113.80
1	G	322	HIS	CA-CB-CG	6.10	119.90	113.80
1	D	322	HIS	CA-CB-CG	6.09	119.89	113.80
1	H	322	HIS	CA-CB-CG	6.09	119.89	113.80
1	H	449	SER	CA-C-N	6.06	125.74	119.56
1	H	449	SER	C-N-CA	6.06	125.74	119.56
1	B	23	THR	CA-C-N	6.04	125.72	119.56
1	B	23	THR	C-N-CA	6.04	125.72	119.56
1	F	23	THR	CA-C-N	6.00	125.68	119.56
1	F	23	THR	C-N-CA	6.00	125.68	119.56
1	C	449	SER	CA-C-N	6.00	126.43	119.47
1	C	449	SER	C-N-CA	6.00	126.43	119.47
1	B	27	THR	CA-C-N	5.99	125.95	119.78
1	B	27	THR	C-N-CA	5.99	125.95	119.78
1	F	27	THR	CA-C-N	5.99	125.95	119.78
1	F	27	THR	C-N-CA	5.99	125.95	119.78
1	F	241	ALA	CA-C-N	5.99	125.67	119.56
1	F	241	ALA	C-N-CA	5.99	125.67	119.56
1	G	449	SER	CA-C-N	5.98	126.40	119.47
1	G	449	SER	C-N-CA	5.98	126.40	119.47
1	A	413	GLY	N-CA-C	-5.97	105.27	112.49
1	E	413	GLY	N-CA-C	-5.97	105.27	112.49
2	P	432	ARG	N-CA-C	5.97	123.00	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	432	ARG	N-CA-C	5.96	122.98	109.81
2	I	55	PRO	N-CA-C	5.95	117.96	110.70
1	B	241	ALA	CA-C-N	5.95	125.63	119.56
1	B	241	ALA	C-N-CA	5.95	125.63	119.56
2	L	432	ARG	N-CA-C	5.95	122.95	109.81
1	G	27	THR	CA-C-N	5.91	125.86	119.78
1	G	27	THR	C-N-CA	5.91	125.86	119.78
1	C	27	THR	CA-C-N	5.89	125.85	119.78
1	C	27	THR	C-N-CA	5.89	125.85	119.78
1	D	45	VAL	CA-C-N	5.88	125.83	119.78
1	D	45	VAL	C-N-CA	5.88	125.83	119.78
1	H	45	VAL	CA-C-N	5.88	125.83	119.78
1	H	45	VAL	C-N-CA	5.88	125.83	119.78
1	H	27	THR	CA-C-N	5.88	125.83	119.78
1	H	27	THR	C-N-CA	5.88	125.83	119.78
2	I	52	GLY	N-CA-C	5.86	124.31	113.76
1	D	27	THR	CA-C-N	5.86	125.81	119.78
1	D	27	THR	C-N-CA	5.86	125.81	119.78
1	B	171	ILE	N-CA-C	5.84	116.29	108.11
1	F	171	ILE	N-CA-C	5.83	116.27	108.11
2	O	433	PRO	N-CA-C	5.82	117.80	110.70
2	Q	372	LEU	CA-C-N	-5.82	112.88	119.28
2	Q	372	LEU	C-N-CA	-5.82	112.88	119.28
2	J	363	VAL	N-CA-C	5.80	115.08	106.85
2	N	372	LEU	CA-C-N	-5.78	112.93	119.28
2	N	372	LEU	C-N-CA	-5.78	112.93	119.28
2	M	372	LEU	CA-C-N	-5.77	112.93	119.28
2	M	372	LEU	C-N-CA	-5.77	112.93	119.28
2	J	324	MET	N-CA-C	5.77	117.65	111.36
2	J	429	LEU	CA-CB-CG	5.76	136.48	116.30
1	B	45	VAL	CA-C-N	5.76	125.72	119.78
1	B	45	VAL	C-N-CA	5.76	125.72	119.78
1	F	45	VAL	CA-C-N	5.76	125.72	119.78
1	F	45	VAL	C-N-CA	5.76	125.72	119.78
2	K	429	LEU	CA-CB-CG	5.75	136.44	116.30
2	L	324	MET	N-CA-C	5.75	117.63	111.36
2	O	372	LEU	CA-C-N	-5.75	112.95	119.28
2	O	372	LEU	C-N-CA	-5.75	112.95	119.28
2	P	429	LEU	CA-CB-CG	5.75	136.44	116.30
2	L	429	LEU	CA-CB-CG	5.75	136.43	116.30
2	P	324	MET	N-CA-C	5.72	117.59	111.36
1	C	164	ARG	N-CA-C	5.71	113.36	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	164	ARG	N-CA-C	5.71	113.36	108.22
1	A	241	ALA	CA-C-N	5.70	125.38	119.56
1	A	241	ALA	C-N-CA	5.70	125.38	119.56
1	E	241	ALA	CA-C-N	5.70	125.38	119.56
1	E	241	ALA	C-N-CA	5.70	125.38	119.56
2	K	324	MET	N-CA-C	5.70	117.57	111.36
1	E	300	ARG	N-CA-C	5.68	117.55	111.36
1	A	300	ARG	N-CA-C	5.67	117.53	111.36
1	D	406	HIS	CA-C-N	5.63	125.30	119.56
1	D	406	HIS	C-N-CA	5.63	125.30	119.56
1	H	406	HIS	CA-C-N	5.63	125.30	119.56
1	H	406	HIS	C-N-CA	5.63	125.30	119.56
2	I	173	ASN	N-CA-C	5.61	118.18	109.60
1	A	85	GLU	CA-C-N	5.58	125.49	119.85
1	A	85	GLU	C-N-CA	5.58	125.49	119.85
1	E	85	GLU	CA-C-N	5.58	125.49	119.85
1	E	85	GLU	C-N-CA	5.58	125.49	119.85
2	O	342	LYS	N-CA-C	5.58	117.37	111.28
1	C	300	ARG	N-CA-C	5.58	117.44	111.36
2	M	342	LYS	N-CA-C	5.57	117.35	111.28
1	G	300	ARG	N-CA-C	5.57	117.43	111.36
2	N	342	LYS	N-CA-C	5.57	117.35	111.28
2	K	304	VAL	CB-CA-C	-5.56	103.04	111.33
1	F	368	MET	CA-C-N	5.54	125.49	119.78
1	F	368	MET	C-N-CA	5.54	125.49	119.78
2	Q	342	LYS	N-CA-C	5.54	117.32	111.28
1	C	406	HIS	CA-C-N	5.53	125.88	119.47
1	C	406	HIS	C-N-CA	5.53	125.88	119.47
1	B	368	MET	CA-C-N	5.52	125.46	119.78
1	B	368	MET	C-N-CA	5.52	125.46	119.78
1	C	114	LEU	CA-C-N	-5.51	112.46	120.29
1	C	114	LEU	C-N-CA	-5.51	112.46	120.29
1	G	114	LEU	CA-C-N	-5.51	112.46	120.29
1	G	114	LEU	C-N-CA	-5.51	112.46	120.29
1	D	120	ASN	CA-CB-CG	-5.51	107.09	112.60
1	G	100	TYR	CA-C-N	5.51	125.44	119.76
1	G	100	TYR	C-N-CA	5.51	125.44	119.76
1	H	120	ASN	CA-CB-CG	-5.51	107.09	112.60
1	G	406	HIS	CA-C-N	5.50	125.85	119.47
1	G	406	HIS	C-N-CA	5.50	125.85	119.47
1	B	406	HIS	CA-C-N	5.50	125.84	119.47
1	B	406	HIS	C-N-CA	5.50	125.84	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	406	HIS	CA-C-N	5.50	125.84	119.47
1	F	406	HIS	C-N-CA	5.50	125.84	119.47
2	L	363	VAL	N-CA-C	5.48	116.00	107.28
1	C	100	TYR	CA-C-N	5.47	125.40	119.76
1	C	100	TYR	C-N-CA	5.47	125.40	119.76
1	A	98	ILE	N-CA-C	5.47	115.77	108.11
1	E	98	ILE	N-CA-C	5.47	115.77	108.11
2	K	363	VAL	N-CA-C	5.47	115.97	107.28
2	P	363	VAL	N-CA-C	5.46	115.97	107.28
1	A	325	SER	N-CA-C	-5.41	107.33	114.04
1	E	325	SER	N-CA-C	-5.41	107.33	114.04
1	C	98	ILE	N-CA-C	5.40	115.67	108.11
1	G	98	ILE	N-CA-C	5.40	115.67	108.11
2	P	306	VAL	N-CA-C	5.39	116.42	108.45
1	D	85	GLU	CA-C-N	5.38	125.29	119.85
1	D	85	GLU	C-N-CA	5.38	125.29	119.85
1	H	85	GLU	CA-C-N	5.38	125.29	119.85
1	H	85	GLU	C-N-CA	5.38	125.29	119.85
2	K	306	VAL	N-CA-C	5.37	116.40	108.45
2	Q	350	TRP	N-CA-C	-5.37	102.93	110.50
2	O	350	TRP	N-CA-C	-5.36	102.94	110.50
1	C	85	GLU	CA-C-N	5.36	125.26	119.85
1	C	85	GLU	C-N-CA	5.36	125.26	119.85
1	G	85	GLU	CA-C-N	5.36	125.26	119.85
1	G	85	GLU	C-N-CA	5.36	125.26	119.85
2	M	350	TRP	N-CA-C	-5.34	102.97	110.50
2	J	306	VAL	N-CA-C	5.33	116.34	108.45
2	J	432	ARG	CA-C-N	5.33	125.87	120.38
2	J	432	ARG	C-N-CA	5.33	125.87	120.38
2	N	350	TRP	N-CA-C	-5.32	103.00	110.50
1	C	42	GLN	CA-C-N	-5.32	114.28	119.76
1	C	42	GLN	C-N-CA	-5.32	114.28	119.76
1	D	241	ALA	CA-C-N	5.31	125.12	119.28
1	D	241	ALA	C-N-CA	5.31	125.12	119.28
1	H	241	ALA	CA-C-N	5.31	125.12	119.28
1	H	241	ALA	C-N-CA	5.31	125.12	119.28
1	A	117	ILE	N-CA-C	5.30	116.07	110.72
1	C	241	ALA	CA-C-N	5.30	125.11	119.28
1	C	241	ALA	C-N-CA	5.30	125.11	119.28
1	E	117	ILE	N-CA-C	5.30	116.07	110.72
1	G	241	ALA	CA-C-N	5.30	125.11	119.28
1	G	241	ALA	C-N-CA	5.30	125.11	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	432	ARG	CA-C-N	5.30	125.83	120.38
2	P	432	ARG	C-N-CA	5.30	125.83	120.38
1	A	449	SER	CA-C-N	5.29	126.23	120.83
1	A	449	SER	C-N-CA	5.29	126.23	120.83
1	E	449	SER	CA-C-N	5.29	126.23	120.83
1	E	449	SER	C-N-CA	5.29	126.23	120.83
2	L	432	ARG	CA-C-N	5.29	125.83	120.38
2	L	432	ARG	C-N-CA	5.29	125.83	120.38
1	A	198	LYS	N-CA-C	5.26	118.07	109.59
1	E	198	LYS	N-CA-C	5.26	118.05	109.59
1	F	198	LYS	N-CA-C	5.25	117.52	109.07
1	D	114	LEU	CA-C-N	-5.24	112.86	120.29
1	D	114	LEU	C-N-CA	-5.24	112.86	120.29
1	H	114	LEU	CA-C-N	-5.24	112.86	120.29
1	H	114	LEU	C-N-CA	-5.24	112.86	120.29
2	J	304	VAL	CB-CA-C	-5.24	103.06	111.59
1	B	198	LYS	N-CA-C	5.22	117.48	109.07
2	K	302	THR	N-CA-C	5.22	117.41	108.90
1	A	164	ARG	N-CA-C	5.21	112.91	108.22
1	E	164	ARG	N-CA-C	5.21	112.91	108.22
2	I	59	GLU	N-CA-C	-5.16	105.66	111.28
1	H	148	PRO	CA-C-N	5.16	126.29	119.84
1	H	148	PRO	C-N-CA	5.16	126.29	119.84
1	D	100	TYR	CA-C-N	5.14	125.06	119.76
1	D	100	TYR	C-N-CA	5.14	125.06	119.76
1	H	100	TYR	CA-C-N	5.14	125.06	119.76
1	H	100	TYR	C-N-CA	5.14	125.06	119.76
2	L	334	VAL	N-CA-C	-5.13	102.89	109.30
1	D	148	PRO	CA-C-N	5.13	126.25	119.84
1	D	148	PRO	C-N-CA	5.13	126.25	119.84
1	A	268	THR	N-CA-C	-5.13	107.41	113.97
1	E	268	THR	N-CA-C	-5.13	107.41	113.97
1	H	284	ASN	N-CA-C	5.12	119.62	113.17
1	A	100	TYR	CA-C-N	5.11	125.03	119.76
1	A	100	TYR	C-N-CA	5.11	125.03	119.76
1	E	100	TYR	CA-C-N	5.11	125.03	119.76
1	E	100	TYR	C-N-CA	5.11	125.03	119.76
1	D	284	ASN	N-CA-C	5.11	119.60	113.17
2	J	334	VAL	N-CA-C	-5.10	102.93	109.30
2	K	334	VAL	N-CA-C	-5.09	102.94	109.30
2	P	334	VAL	N-CA-C	-5.09	102.94	109.30
1	B	372	LEU	CA-C-N	5.09	124.99	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	372	LEU	C-N-CA	5.09	124.99	119.85
1	F	372	LEU	CA-C-N	5.09	124.99	119.85
1	F	372	LEU	C-N-CA	5.09	124.99	119.85
2	O	307	LEU	CA-C-N	-5.08	115.00	120.03
2	O	307	LEU	C-N-CA	-5.08	115.00	120.03
1	C	266	PHE	CA-CB-CG	5.07	118.87	113.80
1	G	266	PHE	CA-CB-CG	5.07	118.87	113.80
2	L	309	VAL	N-CA-C	5.07	116.26	108.71
1	A	266	PHE	CA-CB-CG	5.06	118.86	113.80
1	E	266	PHE	CA-CB-CG	5.06	118.86	113.80
2	Q	307	LEU	CA-C-N	-5.06	115.02	120.03
2	Q	307	LEU	C-N-CA	-5.06	115.02	120.03
1	D	379	ILE	CA-C-N	5.05	130.15	122.11
1	D	379	ILE	C-N-CA	5.05	130.15	122.11
1	D	199	ASP	CA-CB-CG	5.05	117.65	112.60
1	H	199	ASP	CA-CB-CG	5.05	117.65	112.60
1	F	199	ASP	CA-CB-CG	5.04	117.64	112.60
1	H	379	ILE	CA-C-N	5.04	130.12	122.11
1	H	379	ILE	C-N-CA	5.04	130.12	122.11
2	M	307	LEU	CA-C-N	-5.04	115.04	120.03
2	M	307	LEU	C-N-CA	-5.04	115.04	120.03
2	N	307	LEU	CA-C-N	-5.02	115.06	120.03
2	N	307	LEU	C-N-CA	-5.02	115.06	120.03
1	B	199	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3250	0	3166	11	0
1	B	3265	0	3184	17	0
1	C	3253	0	3170	8	0
1	D	3262	0	3185	16	0
1	E	3250	0	3166	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3265	0	3184	11	0
1	G	3253	0	3170	12	0
1	H	3262	0	3185	21	0
2	I	1536	0	1516	30	0
2	J	1133	0	1160	38	0
2	K	1133	0	1160	46	0
2	L	1133	0	1160	39	0
2	M	1124	0	1133	34	0
2	N	1124	0	1133	38	0
2	O	1124	0	1133	32	0
2	P	1133	0	1160	51	0
2	Q	1124	0	1133	39	0
All	All	36624	0	36098	357	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 5.

