



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 04:13 AM UTC

PDB ID : 8SWF / pdb_00008swf
EMDB ID : EMD-40811
Title : Cryo-EM structure of NLRP3 open octamer
Authors : Yu, X.; Matico, R.E.; Miller, R.; Schoubroeck, B.V.; Grauwen, K.; Suarez, J.; Pietrak, B.; Haloi, N.; Yin, Y.; Tresadern, G.J.; Perez-Benito, L.; Lindahl, E.; Bottelbergs, A.; Oehlrich, D.; Opdenbosch, N.V.; Sharma, S.
Deposited on : 2023-05-18
Resolution : 3.39 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:

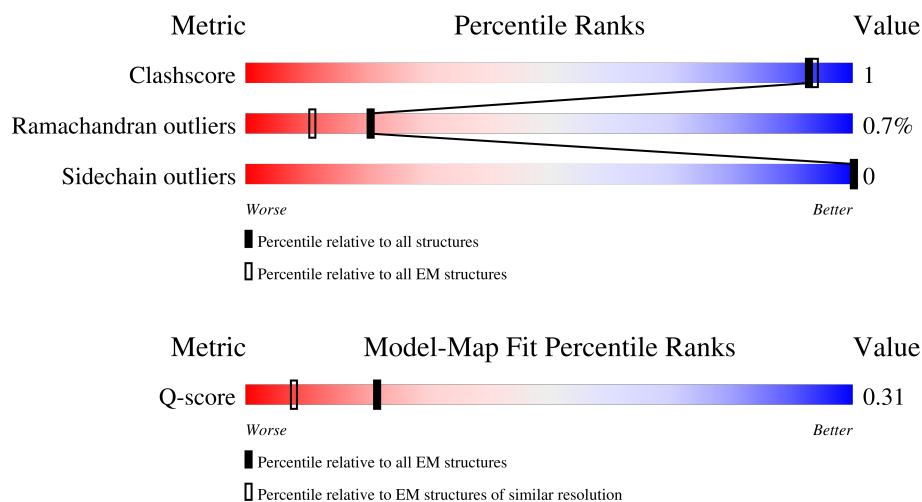
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.39 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	14220 (2.89 - 3.89)

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	910	25% 86% 5% • 8%
1	B	910	26% 86% 5% 8%
1	C	910	51% 87% 5% 8%
1	D	910	25% 85% 6% • 8%

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Mol	Chain	Length	Quality of chain
1	E	910	51% 86% 5% 8%
1	F	910	51% 86% 6% 8%
1	G	910	26% 85% 6% 8%
1	H	910	51% 86% 5% 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 53244 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 NACHT, LRR and PYD domains-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	836	Total	C	N	O	S	0	0
			6667	4246	1133	1230	58		
1	B	836	Total	C	N	O	S	0	0
			6667	4246	1133	1230	58		
1	C	833	Total	C	N	O	S	0	0
			6644	4232	1129	1227	56		
1	D	836	Total	C	N	O	S	0	0
			6667	4246	1133	1230	58		
1	E	833	Total	C	N	O	S	0	0
			6644	4232	1129	1227	56		
1	F	833	Total	C	N	O	S	0	0
			6644	4232	1129	1227	56		
1	G	836	Total	C	N	O	S	0	0
			6667	4246	1133	1230	58		
1	H	833	Total	C	N	O	S	0	0
			6644	4232	1129	1227	56		

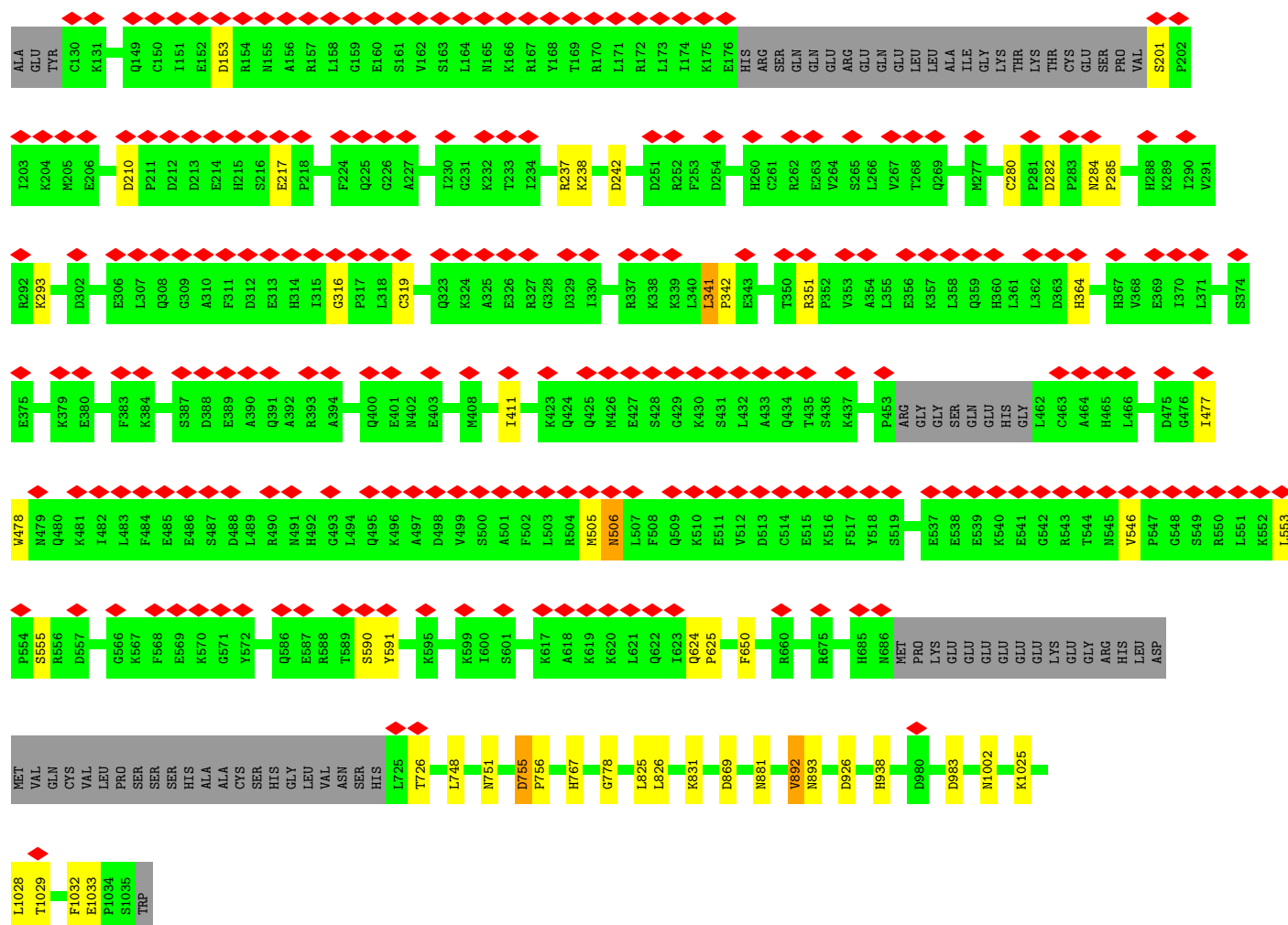
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	ALA	-	expression tag	UNP Q96P20
A	128	GLU	-	expression tag	UNP Q96P20
A	129	TYR	-	expression tag	UNP Q96P20
B	127	ALA	-	expression tag	UNP Q96P20
B	128	GLU	-	expression tag	UNP Q96P20
B	129	TYR	-	expression tag	UNP Q96P20
C	127	ALA	-	expression tag	UNP Q96P20
C	128	GLU	-	expression tag	UNP Q96P20
C	129	TYR	-	expression tag	UNP Q96P20
D	127	ALA	-	expression tag	UNP Q96P20
D	128	GLU	-	expression tag	UNP Q96P20
D	129	TYR	-	expression tag	UNP Q96P20
E	127	ALA	-	expression tag	UNP Q96P20
E	128	GLU	-	expression tag	UNP Q96P20

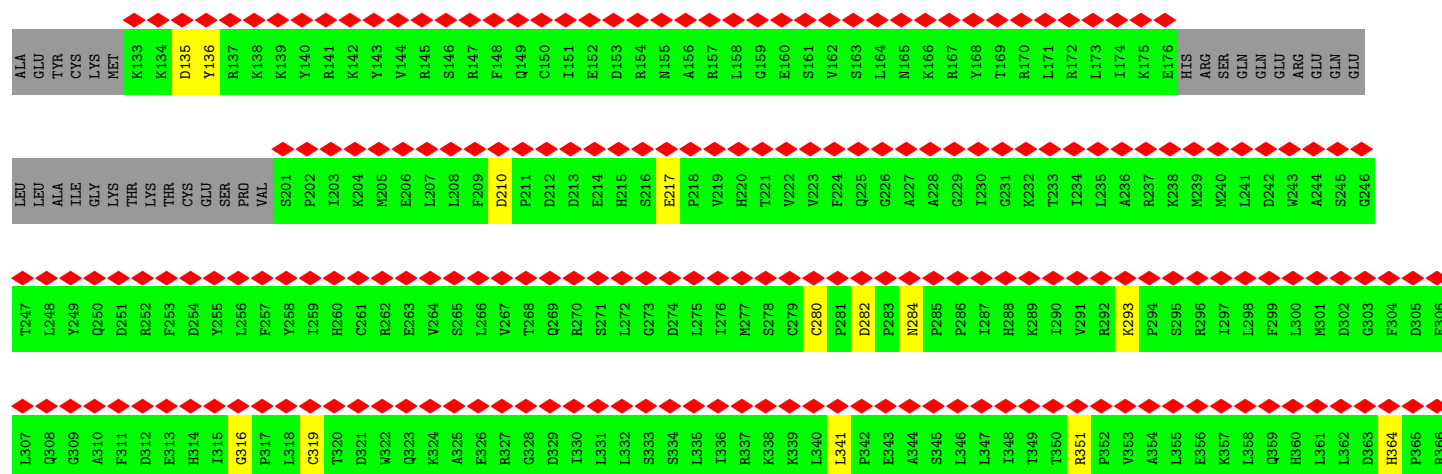
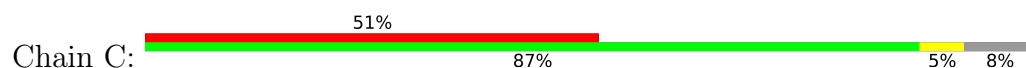
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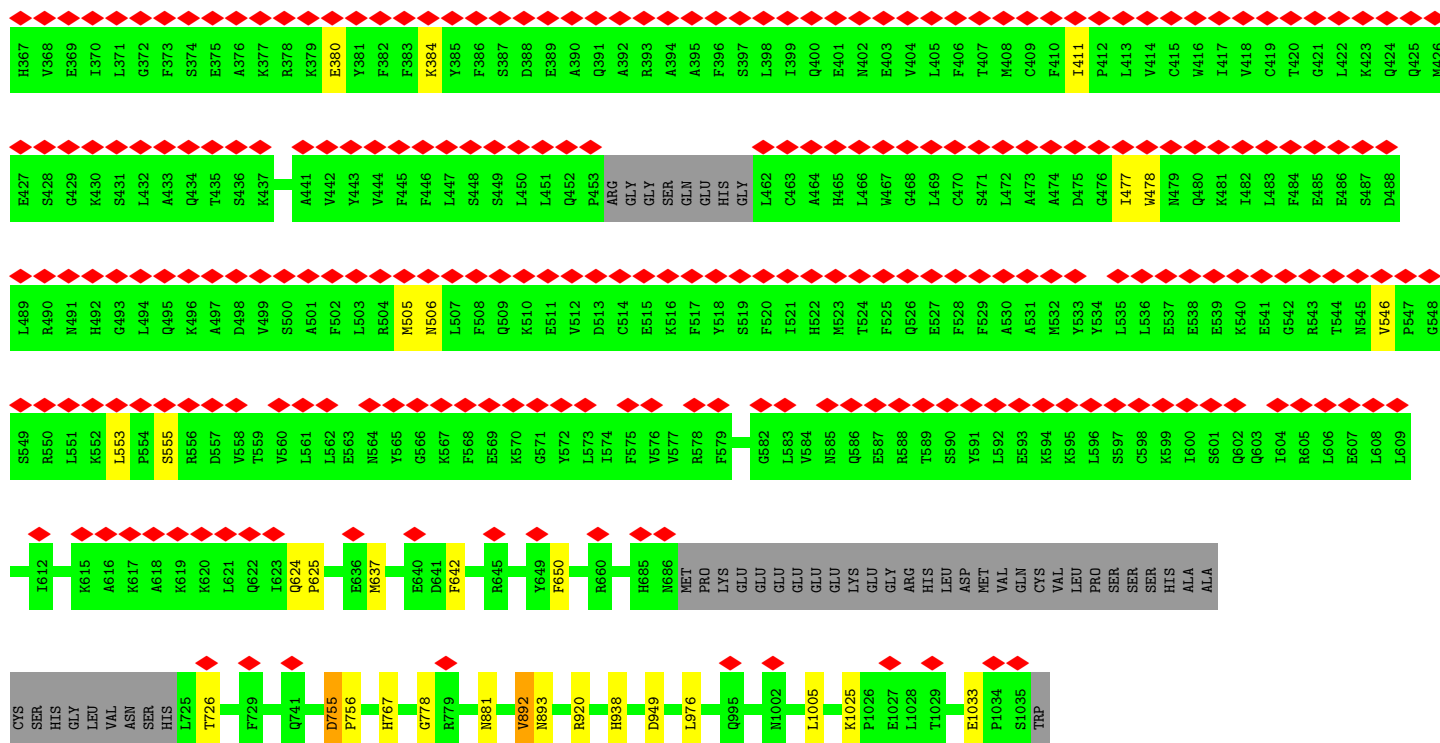
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Chain	Residue	Modelled	Actual	Comment	Reference
E	129	TYR	-	expression tag	UNP Q96P20
F	127	ALA	-	expression tag	UNP Q96P20
F	128	GLU	-	expression tag	UNP Q96P20
F	129	TYR	-	expression tag	UNP Q96P20
G	127	ALA	-	expression tag	UNP Q96P20
G	128	GLU	-	expression tag	UNP Q96P20
G	129	TYR	-	expression tag	UNP Q96P20
H	127	ALA	-	expression tag	UNP Q96P20
H	128	GLU	-	expression tag	UNP Q96P20
H	129	TYR	-	expression tag	UNP Q96P20

