



Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 07:05 PM JST

PDB ID : 8IO2
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.

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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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

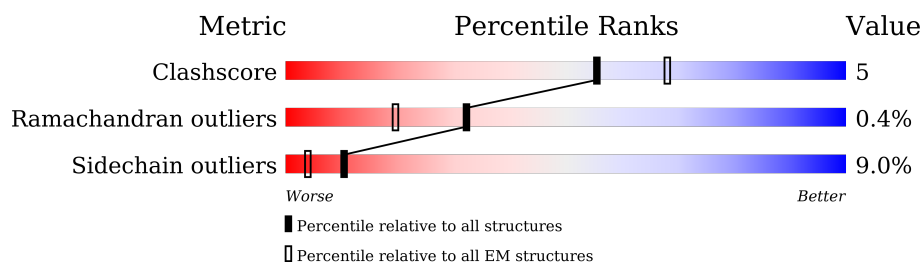
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	
1	E	471	
1	F	471	
1	G	471	
1	H	471	

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Mol	Chain	Length	Quality of chain
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
Q	?	-	LYS	deletion	UNP Q9SR19
Q	?	-	GLU	deletion	UNP Q9SR19

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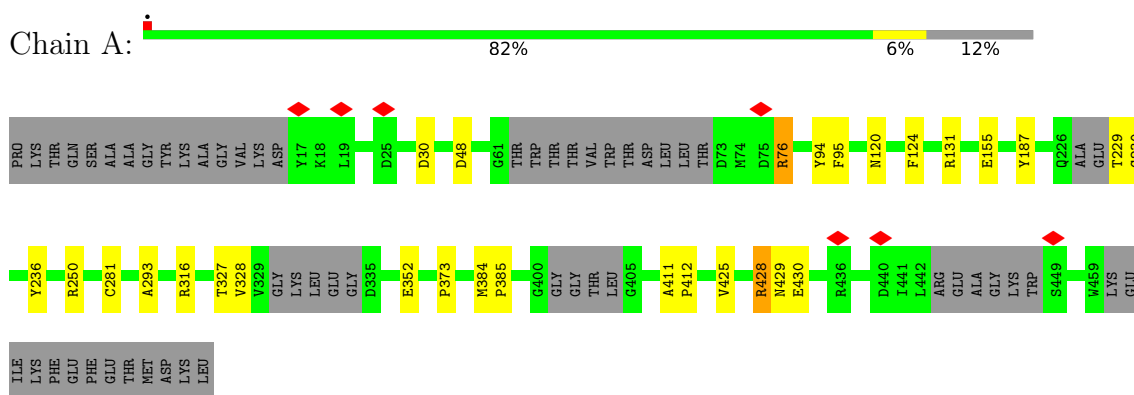
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Chain	Residue	Modelled	Actual	Comment	Reference
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Q	?	-	LYS	deletion	UNP Q9SR19
Q	?	-	LYS	deletion	UNP Q9SR19
Q	?	-	LYS	deletion	UNP Q9SR19
Q	?	-	GLU	deletion	UNP Q9SR19
Q	?	-	GLU	deletion	UNP Q9SR19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

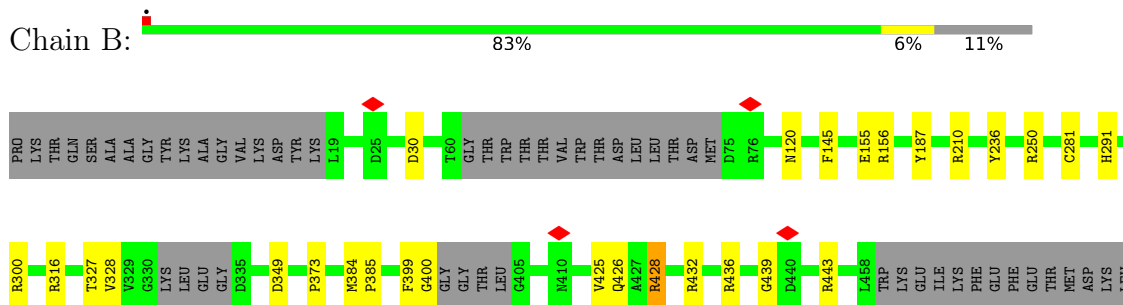
3 Residue-property plots [i](#)

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

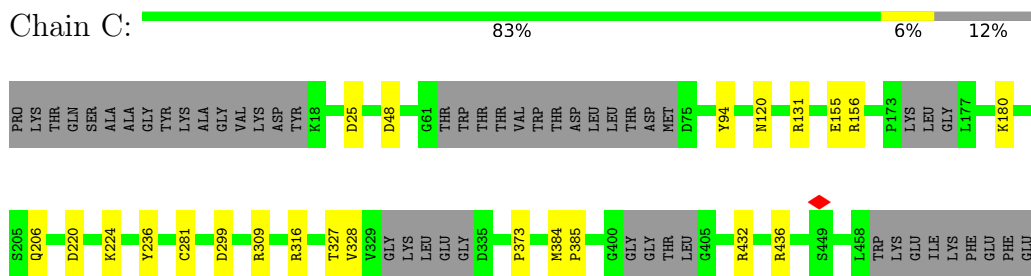
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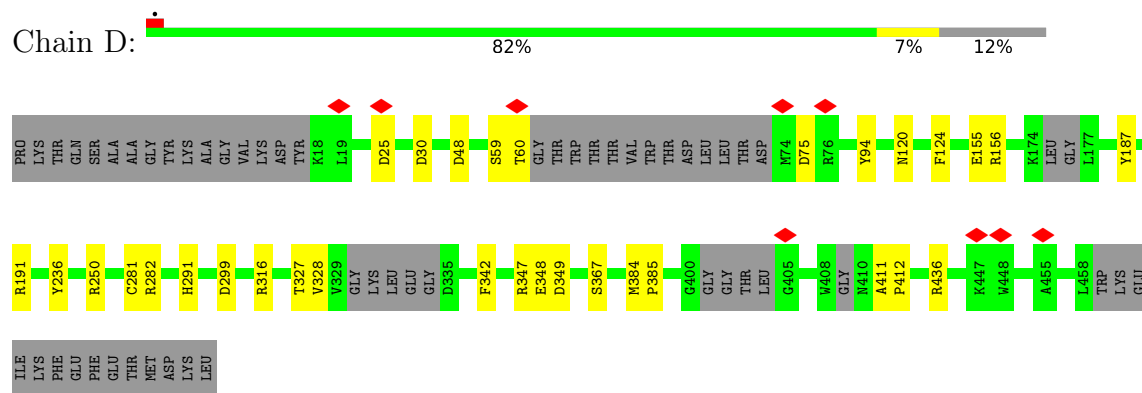
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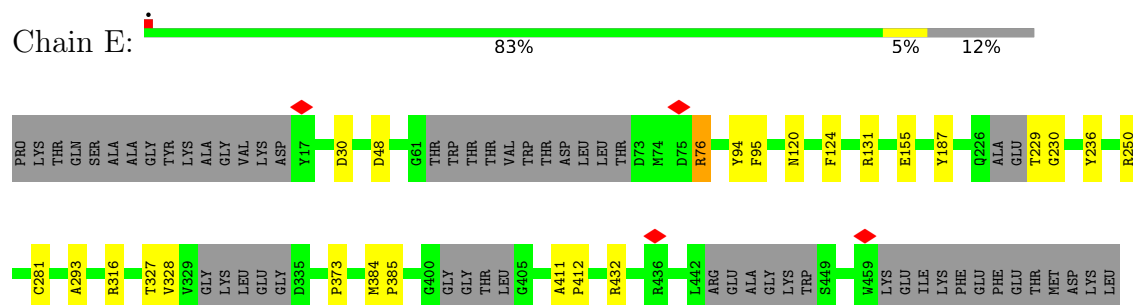
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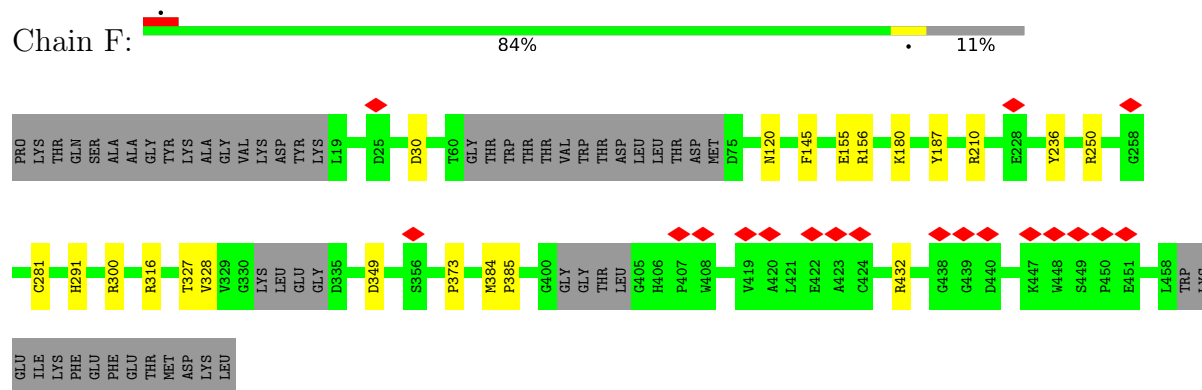
- Molecule 1: Ribulose biphosphate carboxylase large chain



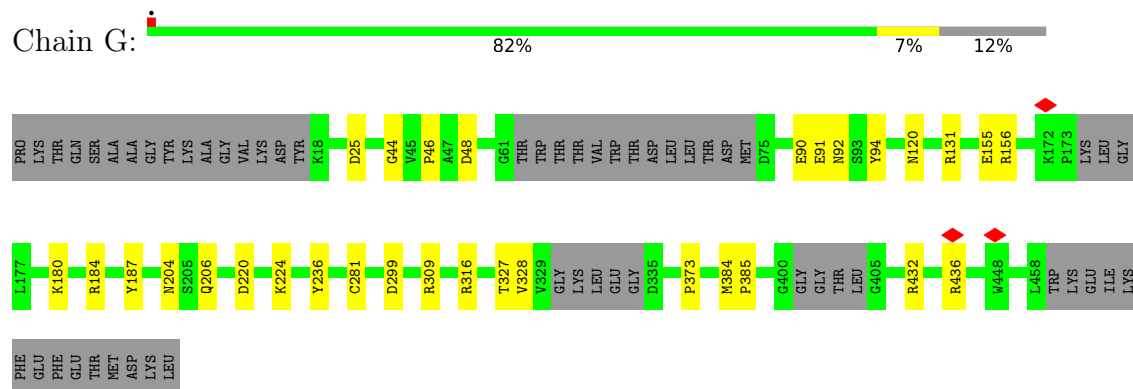
- Molecule 1: Ribulose biphosphate carboxylase large chain