All (357) 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:429:ASN:HB3	2:I:55:PRO:HD2	1.56	0.86
2:K:302:THR:HB	2:N:348:PRO:HB3	1.64	0.79
2:J:304:VAL:HG13	2:M:346:VAL:HB	1.70	0.74
2:K:304:VAL:HG13	2:N:346:VAL:HB	1.70	0.73
2:P:302:THR:HA	2:Q:348:PRO:HB3	1.70	0.72
2:L:304:VAL:HG13	2:O:346:VAL:HB	1.72	0.72
2:I:157:LEU:HD23	2:I:192:GLU:HG3	1.72	0.71
2:L:365:PHE:HB2	2:L:381:LEU:HB2	1.72	0.71
2:P:365:PHE:HB2	2:P:381:LEU:HB2	1.72	0.71
2:K:365:PHE:HB2	2:K:381:LEU:HB2	1.72	0.70
2:J:289:PRO:HD2	2:J:429:LEU:HD12	1.76	0.68
1:A:76:ARG:NH2	1:H:367:SER:OG	2.28	0.67
1:D:367:SER:OG	1:E:76:ARG:NH2	2.27	0.67
2:L:306:VAL:HG22	2:O:346:VAL:HG21	1.77	0.67
2:P:300:GLU:HG2	2:Q:300:GLU:HB3	1.78	0.66
2:J:365:PHE:HB2	2:J:381:LEU:HB2	1.78	0.65
2:L:345:VAL:HG21	2:O:334:VAL:HA	1.80	0.64
2:K:345:VAL:HG21	2:N:334:VAL:HA	1.80	0.63
2:J:345:VAL:HG21	2:M:334:VAL:HA	1.80	0.63
2:L:362:ALA:HB1	2:L:382:LEU:HD11	1.81	0.63
2:L:433:PRO:HA	2:O:331:ASP:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:433:PRO:HA	2:M:331:ASP:HA	1.81	0.62
2:J:362:ALA:HB1	2:J:382:LEU:HD11	1.81	0.62
2:P:345:VAL:HG21	2:Q:334:VAL:HA	1.80	0.62
1:D:59:SER:O	1:D:60:THR:C	2.43	0.62
2:P:362:ALA:HB1	2:P:382:LEU:HD11	1.81	0.62
2:P:306:VAL:HG22	2:Q:346:VAL:HG21	1.82	0.61
2:K:362:ALA:HB1	2:K:382:LEU:HD11	1.81	0.61
2:L:307:LEU:HD11	2:L:347:LEU:HB2	1.82	0.61
2:P:433:PRO:HA	2:Q:331:ASP:HA	1.81	0.61
1:H:59:SER:O	1:H:60:THR:C	2.42	0.61
2:J:306:VAL:HG22	2:M:346:VAL:HG21	1.82	0.60
2:P:401:VAL:HG23	2:P:408:LYS:HG3	1.84	0.59
2:K:306:VAL:HG22	2:N:346:VAL:HG21	1.82	0.59
2:P:303:SER:HB2	2:Q:298:VAL:HA	1.85	0.59
2:L:401:VAL:HG23	2:L:408:LYS:HG3	1.84	0.59
2:P:300:GLU:HB3	2:Q:300:GLU:O	2.02	0.59
2:J:401:VAL:HG23	2:J:408:LYS:HG3	1.84	0.59
2:K:302:THR:HA	2:N:301:ALA:HB2	1.85	0.58
2:J:302:THR:HB	2:M:348:PRO:CB	2.34	0.58
2:L:306:VAL:HG13	2:L:346:VAL:HG12	1.86	0.58
1:H:349:ASP:OD1	1:H:349:ASP:N	2.37	0.57
1:A:352:GLU:OE2	2:I:136:ARG:HB2	2.04	0.56
1:G:91:GLU:HG2	2:P:298:VAL:HG23	1.88	0.56
2:L:305:VAL:H	2:O:346:VAL:HG11	1.71	0.56
2:I:85:SER:O	2:I:87:HIS:ND1	2.31	0.56
1:B:439:GLY:CA	2:K:297:GLU:OE1	2.54	0.56
1:D:349:ASP:N	1:D:349:ASP:OD1	2.37	0.56
2:I:105:GLU:HG2	2:I:132:GLN:HG3	1.86	0.56
2:K:301:ALA:HB1	2:N:297:GLU:HA	1.88	0.56
2:L:302:THR:HB	2:O:348:PRO:CB	2.35	0.56
2:N:311:LYS:HB3	2:N:366:ARG:HH12	1.71	0.56
2:Q:311:LYS:HB3	2:Q:366:ARG:HH12	1.71	0.55
2:P:302:THR:O	2:Q:297:GLU:HB3	2.07	0.55
1:B:436:ARG:HB3	2:K:291:VAL:CG1	2.36	0.55
1:G:92:ASN:HB2	2:P:298:VAL:HG22	1.88	0.55
2:K:433:PRO:HA	2:N:331:ASP:HA	1.89	0.55
2:O:311:LYS:HB3	2:O:366:ARG:HH12	1.71	0.55
2:O:332:PHE:O	2:O:333:LYS:HB2	2.07	0.55
2:J:302:THR:HB	2:M:348:PRO:HB3	1.88	0.55
2:M:311:LYS:HB3	2:M:366:ARG:HH12	1.71	0.55
2:K:347:LEU:HG	2:K:384:VAL:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:170:SER:HB3	2:I:183:MET:HB2	1.88	0.54
2:M:332:PHE:O	2:M:333:LYS:HB2	2.07	0.54
2:P:305:VAL:H	2:Q:346:VAL:HG11	1.72	0.54
2:J:295:PHE:HA	2:M:303:SER:HB2	1.90	0.54
2:K:403:ALA:HB2	2:K:408:LYS:HB3	1.89	0.54
2:P:289:PRO:HD2	2:P:429:LEU:HD12	1.89	0.54
2:N:332:PHE:O	2:N:333:LYS:HB2	2.07	0.54
2:K:295:PHE:HA	2:N:303:SER:HB2	1.90	0.54
2:L:289:PRO:HD2	2:L:429:LEU:HD12	1.89	0.54
2:L:302:THR:HB	2:O:348:PRO:HB3	1.91	0.53
2:K:305:VAL:H	2:N:346:VAL:HG11	1.74	0.53
2:Q:332:PHE:O	2:Q:333:LYS:HB2	2.07	0.53
2:J:403:ALA:HB2	2:J:408:LYS:HB3	1.89	0.53
2:L:347:LEU:HG	2:L:384:VAL:HG21	1.89	0.53
2:L:403:ALA:HB2	2:L:408:LYS:HB3	1.89	0.53
2:J:347:LEU:HG	2:J:384:VAL:HG21	1.89	0.53
2:P:403:ALA:HB2	2:P:408:LYS:HB3	1.89	0.53
2:P:347:LEU:HG	2:P:384:VAL:HG21	1.89	0.53
2:K:289:PRO:HD2	2:K:429:LEU:HD12	1.89	0.53
2:P:431:VAL:HG12	2:Q:331:ASP:HB2	1.91	0.53
1:G:48:ASP:OD1	1:G:48:ASP:N	2.41	0.53
1:C:220:ASP:OD2	1:C:224:LYS:NZ	2.42	0.52
2:J:305:VAL:H	2:M:346:VAL:HG11	1.74	0.52
1:D:48:ASP:N	1:D:48:ASP:OD1	2.42	0.52
2:J:431:VAL:HG12	2:M:331:ASP:HB2	1.91	0.52
1:C:299:ASP:OD1	1:C:299:ASP:C	2.51	0.52
2:K:290:VAL:HG13	2:K:430:VAL:HB	1.91	0.52
2:L:431:VAL:HG12	2:O:331:ASP:HB2	1.91	0.52
2:L:290:VAL:HG13	2:L:430:VAL:HB	1.91	0.52
2:L:295:PHE:HA	2:O:303:SER:HB2	1.90	0.52
1:A:430:GLU:HA	2:I:49:TYR:HB3	1.92	0.52
2:P:290:VAL:HG13	2:P:430:VAL:HB	1.91	0.52
1:B:349:ASP:N	1:B:349:ASP:OD1	2.39	0.52
2:I:109:LEU:O	2:I:114:ARG:NH2	2.40	0.52
1:H:120:ASN:OD1	1:H:120:ASN:N	2.39	0.52
2:K:290:VAL:HG22	2:K:430:VAL:HB	1.92	0.52
1:C:48:ASP:OD1	1:C:48:ASP:N	2.41	0.51
2:I:19:PHE:HB3	2:I:22:LEU:HD12	1.92	0.51
2:I:151:LEU:HD23	2:I:151:LEU:H	1.76	0.51
2:P:290:VAL:HG22	2:P:430:VAL:HB	1.92	0.51
2:M:290:VAL:HG22	2:M:430:VAL:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:19:PHE:HD2	2:I:44:LEU:HD11	1.75	0.51
2:K:346:VAL:HG11	2:N:346:VAL:HG22	1.93	0.51
2:Q:290:VAL:HG22	2:Q:430:VAL:HB	1.93	0.51
1:B:30:ASP:OD1	1:B:30:ASP:N	2.44	0.51
2:P:302:THR:CA	2:Q:348:PRO:HB3	2.41	0.51
1:G:220:ASP:OD2	1:G:224:LYS:NZ	2.42	0.51
2:L:346:VAL:HG11	2:O:346:VAL:HG22	1.93	0.51
2:N:290:VAL:HG22	2:N:430:VAL:HB	1.93	0.51
2:O:290:VAL:HG22	2:O:430:VAL:HB	1.93	0.51
1:F:30:ASP:OD1	1:F:30:ASP:N	2.44	0.50
1:G:299:ASP:OD1	1:G:299:ASP:C	2.51	0.50
2:J:346:VAL:HG11	2:M:346:VAL:HG22	1.93	0.50
1:A:48:ASP:N	1:A:48:ASP:OD1	2.43	0.50
1:B:439:GLY:HA3	2:K:297:GLU:OE1	2.12	0.50
1:F:349:ASP:OD1	1:F:349:ASP:N	2.39	0.50
2:P:346:VAL:HG11	2:Q:346:VAL:HG22	1.93	0.50
2:I:141:TYR:OH	2:I:153:PHE:O	2.29	0.50
2:L:290:VAL:HG22	2:L:430:VAL:HB	1.92	0.50
2:K:307:LEU:HD11	2:K:347:LEU:HB2	1.94	0.49
2:P:307:LEU:HD11	2:P:347:LEU:HB2	1.94	0.49
2:L:383:VAL:HG13	2:L:427:VAL:HG13	1.94	0.49
1:D:299:ASP:C	1:D:299:ASP:OD1	2.55	0.49
2:J:383:VAL:HG13	2:J:427:VAL:HG13	1.94	0.49
2:K:306:VAL:HG13	2:K:346:VAL:HG12	1.95	0.49
2:O:309:VAL:HB	2:O:343:ARG:HB2	1.95	0.49
2:P:292:ARG:HD3	2:P:432:ARG:HB3	1.95	0.49
2:J:292:ARG:HD3	2:J:432:ARG:HB3	1.95	0.49
2:M:309:VAL:HB	2:M:343:ARG:HB2	1.95	0.49
1:B:210:ARG:NE	1:H:282:ARG:HH22	2.11	0.49
1:D:282:ARG:HH22	1:F:210:ARG:NE	2.11	0.49
2:P:306:VAL:HG21	2:P:335:VAL:HG11	1.95	0.49
2:J:306:VAL:HG13	2:J:346:VAL:HG12	1.95	0.49
2:K:383:VAL:HG13	2:K:427:VAL:HG13	1.94	0.48
2:J:306:VAL:HG21	2:J:335:VAL:HG11	1.95	0.48
2:N:309:VAL:HB	2:N:343:ARG:HB2	1.95	0.48
2:P:383:VAL:HG13	2:P:427:VAL:HG13	1.94	0.48
2:P:306:VAL:HG13	2:P:346:VAL:HG12	1.95	0.48
1:A:425:VAL:HG13	1:A:428:ARG:HH21	1.79	0.48
2:I:133:ASP:HA	2:I:136:ARG:HD2	1.96	0.48
2:J:307:LEU:HD11	2:J:347:LEU:HB2	1.94	0.48
2:K:306:VAL:HG21	2:K:335:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:292:ARG:HD3	2:L:432:ARG:HB3	1.95	0.48
2:I:175:ASN:O	2:I:176:PRO:C	2.56	0.48
2:J:290:VAL:HG13	2:J:430:VAL:HB	1.95	0.48
2:P:435:ARG:HD2	2:P:435:ARG:HA	1.58	0.48
1:B:210:ARG:HG3	1:H:282:ARG:HH22	1.79	0.48
1:C:25:ASP:OD1	1:C:25:ASP:N	2.44	0.48
1:H:25:ASP:OD1	1:H:25:ASP:N	2.45	0.48
2:I:139:LYS:HD2	2:I:139:LYS:HA	1.52	0.48
1:F:327:THR:OG1	1:F:328:VAL:N	2.47	0.48
1:H:48:ASP:OD1	1:H:48:ASP:N	2.42	0.48
1:D:282:ARG:HH22	1:F:210:ARG:HG3	1.78	0.48
2:Q:309:VAL:HB	2:Q:343:ARG:HB2	1.95	0.48
1:B:327:THR:OG1	1:B:328:VAL:N	2.47	0.47
1:F:120:ASN:OD1	1:F:120:ASN:N	2.44	0.47
2:I:109:LEU:HB3	2:I:113:GLN:HG3	1.95	0.47
2:M:304:VAL:HG22	2:M:348:PRO:HA	1.96	0.47
1:B:436:ARG:HD3	2:K:291:VAL:HG13	1.95	0.47
1:G:44:GLY:H	2:P:300:GLU:HG3	1.79	0.47
1:E:48:ASP:OD1	1:E:48:ASP:N	2.43	0.47
1:H:299:ASP:OD1	1:H:299:ASP:C	2.55	0.47
2:Q:316:GLU:H	2:Q:316:GLU:HG3	1.47	0.47
1:H:29:LYS:NZ	2:I:129:LYS:HB3	2.29	0.47
1:B:436:ARG:HB3	2:K:291:VAL:HG12	1.96	0.47
1:D:120:ASN:OD1	1:D:120:ASN:N	2.39	0.47
1:H:327:THR:OG1	1:H:328:VAL:N	2.48	0.47
1:D:327:THR:OG1	1:D:328:VAL:N	2.48	0.47
2:M:327:ILE:HB	2:M:336:GLU:HG2	1.97	0.47
2:N:304:VAL:HG22	2:N:348:PRO:HA	1.96	0.47
2:O:304:VAL:HG22	2:O:348:PRO:HA	1.96	0.47
2:P:304:VAL:HG13	2:Q:346:VAL:HB	1.97	0.47
2:Q:304:VAL:HG22	2:Q:348:PRO:HA	1.96	0.47
2:I:55:PRO:HA	2:I:58:ILE:HB	1.96	0.46
2:O:327:ILE:HB	2:O:336:GLU:HG2	1.97	0.46
2:O:308:PRO:HG2	2:O:361:VAL:HG23	1.97	0.46
2:P:299:ALA:O	2:P:301:ALA:N	2.49	0.46
2:J:294:LYS:HA	2:J:294:LYS:HD2	1.33	0.46
2:N:327:ILE:HB	2:N:336:GLU:HG2	1.97	0.46
2:K:431:VAL:HB	2:K:432:ARG:H	1.43	0.46
2:P:312:ALA:HA	2:P:407:LEU:HD12	1.97	0.46
1:H:75:ASP:OD1	1:H:75:ASP:N	2.44	0.46
2:I:58:ILE:HA	2:I:61:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:312:ALA:HA	2:J:407:LEU:HD12	1.97	0.46
2:K:431:VAL:O	2:K:432:ARG:HB2	2.15	0.46
2:L:312:ALA:HA	2:L:407:LEU:HD12	1.97	0.46
2:Q:387:ARG:H	2:Q:387:ARG:HG2	1.42	0.46
2:N:308:PRO:HG2	2:N:361:VAL:HG23	1.97	0.45
1:B:399:PHE:O	1:B:400:GLY:C	2.59	0.45
2:K:312:ALA:HA	2:K:407:LEU:HD12	1.97	0.45
2:Q:308:PRO:HG2	2:Q:361:VAL:HG23	1.97	0.45
2:Q:327:ILE:HB	2:Q:336:GLU:HG2	1.97	0.45
2:K:435:ARG:HD2	2:K:435:ARG:HA	1.52	0.45
2:M:308:PRO:HG2	2:M:361:VAL:HG23	1.97	0.45
2:N:324:MET:HE3	2:N:324:MET:HB3	1.66	0.45
1:E:229:THR:OG1	1:E:230:GLY:N	2.49	0.45
2:M:382:LEU:HB3	2:M:431:VAL:HB	1.99	0.45
2:P:363:VAL:O	2:P:382:LEU:HA	2.17	0.45
1:C:384:MET:N	1:C:385:PRO:CD	2.80	0.45
2:M:323:PRO:HG3	2:M:339:LYS:HB2	1.99	0.45
1:G:384:MET:N	1:G:385:PRO:CD	2.80	0.45
1:B:210:ARG:CD	1:H:282:ARG:HH22	2.29	0.44
2:K:363:VAL:O	2:K:382:LEU:HA	2.17	0.44
2:P:431:VAL:CG1	2:Q:331:ASP:HB2	2.48	0.44
2:O:323:PRO:HG3	2:O:339:LYS:HB2	1.99	0.44
2:I:152:ASP:OD2	2:I:199:ARG:NH2	2.41	0.44
2:L:435:ARG:HD2	2:L:435:ARG:HA	1.58	0.44
2:N:323:PRO:HG3	2:N:339:LYS:HB2	1.99	0.44
1:C:204:ASN:H	1:C:206:GLN:HE22	1.65	0.44
1:D:282:ARG:HH22	1:F:210:ARG:CD	2.29	0.44
2:L:347:LEU:HD21	2:O:332:PHE:CD2	2.52	0.44
1:B:425:VAL:HG13	1:B:428:ARG:HH21	1.82	0.44
2:I:15:ILE:HG13	2:I:16:PRO:HD2	2.00	0.44
2:J:431:VAL:CG1	2:M:331:ASP:HB2	2.47	0.44
2:L:347:LEU:HD22	2:L:347:LEU:HA	1.83	0.44
2:L:431:VAL:CG1	2:O:331:ASP:HB2	2.47	0.44
2:P:294:LYS:HB3	2:P:297:GLU:HB2	1.99	0.44
1:A:327:THR:OG1	1:A:328:VAL:N	2.51	0.44
2:J:435:ARG:HD2	2:J:435:ARG:HA	1.59	0.44
1:D:25:ASP:OD1	1:D:25:ASP:N	2.45	0.44
1:H:384:MET:N	1:H:385:PRO:CD	2.81	0.44
2:K:347:LEU:HD21	2:N:332:PHE:CD2	2.52	0.44
2:L:294:LYS:HD2	2:L:294:LYS:HA	1.33	0.44
2:L:349:SER:O	2:O:300:GLU:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:382:LEU:HB3	2:N:431:VAL:HB	2.00	0.44
2:O:382:LEU:HB3	2:O:431:VAL:HB	1.99	0.44
2:Q:382:LEU:HB3	2:Q:431:VAL:HB	1.99	0.44
1:B:120:ASN:OD1	1:B:120:ASN:N	2.44	0.44
1:G:204:ASN:H	1:G:206:GLN:HE22	1.65	0.44
2:J:347:LEU:HD21	2:M:332:PHE:CD2	2.53	0.44
2:N:387:ARG:H	2:N:387:ARG:HG2	1.42	0.44
2:Q:323:PRO:HG3	2:Q:339:LYS:HB2	1.99	0.44
1:D:384:MET:N	1:D:385:PRO:CD	2.81	0.44
1:G:25:ASP:OD1	1:G:25:ASP:N	2.44	0.44
1:G:120:ASN:OD1	1:G:120:ASN:N	2.48	0.44
2:Q:317:LYS:H	2:Q:317:LYS:HG3	1.52	0.44
2:J:366:ARG:HD2	2:J:366:ARG:HA	1.64	0.43
2:L:363:VAL:O	2:L:382:LEU:HA	2.17	0.43
2:K:349:SER:O	2:N:300:GLU:HA	2.18	0.43
2:J:349:SER:O	2:M:300:GLU:HA	2.18	0.43
2:P:347:LEU:HD21	2:Q:332:PHE:CD2	2.52	0.43
1:D:75:ASP:OD1	1:D:75:ASP:N	2.44	0.43
2:L:415:LEU:HD23	2:L:415:LEU:HA	1.85	0.43
2:P:298:VAL:O	2:Q:302:THR:HG21	2.18	0.43
1:F:399:PHE:O	1:F:400:GLY:C	2.59	0.43
1:B:210:ARG:CD	1:H:282:ARG:NH2	2.81	0.43
1:G:46:PRO:HG3	2:Q:299:ALA:HB1	2.01	0.43
2:K:431:VAL:HG12	2:N:331:ASP:HB2	2.00	0.43
2:Q:324:MET:HE3	2:Q:324:MET:HB3	1.66	0.43
2:P:349:SER:O	2:Q:300:GLU:HA	2.18	0.43
2:K:347:LEU:HD21	2:N:332:PHE:CE2	2.54	0.43
2:L:318:LYS:HG3	2:L:341:TRP:HZ2	1.84	0.43
2:P:294:LYS:HD2	2:P:294:LYS:HA	1.28	0.43
1:D:282:ARG:NH2	1:F:210:ARG:CD	2.81	0.43
2:J:347:LEU:HD21	2:M:332:PHE:CE2	2.54	0.43
2:M:368:ASP:HB3	2:M:381:LEU:HD13	2.01	0.43
1:E:327:THR:OG1	1:E:328:VAL:N	2.51	0.43
2:K:366:ARG:HA	2:K:366:ARG:HD2	1.46	0.43
2:L:382:LEU:H	2:L:431:VAL:HG21	1.84	0.43
2:M:387:ARG:H	2:M:387:ARG:HG2	1.42	0.43
2:P:382:LEU:H	2:P:431:VAL:HG21	1.84	0.43
2:J:382:LEU:H	2:J:431:VAL:HG21	1.84	0.42
1:D:30:ASP:OD2	1:E:30:ASP:OD2	2.38	0.42
1:D:411:ALA:N	1:D:412:PRO:CD	2.82	0.42
2:J:318:LYS:HG3	2:J:341:TRP:HZ2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:318:LYS:HG3	2:K:341:TRP:HZ2	1.84	0.42
2:L:297:GLU:HB2	2:O:302:THR:HG21	2.02	0.42
2:P:347:LEU:HD21	2:Q:332:PHE:CE2	2.54	0.42
2:Q:368:ASP:HB3	2:Q:381:LEU:HD13	2.01	0.42
1:B:384:MET:N	1:B:385:PRO:CD	2.82	0.42
1:H:411:ALA:N	1:H:412:PRO:CD	2.82	0.42
2:I:19:PHE:CD2	2:I:44:LEU:HD11	2.54	0.42
2:P:318:LYS:HG3	2:P:341:TRP:HZ2	1.84	0.42
2:P:415:LEU:HD23	2:P:415:LEU:HA	1.85	0.42
2:L:306:VAL:HG21	2:L:335:VAL:HG11	2.00	0.42
2:M:324:MET:HE3	2:M:324:MET:HB3	1.66	0.42
1:E:384:MET:N	1:E:385:PRO:CD	2.83	0.42
2:P:366:ARG:HD2	2:P:366:ARG:HA	1.46	0.42
1:A:384:MET:N	1:A:385:PRO:CD	2.83	0.42
2:L:370:LYS:HD3	2:L:370:LYS:HA	1.79	0.42
2:M:383:VAL:HG13	2:M:427:VAL:HG13	2.02	0.42
2:O:324:MET:HE3	2:O:324:MET:HB3	1.66	0.42
2:O:387:ARG:H	2:O:387:ARG:HG2	1.42	0.42
1:A:411:ALA:N	1:A:412:PRO:CD	2.82	0.42
2:I:136:ARG:HE	2:I:136:ARG:HB3	1.34	0.42
2:N:317:LYS:H	2:N:317:LYS:HG3	1.52	0.42
2:O:383:VAL:HG13	2:O:427:VAL:HG13	2.02	0.42
2:P:370:LYS:HD3	2:P:370:LYS:HA	1.79	0.42
1:A:30:ASP:OD2	1:H:30:ASP:OD2	2.37	0.42
1:C:327:THR:OG1	1:C:328:VAL:N	2.53	0.42
2:L:318:LYS:HD2	2:L:318:LYS:HA	1.90	0.42
2:L:347:LEU:HD21	2:O:332:PHE:CE2	2.54	0.42
2:M:316:GLU:H	2:M:316:GLU:HG3	1.47	0.42
1:E:411:ALA:N	1:E:412:PRO:CD	2.82	0.42
1:G:327:THR:OG1	1:G:328:VAL:N	2.53	0.42
2:I:165:LEU:HD12	2:I:168:ARG:HH21	1.85	0.42
2:N:383:VAL:HG13	2:N:427:VAL:HG13	2.02	0.42
1:A:120:ASN:OD1	1:A:120:ASN:N	2.51	0.42
2:N:316:GLU:H	2:N:316:GLU:HG3	1.47	0.42
2:O:368:ASP:HB3	2:O:381:LEU:HD13	2.01	0.42
2:Q:383:VAL:HG13	2:Q:427:VAL:HG13	2.02	0.42
2:K:297:GLU:HB2	2:N:302:THR:HG21	2.02	0.41
2:L:382:LEU:N	2:L:431:VAL:HG11	2.35	0.41
1:F:384:MET:N	1:F:385:PRO:CD	2.82	0.41
2:P:318:LYS:HD2	2:P:318:LYS:HA	1.90	0.41
2:Q:316:GLU:HA	2:Q:319:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:61:LEU:HD22	2:I:61:LEU:HA	1.85	0.41
2:I:78:VAL:HG13	2:I:114:ARG:HD3	2.01	0.41
2:K:431:VAL:CG1	2:N:331:ASP:HB2	2.51	0.41
2:N:342:LYS:HZ3	2:N:342:LYS:HG3	1.69	0.41
1:H:399:PHE:O	1:H:400:GLY:C	2.62	0.41
2:N:342:LYS:HZ3	2:N:342:LYS:H	1.69	0.41
1:F:265:ASP:OD1	1:F:265:ASP:C	2.62	0.41
1:H:265:ASP:OD1	1:H:265:ASP:C	2.64	0.41
2:O:392:VAL:HG12	2:O:416:LYS:HE2	2.02	0.41
2:P:382:LEU:N	2:P:431:VAL:HG11	2.35	0.41
1:B:265:ASP:OD1	1:B:265:ASP:C	2.62	0.41
2:I:118:ALA:HA	2:I:121:ILE:HG12	2.02	0.41
2:M:292:ARG:NH2	2:M:435:ARG:HE	2.19	0.41
2:M:390:ASN:HB2	2:M:423:SER:O	2.21	0.41
2:N:368:ASP:HB3	2:N:381:LEU:HD13	2.01	0.41
2:O:316:GLU:H	2:O:316:GLU:HG3	1.47	0.41
2:O:316:GLU:HA	2:O:319:ILE:HD12	2.03	0.41
2:Q:392:VAL:HG12	2:Q:416:LYS:HE2	2.02	0.41
2:N:390:ASN:HB2	2:N:423:SER:O	2.21	0.41
2:J:347:LEU:HD22	2:J:347:LEU:HA	1.83	0.41
2:J:433:PRO:O	2:J:434:PRO:C	2.64	0.41
2:K:318:LYS:HD2	2:K:318:LYS:HA	1.90	0.41
2:M:392:VAL:HG12	2:M:416:LYS:HE2	2.02	0.41
2:P:290:VAL:HG22	2:P:430:VAL:CG2	2.51	0.41
2:P:301:ALA:N	2:Q:302:THR:H	2.18	0.41
2:Q:322:ALA:HA	2:Q:323:PRO:HD3	1.98	0.41
2:J:297:GLU:HB2	2:M:302:THR:HG21	2.02	0.41
2:M:389:ARG:H	2:M:389:ARG:HG2	1.72	0.41
2:O:390:ASN:HB2	2:O:423:SER:O	2.21	0.41
1:C:120:ASN:OD1	1:C:120:ASN:N	2.48	0.40
1:H:352:GLU:OE2	2:I:177:SER:HA	2.21	0.40
2:N:392:VAL:HG12	2:N:416:LYS:HE2	2.02	0.40
2:I:104:TYR:O	2:I:107:ARG:HD3	2.21	0.40
2:I:133:ASP:OD1	2:I:136:ARG:NH1	2.53	0.40
2:K:289:PRO:O	2:K:430:VAL:N	2.45	0.40
2:K:342:LYS:HZ2	2:K:342:LYS:HG3	1.76	0.40
2:N:319:ILE:H	2:N:319:ILE:HG13	1.75	0.40
2:P:433:PRO:O	2:P:434:PRO:C	2.63	0.40
1:H:148:PRO:HA	1:H:149:PRO:HD3	1.97	0.40
2:J:304:VAL:H	2:J:304:VAL:HG23	1.60	0.40
2:K:290:VAL:HG22	2:K:430:VAL:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:370:LYS:HD3	2:K:370:LYS:HA	1.79	0.40
2:P:384:VAL:HG23	2:Q:332:PHE:CZ	2.56	0.40
2:K:384:VAL:HG23	2:N:332:PHE:CZ	2.56	0.40
2:M:333:LYS:O	2:M:334:VAL:C	2.65	0.40
2:N:316:GLU:HA	2:N:319:ILE:HD12	2.03	0.40
2:J:370:LYS:HD3	2:J:370:LYS:HA	1.78	0.40
2:J:382:LEU:N	2:J:431:VAL:HG11	2.35	0.40
2:K:319:ILE:HG21	2:K:424:LEU:HB3	2.04	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	403/471 (86%)	394 (98%)	8 (2%)	1 (0%)	43	73
1	B	410/471 (87%)	406 (99%)	4 (1%)	0	100	100
1	C	406/471 (86%)	401 (99%)	5 (1%)	0	100	100
1	D	404/471 (86%)	400 (99%)	4 (1%)	0	100	100
1	E	403/471 (86%)	394 (98%)	8 (2%)	1 (0%)	43	73
1	F	410/471 (87%)	406 (99%)	4 (1%)	0	100	100
1	G	406/471 (86%)	401 (99%)	5 (1%)	0	100	100
1	H	404/471 (86%)	400 (99%)	4 (1%)	0	100	100
2	I	193/346 (56%)	179 (93%)	13 (7%)	1 (0%)	24	57
2	J	145/346 (42%)	137 (94%)	6 (4%)	2 (1%)	9	34
2	K	145/346 (42%)	140 (97%)	2 (1%)	3 (2%)	5	25
2	L	145/346 (42%)	136 (94%)	7 (5%)	2 (1%)	9	34
2	M	148/346 (43%)	142 (96%)	5 (3%)	1 (1%)	18	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	148/346 (43%)	142 (96%)	5 (3%)	1 (1%)	18	49
2	O	148/346 (43%)	142 (96%)	5 (3%)	1 (1%)	18	49
2	P	145/346 (42%)	137 (94%)	5 (3%)	3 (2%)	5	25
2	Q	148/346 (43%)	142 (96%)	5 (3%)	1 (1%)	18	49
All	All	4611/6882 (67%)	4499 (98%)	95 (2%)	17 (0%)	31	61