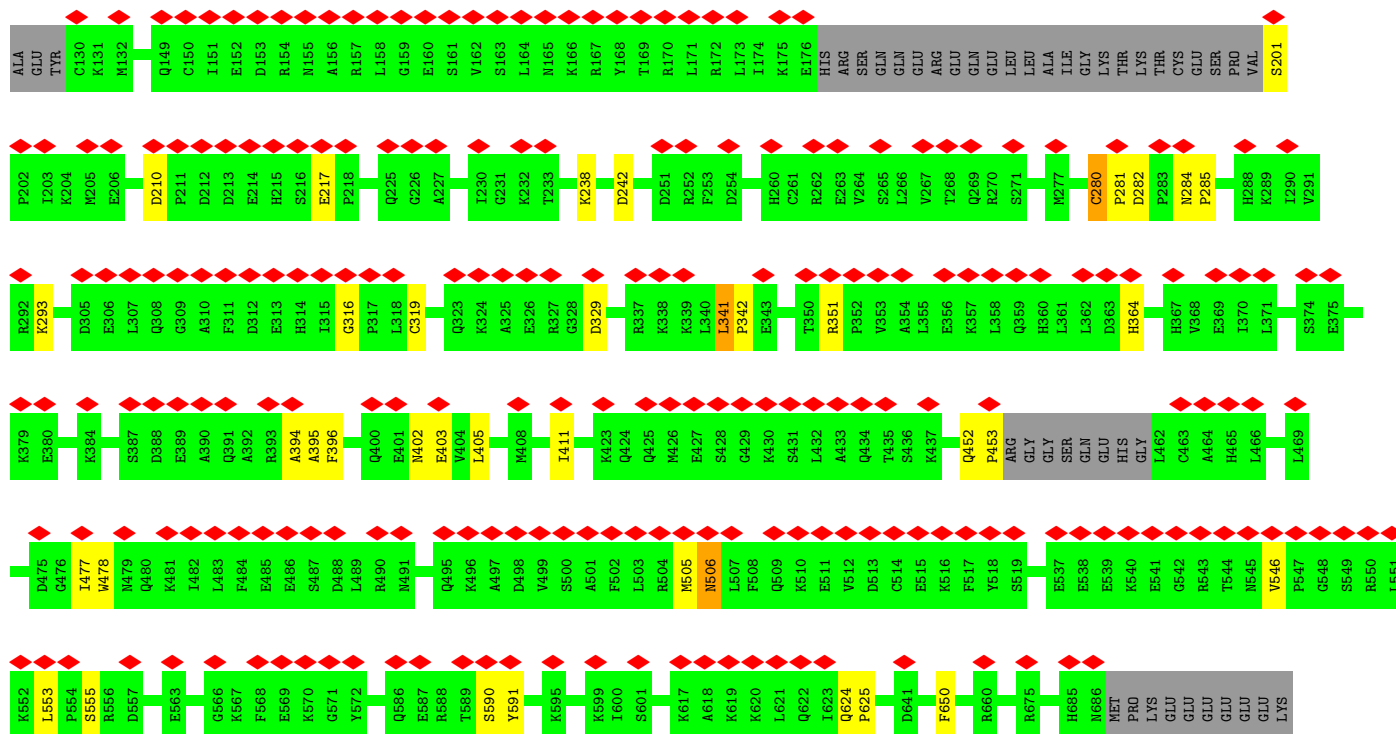
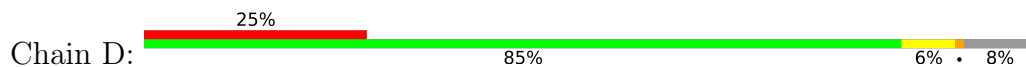


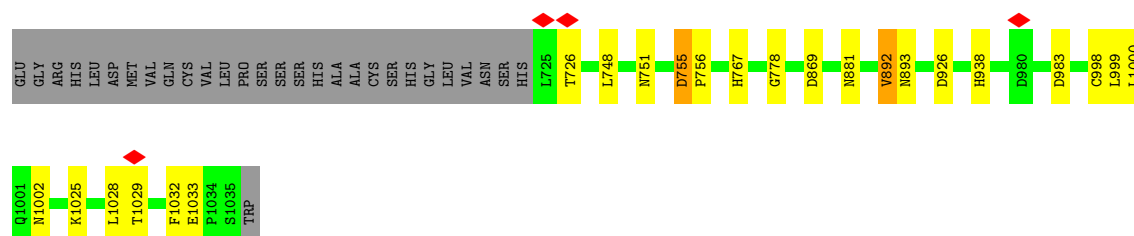
• Molecule 1: NACHT, LRR and PYD domains-containing protein 3



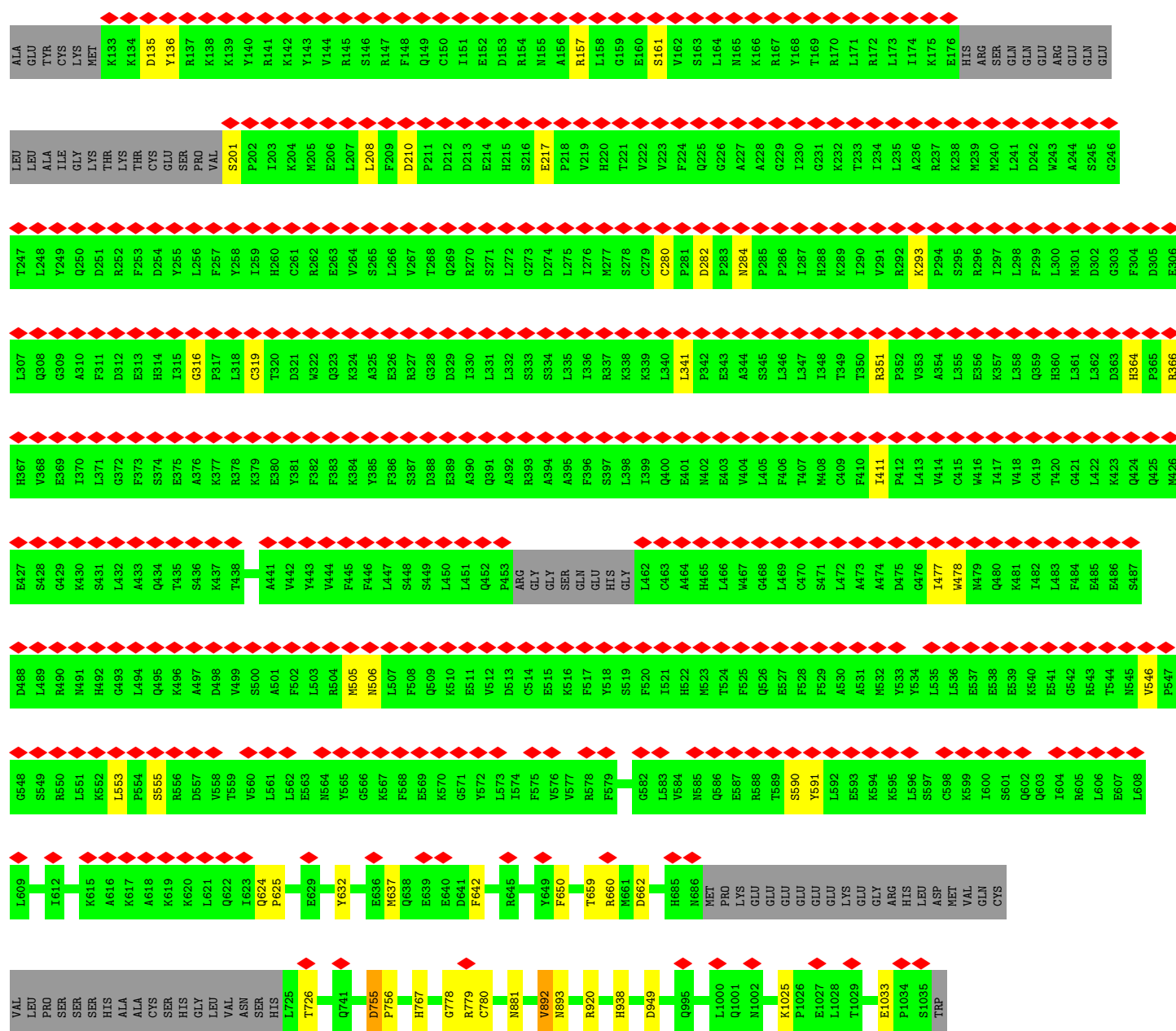
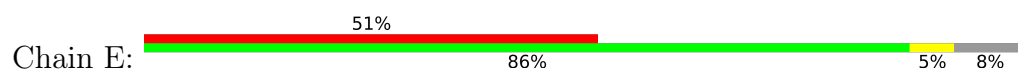


• Molecule 1: NACHT, LRR and PYD domains-containing protein 3

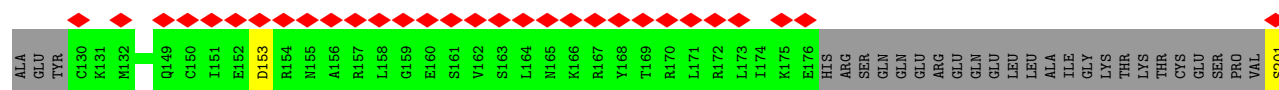




- Molecule 1: NACHT, LRR and PYD domains-containing protein 3



- Molecule 1: NACHT, LRR and PYD domains-containing protein 3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	466664	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 ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.360	Depositor
Minimum map value	-1.507	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	262.4, 262.4, 262.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.66	0/6786	0.87	44/9140 (0.5%)
1	B	0.66	0/6786	0.86	44/9140 (0.5%)
1	C	0.65	0/6763	0.85	40/9111 (0.4%)
1	D	0.66	0/6786	0.87	44/9140 (0.5%)
1	E	0.65	0/6763	0.86	42/9111 (0.5%)
1	F	0.68	4/6763 (0.1%)	0.89	46/9111 (0.5%)
1	G	0.66	0/6786	0.86	44/9140 (0.5%)
1	H	0.65	0/6763	0.86	40/9111 (0.4%)
All	All	0.66	4/54196 (0.0%)	0.87	344/73004 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	394	ALA	C-O	7.13	1.32	1.24
1	F	395	ALA	N-CA	-6.37	1.38	1.46
1	F	395	ALA	C-O	-5.29	1.18	1.24
1	F	394	ALA	C-N	-5.19	1.27	1.33

