



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:19 PM UTC

PDB ID : 6WJV / pdb_00006wjv
EMDB ID : EMD-21701
Title : Structure of the *Saccharomyces cerevisiae* polymerase epsilon holoenzyme
Authors : Yuan, Z.; Georgescu, R.; Schauer, G.D.; O'Donnell, M.; Li, H.
Deposited on : 2020-04-14
Resolution : 3.50 Å (reported)

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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

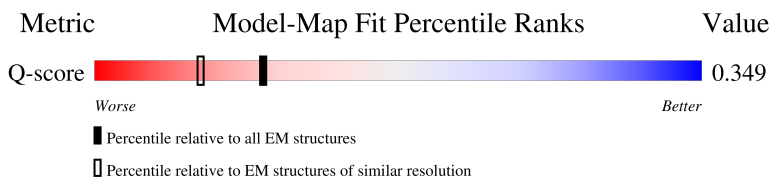
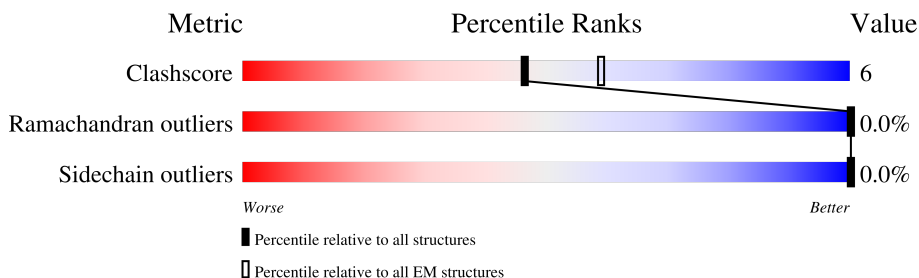
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	2222	55% 74% 14% 12%
2	2	689	50% 11% 38%
3	3	201	15% 37% 5% 58%
4	4	196	23% 44% 10% 45%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19593 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 DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1951	Total	C	N	O	S	0	0
			14886	9527	2476	2813	70		

- Molecule 2 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	424	Total	C	N	O	S	0	0
			3225	2055	545	610	15		

- Molecule 3 is a protein called DNA polymerase epsilon subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	85	Total	C	N	O	S	0	0
			652	417	107	126	2		

- Molecule 4 is a protein called DNA polymerase epsilon subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	107	Total	C	N	O	S	0	0
			829	521	146	161	1		

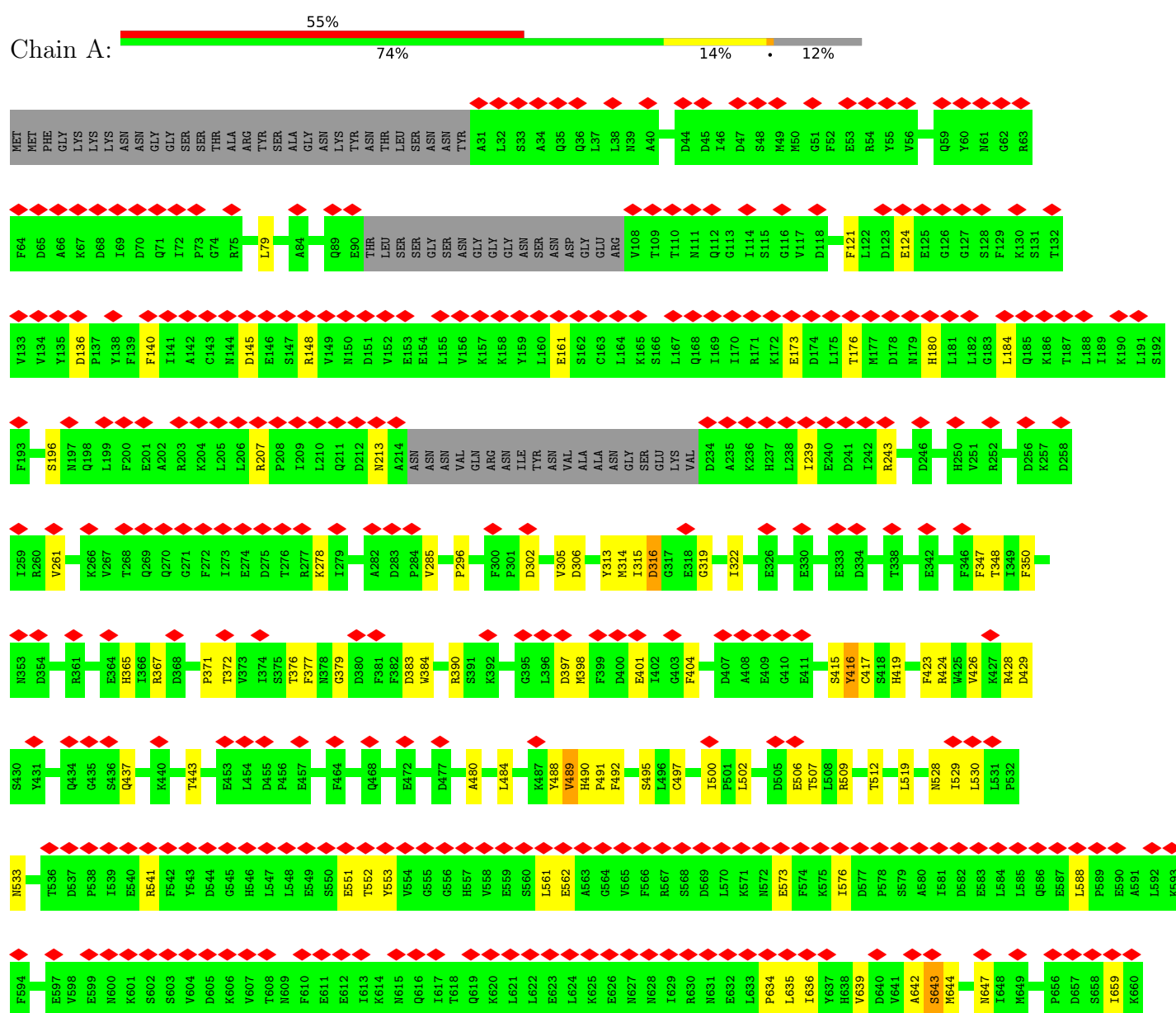
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