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	176	PRO
2	K	301	ALA
2	K	431	VAL
2	M	333	LYS
2	N	333	LYS
2	O	333	LYS
2	P	300	GLU
2	Q	333	LYS
1	A	293	ALA
1	E	293	ALA
2	K	432	ARG
2	P	301	ALA
2	J	301	ALA
2	L	301	ALA
2	J	432	ARG
2	L	432	ARG
2	P	432	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	338/382 (88%)	337 (100%)	1 (0%)	86	87
1	B	338/382 (88%)	334 (99%)	4 (1%)	63	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	337/382 (88%)	335 (99%)	2 (1%)	78	83
1	D	339/382 (89%)	339 (100%)	0	100	100
1	E	338/382 (88%)	338 (100%)	0	100	100
1	F	338/382 (88%)	337 (100%)	1 (0%)	86	87
1	G	337/382 (88%)	335 (99%)	2 (1%)	78	83
1	H	339/382 (89%)	339 (100%)	0	100	100
2	I	166/291 (57%)	150 (90%)	16 (10%)	8	30
2	J	119/291 (41%)	71 (60%)	48 (40%)	0	0
2	K	119/291 (41%)	73 (61%)	46 (39%)	0	0
2	L	119/291 (41%)	71 (60%)	48 (40%)	0	0
2	M	115/291 (40%)	78 (68%)	37 (32%)	0	0
2	N	115/291 (40%)	78 (68%)	37 (32%)	0	0
2	O	115/291 (40%)	78 (68%)	37 (32%)	0	0
2	P	119/291 (41%)	71 (60%)	48 (40%)	0	0
2	Q	115/291 (40%)	78 (68%)	37 (32%)	0	0
All	All	3806/5675 (67%)	3442 (90%)	364 (10%)	10	30