All (344) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	394	ALA	CA-C-N	8.26	131.18	120.44
1	F	394	ALA	C-N-CA	8.26	131.18	120.44
1	B	1025	LYS	CA-C-N	7.47	127.18	119.56
1	B	1025	LYS	C-N-CA	7.47	127.18	119.56
1	C	553	LEU	CA-C-N	7.44	126.98	119.24
1	C	553	LEU	C-N-CA	7.44	126.98	119.24
1	A	1025	LYS	CA-C-N	7.42	127.13	119.56
1	A	1025	LYS	C-N-CA	7.42	127.13	119.56
1	G	1025	LYS	CA-C-N	7.41	127.12	119.56
1	G	1025	LYS	C-N-CA	7.41	127.12	119.56
1	D	1025	LYS	CA-C-N	7.37	127.08	119.56
1	D	1025	LYS	C-N-CA	7.37	127.08	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	351	ARG	CA-C-N	7.32	127.03	119.56
1	H	351	ARG	C-N-CA	7.32	127.03	119.56
1	F	553	LEU	CA-C-N	7.26	126.79	119.24
1	F	553	LEU	C-N-CA	7.26	126.79	119.24
1	H	1025	LYS	CA-C-N	7.26	126.96	119.56
1	H	1025	LYS	C-N-CA	7.26	126.96	119.56
1	E	1025	LYS	CA-C-N	7.25	126.95	119.56
1	E	1025	LYS	C-N-CA	7.25	126.95	119.56
1	F	1025	LYS	CA-C-N	7.22	126.92	119.56
1	F	1025	LYS	C-N-CA	7.22	126.92	119.56
1	G	280	CYS	CA-C-N	7.21	126.92	119.56
1	G	280	CYS	C-N-CA	7.21	126.92	119.56
1	D	280	CYS	CA-C-N	7.21	126.92	119.56
1	D	280	CYS	C-N-CA	7.21	126.92	119.56
1	C	1025	LYS	CA-C-N	7.20	126.90	119.56
1	C	1025	LYS	C-N-CA	7.20	126.90	119.56
1	F	351	ARG	CA-C-N	7.18	126.89	119.56
1	F	351	ARG	C-N-CA	7.18	126.89	119.56
1	B	280	CYS	CA-C-N	7.18	126.88	119.56
1	B	280	CYS	C-N-CA	7.18	126.88	119.56
1	E	351	ARG	CA-C-N	7.13	126.83	119.56
1	E	351	ARG	C-N-CA	7.13	126.83	119.56
1	H	293	LYS	CA-C-N	7.10	127.06	120.03
1	H	293	LYS	C-N-CA	7.10	127.06	120.03
1	A	280	CYS	CA-C-N	7.08	126.78	119.56
1	A	280	CYS	C-N-CA	7.08	126.78	119.56
1	H	364	HIS	CA-C-N	7.08	127.25	120.31
1	H	364	HIS	C-N-CA	7.08	127.25	120.31
1	B	293	LYS	CA-C-N	7.06	126.99	120.21
1	B	293	LYS	C-N-CA	7.06	126.99	120.21
1	F	293	LYS	CA-C-N	7.02	126.98	120.03
1	F	293	LYS	C-N-CA	7.02	126.98	120.03
1	F	364	HIS	CA-C-N	6.98	127.43	120.52
1	F	364	HIS	C-N-CA	6.98	127.43	120.52
1	B	553	LEU	CA-C-N	6.98	127.27	119.32
1	B	553	LEU	C-N-CA	6.98	127.27	119.32
1	D	341	LEU	CA-C-N	6.96	127.00	119.90
1	D	341	LEU	C-N-CA	6.96	127.00	119.90
1	F	201	SER	CA-C-N	6.92	126.89	119.76
1	F	201	SER	C-N-CA	6.92	126.89	119.76
1	G	364	HIS	CA-C-N	6.89	127.06	120.31
1	G	364	HIS	C-N-CA	6.89	127.06	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	293	LYS	CA-C-N	6.88	126.82	120.21
1	D	293	LYS	C-N-CA	6.88	126.82	120.21
1	D	364	HIS	CA-C-N	6.88	127.05	120.31
1	D	364	HIS	C-N-CA	6.88	127.05	120.31
1	A	293	LYS	CA-C-N	6.88	126.81	120.21
1	A	293	LYS	C-N-CA	6.88	126.81	120.21
1	H	217	GLU	CA-C-N	6.87	126.85	119.78
1	H	217	GLU	C-N-CA	6.87	126.85	119.78
1	A	364	HIS	CA-C-N	6.86	127.04	120.31
1	A	364	HIS	C-N-CA	6.86	127.04	120.31
1	E	364	HIS	CA-C-N	6.86	127.31	120.52
1	E	364	HIS	C-N-CA	6.86	127.31	120.52
1	C	364	HIS	CA-C-N	6.84	127.30	120.52
1	C	364	HIS	C-N-CA	6.84	127.30	120.52
1	B	364	HIS	CA-C-N	6.82	126.99	120.31
1	B	364	HIS	C-N-CA	6.82	126.99	120.31
1	D	553	LEU	CA-C-N	6.81	127.09	119.32
1	D	553	LEU	C-N-CA	6.81	127.09	119.32
1	C	217	GLU	CA-C-N	6.79	126.78	119.78
1	C	217	GLU	C-N-CA	6.79	126.78	119.78
1	H	316	GLY	CA-C-N	6.79	126.70	119.85
1	H	316	GLY	C-N-CA	6.79	126.70	119.85
1	A	553	LEU	CA-C-N	6.78	127.05	119.32
1	A	553	LEU	C-N-CA	6.78	127.05	119.32
1	H	210	ASP	CA-C-N	6.78	126.76	119.78
1	H	210	ASP	C-N-CA	6.78	126.76	119.78
1	C	293	LYS	CA-C-N	6.77	126.74	120.03
1	C	293	LYS	C-N-CA	6.77	126.74	120.03
1	F	217	GLU	CA-C-N	6.75	126.74	119.78
1	F	217	GLU	C-N-CA	6.75	126.74	119.78
1	D	210	ASP	CA-C-N	6.75	126.73	119.78
1	D	210	ASP	C-N-CA	6.75	126.73	119.78
1	A	210	ASP	CA-C-N	6.75	126.73	119.78
1	A	210	ASP	C-N-CA	6.75	126.73	119.78
1	E	282	ASP	CA-C-N	6.75	126.89	119.87
1	E	282	ASP	C-N-CA	6.75	126.89	119.87
1	E	217	GLU	CA-C-N	6.74	126.72	119.78
1	E	217	GLU	C-N-CA	6.74	126.72	119.78
1	F	282	ASP	CA-C-N	6.73	126.87	119.87
1	F	282	ASP	C-N-CA	6.73	126.87	119.87
1	E	316	GLY	CA-C-N	6.72	126.64	119.85
1	E	316	GLY	C-N-CA	6.72	126.64	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	ASP	CA-C-N	6.72	126.70	119.78
1	B	210	ASP	C-N-CA	6.72	126.70	119.78
1	C	282	ASP	CA-C-N	6.72	126.86	119.87
1	C	282	ASP	C-N-CA	6.72	126.86	119.87
1	F	316	GLY	CA-C-N	6.72	126.64	119.85
1	F	316	GLY	C-N-CA	6.72	126.64	119.85
1	C	316	GLY	CA-C-N	6.72	126.64	119.85
1	C	316	GLY	C-N-CA	6.72	126.64	119.85
1	H	282	ASP	CA-C-N	6.69	126.83	119.87
1	H	282	ASP	C-N-CA	6.69	126.83	119.87
1	F	1033	GLU	CA-C-N	6.66	126.29	119.56
1	F	1033	GLU	C-N-CA	6.66	126.29	119.56
1	G	316	GLY	CA-C-N	6.66	126.42	119.76
1	G	316	GLY	C-N-CA	6.66	126.42	119.76
1	E	293	LYS	CA-C-N	6.65	126.62	120.03
1	E	293	LYS	C-N-CA	6.65	126.62	120.03
1	C	1033	GLU	CA-C-N	6.65	126.27	119.56
1	C	1033	GLU	C-N-CA	6.65	126.27	119.56
1	C	351	ARG	CA-C-N	6.62	127.15	119.47
1	C	351	ARG	C-N-CA	6.62	127.15	119.47
1	A	316	GLY	CA-C-N	6.61	126.37	119.76
1	A	316	GLY	C-N-CA	6.61	126.37	119.76
1	B	316	GLY	CA-C-N	6.61	126.37	119.76
1	B	316	GLY	C-N-CA	6.61	126.37	119.76
1	H	553	LEU	CA-C-N	6.56	126.80	119.32
1	H	553	LEU	C-N-CA	6.56	126.80	119.32
1	G	210	ASP	CA-C-N	6.55	126.53	119.78
1	G	210	ASP	C-N-CA	6.55	126.53	119.78
1	D	316	GLY	CA-C-N	6.54	126.31	119.76
1	D	316	GLY	C-N-CA	6.54	126.31	119.76
1	H	1033	GLU	CA-C-N	6.54	126.17	119.56
1	H	1033	GLU	C-N-CA	6.54	126.17	119.56
1	G	201	SER	CA-C-N	6.50	126.46	119.76
1	G	201	SER	C-N-CA	6.50	126.46	119.76
1	C	210	ASP	CA-C-N	6.49	126.47	119.78
1	C	210	ASP	C-N-CA	6.49	126.47	119.78
1	A	351	ARG	CA-C-N	6.49	126.18	119.56
1	A	351	ARG	C-N-CA	6.49	126.18	119.56
1	E	553	LEU	CA-C-N	6.49	126.72	119.32
1	E	553	LEU	C-N-CA	6.49	126.72	119.32
1	E	201	SER	CA-C-N	6.49	126.44	119.76
1	E	201	SER	C-N-CA	6.49	126.44	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1033	GLU	CA-C-N	6.48	126.11	119.56
1	E	1033	GLU	C-N-CA	6.48	126.11	119.56
1	G	282	ASP	CA-C-N	6.48	126.61	119.87
1	G	282	ASP	C-N-CA	6.48	126.61	119.87
1	G	293	LYS	CA-C-N	6.47	126.44	120.03
1	G	293	LYS	C-N-CA	6.47	126.44	120.03
1	D	201	SER	CA-C-N	6.47	126.43	119.76
1	D	201	SER	C-N-CA	6.47	126.43	119.76
1	E	210	ASP	CA-C-N	6.46	126.44	119.78
1	E	210	ASP	C-N-CA	6.46	126.44	119.78
1	F	210	ASP	CA-C-N	6.44	126.42	119.78
1	F	210	ASP	C-N-CA	6.44	126.42	119.78
1	D	282	ASP	CA-C-N	6.38	126.51	119.87
1	D	282	ASP	C-N-CA	6.38	126.51	119.87
1	A	217	GLU	CA-C-N	6.35	126.32	119.78
1	A	217	GLU	C-N-CA	6.35	126.32	119.78
1	G	881	ASN	CA-C-N	6.33	126.02	119.82
1	G	881	ASN	C-N-CA	6.33	126.02	119.82
1	H	881	ASN	CA-C-N	6.31	126.00	119.82
1	H	881	ASN	C-N-CA	6.31	126.00	119.82
1	G	217	GLU	CA-C-N	6.29	126.26	119.78
1	G	217	GLU	C-N-CA	6.29	126.26	119.78
1	A	282	ASP	CA-C-N	6.29	126.41	119.87
1	A	282	ASP	C-N-CA	6.29	126.41	119.87
1	D	881	ASN	CA-C-N	6.29	125.98	119.82
1	D	881	ASN	C-N-CA	6.29	125.98	119.82
1	G	938	HIS	CA-C-N	6.28	125.96	119.56
1	G	938	HIS	C-N-CA	6.28	125.96	119.56
1	D	217	GLU	CA-C-N	6.28	126.24	119.78
1	D	217	GLU	C-N-CA	6.28	126.24	119.78
1	A	201	SER	CA-C-N	6.27	126.21	119.76
1	A	201	SER	C-N-CA	6.27	126.21	119.76
1	B	938	HIS	CA-C-N	6.26	125.95	119.56