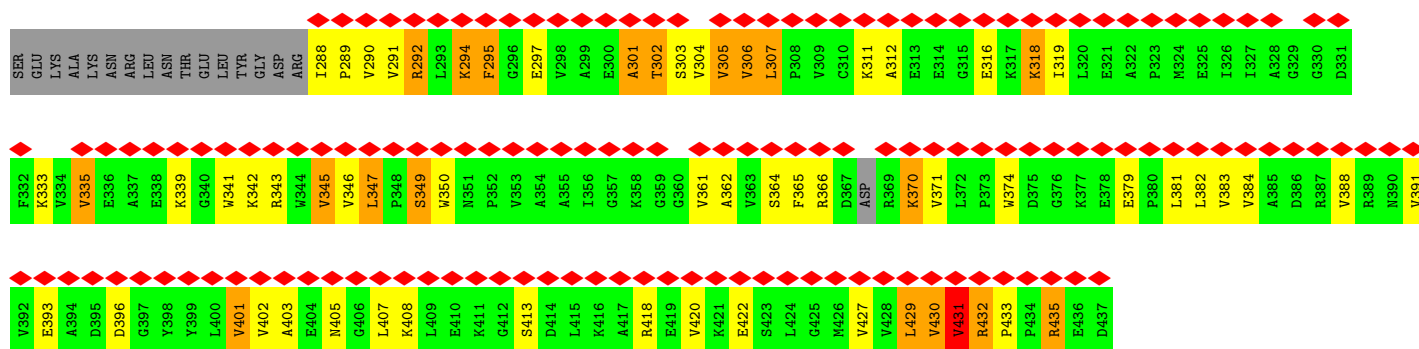


- Molecule 1: Ribulose biphosphate carboxylase large chain

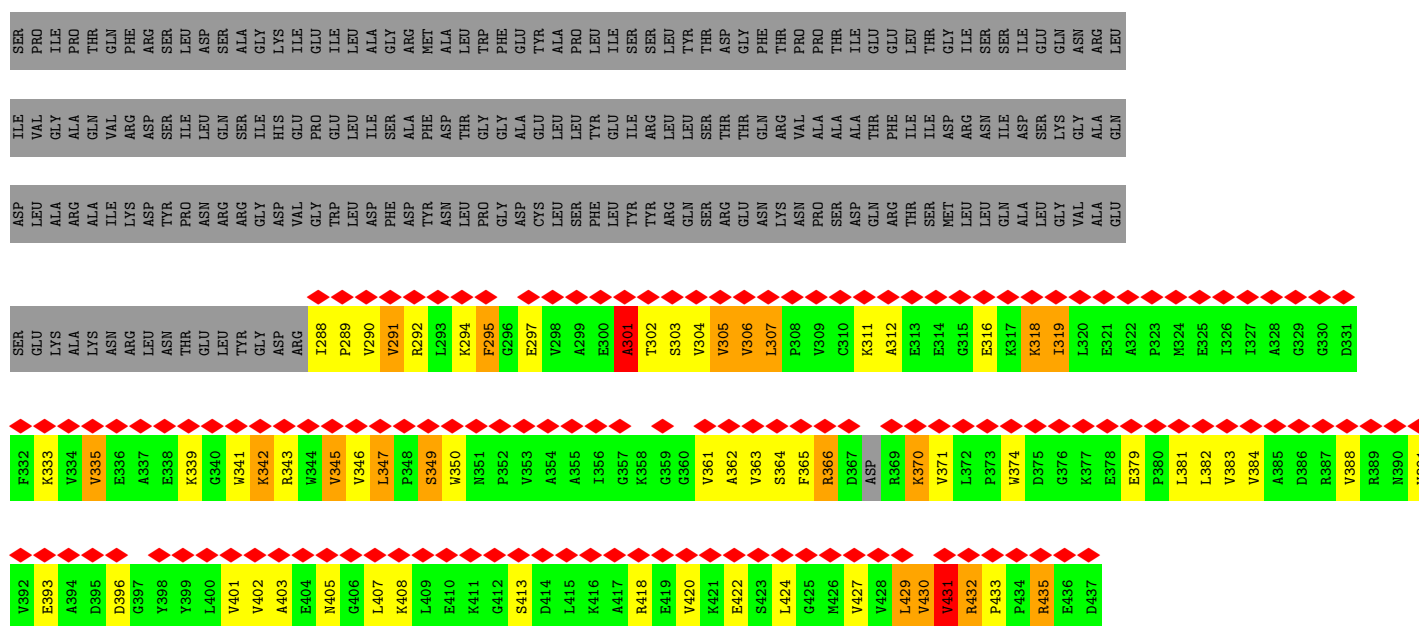
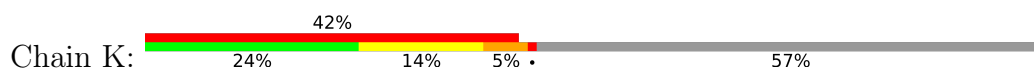


- Molecule 1: Ribulose biphosphate carboxylase large chain

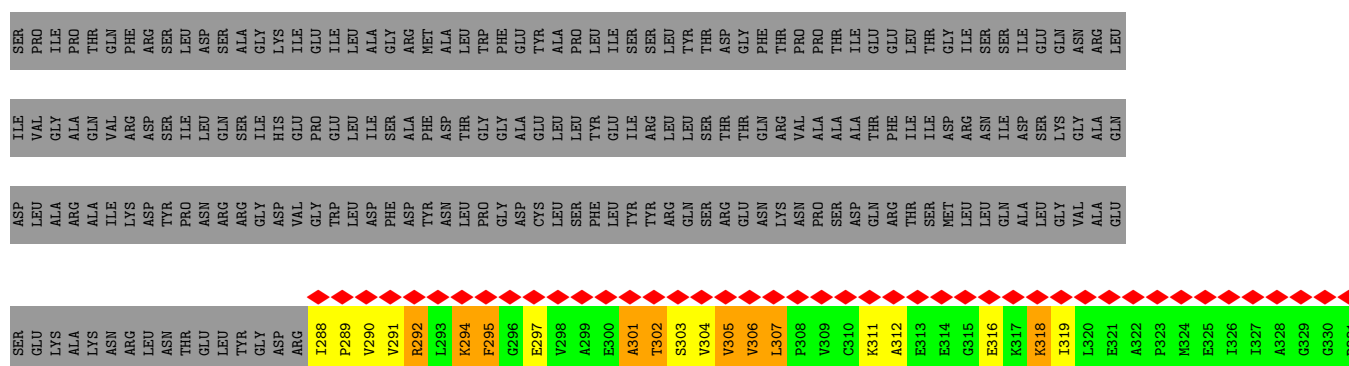
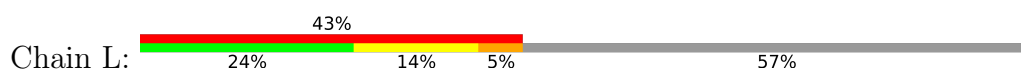


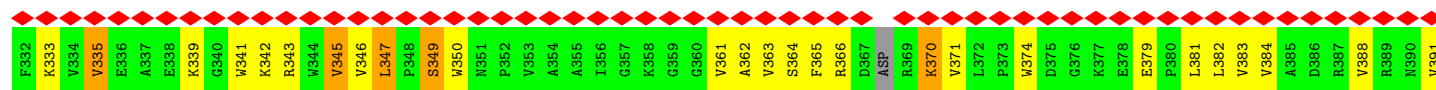


• Molecule 2: Rubisco accumulation factor 1.2, chloroplastic

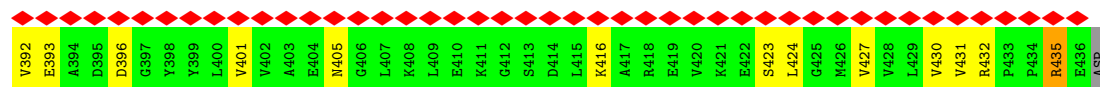
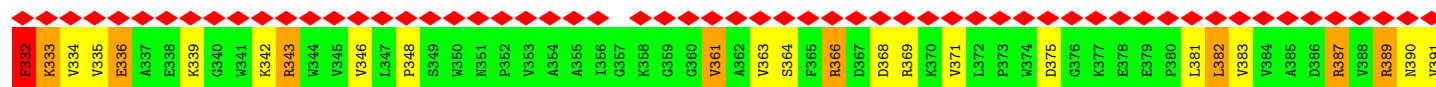
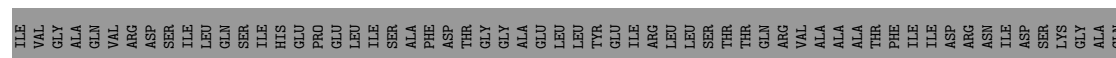
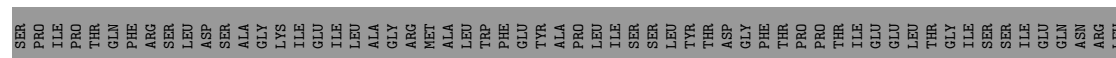
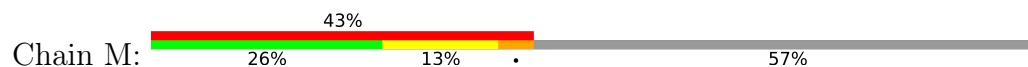