All (364) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	428	ARG
1	B	180	LYS
1	B	426	GLN
1	B	428	ARG
1	B	443	ARG
1	C	91	GLU
1	C	180	LYS
1	F	180	LYS
1	G	90	GLU
1	G	180	LYS
2	I	45	ILE
2	I	48	LEU
2	I	51	ASP
2	I	54	THR
2	I	57	THR
2	I	59	GLU
2	I	60	GLU

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Mol	Chain	Res	Type
2	I	61	LEU
2	I	134	LEU
2	I	136	ARG
2	I	139	LYS
2	I	171	ARG
2	I	172	GLU
2	I	174	LYS
2	I	179	GLN
2	I	181	THR
2	J	288	ILE
2	J	290	VAL
2	J	291	VAL
2	J	292	ARG
2	J	294	LYS
2	J	295	PHE
2	J	298	VAL
2	J	302	THR
2	J	303	SER
2	J	305	VAL
2	J	306	VAL
2	J	307	LEU
2	J	311	LYS
2	J	313	GLU
2	J	314	GLU
2	J	316	GLU
2	J	318	LYS
2	J	319	ILE
2	J	333	LYS
2	J	335	VAL
2	J	338	GLU
2	J	339	LYS
2	J	342	LYS
2	J	343	ARG
2	J	345	VAL
2	J	347	LEU
2	J	349	SER
2	J	361	VAL
2	J	364	SER
2	J	366	ARG
2	J	370	LYS
2	J	371	VAL
2	J	379	GLU