1	B	938	HIS	C-N-CA	6.26	125.95	119.56
1	E	881	ASN	CA-C-N	6.25	125.95	119.82
1	E	881	ASN	C-N-CA	6.25	125.95	119.82
1	B	881	ASN	CA-C-N	6.25	125.95	119.82
1	B	881	ASN	C-N-CA	6.25	125.95	119.82
1	C	881	ASN	CA-C-N	6.24	125.94	119.82
1	C	881	ASN	C-N-CA	6.24	125.94	119.82
1	G	341	LEU	CA-C-N	6.24	126.19	119.76
1	G	341	LEU	C-N-CA	6.24	126.19	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	881	ASN	CA-C-N	6.23	125.93	119.82
1	F	881	ASN	C-N-CA	6.23	125.93	119.82
1	G	351	ARG	CA-C-N	6.23	126.70	119.47
1	G	351	ARG	C-N-CA	6.23	126.70	119.47
1	B	217	GLU	CA-C-N	6.22	126.19	119.78
1	B	217	GLU	C-N-CA	6.22	126.19	119.78
1	B	282	ASP	CA-C-N	6.22	126.34	119.87
1	B	282	ASP	C-N-CA	6.22	126.34	119.87
1	A	881	ASN	CA-C-N	6.18	125.88	119.82
1	A	881	ASN	C-N-CA	6.18	125.88	119.82
1	E	341	LEU	CA-C-N	6.16	126.18	119.90
1	E	341	LEU	C-N-CA	6.16	126.18	119.90
1	D	938	HIS	CA-C-N	6.16	125.84	119.56
1	D	938	HIS	C-N-CA	6.16	125.84	119.56
1	B	351	ARG	CA-C-N	6.15	126.60	119.47
1	B	351	ARG	C-N-CA	6.15	126.60	119.47
1	E	938	HIS	CA-C-N	6.12	125.80	119.56
1	E	938	HIS	C-N-CA	6.12	125.80	119.56
1	D	351	ARG	CA-C-N	6.11	126.56	119.47
1	D	351	ARG	C-N-CA	6.11	126.56	119.47
1	A	1033	GLU	CA-C-N	6.10	125.72	119.56
1	A	1033	GLU	C-N-CA	6.10	125.72	119.56
1	E	650	PHE	CA-C-N	6.10	125.72	119.56
1	E	650	PHE	C-N-CA	6.10	125.72	119.56
1	A	341	LEU	CA-C-N	6.09	126.03	119.76
1	A	341	LEU	C-N-CA	6.09	126.03	119.76
1	D	1033	GLU	CA-C-N	6.09	125.71	119.56
1	D	1033	GLU	C-N-CA	6.09	125.71	119.56
1	H	650	PHE	CA-C-N	6.08	125.70	119.56
1	H	650	PHE	C-N-CA	6.08	125.70	119.56
1	F	650	PHE	CA-C-N	6.06	125.74	119.56
1	F	650	PHE	C-N-CA	6.06	125.74	119.56
1	E	767	HIS	CA-C-N	6.05	126.49	119.47
1	E	767	HIS	C-N-CA	6.05	126.49	119.47
1	B	767	HIS	CA-C-N	6.03	126.47	119.47
1	B	767	HIS	C-N-CA	6.03	126.47	119.47
1	C	650	PHE	CA-C-N	6.03	125.71	119.56
1	C	650	PHE	C-N-CA	6.03	125.71	119.56
1	G	1033	GLU	CA-C-N	6.03	125.65	119.56
1	G	1033	GLU	C-N-CA	6.03	125.65	119.56
1	H	767	HIS	CA-C-N	6.03	126.46	119.47
1	H	767	HIS	C-N-CA	6.03	126.46	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	767	HIS	CA-C-N	6.01	126.44	119.47
1	C	767	HIS	C-N-CA	6.01	126.44	119.47
1	C	938	HIS	CA-C-N	5.99	125.67	119.56
1	C	938	HIS	C-N-CA	5.99	125.67	119.56
1	H	938	HIS	CA-C-N	5.99	125.67	119.56
1	H	938	HIS	C-N-CA	5.99	125.67	119.56
1	B	341	LEU	CA-C-N	5.99	125.92	119.76
1	B	341	LEU	C-N-CA	5.99	125.92	119.76
1	F	767	HIS	CA-C-N	5.98	126.41	119.47
1	F	767	HIS	C-N-CA	5.98	126.41	119.47
1	D	767	HIS	CA-C-N	5.98	126.41	119.47
1	D	767	HIS	C-N-CA	5.98	126.41	119.47
1	G	553	LEU	CA-C-N	5.97	126.13	119.32
1	G	553	LEU	C-N-CA	5.97	126.13	119.32
1	G	767	HIS	CA-C-N	5.97	126.40	119.47
1	G	767	HIS	C-N-CA	5.97	126.40	119.47
1	B	1033	GLU	CA-C-N	5.95	125.57	119.56
1	B	1033	GLU	C-N-CA	5.95	125.57	119.56
1	F	938	HIS	CA-C-N	5.93	125.61	119.56
1	F	938	HIS	C-N-CA	5.93	125.61	119.56
1	B	201	SER	CA-C-N	5.92	125.85	119.76
1	B	201	SER	C-N-CA	5.92	125.85	119.76
1	A	938	HIS	CA-C-N	5.89	125.57	119.56
1	A	938	HIS	C-N-CA	5.89	125.57	119.56
1	A	767	HIS	CA-C-N	5.85	126.26	119.47
1	A	767	HIS	C-N-CA	5.85	126.26	119.47
1	F	341	LEU	CA-C-N	5.83	125.85	119.90
1	F	341	LEU	C-N-CA	5.83	125.85	119.90
1	B	411	ILE	CA-C-N	5.83	125.97	119.32
1	B	411	ILE	C-N-CA	5.83	125.97	119.32
1	F	546	VAL	CA-C-N	5.79	126.19	119.47
1	F	546	VAL	C-N-CA	5.79	126.19	119.47
1	G	411	ILE	CA-C-N	5.79	125.92	119.32
1	G	411	ILE	C-N-CA	5.79	125.92	119.32
1	D	546	VAL	CA-C-N	5.77	126.17	119.47
1	D	546	VAL	C-N-CA	5.77	126.17	119.47
1	E	546	VAL	CA-C-N	5.76	126.15	119.47
1	E	546	VAL	C-N-CA	5.76	126.15	119.47
1	G	546	VAL	CA-C-N	5.75	126.14	119.47
1	G	546	VAL	C-N-CA	5.75	126.14	119.47
1	B	546	VAL	CA-C-N	5.73	126.11	119.47
1	B	546	VAL	C-N-CA	5.73	126.11	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	546	VAL	CA-C-N	5.73	126.11	119.47
1	C	546	VAL	C-N-CA	5.73	126.11	119.47
1	D	755	ASP	CA-C-N	5.72	125.39	119.56
1	D	755	ASP	C-N-CA	5.72	125.39	119.56
1	A	546	VAL	CA-C-N	5.70	126.08	119.47
1	A	546	VAL	C-N-CA	5.70	126.08	119.47
1	G	755	ASP	CA-C-N	5.68	125.35	119.56
1	G	755	ASP	C-N-CA	5.68	125.35	119.56
1	H	284	ASN	CA-C-N	5.64	126.19	120.38
1	H	284	ASN	C-N-CA	5.64	126.19	120.38
1	A	650	PHE	CA-C-N	5.63	125.47	119.28
1	A	650	PHE	C-N-CA	5.63	125.47	119.28
1	E	284	ASN	CA-C-N	5.63	126.18	120.38
1	E	284	ASN	C-N-CA	5.63	126.18	120.38
1	A	755	ASP	CA-C-N	5.62	125.30	119.56
1	A	755	ASP	C-N-CA	5.62	125.30	119.56
1	F	284	ASN	CA-C-N	5.61	126.16	120.38
1	F	284	ASN	C-N-CA	5.61	126.16	120.38
1	A	411	ILE	CA-C-N	5.60	125.70	119.32
1	A	411	ILE	C-N-CA	5.60	125.70	119.32
1	C	284	ASN	CA-C-N	5.59	126.14	120.38
1	C	284	ASN	C-N-CA	5.59	126.14	120.38
1	B	650	PHE	CA-C-N	5.58	125.42	119.28
1	B	650	PHE	C-N-CA	5.58	125.42	119.28
1	D	650	PHE	CA-C-N	5.58	125.41	119.28
1	D	650	PHE	C-N-CA	5.58	125.41	119.28
1	F	280	CYS	CA-C-N	5.56	126.79	119.84
1	F	280	CYS	C-N-CA	5.56	126.79	119.84
1	F	411	ILE	CA-C-N	5.56	125.66	119.32
1	F	411	ILE	C-N-CA	5.56	125.66	119.32
1	G	650	PHE	CA-C-N	5.56	125.40	119.28
1	G	650	PHE	C-N-CA	5.56	125.40	119.28
1	D	411	ILE	CA-C-N	5.56	125.66	119.32
1	D	411	ILE	C-N-CA	5.56	125.66	119.32
1	E	411	ILE	CA-C-N	5.55	125.65	119.32
1	E	411	ILE	C-N-CA	5.55	125.65	119.32
1	H	280	CYS	CA-C-N	5.53	126.75	119.84
1	H	280	CYS	C-N-CA	5.53	126.75	119.84
1	H	411	ILE	CA-C-N	5.53	125.62	119.32
1	H	411	ILE	C-N-CA	5.53	125.62	119.32
1	C	280	CYS	CA-C-N	5.52	126.74	119.84
1	C	280	CYS	C-N-CA	5.52	126.74	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	755	ASP	CA-C-N	5.50	125.17	119.56
1	F	755	ASP	C-N-CA	5.50	125.17	119.56
1	H	755	ASP	CA-C-N	5.49	125.16	119.56
1	H	755	ASP	C-N-CA	5.49	125.16	119.56
1	E	280	CYS	CA-C-N	5.48	126.69	119.84
1	E	280	CYS	C-N-CA	5.48	126.69	119.84
1	E	755	ASP	CA-C-N	5.45	125.12	119.56
1	E	755	ASP	C-N-CA	5.45	125.12	119.56
1	C	411	ILE	CA-C-N	5.44	125.53	119.32
1	C	411	ILE	C-N-CA	5.44	125.53	119.32
1	B	284	ASN	CA-C-N	5.43	125.97	120.38
1	B	284	ASN	C-N-CA	5.43	125.97	120.38
1	C	755	ASP	CA-C-N	5.42	125.09	119.56
1	C	755	ASP	C-N-CA	5.42	125.09	119.56
1	B	755	ASP	CA-C-N	5.42	125.09	119.56
1	B	755	ASP	C-N-CA	5.42	125.09	119.56
1	G	284	ASN	CA-C-N	5.42	125.96	120.38
1	G	284	ASN	C-N-CA	5.42	125.96	120.38
1	A	285	PRO	CA-C-N	5.33	126.50	119.84
1	A	285	PRO	C-N-CA	5.33	126.50	119.84
1	D	284	ASN	CA-C-N	5.32	125.86	120.38
1	D	284	ASN	C-N-CA	5.32	125.86	120.38
1	D	285	PRO	CA-C-N	5.26	126.41	119.84
1	D	285	PRO	C-N-CA	5.26	126.41	119.84
1	B	285	PRO	CA-C-N	5.23	126.38	119.84
1	B	285	PRO	C-N-CA	5.23	126.38	119.84
1	F	285	PRO	CA-C-N	5.21	126.35	119.84
1	F	285	PRO	C-N-CA	5.21	126.35	119.84
1	A	284	ASN	CA-C-N	5.21	125.74	120.38
1	A	284	ASN	C-N-CA	5.21	125.74	120.38
1	H	341	LEU	CA-C-N	5.20	125.13	119.78
1	H	341	LEU	C-N-CA	5.20	125.13	119.78
1	G	285	PRO	CA-C-N	5.16	126.29	119.84
1	G	285	PRO	C-N-CA	5.16	126.29	119.84
1	H	546	VAL	CA-C-N	5.10	126.21	119.84
1	H	546	VAL	C-N-CA	5.10	126.21	119.84
1	C	341	LEU	CA-C-N	5.07	124.98	119.76
1	C	341	LEU	C-N-CA	5.07	124.98	119.76