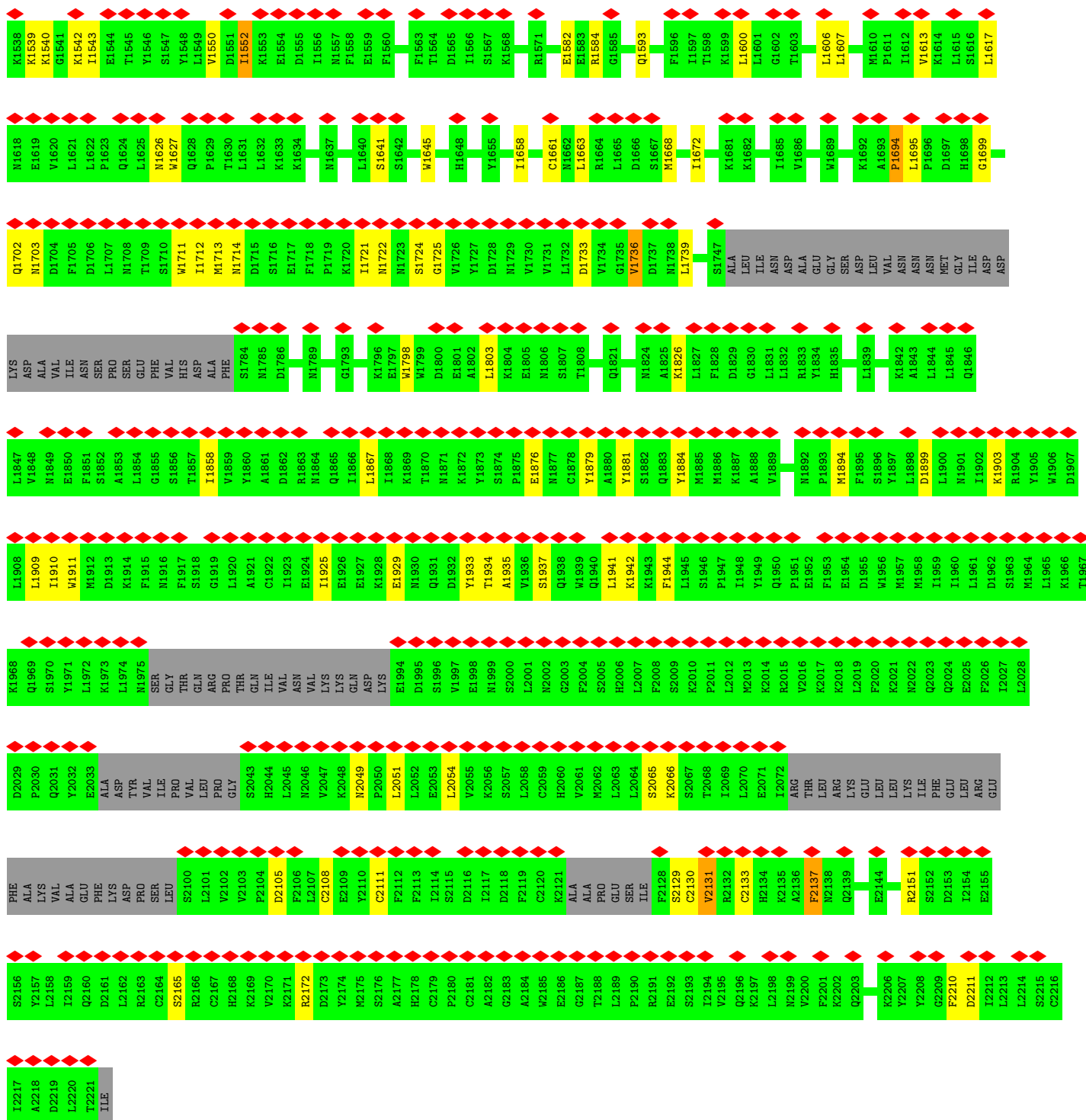
3 Residue-property plots

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

- Molecule 1: DNA polymerase epsilon catalytic subunit A



M1470	PHE	E1315	GLU	P1130	L1045	L981	K917	I857	A788	L721	A661
A1471	LYS	A1318	GLU	S1131	L1046	K982	H921	I858	K789	T722	E662
E1472	THR	A1319	ASP	L1132	C1047	G983	Q922	Q859	T790	F723	R663
M1473	LEU	W1322	LEU	E1133	E1048	F984	Y923	M860	K791	D724	ASP
E1474	PRO		VAL	L1134	N1049	E985	Q924	A861	K792	E725	ALA
R1475	LEU		LEU	D1135	R1050	L986	E925	R862	G793	L726	SER
Y1476	SER		PRO	D1136	R1051	K987	L926	A863	N794	E727	CYS
L1477	GLU		GLU	I1137	M1052	R988	E926	V965	L795	S727	ASP
S1478	ILE		ILE	R1138	S1053	R989	K927	E866	A796	Y728	PHE
G1479	THR		THR	R1139	K1054	G990	D928	E867	S796	A729	ASN
F1480	SER		LEU	I1140	T1055	E991	P929	V868	K797	D730	ARG
S1481	ASN		ASN	I1141	L1056	L992	E930	E869	I798	Q731	PRO
S1481	VAL		VAL	D1142	K1057	Q993	L930	R870	D799	V732	GLY
M1482	PRO		PRO	W143	E1058	L994	N931	P871	S801	I733	LYS
D1483	GLU		GLU		Y1059	L995	Y932	E871	S801	H734	CYS
I1484	ASP		THR		E1060	K996	I933	L872	D802	I735	
G1485	THR		MET		G1061	N997	Y934	E873	K903	K736	