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Mol	Chain	Res	Type
2	J	388	VAL
2	J	391	VAL
2	J	393	GLU
2	J	396	ASP
2	J	401	VAL
2	J	402	VAL
2	J	405	ASN
2	J	408	LYS
2	J	413	SER
2	J	418	ARG
2	J	420	VAL
2	J	422	GLU
2	J	430	VAL
2	J	431	VAL
2	J	435	ARG
2	K	288	ILE
2	K	291	VAL
2	K	292	ARG
2	K	294	LYS
2	K	295	PHE
2	K	298	VAL
2	K	305	VAL
2	K	306	VAL
2	K	307	LEU
2	K	311	LYS
2	K	313	GLU
2	K	314	GLU
2	K	316	GLU
2	K	318	LYS
2	K	319	ILE
2	K	333	LYS
2	K	335	VAL
2	K	338	GLU
2	K	339	LYS
2	K	342	LYS
2	K	343	ARG
2	K	345	VAL
2	K	347	LEU
2	K	349	SER
2	K	361	VAL
2	K	363	VAL
2	K	364	SER

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Mol	Chain	Res	Type
2	K	366	ARG
2	K	370	LYS
2	K	371	VAL
2	K	379	GLU
2	K	388	VAL
2	K	391	VAL
2	K	393	GLU
2	K	396	ASP
2	K	401	VAL
2	K	402	VAL
2	K	405	ASN
2	K	408	LYS
2	K	413	SER
2	K	418	ARG
2	K	420	VAL
2	K	422	GLU
2	K	430	VAL
2	K	431	VAL
2	K	435	ARG
2	L	288	ILE
2	L	291	VAL
2	L	292	ARG
2	L	294	LYS
2	L	295	PHE
2	L	298	VAL
2	L	302	THR
2	L	303	SER
2	L	305	VAL
2	L	306	VAL
2	L	307	LEU
2	L	311	LYS
2	L	313	GLU
2	L	314	GLU
2	L	316	GLU
2	L	318	LYS
2	L	319	ILE
2	L	333	LYS
2	L	335	VAL
2	L	338	GLU
2	L	339	LYS
2	L	342	LYS
2	L	343	ARG

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Mol	Chain	Res	Type
2	L	345	VAL
2	L	347	LEU
2	L	349	SER
2	L	361	VAL
2	L	363	VAL
2	L	364	SER
2	L	366	ARG
2	L	370	LYS
2	L	371	VAL
2	L	379	GLU
2	L	388	VAL
2	L	391	VAL
2	L	393	GLU
2	L	396	ASP
2	L	401	VAL
2	L	402	VAL
2	L	405	ASN
2	L	408	LYS
2	L	413	SER
2	L	418	ARG
2	L	420	VAL
2	L	422	GLU
2	L	430	VAL
2	L	431	VAL
2	L	435	ARG
2	M	288	ILE
2	M	300	GLU
2	M	303	SER
2	M	304	VAL
2	M	305	VAL
2	M	306	VAL
2	M	313	GLU
2	M	316	GLU
2	M	317	LYS
2	M	318	LYS
2	M	324	MET
2	M	326	ILE
2	M	331	ASP
2	M	332	PHE
2	M	335	VAL
2	M	336	GLU
2	M	342	LYS

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Mol	Chain	Res	Type
2	M	343	ARG
2	M	345	VAL
2	M	347	LEU
2	M	353	VAL
2	M	361	VAL
2	M	363	VAL
2	M	364	SER
2	M	369	ARG
2	M	371	VAL
2	M	375	ASP
2	M	382	LEU
2	M	387	ARG
2	M	389	ARG
2	M	391	VAL
2	M	393	GLU
2	M	396	ASP
2	M	401	VAL
2	M	402	VAL
2	M	424	LEU
2	M	435	ARG
2	N	288	ILE
2	N	300	GLU
2	N	303	SER
2	N	304	VAL
2	N	305	VAL
2	N	306	VAL
2	N	313	GLU
2	N	316	GLU
2	N	317	LYS
2	N	318	LYS
2	N	324	MET
2	N	326	ILE
2	N	331	ASP
2	N	332	PHE
2	N	335	VAL
2	N	336	GLU
2	N	342	LYS
2	N	343	ARG
2	N	345	VAL
2	N	347	LEU
2	N	353	VAL
2	N	361	VAL

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Mol	Chain	Res	Type
2	N	363	VAL
2	N	364	SER
2	N	369	ARG
2	N	371	VAL
2	N	375	ASP
2	N	382	LEU
2	N	387	ARG
2	N	389	ARG
2	N	391	VAL
2	N	393	GLU
2	N	396	ASP
2	N	401	VAL
2	N	402	VAL
2	N	424	LEU
2	N	435	ARG
2	O	288	ILE
2	O	300	GLU
2	O	303	SER
2	O	304	VAL
2	O	305	VAL
2	O	306	VAL
2	O	313	GLU
2	O	316	GLU
2	O	317	LYS
2	O	318	LYS
2	O	324	MET
2	O	326	ILE
2	O	331	ASP
2	O	332	PHE
2	O	335	VAL
2	O	336	GLU
2	O	342	LYS
2	O	343	ARG
2	O	345	VAL
2	O	347	LEU
2	O	353	VAL
2	O	361	VAL
2	O	363	VAL
2	O	364	SER
2	O	369	ARG
2	O	371	VAL
2	O	375	ASP

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Mol	Chain	Res	Type
2	O	382	LEU
2	O	387	ARG
2	O	389	ARG
2	O	391	VAL
2	O	393	GLU
2	O	396	ASP
2	O	401	VAL
2	O	402	VAL
2	O	424	LEU
2	O	435	ARG
2	P	288	ILE
2	P	291	VAL
2	P	292	ARG
2	P	294	LYS
2	P	295	PHE
2	P	297	GLU
2	P	298	VAL
2	P	300	GLU
2	P	303	SER
2	P	305	VAL
2	P	306	VAL
2	P	307	LEU
2	P	311	LYS
2	P	313	GLU
2	P	314	GLU
2	P	316	GLU
2	P	318	LYS
2	P	319	ILE
2	P	333	LYS
2	P	335	VAL
2	P	339	LYS
2	P	342	LYS
2	P	343	ARG
2	P	345	VAL
2	P	347	LEU
2	P	349	SER
2	P	361	VAL
2	P	363	VAL
2	P	364	SER
2	P	366	ARG
2	P	370	LYS
2	P	371	VAL

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Mol	Chain	Res	Type
2	P	379	GLU
2	P	388	VAL
2	P	391	VAL
2	P	393	GLU
2	P	396	ASP
2	P	401	VAL
2	P	402	VAL
2	P	405	ASN
2	P	408	LYS
2	P	413	SER
2	P	418	ARG
2	P	420	VAL
2	P	422	GLU
2	P	430	VAL
2	P	431	VAL
2	P	435	ARG
2	Q	288	ILE
2	Q	300	GLU
2	Q	303	SER
2	Q	304	VAL
2	Q	305	VAL
2	Q	306	VAL
2	Q	313	GLU
2	Q	316	GLU
2	Q	317	LYS
2	Q	318	LYS
2	Q	324	MET
2	Q	326	ILE
2	Q	331	ASP
2	Q	332	PHE
2	Q	335	VAL
2	Q	336	GLU
2	Q	342	LYS
2	Q	343	ARG
2	Q	345	VAL
2	Q	347	LEU
2	Q	353	VAL
2	Q	361	VAL
2	Q	363	VAL
2	Q	364	SER
2	Q	369	ARG
2	Q	371	VAL

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Mol	Chain	Res	Type
2	Q	375	ASP
2	Q	382	LEU
2	Q	387	ARG
2	Q	389	ARG
2	Q	391	VAL
2	Q	393	GLU
2	Q	396	ASP
2	Q	401	VAL
2	Q	402	VAL
2	Q	424	LEU
2	Q	435	ARG

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

Mol	Chain	Res	Type
1	A	383	HIS
1	B	264	HIS
1	C	202	ASN
1	C	264	HIS
1	C	274	ASN
1	D	204	ASN
1	E	383	HIS
1	F	181	ASN
1	F	206	GLN
1	F	264	HIS
1	G	202	ASN
1	G	206	GLN
1	G	264	HIS
1	G	274	ASN
2	I	18	GLN
2	I	77	GLN
2	M	405	ASN
2	N	405	ASN
2	O	405	ASN
2	Q	405	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

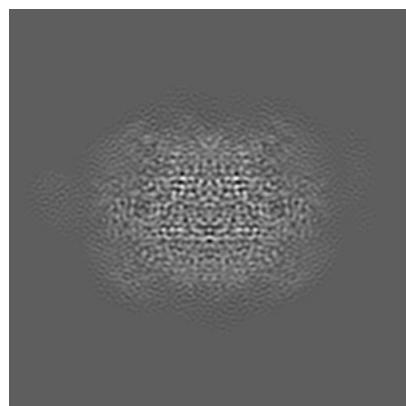
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35605. These allow visual inspection of the internal detail of the map and identification of artifacts.

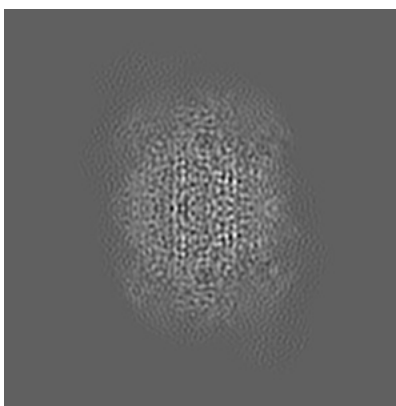
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

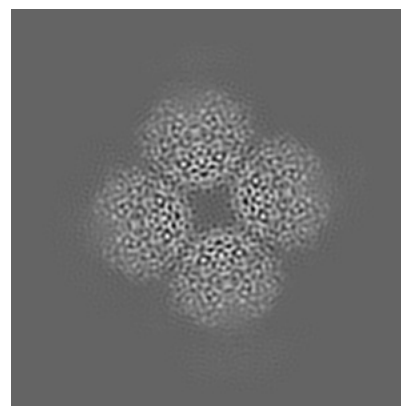
6.1.1 Primary map



X

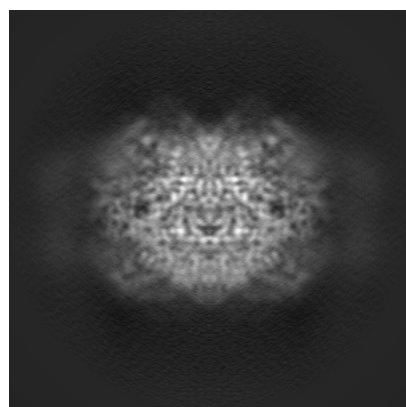


Y

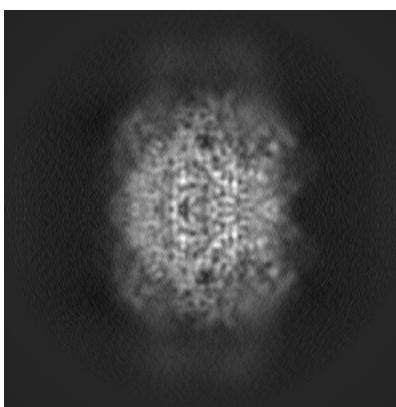


Z

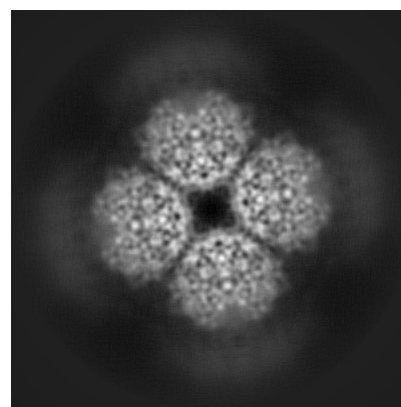
6.1.2 Raw map



X



Y

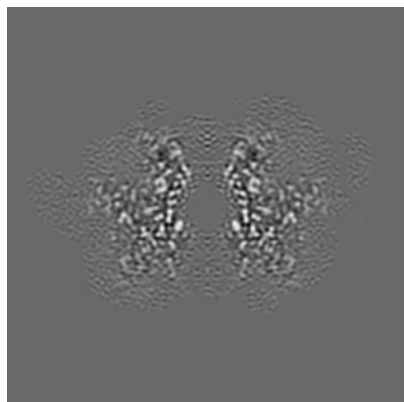


Z

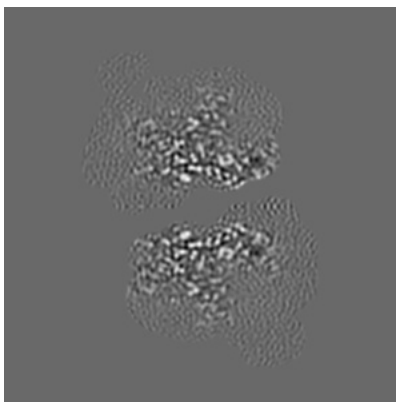
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