• Molecule 2: Rubisco accumulation factor 1.2, chloroplastic

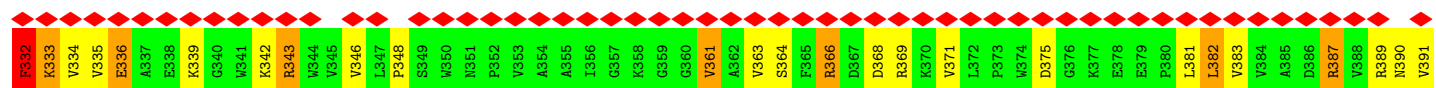
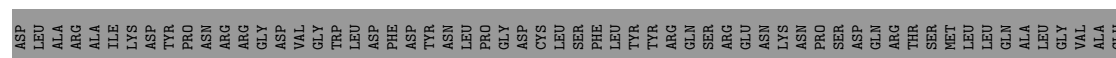
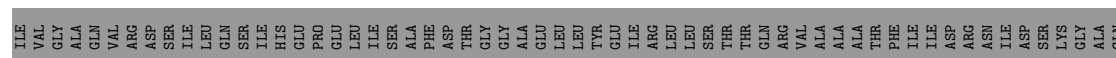
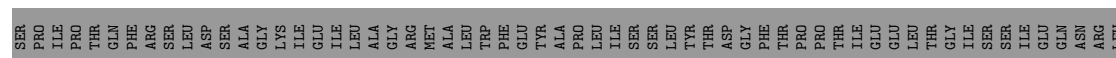




- Molecule 2: Rubisco accumulation factor 1.2, chloroplastic



- Molecule 2: Rubisco accumulation factor 1.2, chloroplastic

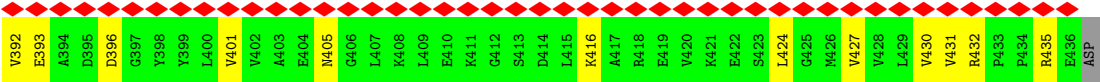
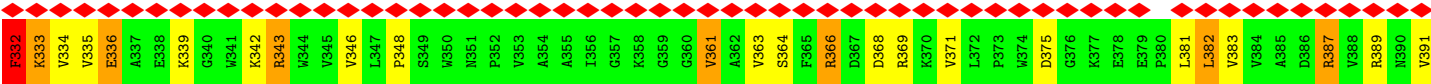




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TRP
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GLY
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ALA
PRO
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ILE
SER
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4 Experimental 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 (\AA)	216.31999, 216.31999, 216.31999	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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	11/3328 (0.3%)	0.89	5/4502 (0.1%)
1	B	1.12	8/3344 (0.2%)	0.94	8/4526 (0.2%)
1	C	1.12	6/3331 (0.2%)	0.91	9/4507 (0.2%)
1	D	1.16	10/3339 (0.3%)	0.95	10/4515 (0.2%)
1	E	1.13	11/3328 (0.3%)	0.91	7/4502 (0.2%)
1	F	1.13	8/3344 (0.2%)	0.94	8/4526 (0.2%)
1	G	1.12	6/3331 (0.2%)	0.91	9/4507 (0.2%)
1	H	1.16	10/3339 (0.3%)	0.95	10/4515 (0.2%)
2	I	0.33	0/1564	0.61	0/2120
2	J	0.42	0/1153	0.89	4/1565 (0.3%)
2	K	0.39	0/1153	0.80	3/1565 (0.2%)
2	L	0.42	0/1153	0.88	4/1565 (0.3%)
2	M	0.35	0/1145	0.69	2/1560 (0.1%)
2	N	0.35	0/1145	0.69	2/1560 (0.1%)
2	O	0.36	0/1145	0.70	2/1560 (0.1%)
2	P	0.45	0/1153	1.00	7/1565 (0.4%)
2	Q	0.35	0/1145	0.69	2/1560 (0.1%)
All	All	0.98	70/37440 (0.2%)	0.88	92/50720 (0.2%)

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	342	PHE	CB-CG	-12.01	1.30	1.51
1	H	342	PHE	CB-CG	-12.01	1.30	1.51
1	A	187	TYR	CG-CD1	-7.43	1.29	1.39
1	E	187	TYR	CG-CD1	-7.43	1.29	1.39
1	A	155	GLU	CG-CD	-7.17	1.41	1.51
1	E	155	GLU	CG-CD	-7.17	1.41	1.51
1	B	155	GLU	CG-CD	-7.09	1.41	1.51
1	F	155	GLU	CG-CD	-7.09	1.41	1.51
1	D	281	CYS	CB-SG	-6.56	1.71	1.82
1	H	281	CYS	CB-SG	-6.53	1.71	1.82
1	D	155	GLU	CG-CD	-6.33	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	155	GLU	CG-CD	-6.33	1.42	1.51
1	C	281	CYS	CB-SG	-6.27	1.71	1.82
1	G	281	CYS	CB-SG	-6.27	1.71	1.82
1	C	155	GLU	CG-CD	-6.25	1.42	1.51
1	G	155	GLU	CG-CD	-6.21	1.42	1.51
1	A	187	TYR	CD1-CE1	-6.14	1.30	1.39
1	E	187	TYR	CD1-CE1	-6.14	1.30	1.39
1	C	236	TYR	CG-CD2	-6.11	1.31	1.39
1	G	236	TYR	CG-CD2	-6.11	1.31	1.39
1	B	236	TYR	CE2-CZ	-6.06	1.30	1.38
1	F	236	TYR	CE2-CZ	-6.06	1.30	1.38
1	A	187	TYR	CB-CG	-5.98	1.42	1.51
1	E	187	TYR	CB-CG	-5.98	1.42	1.51
1	B	236	TYR	CG-CD2	-5.97	1.31	1.39
1	F	236	TYR	CG-CD2	-5.97	1.31	1.39
1	D	236	TYR	CG-CD2	-5.91	1.31	1.39
1	H	236	TYR	CG-CD2	-5.88	1.31	1.39
1	A	236	TYR	CG-CD2	-5.83	1.31	1.39
1	E	236	TYR	CG-CD2	-5.83	1.31	1.39
1	A	236	TYR	CE2-CZ	-5.78	1.31	1.38
1	E	236	TYR	CE2-CZ	-5.78	1.31	1.38
1	C	236	TYR	CE2-CZ	-5.75	1.31	1.38
1	G	236	TYR	CE2-CZ	-5.75	1.31	1.38
1	D	236	TYR	CE2-CZ	-5.74	1.31	1.38
1	E	94	TYR	CB-CG	-5.71	1.43	1.51
1	A	94	TYR	CB-CG	-5.69	1.43	1.51
1	H	236	TYR	CE2-CZ	-5.69	1.31	1.38
1	A	281	CYS	CB-SG	-5.55	1.72	1.81
1	E	281	CYS	CB-SG	-5.55	1.72	1.81
1	D	94	TYR	CB-CG	-5.50	1.43	1.51
1	H	94	TYR	CB-CG	-5.50	1.43	1.51
1	C	94	TYR	CB-CG	-5.44	1.43	1.51
1	G	94	TYR	CB-CG	-5.44	1.43	1.51
1	D	124	PHE	CB-CG	-5.41	1.42	1.51
1	H	124	PHE	CB-CG	-5.41	1.42	1.51
1	B	281	CYS	CB-SG	-5.29	1.73	1.81
1	F	281	CYS	CB-SG	-5.29	1.73	1.81
1	C	373	PRO	N-CD	-5.22	1.40	1.47
1	G	373	PRO	N-CD	-5.22	1.40	1.47
1	E	373	PRO	N-CD	-5.21	1.40	1.47
1	H	291	HIS	CB-CG	-5.21	1.40	1.50
1	D	291	HIS	CB-CG	-5.19	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	373	PRO	N-CD	-5.18	1.40	1.47
1	B	145	PHE	CB-CG	-5.16	1.42	1.51
1	F	145	PHE	CB-CG	-5.16	1.42	1.51
1	B	373	PRO	N-CD	-5.12	1.40	1.47
1	F	373	PRO	N-CD	-5.12	1.40	1.47
1	A	124	PHE	CB-CG	-5.12	1.42	1.51
1	E	124	PHE	CB-CG	-5.12	1.42	1.51
1	D	155	GLU	CD-OE1	-5.05	1.20	1.25
1	H	155	GLU	CD-OE1	-5.05	1.20	1.25
1	A	95	PHE	CB-CG	-5.04	1.42	1.51
1	E	95	PHE	CB-CG	-5.04	1.42	1.51
1	B	291	HIS	CB-CG	-5.01	1.41	1.50
1	F	291	HIS	CB-CG	-5.01	1.41	1.50
1	B	155	GLU	CD-OE2	-5.01	1.20	1.25
1	F	155	GLU	CD-OE2	-5.01	1.20	1.25
1	D	348	GLU	CD-OE2	-5.00	1.20	1.25
1	H	348	GLU	CD-OE2	-5.00	1.20	1.25