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	6667	0	6735	21	0
1	B	6667	0	6735	19	0
1	C	6644	0	6708	11	0
1	D	6667	0	6735	25	0
1	E	6644	0	6708	17	0
1	F	6644	0	6708	17	0
1	G	6667	0	6735	21	0
1	H	6644	0	6708	17	0
All	All	53244	0	53772	147	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 1.

All (147) 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:D:238:LYS:NZ	1:D:242:ASP:OD1	2.34	0.59
1:G:238:LYS:NZ	1:G:242:ASP:OD1	2.36	0.58
1:A:238:LYS:NZ	1:A:242:ASP:OD1	2.35	0.58
1:A:402:ASN:HD21	1:A:405:LEU:H	1.52	0.58
1:B:238:LYS:NZ	1:B:242:ASP:OD1	2.35	0.58
1:D:402:ASN:HD21	1:D:405:LEU:H	1.53	0.56
1:B:1028:LEU:O	1:B:1029:THR:C	2.52	0.53
1:H:632:TYR:OH	1:H:662:ASP:OD1	2.26	0.53
1:A:1028:LEU:O	1:A:1029:THR:C	2.53	0.52
1:D:1028:LEU:O	1:D:1029:THR:C	2.52	0.52
1:D:505:MET:O	1:D:506:ASN:C	2.52	0.52
1:A:505:MET:O	1:A:506:ASN:C	2.53	0.51
1:G:505:MET:O	1:G:506:ASN:C	2.54	0.51
1:F:632:TYR:OH	1:F:662:ASP:OD1	2.29	0.51
1:B:505:MET:O	1:B:506:ASN:C	2.52	0.51
1:E:632:TYR:OH	1:E:662:ASP:OD1	2.29	0.51
1:G:624:GLN:HB3	1:G:625:PRO:CD	2.41	0.50
1:G:1028:LEU:O	1:G:1029:THR:C	2.54	0.50
1:G:624:GLN:HB3	1:G:625:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:GLN:HB3	1:A:625:PRO:CD	2.43	0.49
1:B:624:GLN:HB3	1:B:625:PRO:CD	2.43	0.49
1:D:624:GLN:HB3	1:D:625:PRO:CD	2.43	0.49
1:D:926:ASP:OD1	1:D:926:ASP:N	2.45	0.49
1:A:926:ASP:OD1	1:A:926:ASP:N	2.46	0.48
1:A:983:ASP:N	1:A:983:ASP:OD1	2.43	0.48
1:E:505:MET:O	1:E:506:ASN:C	2.56	0.48
1:D:402:ASN:ND2	1:D:405:LEU:H	2.12	0.47
1:H:505:MET:O	1:H:506:ASN:C	2.57	0.47
1:A:402:ASN:ND2	1:A:405:LEU:H	2.12	0.47
1:B:831:LYS:NZ	1:G:1019:GLU:OE2	2.48	0.47
1:E:135:ASP:OD1	1:E:136:TYR:N	2.47	0.47
1:H:380:GLU:OE1	1:H:384:LYS:NZ	2.48	0.47
1:H:590:SER:OG	1:H:591:TYR:N	2.48	0.47
1:C:505:MET:O	1:C:506:ASN:C	2.58	0.47
1:E:624:GLN:HB3	1:E:625:PRO:HD2	1.96	0.47
1:F:135:ASP:OD1	1:F:136:TYR:N	2.48	0.46
1:B:983:ASP:OD1	1:B:983:ASP:N	2.44	0.46
1:H:135:ASP:OD1	1:H:136:TYR:N	2.48	0.46
1:C:135:ASP:OD1	1:C:136:TYR:N	2.48	0.46
1:D:983:ASP:OD1	1:D:983:ASP:N	2.45	0.46
1:D:998:CYS:O	1:D:1000:LEU:N	2.49	0.46
1:F:505:MET:O	1:F:506:ASN:C	2.58	0.46
1:F:624:GLN:HB3	1:F:625:PRO:HD2	1.96	0.46
1:G:590:SER:OG	1:G:591:TYR:N	2.49	0.46
1:G:983:ASP:N	1:G:983:ASP:OD1	2.44	0.46
1:C:380:GLU:OE1	1:C:384:LYS:NZ	2.48	0.46
1:D:748:LEU:O	1:D:751:ASN:ND2	2.49	0.46
1:B:590:SER:OG	1:B:591:TYR:N	2.49	0.46
1:E:590:SER:OG	1:E:591:TYR:N	2.49	0.46
1:C:976:LEU:O	1:C:1005:LEU:N	2.44	0.45
1:H:976:LEU:O	1:H:1005:LEU:N	2.44	0.45
1:H:624:GLN:HB3	1:H:625:PRO:HD2	1.98	0.45
1:F:590:SER:OG	1:F:591:TYR:N	2.49	0.45
1:G:926:ASP:N	1:G:926:ASP:OD1	2.46	0.45
1:B:748:LEU:O	1:B:751:ASN:ND2	2.49	0.45
1:D:341:LEU:N	1:D:342:PRO:HD3	2.32	0.45
1:A:748:LEU:O	1:A:751:ASN:ND2	2.50	0.45
1:E:624:GLN:HB3	1:E:625:PRO:CD	2.46	0.45
1:D:590:SER:OG	1:D:591:TYR:N	2.49	0.45
1:B:926:ASP:N	1:B:926:ASP:OD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:748:LEU:O	1:G:751:ASN:ND2	2.49	0.45
1:F:624:GLN:HB3	1:F:625:PRO:CD	2.47	0.44
1:A:755:ASP:N	1:A:756:PRO:CD	2.80	0.44
1:D:755:ASP:N	1:D:756:PRO:CD	2.80	0.44
1:F:920:ARG:HB2	1:F:949:ASP:HB3	2.00	0.44
1:B:624:GLN:HB3	1:B:625:PRO:HD2	1.99	0.44
1:E:920:ARG:HB2	1:E:949:ASP:HB3	2.00	0.44
1:D:624:GLN:HB3	1:D:625:PRO:HD2	2.00	0.44
1:A:624:GLN:HB3	1:A:625:PRO:HD2	2.00	0.44
1:G:380:GLU:OE1	1:G:384:LYS:NZ	2.51	0.44
1:G:755:ASP:N	1:G:756:PRO:CD	2.80	0.43
1:B:755:ASP:N	1:B:756:PRO:CD	2.80	0.43
1:A:869:ASP:OD1	1:A:869:ASP:N	2.50	0.43
1:C:920:ARG:HB2	1:C:949:ASP:HB3	2.00	0.43
1:D:1002:ASN:OD1	1:D:1002:ASN:N	2.51	0.43
1:F:892:VAL:HG12	1:F:893:ASN:N	2.33	0.43
1:B:153:ASP:OD2	1:B:237:ARG:NH2	2.50	0.43
1:C:624:GLN:HB3	1:C:625:PRO:HD2	2.01	0.43
1:D:394:ALA:O	1:D:395:ALA:HB3	2.18	0.43
1:E:157:ARG:NH1	1:E:161:SER:O	2.50	0.43
1:D:869:ASP:OD1	1:D:869:ASP:N	2.51	0.43
1:G:153:ASP:OD2	1:G:237:ARG:NH2	2.50	0.43
1:E:778:GLY:O	1:E:780:CYS:N	2.52	0.43
1:E:892:VAL:HG12	1:E:893:ASN:N	2.34	0.43
1:H:920:ARG:HB2	1:H:949:ASP:HB3	2.00	0.43
1:A:477:ILE:HG13	1:A:478:TRP:N	2.34	0.43
1:B:1002:ASN:OD1	1:B:1002:ASN:N	2.52	0.43
1:D:402:ASN:OD1	1:D:403:GLU:N	2.51	0.43
1:H:892:VAL:HG12	1:H:893:ASN:N	2.34	0.43
1:F:157:ARG:NH1	1:F:161:SER:O	2.51	0.43
1:C:892:VAL:HG12	1:C:893:ASN:N	2.34	0.43
1:A:319:CYS:O	1:A:319:CYS:SG	2.77	0.42
1:B:341:LEU:N	1:B:342:PRO:HD3	2.34	0.42
1:F:755:ASP:N	1:F:756:PRO:CD	2.83	0.42
1:B:319:CYS:SG	1:B:319:CYS:O	2.78	0.42
1:F:477:ILE:HG13	1:F:478:TRP:N	2.34	0.42
1:F:659:THR:OG1	1:F:660:ARG:N	2.52	0.42
1:A:1031:VAL:O	1:A:1032:PHE:HB3	2.20	0.42
1:E:208:LEU:O	1:E:366:ARG:NH1	2.52	0.42
1:G:1031:VAL:O	1:G:1032:PHE:HB3	2.20	0.42
1:H:624:GLN:HB3	1:H:625:PRO:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LEU:N	1:A:342:PRO:HD3	2.34	0.42
1:C:477:ILE:HG13	1:C:478:TRP:N	2.35	0.42
1:D:477:ILE:HG13	1:D:478:TRP:N	2.35	0.42
1:E:755:ASP:HB2	1:E:756:PRO:HD3	2.02	0.42
1:G:869:ASP:OD1	1:G:869:ASP:N	2.51	0.42
1:H:659:THR:OG1	1:H:660:ARG:N	2.53	0.42
1:D:892:VAL:HG12	1:D:893:ASN:N	2.35	0.42
1:F:319:CYS:SG	1:F:319:CYS:O	2.78	0.42
1:D:319:CYS:SG	1:D:319:CYS:O	2.78	0.41
1:A:892:VAL:HG12	1:A:893:ASN:N	2.36	0.41
1:G:319:CYS:O	1:G:319:CYS:SG	2.78	0.41
1:H:477:ILE:HG13	1:H:478:TRP:N	2.36	0.41
1:A:402:ASN:OD1	1:A:403:GLU:N	2.53	0.41
1:F:755:ASP:HB2	1:F:756:PRO:HD3	2.03	0.41
1:E:755:ASP:N	1:E:756:PRO:CD	2.84	0.41
1:E:319:CYS:SG	1:E:319:CYS:O	2.78	0.41
1:E:659:THR:OG1	1:E:660:ARG:N	2.53	0.41
1:F:380:GLU:OE1	1:F:384:LYS:NZ	2.54	0.41
1:F:637:MET:SD	1:F:642:PHE:CD2	3.14	0.41
1:H:319:CYS:SG	1:H:319:CYS:O	2.78	0.41
1:H:804:ASP:OD1	1:H:804:ASP:C	2.64	0.41
1:B:477:ILE:HG13	1:B:478:TRP:N	2.35	0.41
1:C:319:CYS:SG	1:C:319:CYS:O	2.78	0.41
1:G:477:ILE:HG13	1:G:478:TRP:N	2.35	0.41
1:D:452:GLN:N	1:D:453:PRO:CD	2.84	0.41
1:E:477:ILE:HG13	1:E:478:TRP:N	2.35	0.41
1:G:341:LEU:N	1:G:342:PRO:HD3	2.35	0.41
1:G:533:TYR:O	1:G:556:ARG:NH1	2.54	0.41
1:H:251:ASP:OD1	1:H:251:ASP:N	2.52	0.41
1:H:555:SER:OG	1:H:556:ARG:N	2.54	0.41
1:H:755:ASP:N	1:H:756:PRO:CD	2.82	0.41
1:B:892:VAL:HG12	1:B:893:ASN:N	2.35	0.41
1:A:659:THR:OG1	1:A:660:ARG:N	2.54	0.41
1:D:394:ALA:O	1:D:396:PHE:N	2.53	0.41
1:F:804:ASP:OD1	1:F:804:ASP:C	2.64	0.41
1:B:869:ASP:OD1	1:B:869:ASP:N	2.50	0.40
1:D:280:CYS:HB2	1:D:281:PRO:CD	2.51	0.40
1:E:637:MET:SD	1:E:642:PHE:CD2	3.14	0.40
1:G:825:LEU:O	1:G:826:LEU:HB2	2.22	0.40
1:A:329:ASP:OD1	1:A:329:ASP:N	2.53	0.40
1:B:825:LEU:O	1:B:826:LEU:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:GLN:N	1:A:453:PRO:CD	2.85	0.40
1:C:755:ASP:HB2	1:C:756:PRO:HD3	2.02	0.40
1:C:637:MET:SD	1:C:642:PHE:CD2	3.15	0.40
1:D:329:ASP:OD1	1:D:329:ASP:N	2.53	0.40
1:G:452:GLN:N	1:G:453:PRO:CD	2.85	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	820/910 (90%)	783 (96%)	30 (4%)	7 (1%)	14	42
1	B	820/910 (90%)	784 (96%)	30 (4%)	6 (1%)	18	47
1	C	817/910 (90%)	780 (96%)	33 (4%)	4 (0%)	24	54
1	D	820/910 (90%)	780 (95%)	33 (4%)	7 (1%)	14	42
1	E	817/910 (90%)	783 (96%)	30 (4%)	4 (0%)	24	54
1	F	817/910 (90%)	783 (96%)	29 (4%)	5 (1%)	21	50
1	G	820/910 (90%)	783 (96%)	29 (4%)	8 (1%)	12	40
1	H	817/910 (90%)	781 (96%)	31 (4%)	5 (1%)	21	50
All	All	6548/7280 (90%)	6257 (96%)	245 (4%)	46 (1%)	20	47

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	892	VAL
1	A	1032	PHE
1	B	892	VAL
1	C	892	VAL
1	D	892	VAL

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Mol	Chain	Res	Type
1	D	999	LEU
1	D	1032	PHE
1	E	555	SER
1	E	892	VAL
1	F	892	VAL
1	G	892	VAL
1	G	1032	PHE
1	H	892	VAL
1	A	555	SER
1	A	1029	THR
1	B	555	SER
1	B	1032	PHE
1	C	555	SER
1	C	726	THR
1	D	555	SER
1	E	726	THR
1	F	555	SER
1	F	726	THR
1	G	555	SER
1	G	1029	THR
1	H	555	SER
1	A	726	THR
1	B	506	ASN
1	B	726	THR
1	D	726	THR
1	E	779	ARG
1	H	726	THR
1	A	506	ASN
1	D	506	ASN
1	F	506	ASN
1	G	506	ASN
1	G	726	THR
1	B	778	GLY
1	G	949	ASP
1	H	506	ASN
1	C	778	GLY
1	F	778	GLY
1	G	778	GLY
1	H	778	GLY
1	A	778	GLY
1	D	778	GLY

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	758/822 (92%)	758 (100%)	0	100	100
1	B	758/822 (92%)	758 (100%)	0	100	100
1	C	755/822 (92%)	755 (100%)	0	100	100
1	D	758/822 (92%)	758 (100%)	0	100	100
1	E	755/822 (92%)	755 (100%)	0	100	100
1	F	755/822 (92%)	755 (100%)	0	100	100
1	G	758/822 (92%)	758 (100%)	0	100	100
1	H	755/822 (92%)	755 (100%)	0	100	100
All	All	6052/6576 (92%)	6052 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	314	HIS
1	A	360	HIS
1	A	391	GLN
1	A	425	GLN
1	A	495	GLN
1	A	622	GLN
1	A	638	GLN
1	A	798	GLN
1	A	1002	ASN
1	B	269	GLN
1	B	314	HIS
1	B	323	GLN
1	B	400	GLN
1	B	434	GLN
1	B	495	GLN
1	B	638	GLN
1	B	784	HIS

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Mol	Chain	Res	Type
1	C	314	HIS
1	C	495	GLN
1	C	644	GLN
1	C	672	ASN
1	C	686	ASN
1	D	314	HIS
1	D	391	GLN
1	D	434	GLN
1	D	495	GLN
1	D	798	GLN
1	E	314	HIS
1	E	495	GLN
1	E	644	GLN
1	E	672	ASN
1	E	956	HIS
1	F	314	HIS
1	F	495	GLN
1	F	686	ASN
1	G	314	HIS
1	G	400	GLN
1	G	509	GLN
1	G	622	GLN
1	G	638	GLN
1	G	956	HIS
1	G	1002	ASN
1	H	314	HIS
1	H	495	GLN
1	H	956	HIS

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 [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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	4
1	C	4
1	H	4
1	F	4
1	A	4
1	G	4
1	D	4
1	B	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	370:ILE	C	371:LEU	N	5.54
1	C	370:ILE	C	371:LEU	N	5.46
1	H	370:ILE	C	371:LEU	N	5.46
1	F	370:ILE	C	371:LEU	N	5.42
1	H	437:LYS	C	438:THR	N	5.17
1	F	437:LYS	C	438:THR	N	5.16
1	E	437:LYS	C	438:THR	N	5.12
1	A	370:ILE	C	371:LEU	N	4.97
1	G	370:ILE	C	371:LEU	N	4.94
1	D	437:LYS	C	438:THR	N	4.88
1	D	370:ILE	C	371:LEU	N	4.80
1	A	437:LYS	C	438:THR	N	4.76
1	B	370:ILE	C	371:LEU	N	4.76
1	G	437:LYS	C	438:THR	N	4.76
1	C	437:LYS	C	438:THR	N	4.75
1	B	437:LYS	C	438:THR	N	4.74
1	A	537:GLU	C	538:GLU	N	4.09
1	D	537:GLU	C	538:GLU	N	4.09

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	537:GLU	C	538:GLU	N	4.08
1	G	537:GLU	C	538:GLU	N	4.04
1	H	552:LYS	C	553:LEU	N	3.68
1	A	552:LYS	C	553:LEU	N	3.61
1	G	552:LYS	C	553:LEU	N	3.58
1	B	552:LYS	C	553:LEU	N	3.56
1	E	552:LYS	C	553:LEU	N	3.55
1	D	552:LYS	C	553:LEU	N	3.54
1	F	552:LYS	C	553:LEU	N	3.51
1	H	537:GLU	C	538:GLU	N	3.50
1	E	537:GLU	C	538:GLU	N	3.42
1	F	537:GLU	C	538:GLU	N	3.42
1	C	552:LYS	C	553:LEU	N	3.41
1	C	537:GLU	C	538:GLU	N	3.39

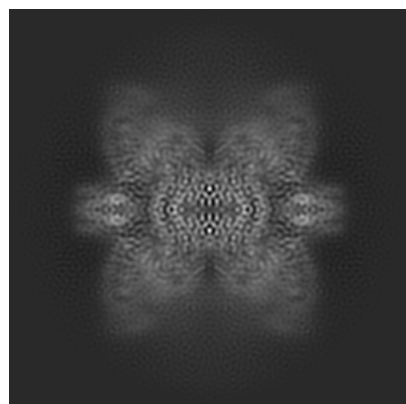
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40811. These allow visual inspection of the internal detail of the map and identification of artifacts.