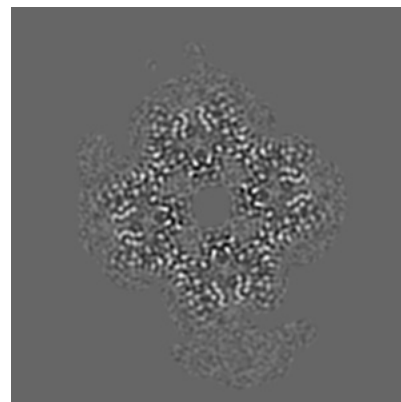
6.2.1 Primary map



X Index: 208

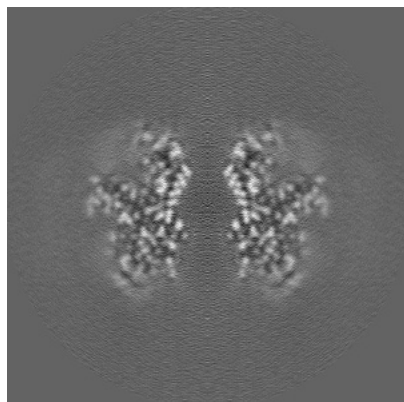


Y Index: 208

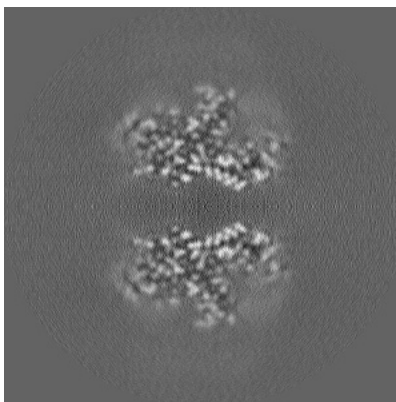


Z Index: 208

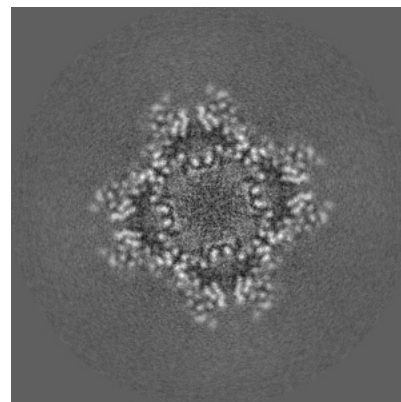
6.2.2 Raw map



X Index: 208



Y Index: 208

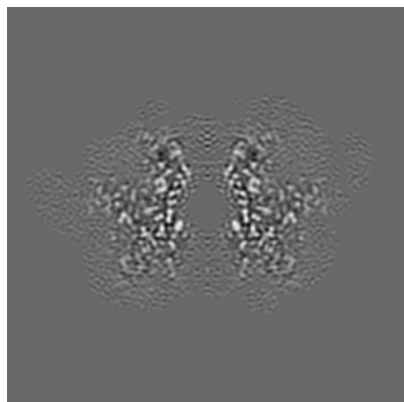


Z Index: 208

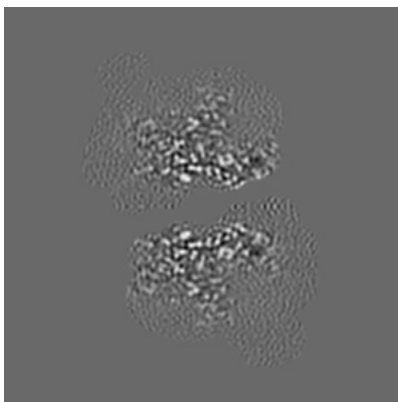
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

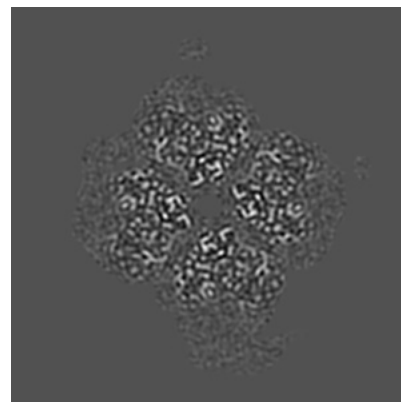
6.3.1 Primary map



X Index: 208

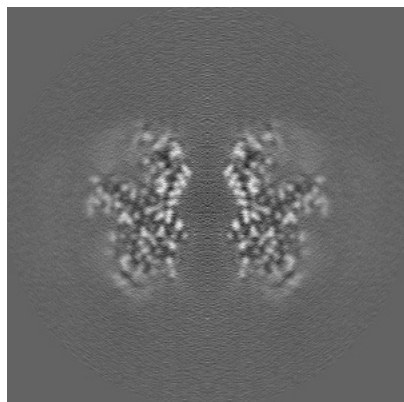


Y Index: 208

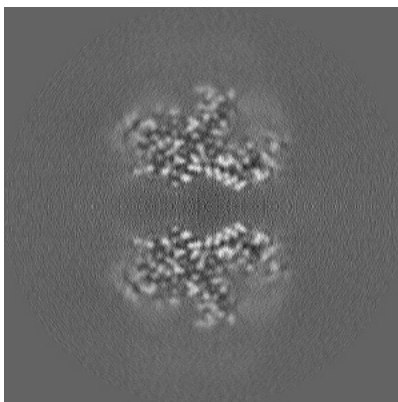


Z Index: 193

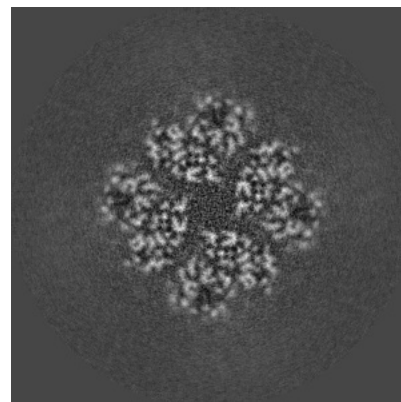
6.3.2 Raw map



X Index: 208



Y Index: 208

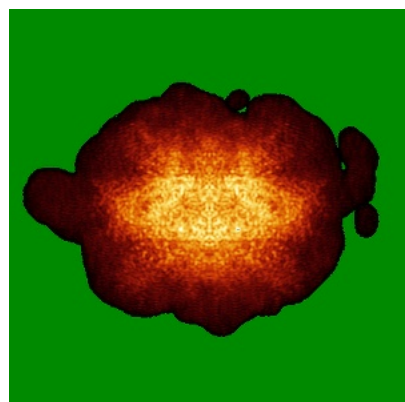


Z Index: 223

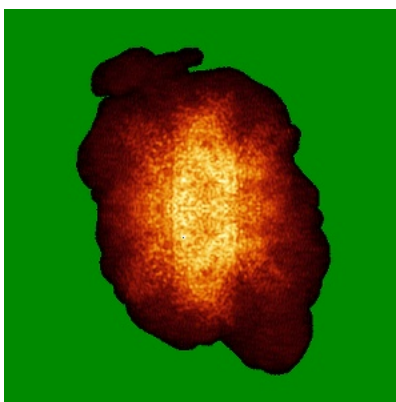
The images above show the largest variance slices of the map in three orthogonal directions.

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

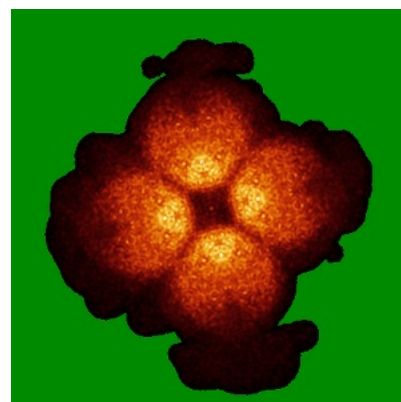
6.4.1 Primary map



X

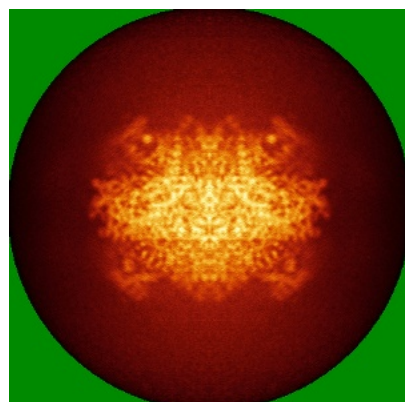


Y

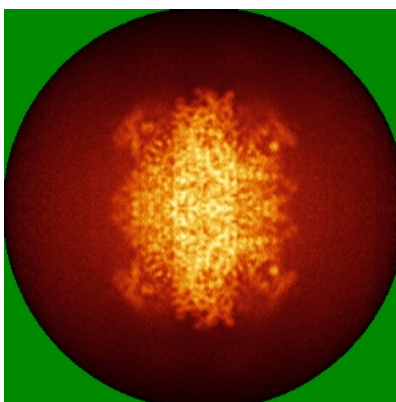


Z

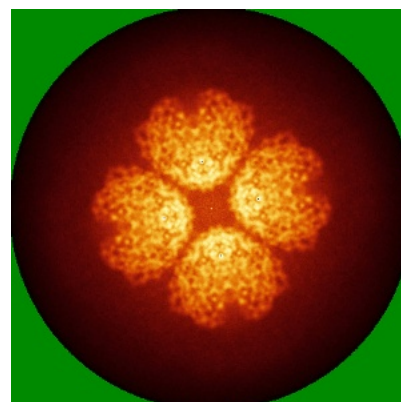
6.4.2 Raw map



X



Y

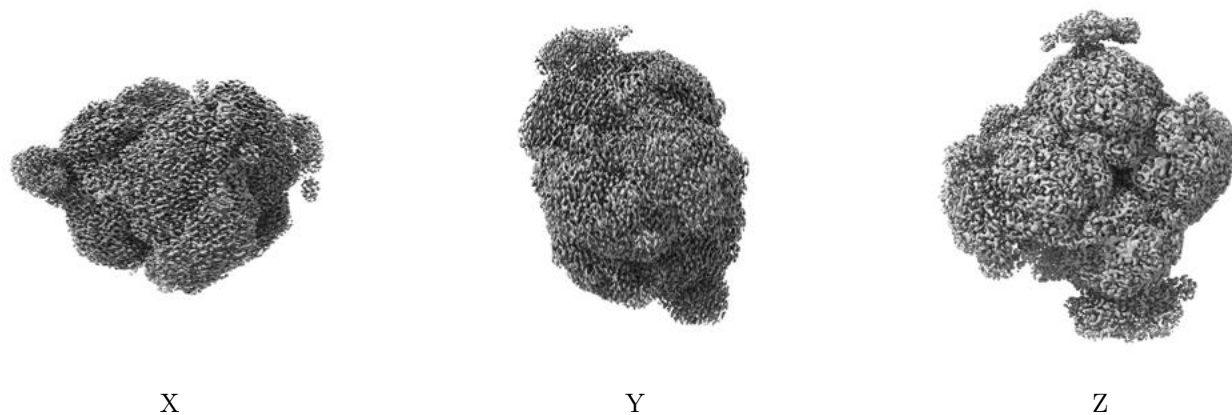


Z

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

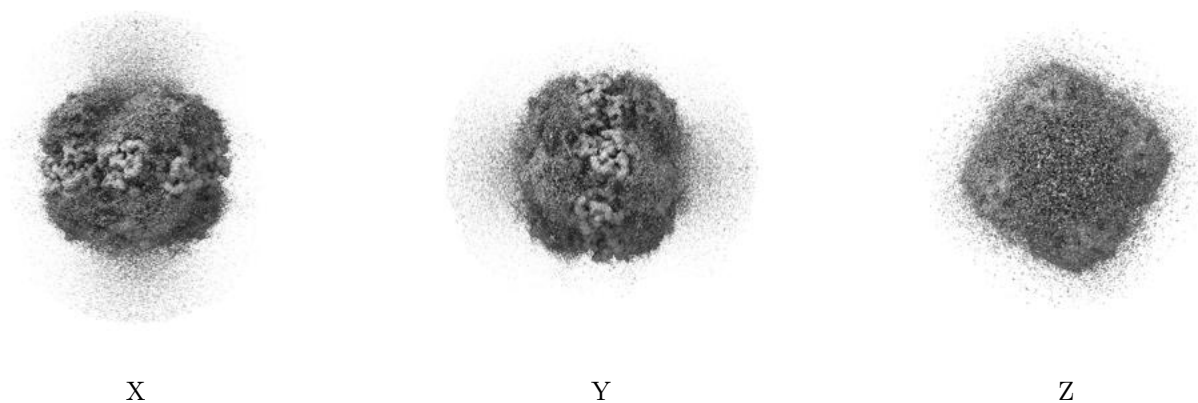
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. 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.