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	250	ARG	NE-CZ-NH1	12.02	126.31	120.30
1	H	250	ARG	NE-CZ-NH1	12.00	126.30	120.30
1	B	250	ARG	NE-CZ-NH1	11.85	126.22	120.30
1	F	250	ARG	NE-CZ-NH1	11.85	126.22	120.30
2	P	298	VAL	N-CA-C	-11.47	80.04	111.00
1	B	156	ARG	NE-CZ-NH2	-10.93	114.83	120.30
1	F	156	ARG	NE-CZ-NH2	-10.93	114.83	120.30
1	C	156	ARG	NE-CZ-NH2	-10.67	114.97	120.30
1	G	156	ARG	NE-CZ-NH2	-10.67	114.97	120.30
1	D	156	ARG	NE-CZ-NH2	-10.57	115.02	120.30
1	H	156	ARG	NE-CZ-NH2	-10.57	115.02	120.30
2	P	431	VAL	N-CA-C	10.30	138.82	111.00
2	L	431	VAL	N-CA-C	10.29	138.79	111.00
2	J	431	VAL	N-CA-C	10.29	138.77	111.00
2	P	301	ALA	N-CA-C	9.82	137.52	111.00
2	P	302	THR	N-CA-C	9.39	136.36	111.00
2	J	429	LEU	CA-CB-CG	9.21	136.48	115.30
2	K	429	LEU	CA-CB-CG	9.19	136.44	115.30
2	P	429	LEU	CA-CB-CG	9.19	136.44	115.30
2	L	429	LEU	CA-CB-CG	9.19	136.43	115.30
1	A	187	TYR	CB-CG-CD1	-9.12	115.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	187	TYR	CB-CG-CD1	-9.12	115.53	121.00
1	D	156	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	H	156	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	E	432	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	C	156	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	G	436	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	G	156	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	C	436	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	B	156	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	F	156	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	D	191	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	H	191	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	D	250	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	H	250	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	B	250	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	F	250	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	H	436	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	D	436	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	C	309	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	G	309	ARG	NE-CZ-NH2	-7.13	116.73	120.30
2	P	300	GLU	CB-CA-C	6.84	124.08	110.40
2	L	301	ALA	N-CA-C	6.66	128.99	111.00
2	J	301	ALA	N-CA-C	6.65	128.95	111.00
1	D	316	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	H	316	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	B	316	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	F	316	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	316	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	E	316	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	C	432	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	G	432	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	C	316	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	G	316	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	D	342	PHE	CB-CA-C	-6.08	98.25	110.40
1	H	342	PHE	CB-CA-C	-6.08	98.25	110.40
2	N	329	GLY	N-CA-C	-5.99	98.12	113.10
2	O	329	GLY	N-CA-C	-5.99	98.14	113.10
2	Q	329	GLY	N-CA-C	-5.98	98.15	113.10
1	C	131	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	G	131	ARG	NE-CZ-NH2	5.97	123.29	120.30
1	C	187	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	G	187	TYR	CB-CG-CD2	-5.97	117.42	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	329	GLY	N-CA-C	-5.97	98.19	113.10
2	P	431	VAL	CB-CA-C	-5.91	100.18	111.40
2	L	431	VAL	CB-CA-C	-5.90	100.18	111.40
2	J	431	VAL	CB-CA-C	-5.90	100.19	111.40
1	B	432	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	76	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	E	76	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	F	432	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	C	184	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	G	184	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	B	300	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	F	300	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	187	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	H	187	TYR	CB-CG-CD2	-5.59	117.65	121.00
2	K	431	VAL	N-CA-C	5.53	125.94	111.00
2	M	332	PHE	N-CA-CB	5.42	120.36	110.60
2	O	332	PHE	N-CA-CB	5.42	120.35	110.60
2	N	332	PHE	N-CA-CB	5.41	120.34	110.60
2	Q	332	PHE	N-CA-CB	5.38	120.29	110.60
1	E	432	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	K	301	ALA	N-CA-C	5.29	125.29	111.00
1	A	131	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	E	131	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	250	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	E	250	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	187	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	F	187	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	D	347	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	H	347	ARG	NE-CZ-NH1	5.15	122.87	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3250	0	3166	12	0
1	B	3265	0	3184	16	0
1	C	3253	0	3170	8	0
1	D	3262	0	3185	16	0
1	E	3250	0	3166	8	0
1	F	3265	0	3184	9	0
1	G	3253	0	3170	12	0
1	H	3262	0	3185	19	0
2	I	1536	0	1516	30	0
2	J	1133	0	1160	37	0
2	K	1133	0	1160	46	0
2	L	1133	0	1160	39	0
2	M	1124	0	1133	32	0
2	N	1124	0	1133	36	0
2	O	1124	0	1133	32	0
2	P	1133	0	1160	50	0
2	Q	1124	0	1133	38	0
All	All	36624	0	36098	347	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 (347) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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:D:59:SER:O	1:D:60:THR:C	2.43	0.57
1:H:349:ASP:OD1	1:H:349:ASP:N	2.37	0.57
1:H:59:SER:O	1:H:60:THR:C	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:Q:332:PHE:O	2:Q:333:LYS:HB2	2.07	0.53
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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:G:220:ASP:OD2	1:G:224:LYS:NZ	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:306:VAL:HG21	2:K:335:VAL:HG11	1.95	0.48
2:L:292:ARG:HD3	2:L:432:ARG:HB3	1.95	0.48
1:C:299:ASP:OD1	1:C:299:ASP:C	2.51	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
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
1:B:120:ASN:N	1:B:120:ASN:OD1	2.44	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:58:ILE:HA	2:I:61:LEU:HB2	1.98	0.46
1:G:299:ASP:OD1	1:G:299:ASP:C	2.51	0.46
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
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
1:A:229:THR:OG1	1:A:230:GLY:N	2.49	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
1:D:299:ASP:C	1:D:299:ASP:OD1	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:I:175:ASN:O	2:I:176:PRO:C	2.56	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:N	1:D:75:ASP:OD1	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: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:N:324:MET:HE3	2:N:324:MET:HB3	1.94	0.43
2:P:349:SER:O	2:Q:300:GLU:HA	2.18	0.43
1:E:120:ASN:N	1:E:120:ASN:OD1	2.51	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:C:120:ASN:OD1	1:C:120:ASN:N	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:299:ASP:OD1	1:H:299:ASP:C	2.55	0.42
2:J:318:LYS:HG3	2:J:341:TRP:HZ2	1.84	0.42
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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:HA	2:O:319:ILE:HD12	2.03	0.41
2:O:316:GLU:H	2:O:316:GLU:HG3	1.47	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: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
1:B:399:PHE:O	1:B:400:GLY:C	2.59	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: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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:319:ILE:HG21	2:K:424:LEU:HB3	2.04	0.40
2:O:324:MET:HE3	2:O:324:MET:HB3	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/471 (86%)	394 (98%)	8 (2%)	1 (0%)	44	74
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%)	44	74
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%)	25	58
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%)	19	51
2	N	148/346 (43%)	142 (96%)	5 (3%)	1 (1%)	19	51
2	O	148/346 (43%)	142 (96%)	5 (3%)	1 (1%)	19	51
2	P	145/346 (42%)	137 (94%)	5 (3%)	3 (2%)	5	25
2	Q	148/346 (43%)	142 (96%)	5 (3%)	1 (1%)	19	51
All	All	4611/6882 (67%)	4499 (98%)	95 (2%)	17 (0%)	32	63

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%)	91	95
1	B	338/382 (88%)	335 (99%)	3 (1%)	75	88
1	C	337/382 (88%)	336 (100%)	1 (0%)	91	95
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%)	91	95
1	G	337/382 (88%)	335 (99%)	2 (1%)	84	91
1	H	339/382 (89%)	339 (100%)	0	100	100
2	I	166/291 (57%)	149 (90%)	17 (10%)	6	23
2	J	119/291 (41%)	76 (64%)	43 (36%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	119/291 (41%)	76 (64%)	43 (36%)	0	0
2	L	119/291 (41%)	75 (63%)	44 (37%)	0	0
2	M	115/291 (40%)	79 (69%)	36 (31%)	0	0
2	N	115/291 (40%)	80 (70%)	35 (30%)	0	0
2	O	115/291 (40%)	80 (70%)	35 (30%)	0	0
2	P	119/291 (41%)	74 (62%)	45 (38%)	0	0
2	Q	115/291 (40%)	79 (69%)	36 (31%)	0	0
All	All	3806/5675 (67%)	3464 (91%)	342 (9%)	10	29

All (342) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	428	ARG
1	B	426	GLN
1	B	428	ARG
1	B	443	ARG
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
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	175	ASN
2	I	179	GLN
2	I	181	THR
2	J	288	ILE
2	J	291	VAL
2	J	292	ARG

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Mol	Chain	Res	Type
2	J	294	LYS
2	J	295	PHE
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	316	GLU
2	J	318	LYS
2	J	319	ILE
2	J	333	LYS
2	J	335	VAL
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	350	TRP
2	J	361	VAL
2	J	364	SER
2	J	370	LYS
2	J	371	VAL
2	J	374	TRP
2	J	379	GLU
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	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

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Mol	Chain	Res	Type
2	K	292	ARG
2	K	294	LYS
2	K	295	PHE
2	K	303	SER
2	K	305	VAL
2	K	306	VAL
2	K	307	LEU
2	K	311	LYS
2	K	316	GLU
2	K	318	LYS
2	K	319	ILE
2	K	333	LYS
2	K	335	VAL
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	350	TRP
2	K	361	VAL
2	K	364	SER
2	K	366	ARG
2	K	370	LYS
2	K	371	VAL
2	K	374	TRP
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	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

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Mol	Chain	Res	Type
2	L	291	VAL
2	L	292	ARG
2	L	294	LYS
2	L	295	PHE
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	316	GLU
2	L	318	LYS
2	L	319	ILE
2	L	333	LYS
2	L	335	VAL
2	L	339	LYS
2	L	342	LYS
2	L	343	ARG
2	L	345	VAL
2	L	347	LEU
2	L	349	SER
2	L	350	TRP
2	L	361	VAL
2	L	364	SER
2	L	366	ARG
2	L	370	LYS
2	L	371	VAL
2	L	374	TRP
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	413	SER
2	L	418	ARG
2	L	420	VAL
2	L	422	GLU
2	L	430	VAL
2	L	431	VAL

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Mol	Chain	Res	Type
2	L	435	ARG
2	M	288	ILE
2	M	292	ARG
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
2	M	343	ARG
2	M	361	VAL
2	M	363	VAL
2	M	364	SER
2	M	366	ARG
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	405	ASN
2	M	424	LEU
2	M	432	ARG
2	M	435	ARG
2	N	288	ILE
2	N	303	SER
2	N	304	VAL
2	N	305	VAL
2	N	306	VAL

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Mol	Chain	Res	Type
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	361	VAL
2	N	363	VAL
2	N	364	SER
2	N	366	ARG
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	405	ASN
2	N	424	LEU
2	N	432	ARG
2	N	435	ARG
2	O	288	ILE
2	O	292	ARG
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

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Mol	Chain	Res	Type
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	361	VAL
2	O	363	VAL
2	O	364	SER
2	O	366	ARG
2	O	369	ARG
2	O	371	VAL
2	O	375	ASP
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	405	ASN
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	300	GLU
2	P	303	SER
2	P	305	VAL
2	P	306	VAL
2	P	307	LEU
2	P	311	LYS
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

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Mol	Chain	Res	Type
2	P	343	ARG
2	P	345	VAL
2	P	347	LEU
2	P	349	SER
2	P	350	TRP
2	P	361	VAL
2	P	364	SER
2	P	366	ARG
2	P	370	LYS
2	P	371	VAL
2	P	374	TRP
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	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	292	ARG
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

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Mol	Chain	Res	Type
2	Q	342	LYS
2	Q	343	ARG
2	Q	361	VAL
2	Q	363	VAL
2	Q	364	SER
2	Q	366	ARG
2	Q	369	ARG
2	Q	371	VAL
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	405	ASN
2	Q	424	LEU
2	Q	432	ARG
2	Q	435	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	426	GLN
2	I	70	ASN
2	I	77	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.