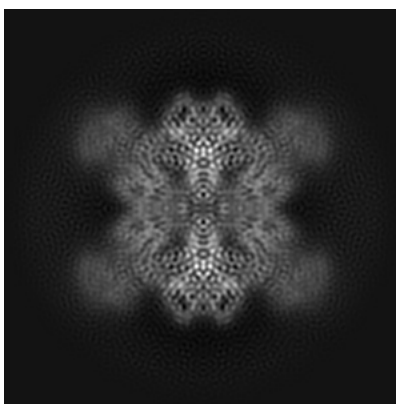
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

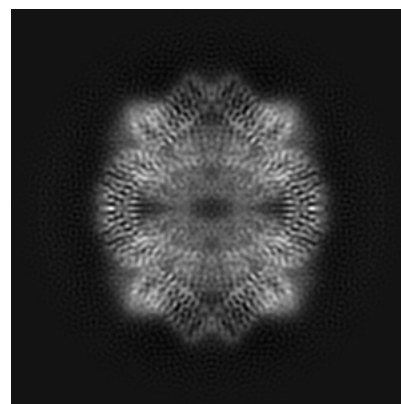
6.1.1 Primary map



X

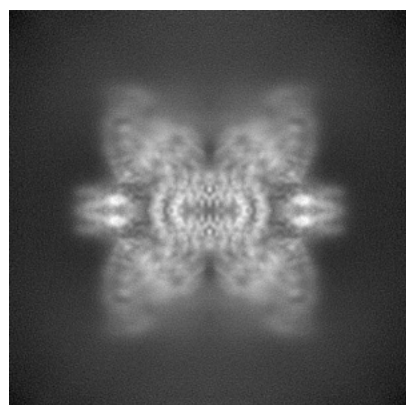


Y

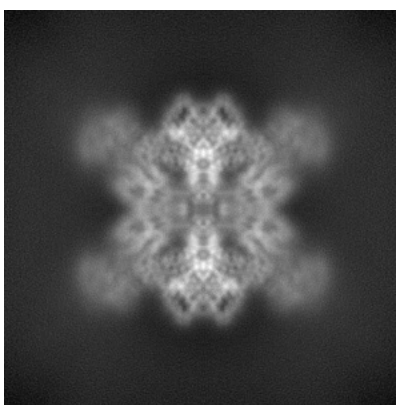


Z

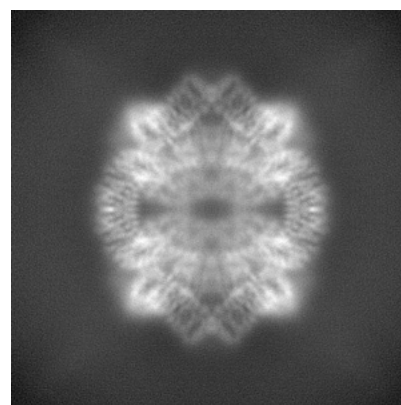
6.1.2 Raw map



X



Y

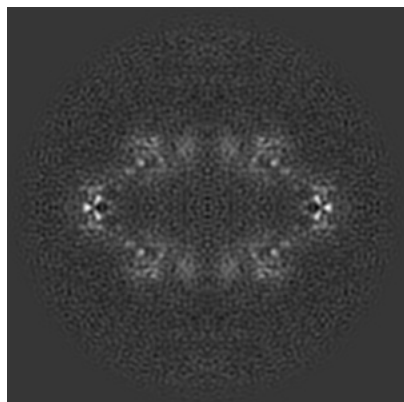


Z

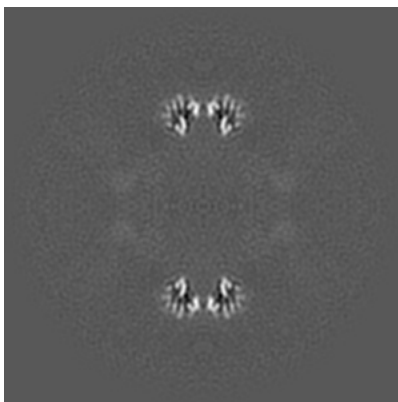
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

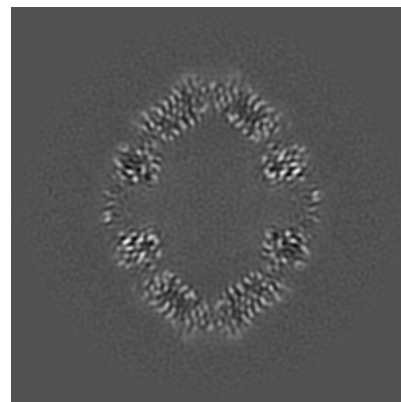
6.2.1 Primary map



X Index: 160

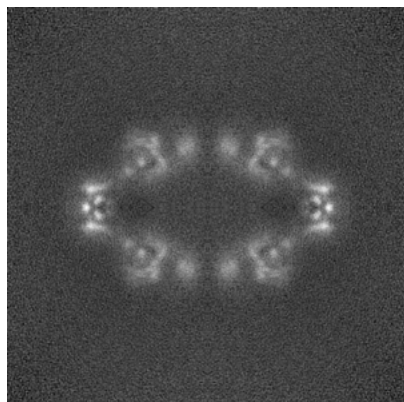


Y Index: 160

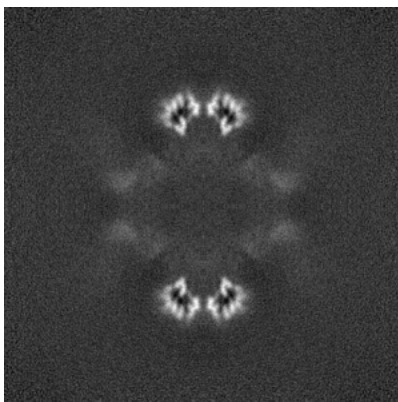


Z Index: 160

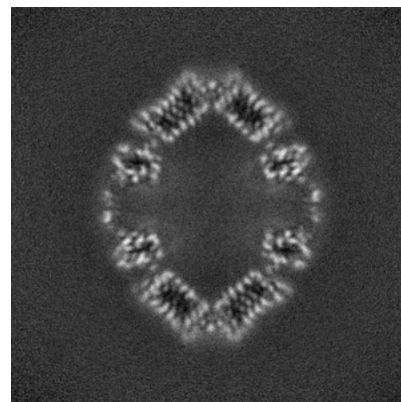
6.2.2 Raw map



X Index: 160



Y Index: 160

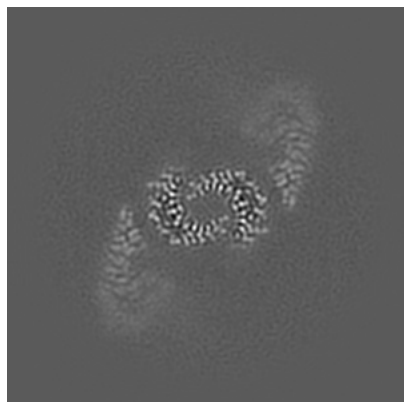


Z Index: 160

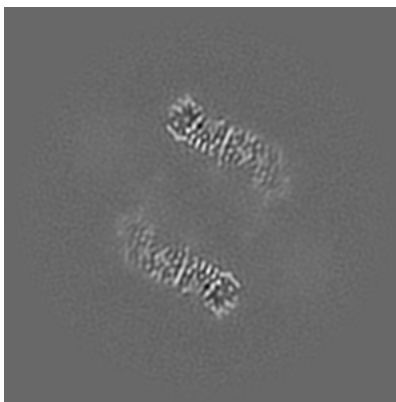
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

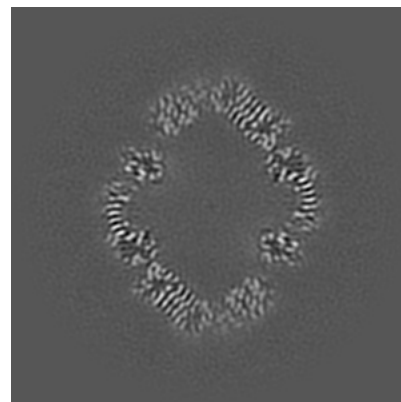
6.3.1 Primary map



X Index: 98

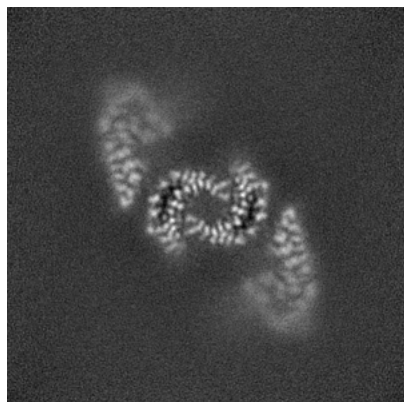


Y Index: 184

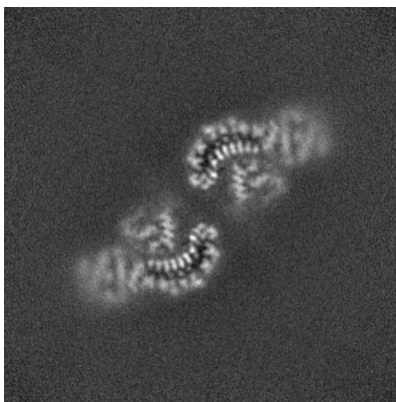


Z Index: 152

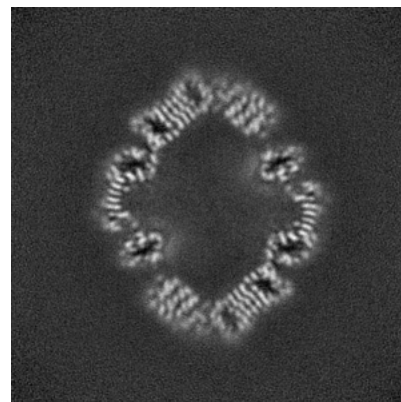
6.3.2 Raw map



X Index: 221



Y Index: 93

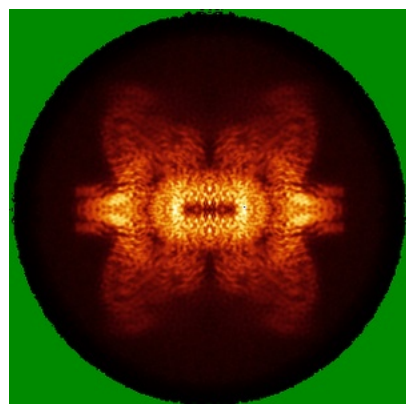


Z Index: 166

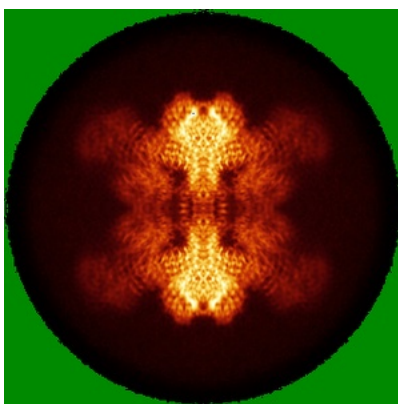
The images above show the largest variance slices of the map in three orthogonal directions.

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

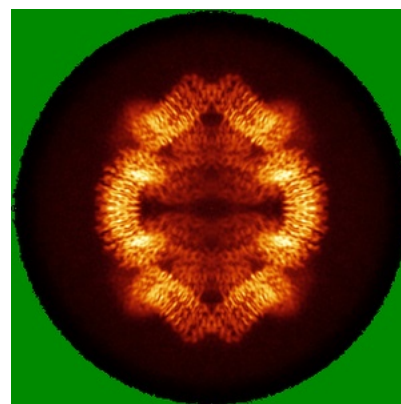
6.4.1 Primary map



X

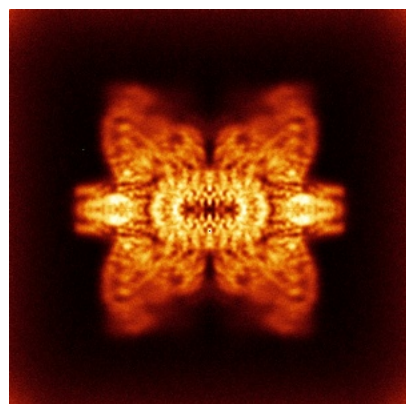


Y

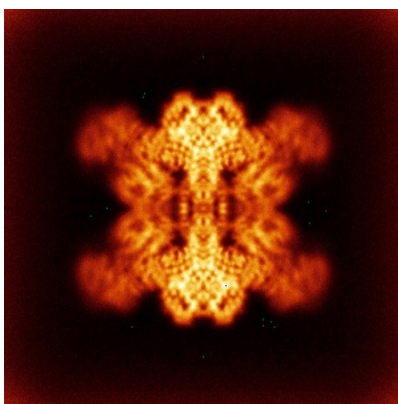


Z

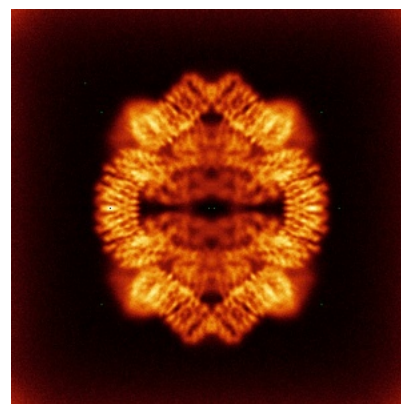
6.4.2 Raw map



X



Y

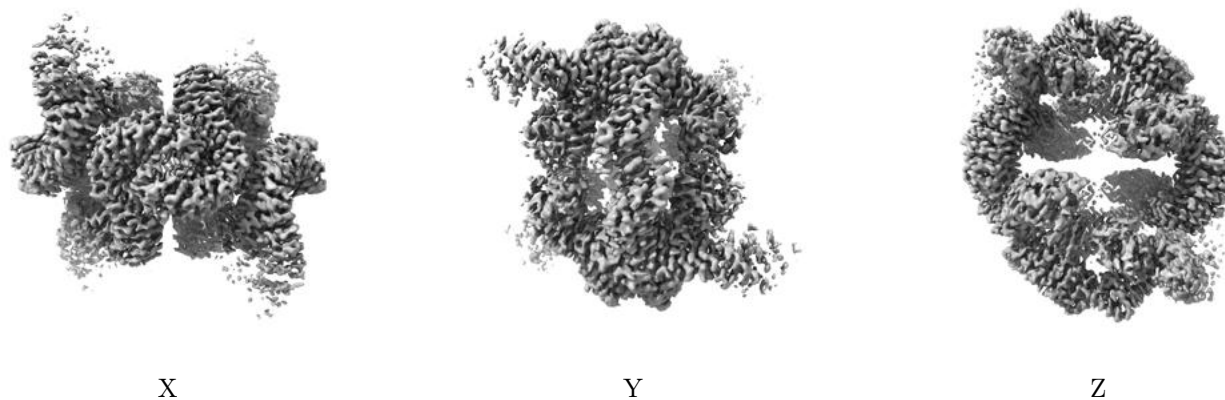


Z

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.