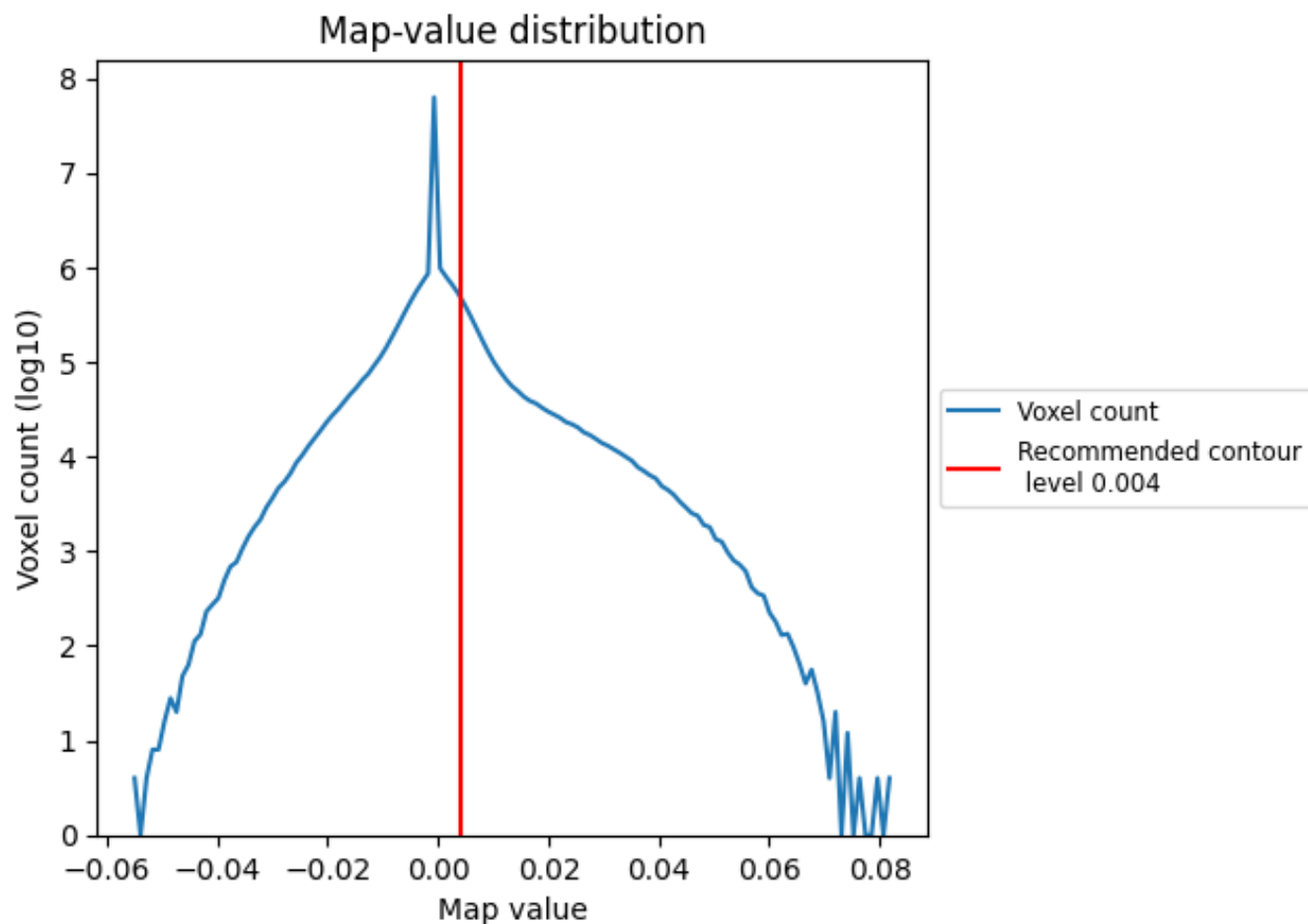
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

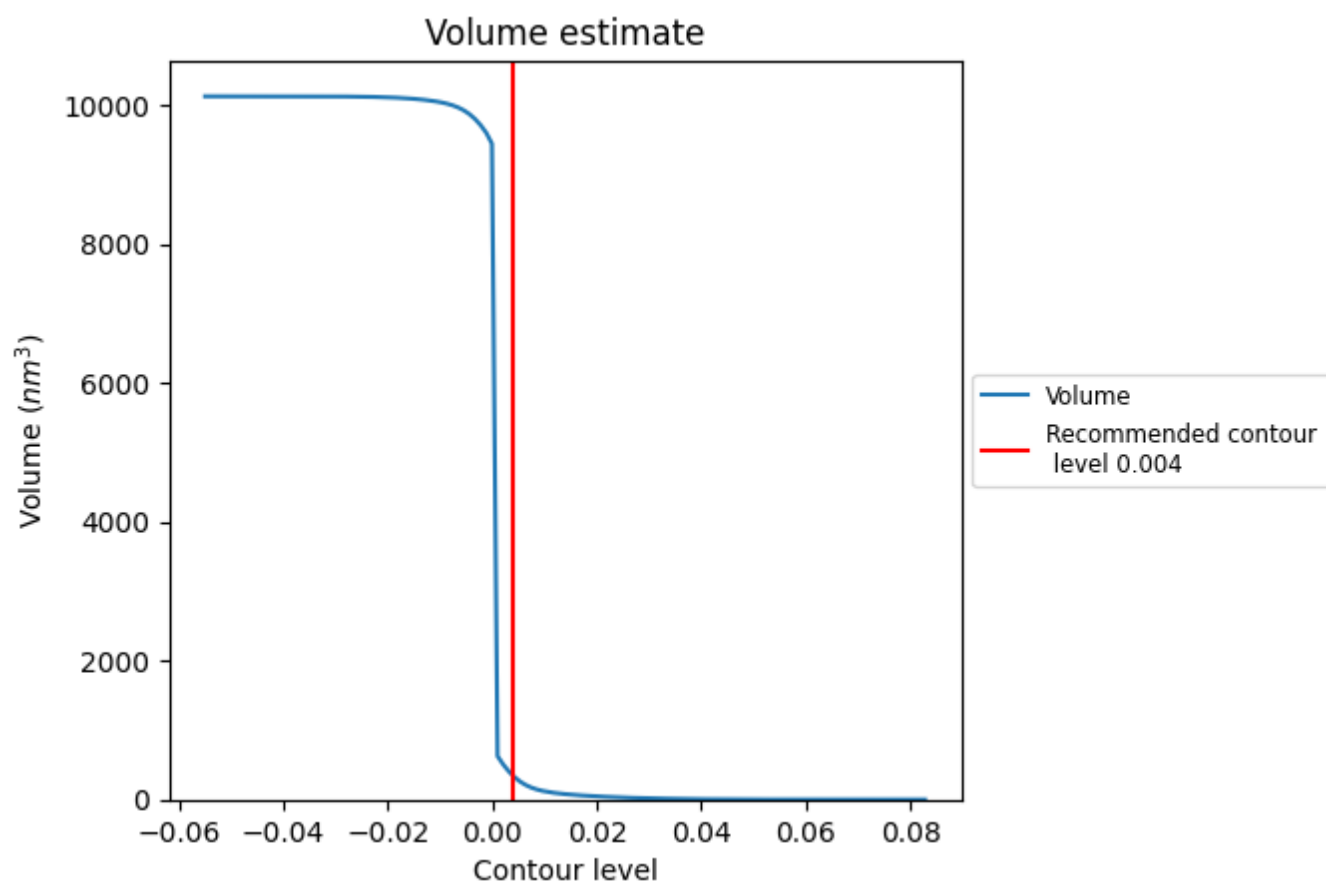
This section contains the results of statistical analysis of the map.

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.

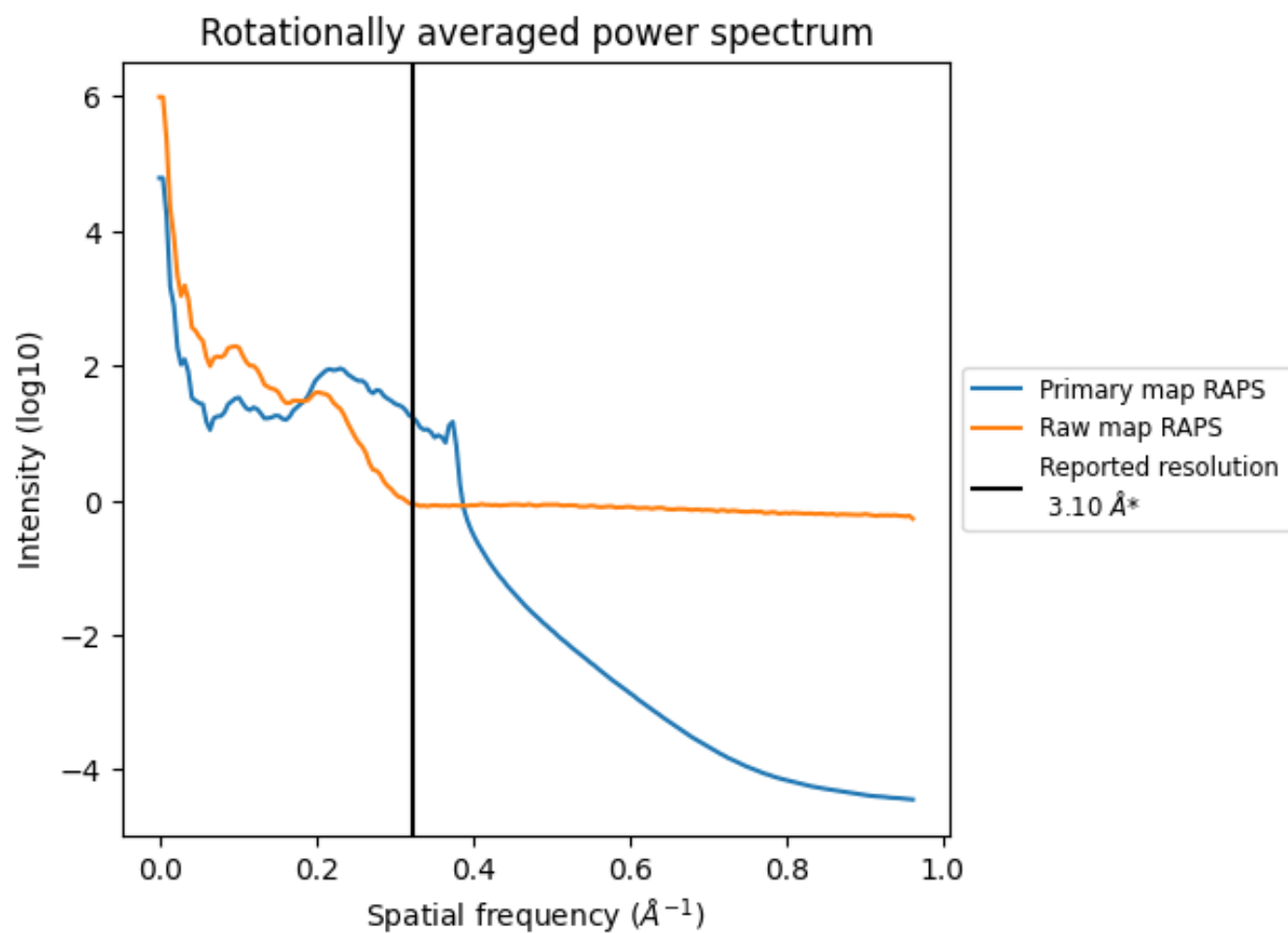
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 344 nm³; this corresponds to an approximate mass of 311 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 [i](#)