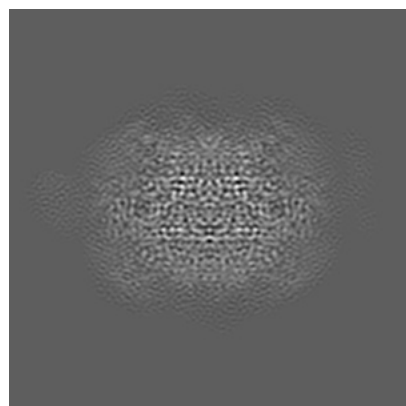
6 Map visualisation [i](#)

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

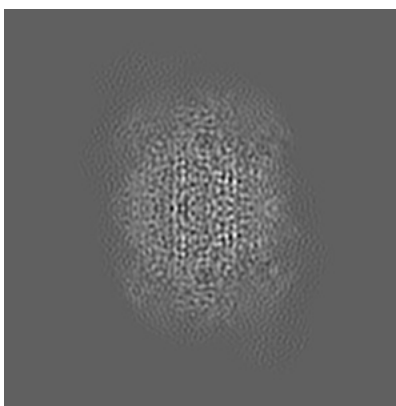
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

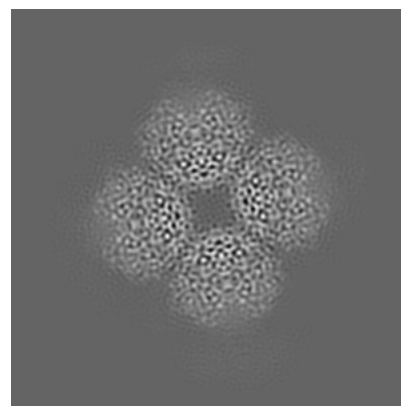
6.1.1 Primary map



X

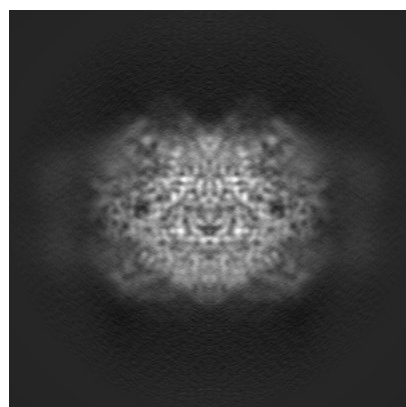


Y

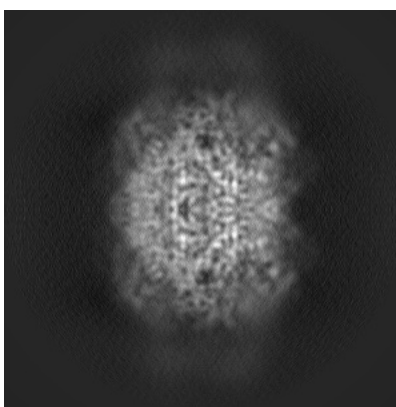


Z

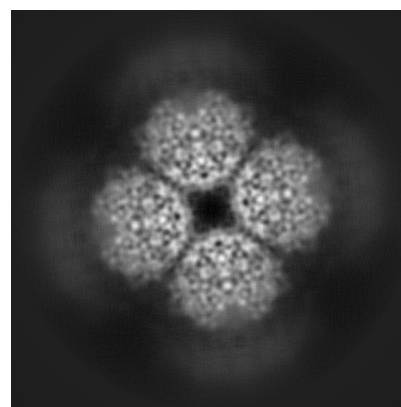
6.1.2 Raw map



X



Y

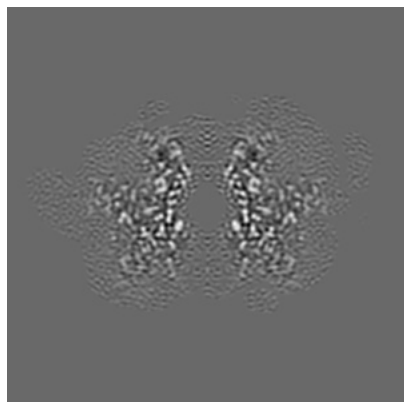


Z

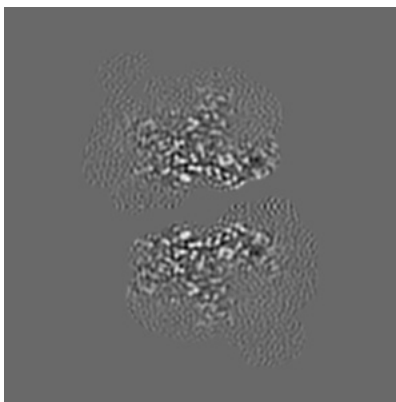
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

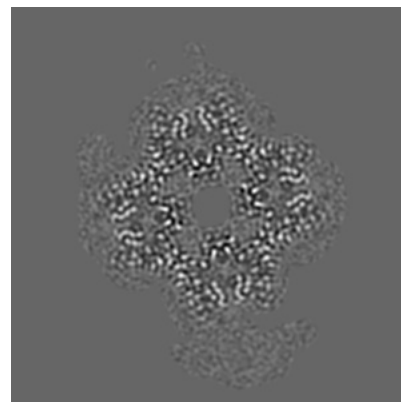
6.2.1 Primary map



X Index: 208

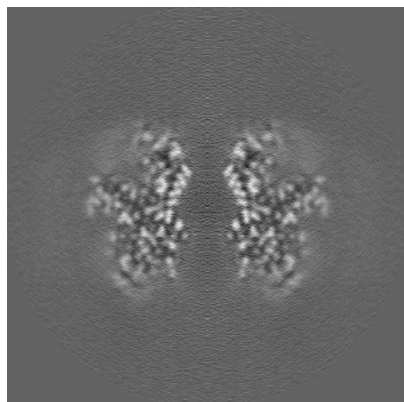


Y Index: 208

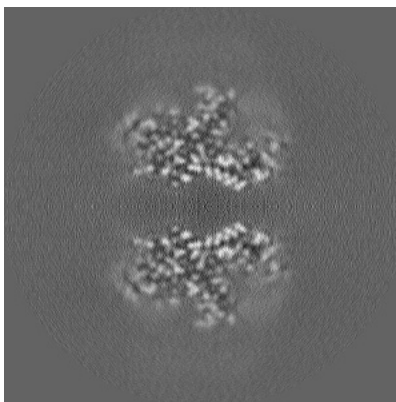


Z Index: 208

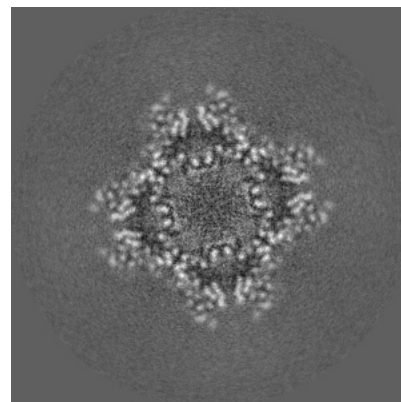
6.2.2 Raw map



X Index: 208



Y Index: 208

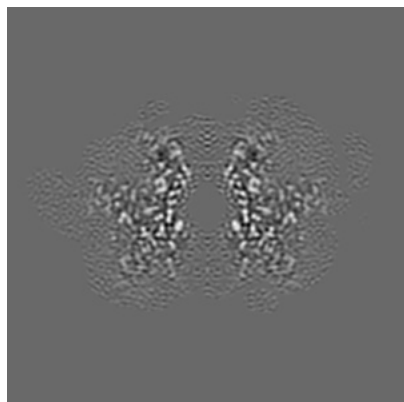


Z Index: 208

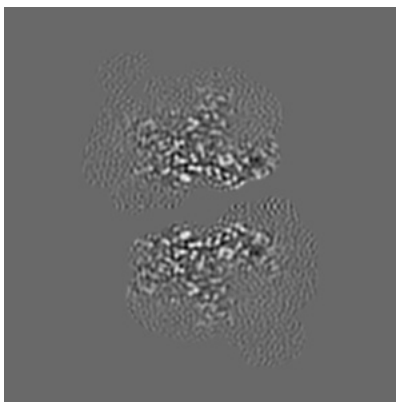
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

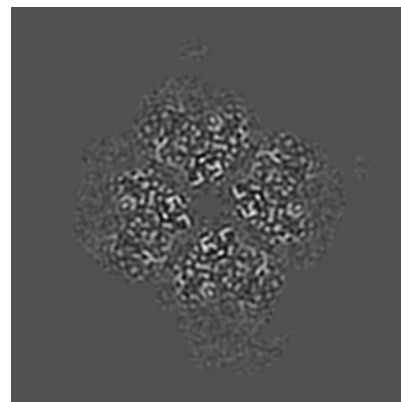
6.3.1 Primary map



X Index: 208

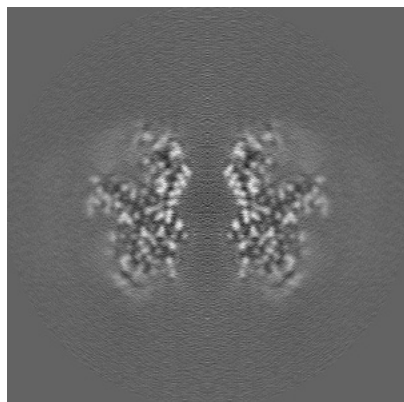


Y Index: 208

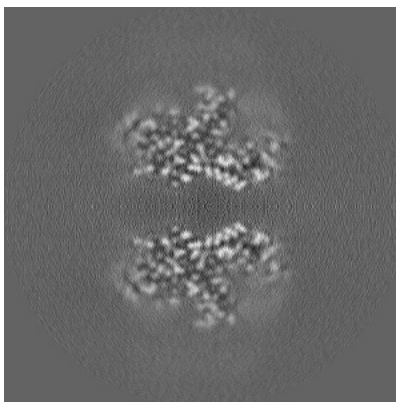


Z Index: 193

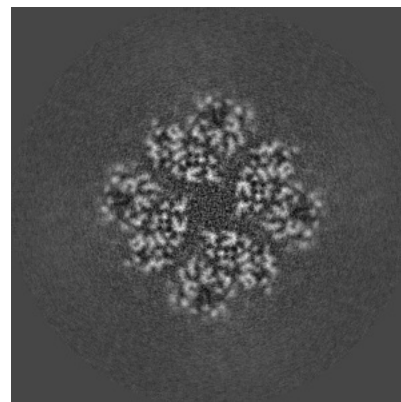
6.3.2 Raw map



X Index: 208



Y Index: 208

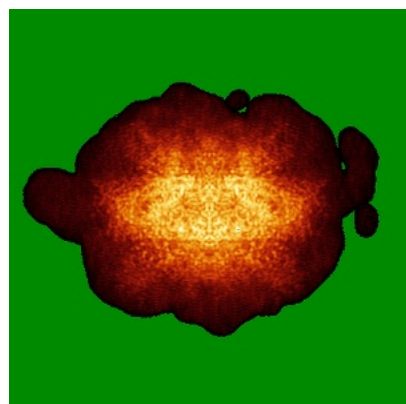


Z Index: 223

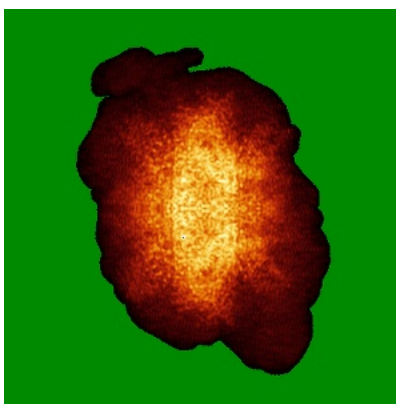
The images above show the largest variance slices of the map in three orthogonal directions.