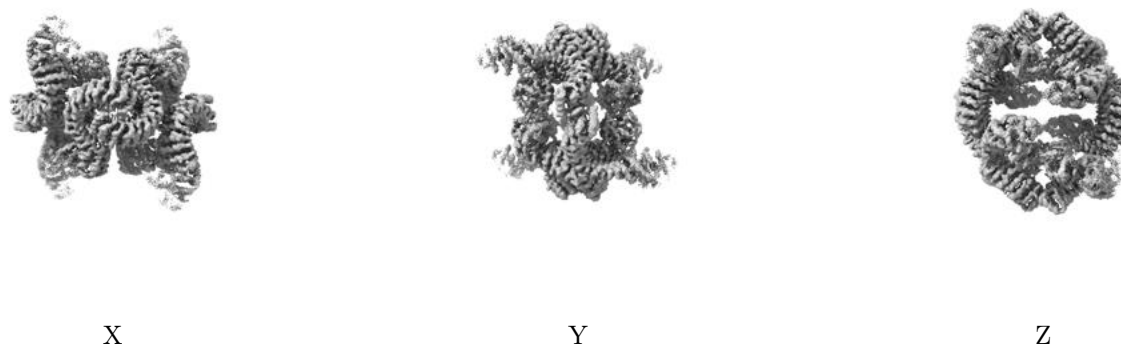
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

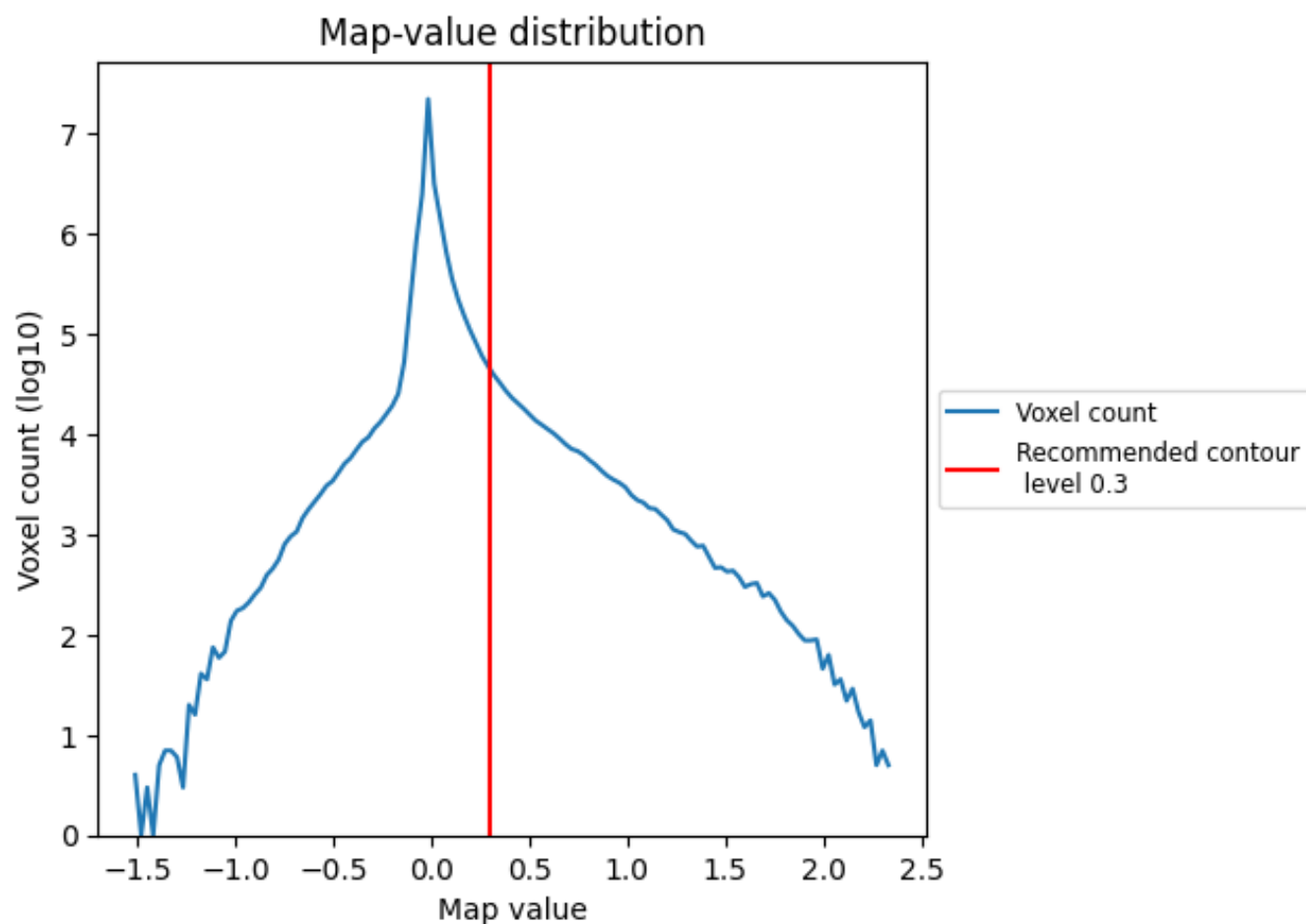
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

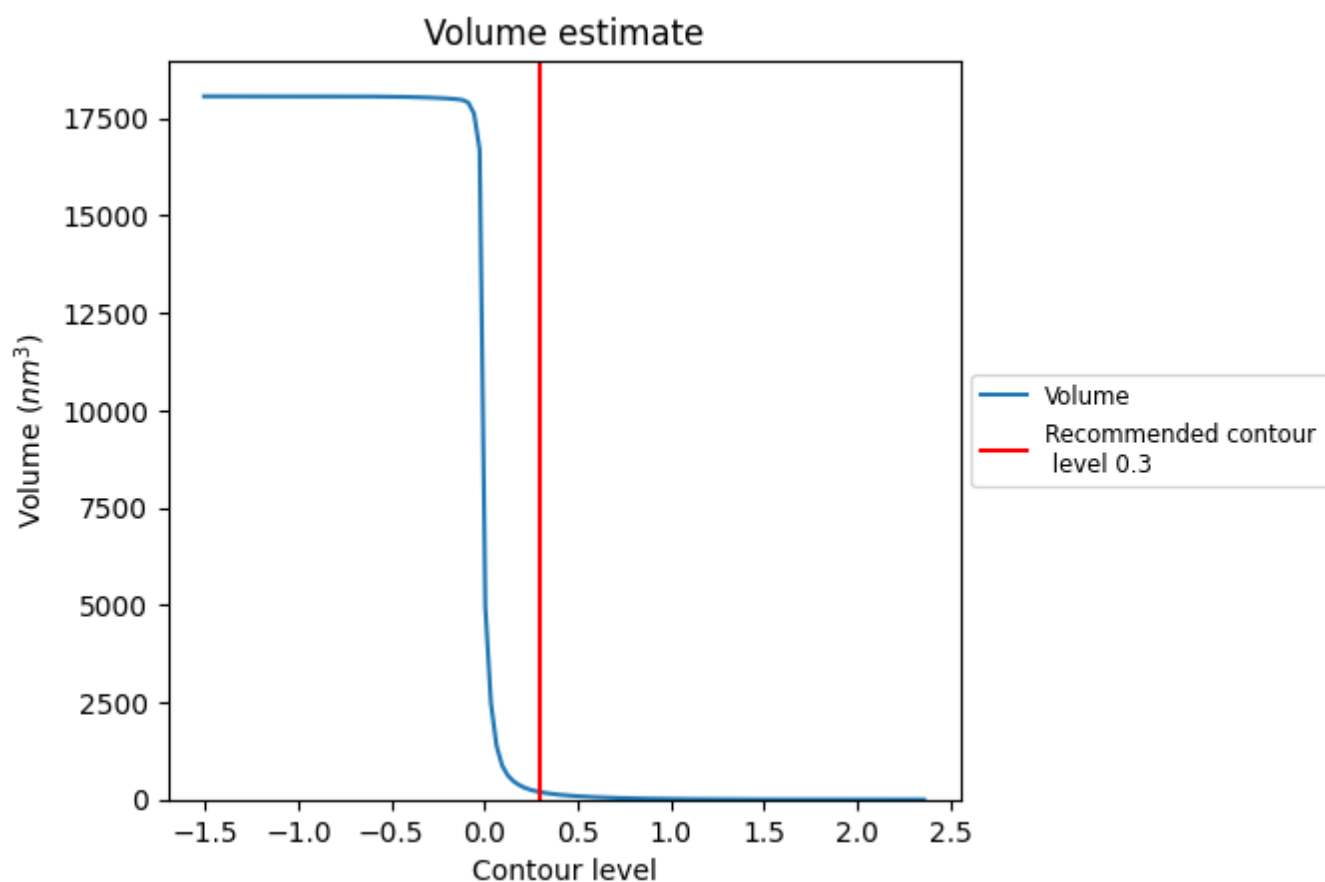
This section contains the results of statistical analysis of the map.

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.

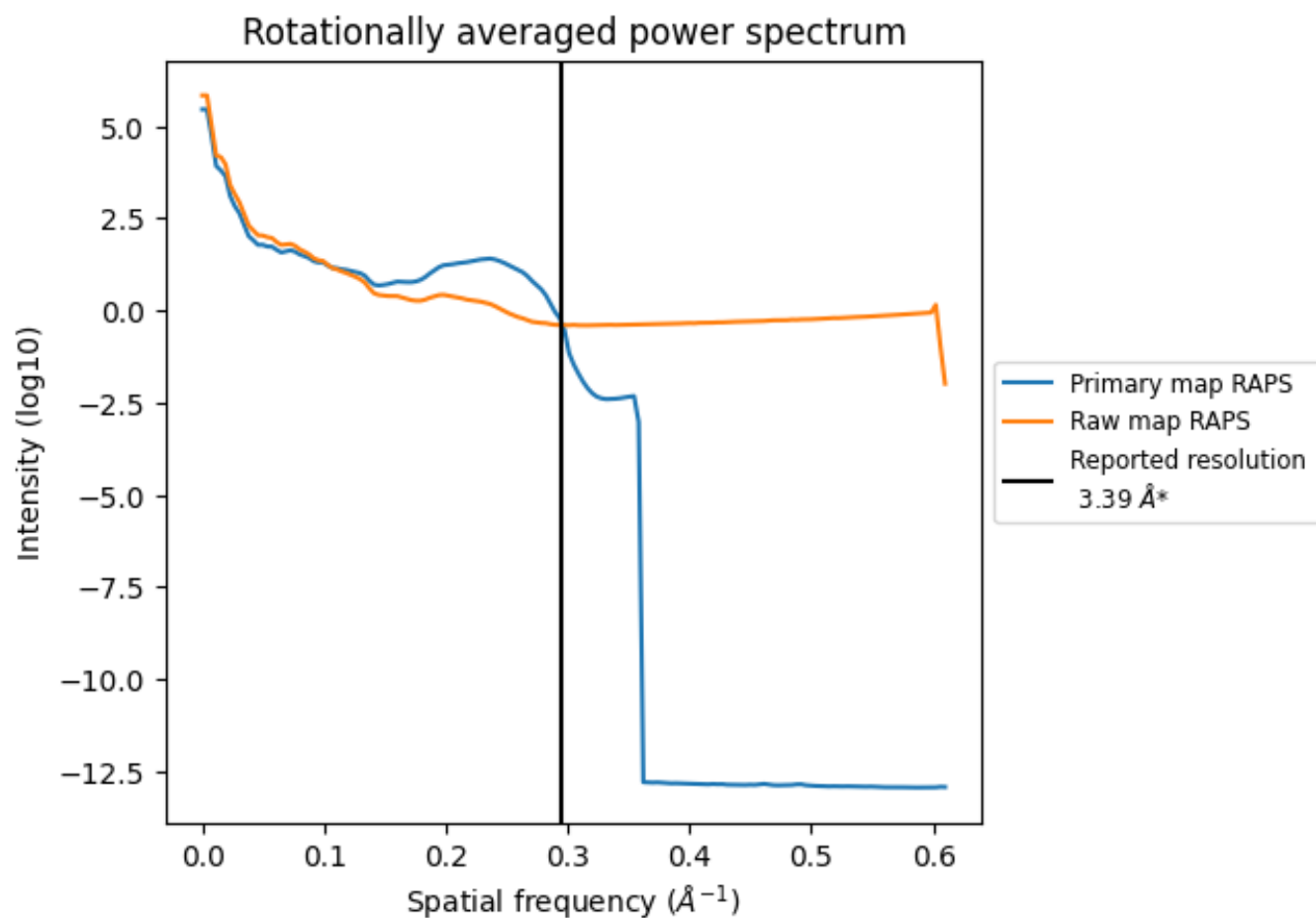
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm³; this corresponds to an approximate mass of 173 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 ⓘ