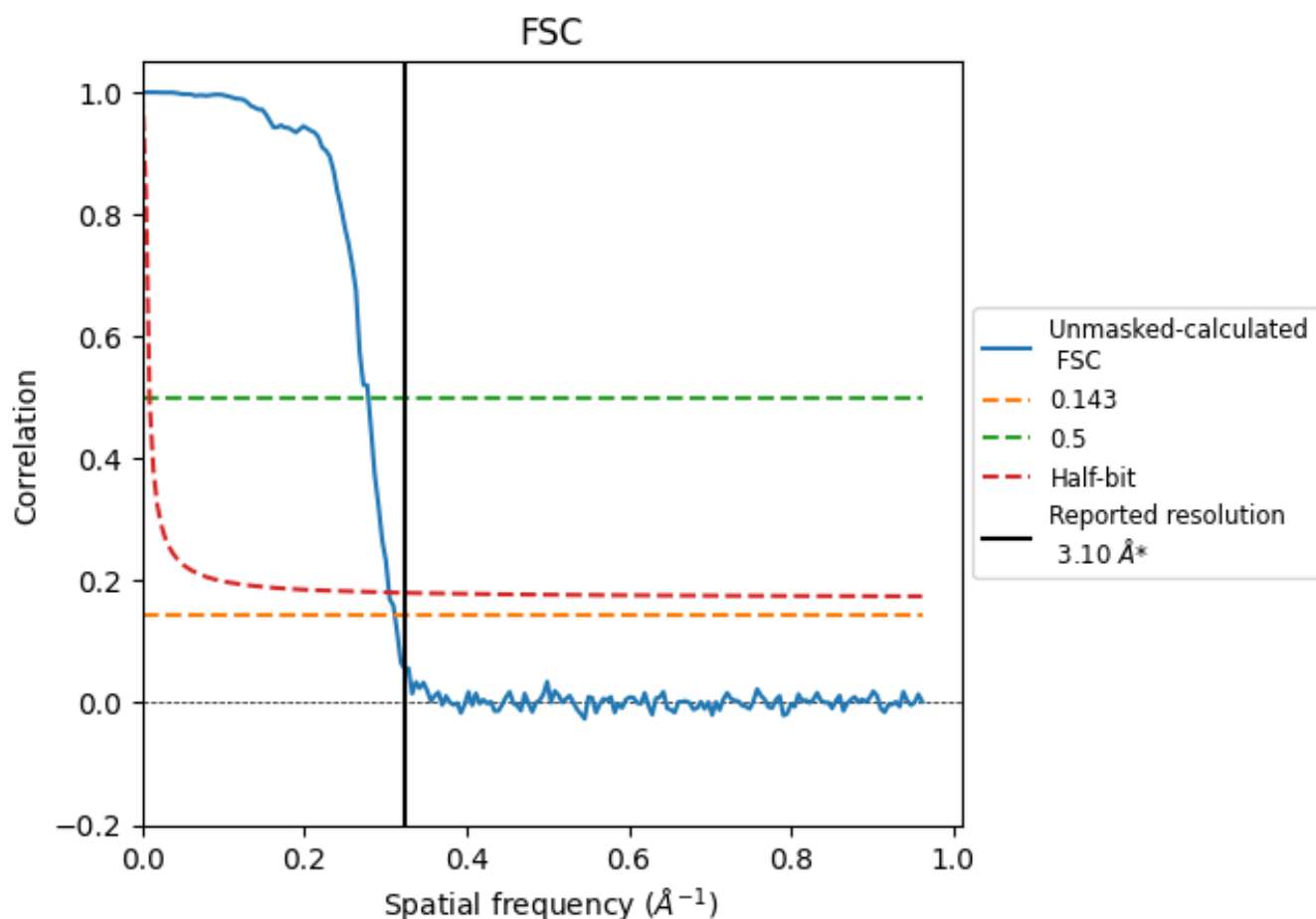


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

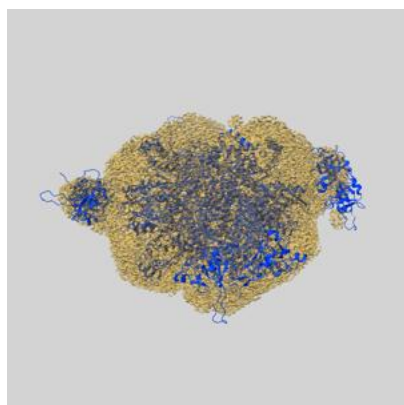
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.21	3.59	3.29

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

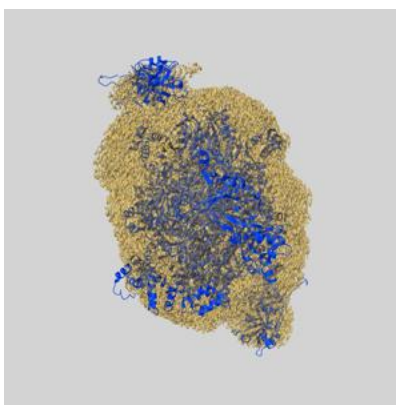
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35605 and PDB model 8IO2. Per-residue inclusion information can be found in section 3 on page 10.

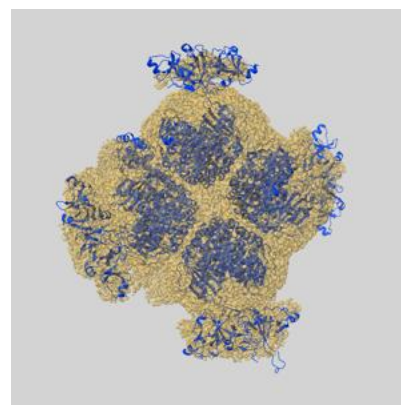
9.1 Map-model overlay [i](#)



X



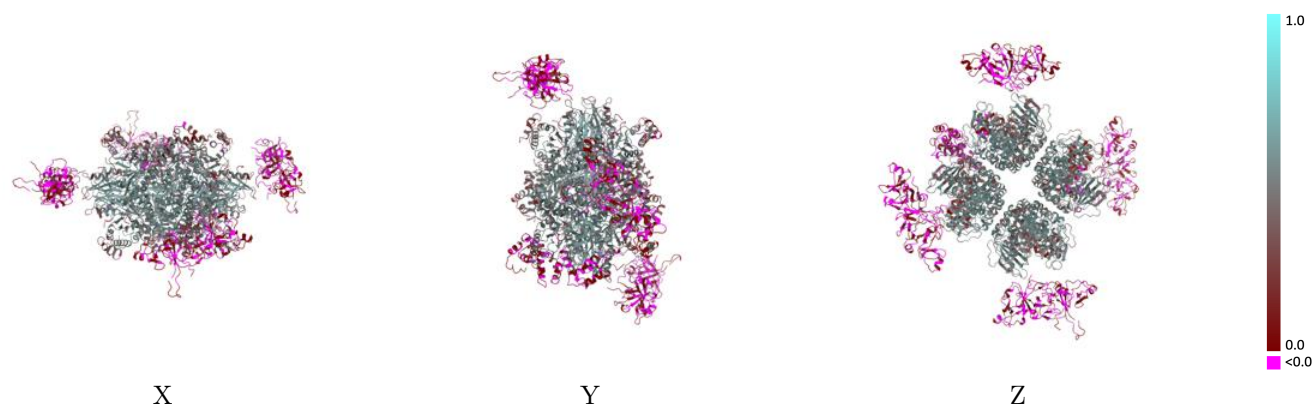
Y



Z

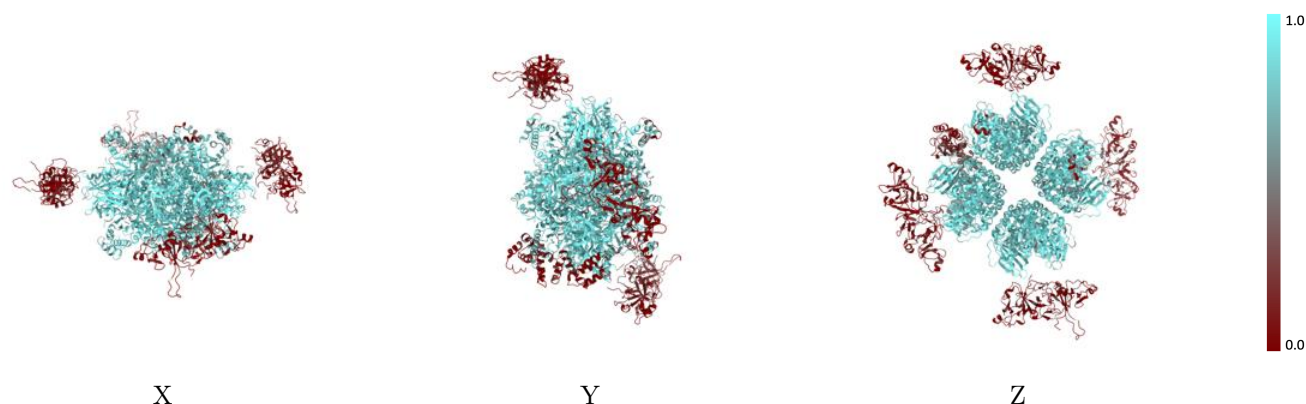
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



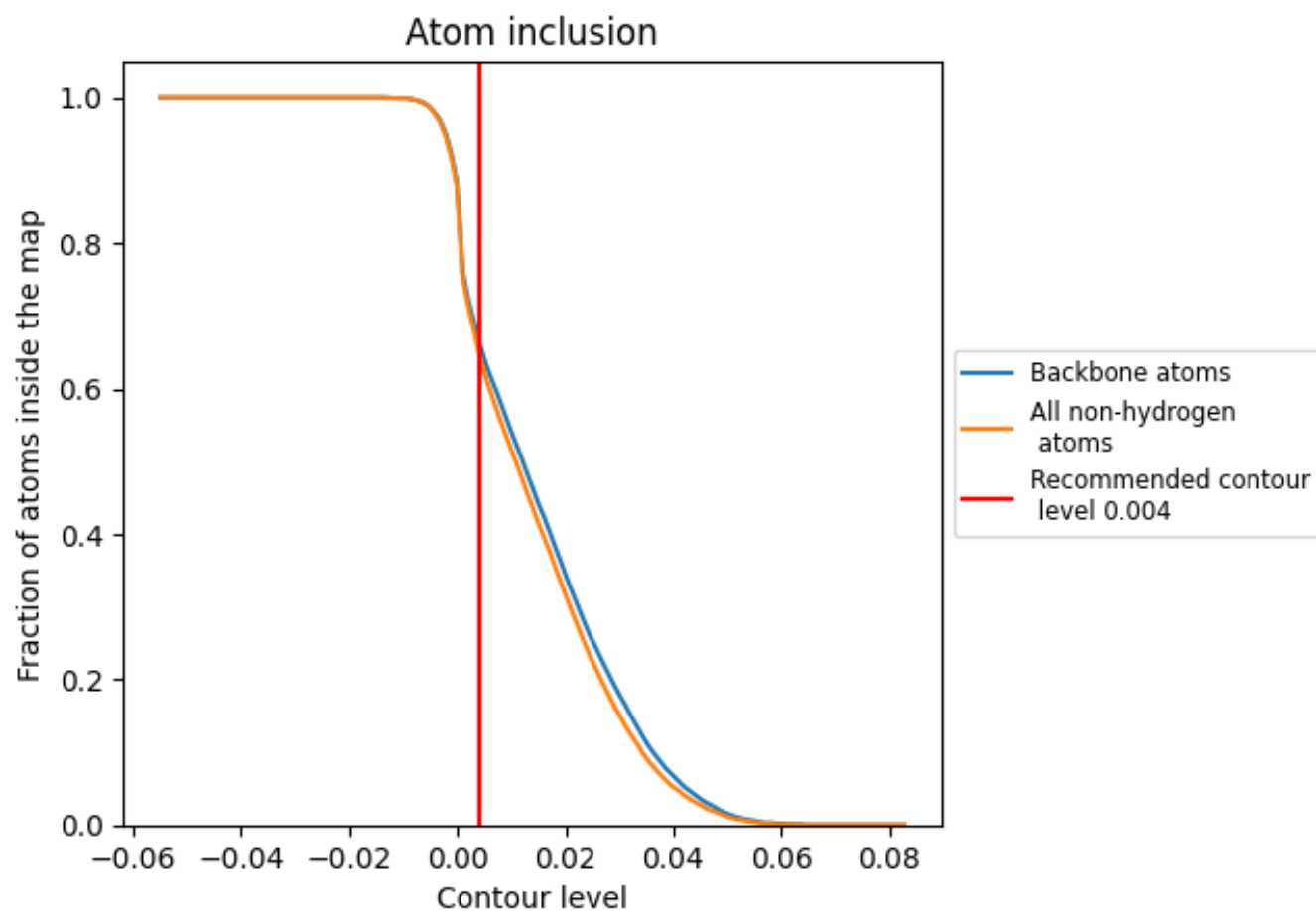
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 65% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6500	0.3620
A	0.8820	0.5030
B	0.8830	0.5050
C	0.8950	0.5110
D	0.8720	0.4940
E	0.8950	0.4980
F	0.8530	0.4820
G	0.8910	0.5050
H	0.8630	0.4870
I	0.1170	0.0350
J	0.0690	0.0300
K	0.1180	0.0280
L	0.0810	0.0140
M	0.0680	0.0140
N	0.1040	0.0380
O	0.1190	0.0470
P	0.0450	0.0200
Q	0.0400	0.0180

1.0

0.0

<0.0