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

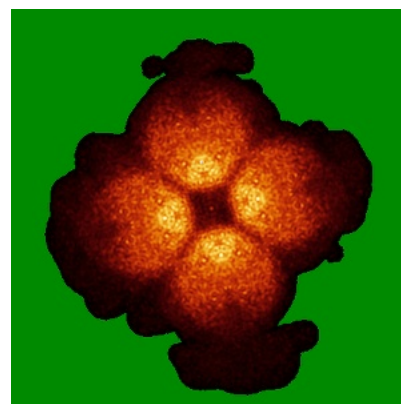
6.4.1 Primary map



X

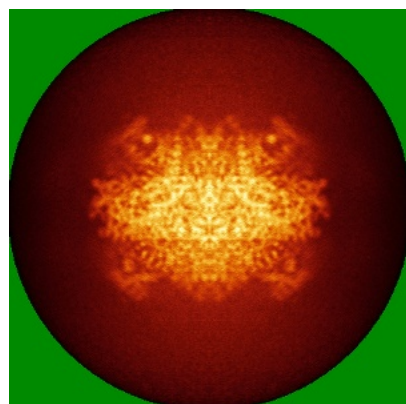


Y

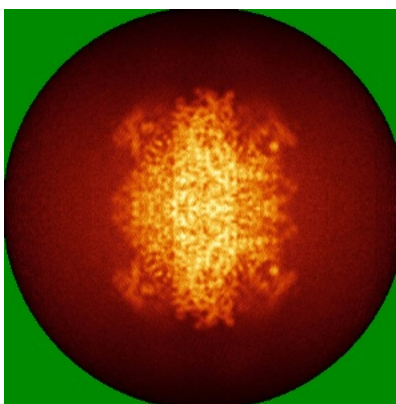


Z

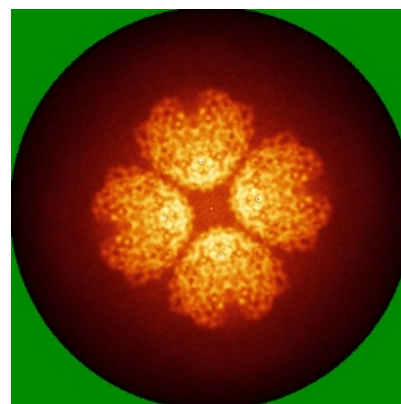
6.4.2 Raw map



X



Y

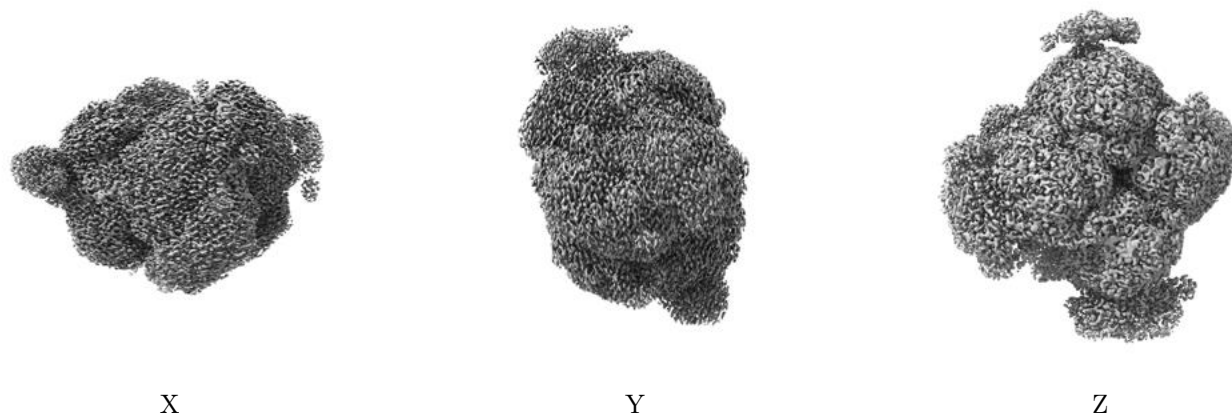


Z

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.

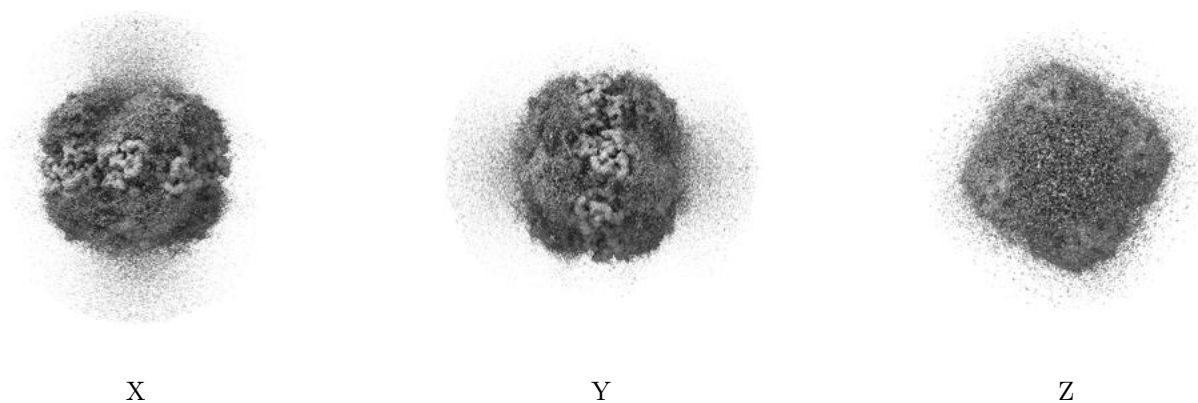
6.5 Orthogonal surface views [i](#)

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.

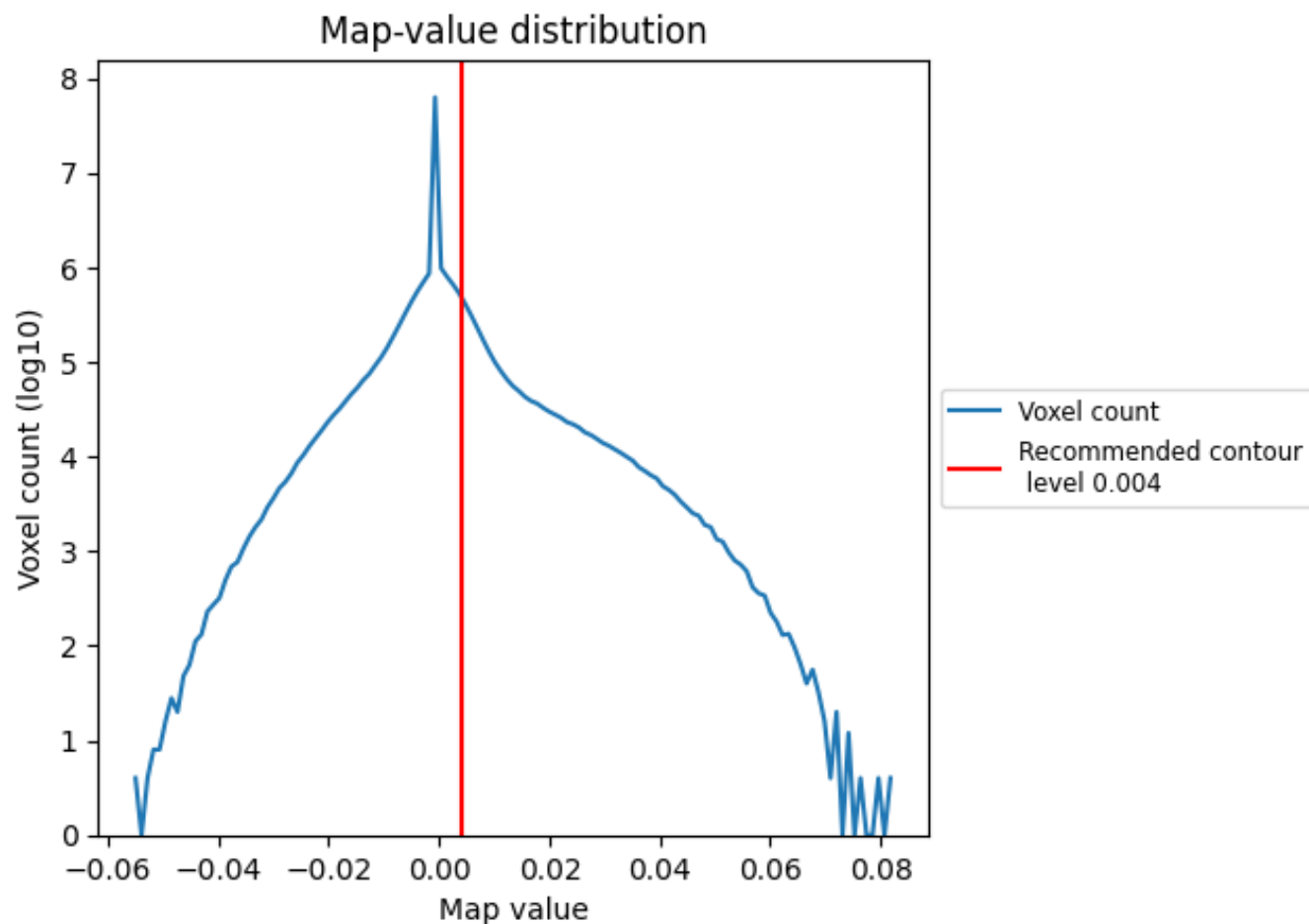
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