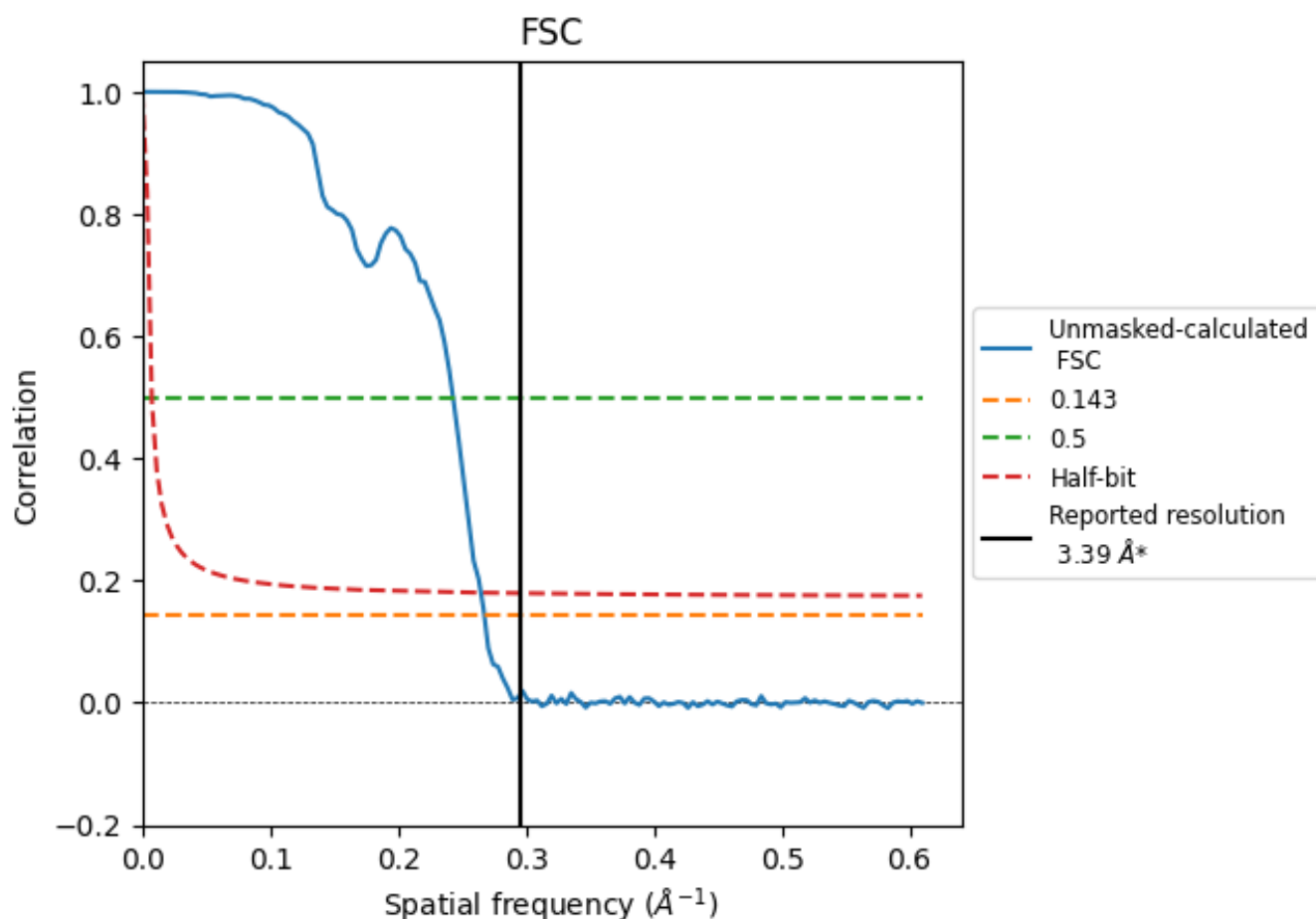


*Reported resolution corresponds to spatial frequency of 0.295 Å⁻¹

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 0.295 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

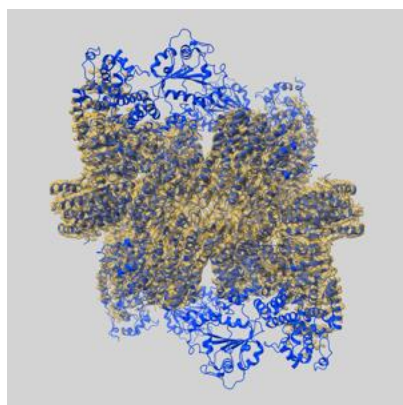
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.39	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.74	4.12	3.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.74 differs from the reported value 3.39 by more than 10 %

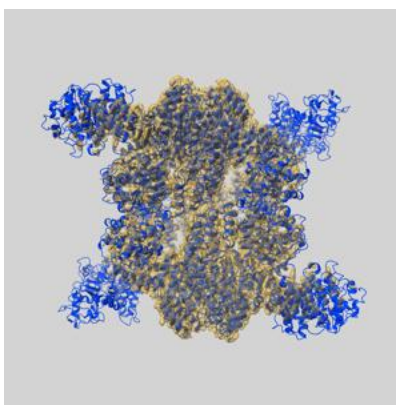
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40811 and PDB model 8SWF. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

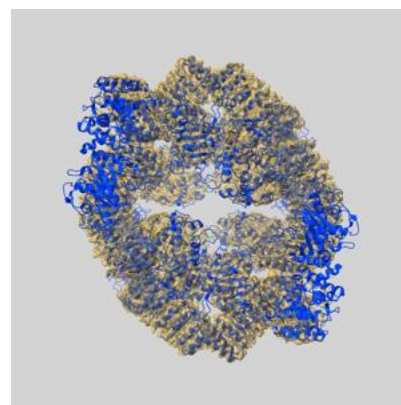
9.1 Map-model overlay [i](#)



X



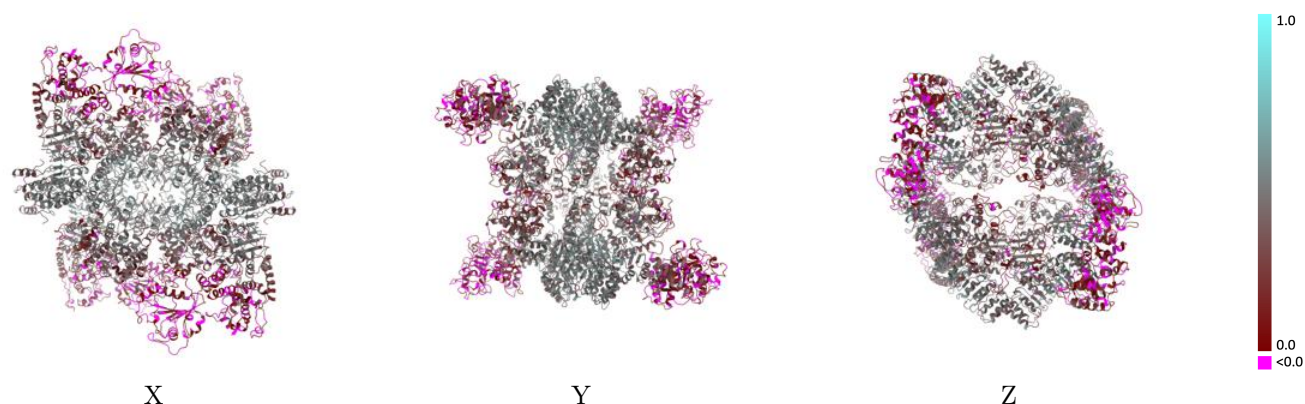
Y



Z

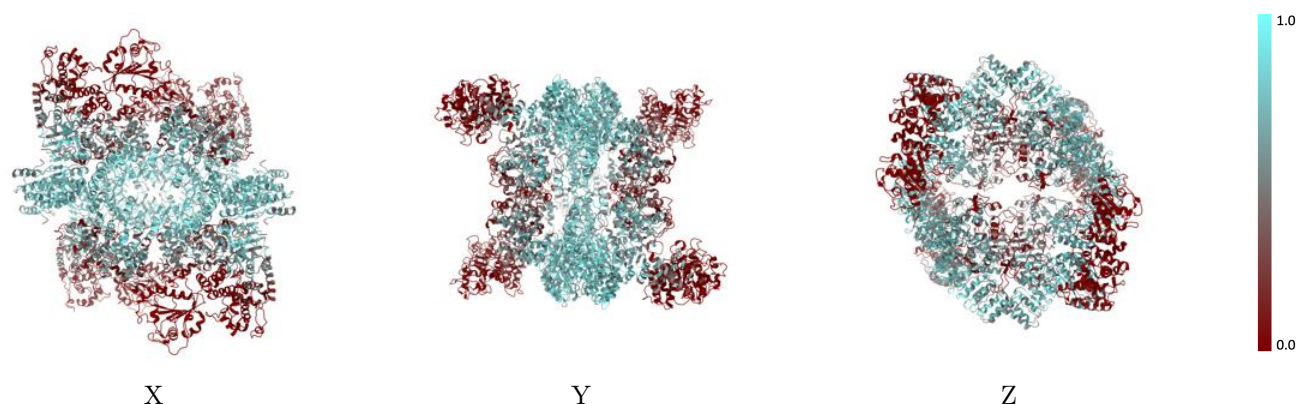
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



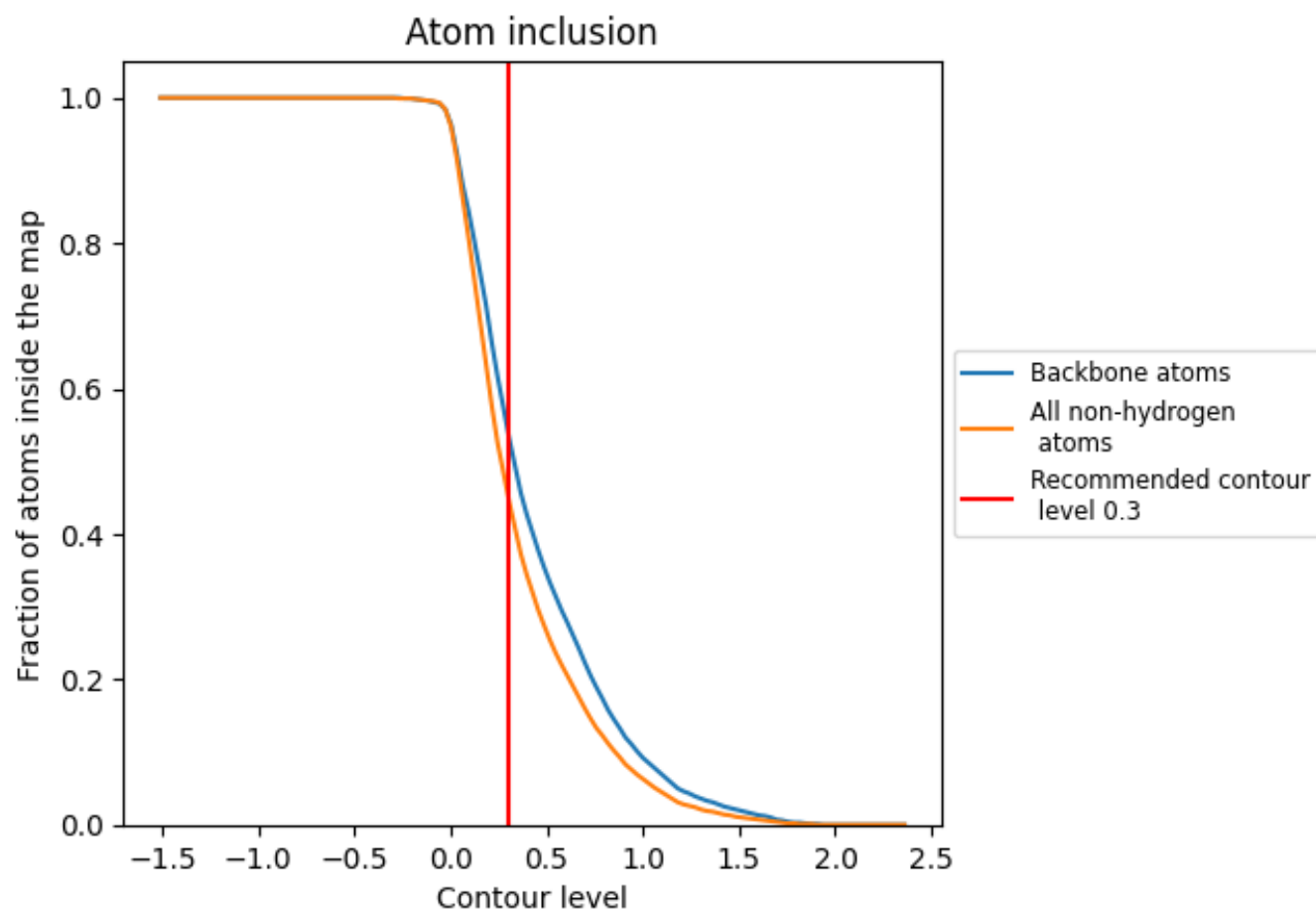
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 45% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4510	0.3100
A	0.5640	0.3790
B	0.5660	0.3810
C	0.3380	0.2410
D	0.5650	0.3800
E	0.3360	0.2400
F	0.3360	0.2400
G	0.5650	0.3780
H	0.3360	0.2380

1.0

0.0

<0.0