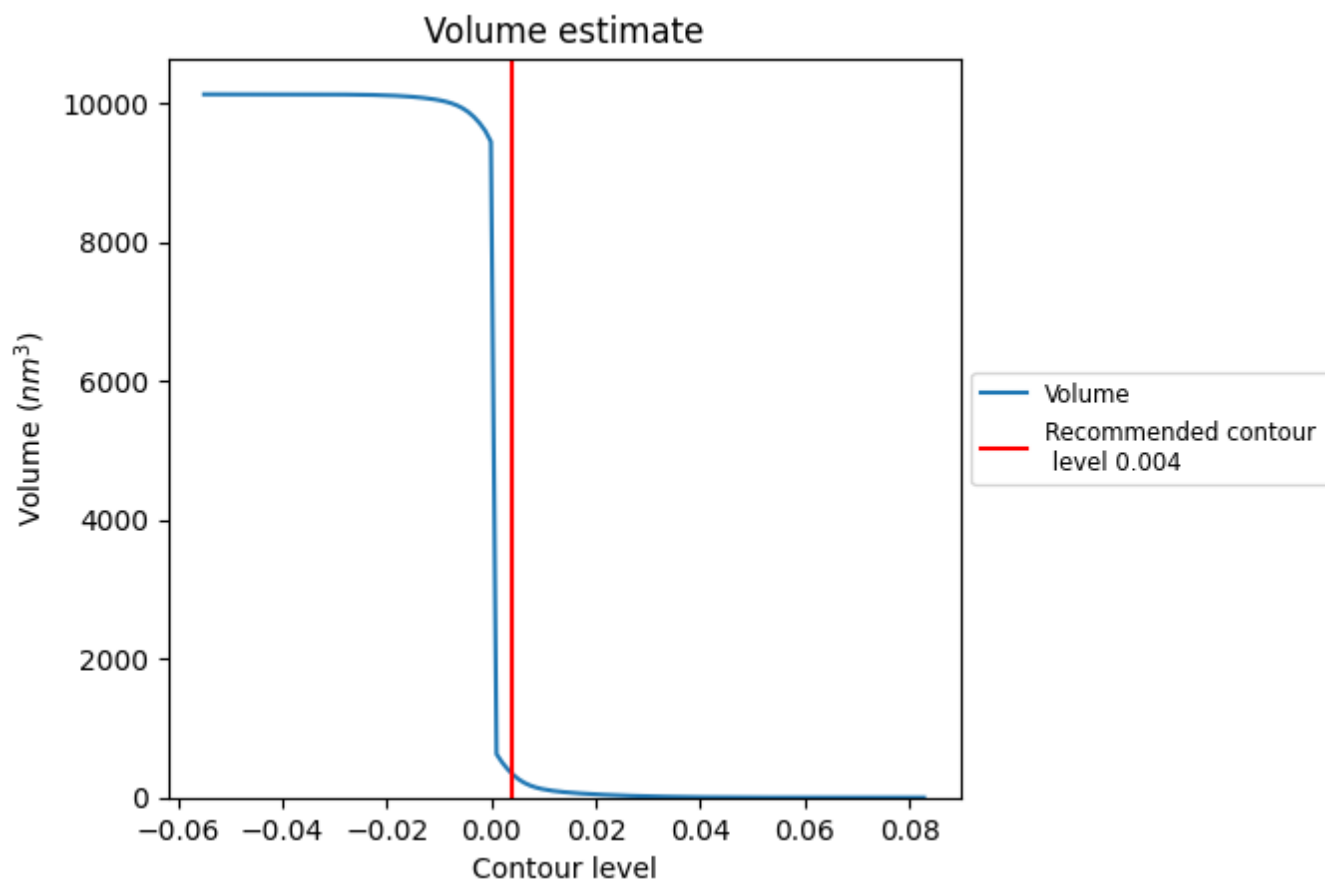
This section contains the results of statistical analysis of the map.

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.

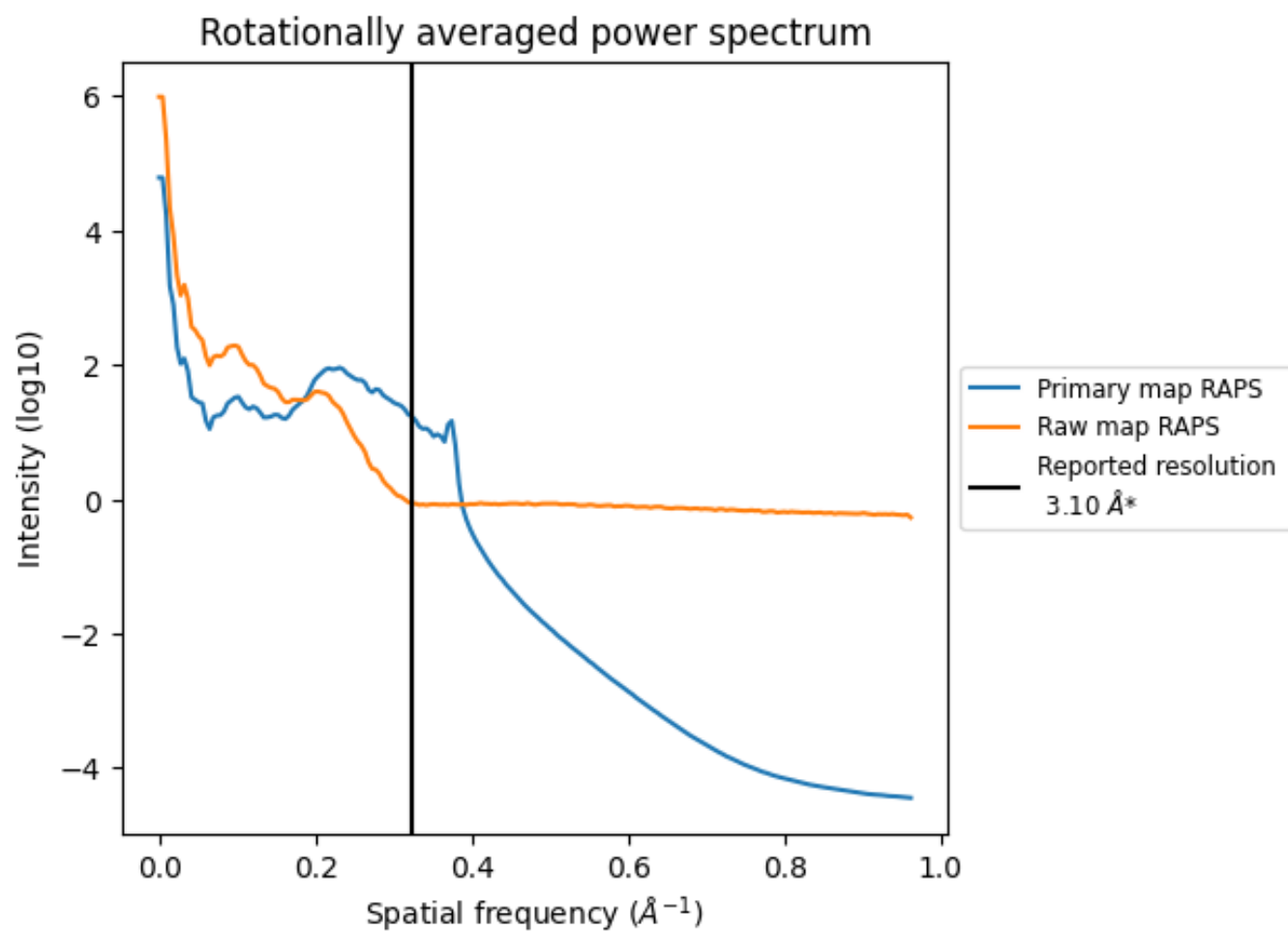
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 344 nm^3 ; 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 ⓘ

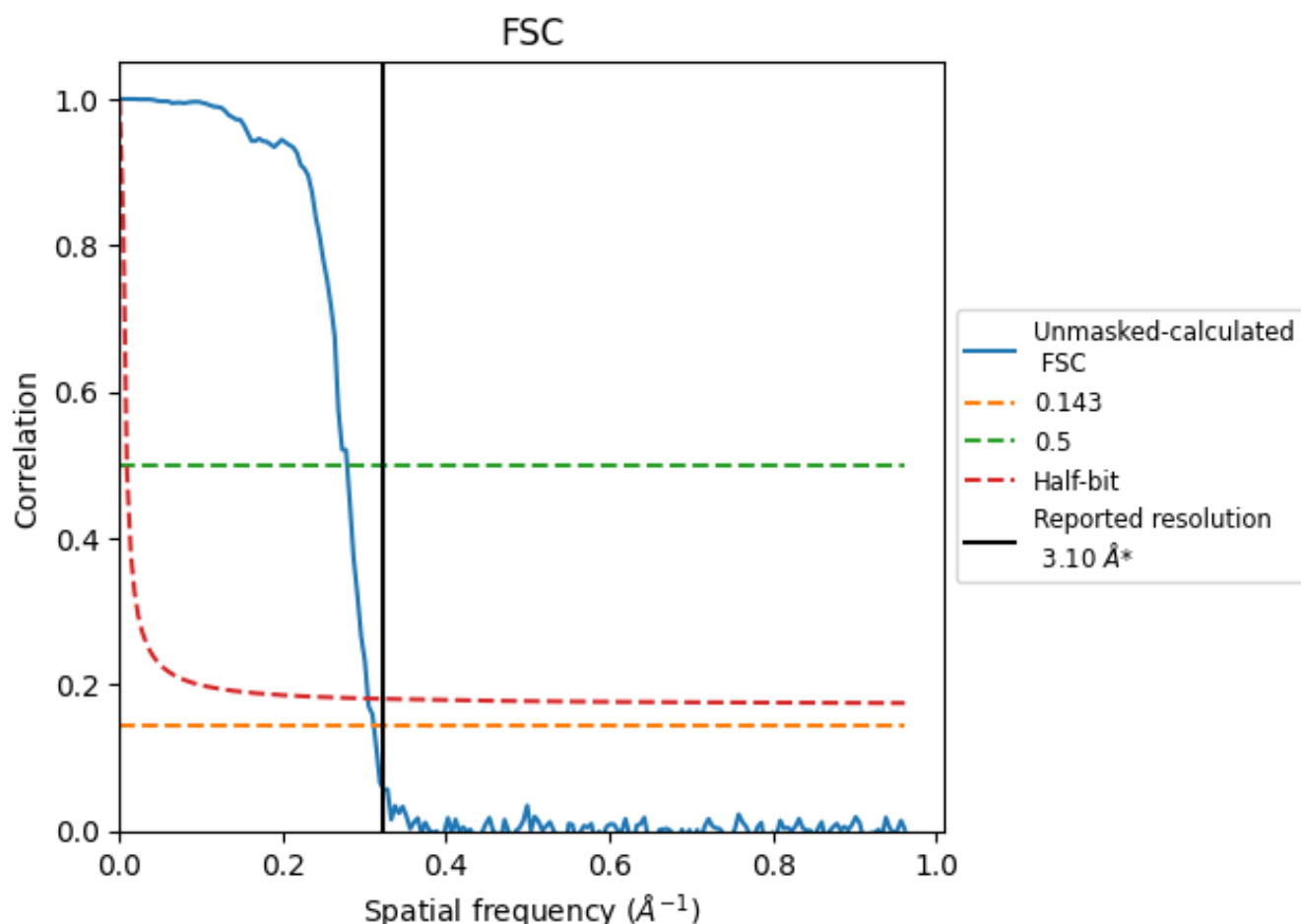


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

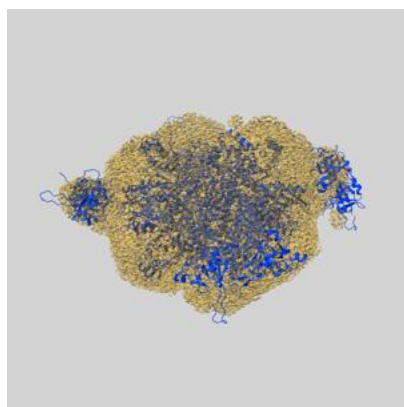
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.21	3.59	3.29

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

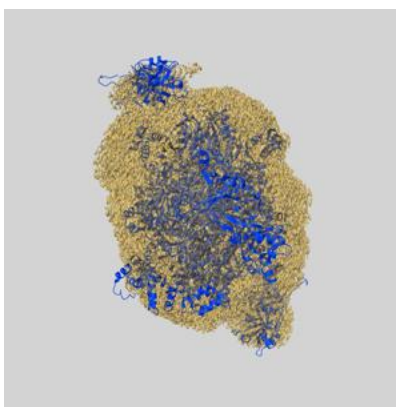
9 Map-model fit [i](#)

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.

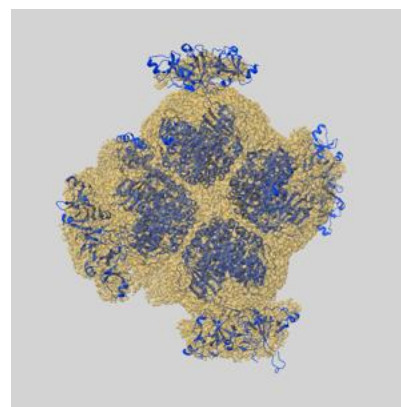
9.1 Map-model overlay [i](#)



X



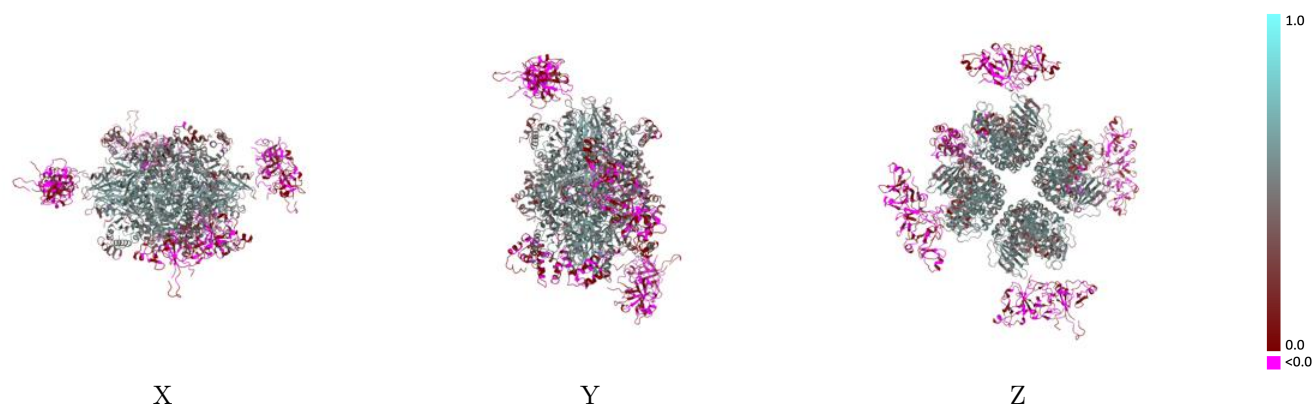
Y



Z

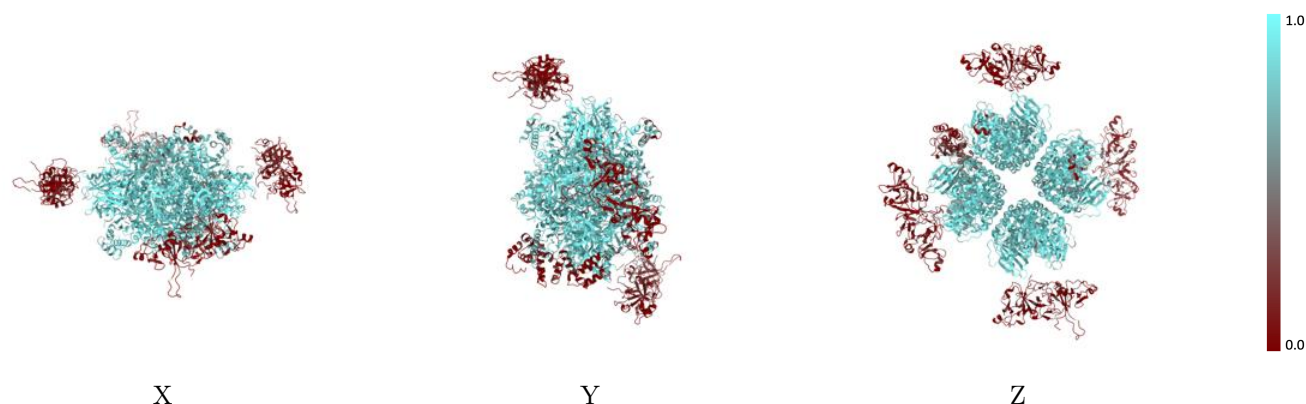
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



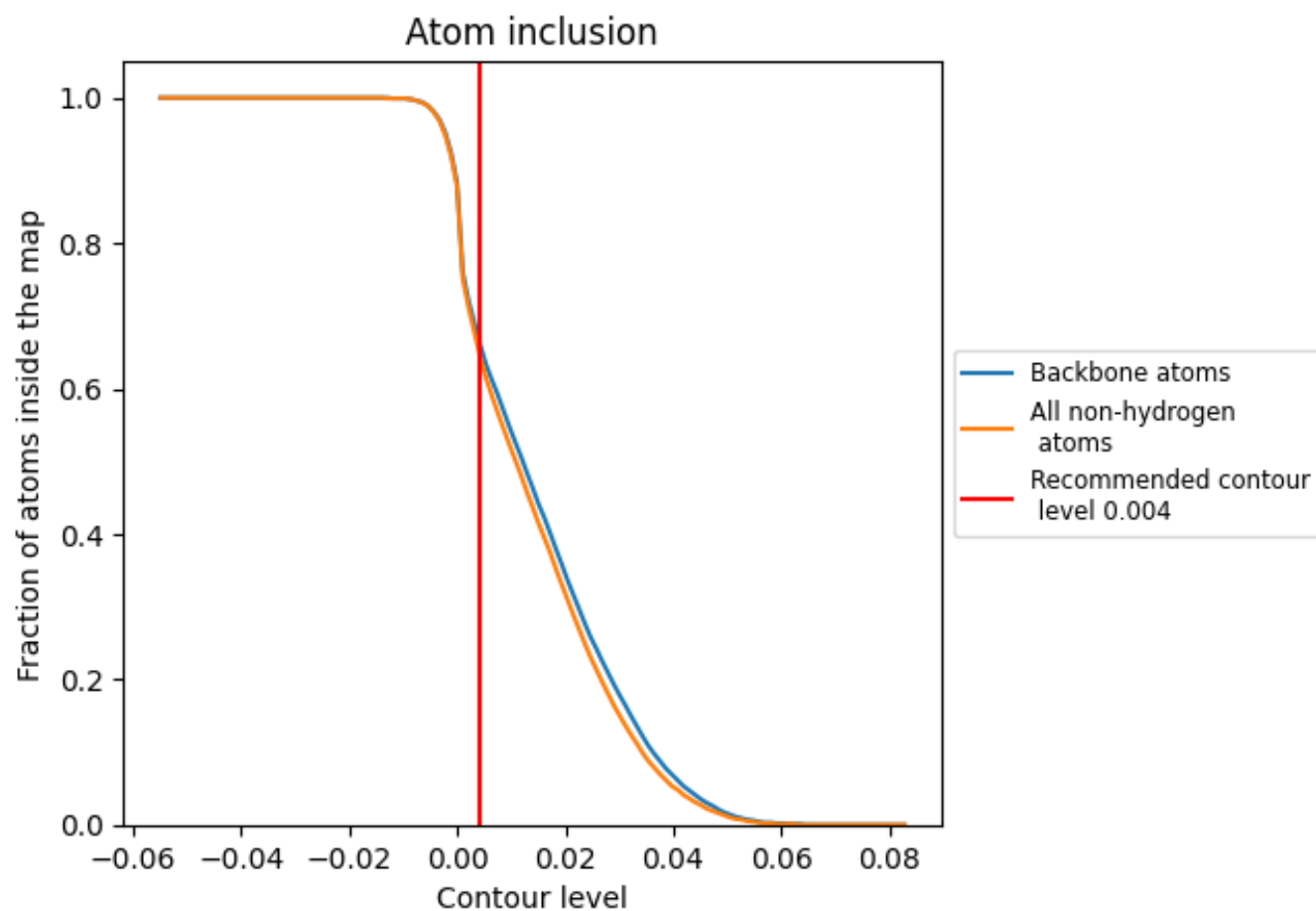
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.0130
N	 0.1040	 0.0380
O	 0.1190	 0.0470
P	 0.0450	 0.0200
Q	 0.0400	 0.0190