Y1486	GLY		GLY		R1071	Q999	E935	L874	H904	K737	
F1490	ILE		ILE		R1072	S1000	H937	D875	A805	R738	
F1491	LYS		LYS		L1073	D1001	S938	T876	R806	L739	
T1492	ASP		ASP		D1075	I1002	E939	G877	D807	T740	
S1493	ILE		ILE		L1076	F1003	N940	I879	E741	E742	
I1494	ASP		ASP		D1077	K1004	T941	W880	F486	S743	
G1495	THR		THR		L1078	V1005	I942	C881	K310	K744	
Y1496	GLU		GLU		M1081	F1006	F943	I882	K811	K745	
M1482	PRO		PRO		V1082	L1007	E945	L883	M812	V746	
F1498	VAL		VAL		K1083	D1008	Y946	K885	F690	Y747	
F1502	GLU		GLU		D1084	E1008	D947	S886	P691	Y747	
K1503	ASP		ASP		S1094	G1009	G948	S887	S692	H748	
G1506	ALA		ALA		S1095	D1010	P949	P888	K693	R749	
D1507	LYS		LYS		K1096	T1011	Y950	E889	M694	V750	
L1512	ILE		ILE		F1097	L1012	K951	T890	D695	K751	
V1513	ILE		ILE		Q1098	E1013	A952	Y891	E696	V752	
L1514	ARG		ARG		N1099	G1014	N953	F992	Y697	S753	
K1515	THR		THR		P1101	I015	F954	F993	M698	E754	
P1516	LYS		LYS		A1106	I016	L955	T894	M699	I755	
S1517	LYS		LYS			S1017	F956	F830	I700	V756	
M1518	LYS		LYS			A1018	S957	Y831	K701	E757	
Q1519	ALA		ALA			I019	S958	G832	R702	R758	
S1520	VAL		VAL			A1020	E960	N997	A703	E759	
Q1521	SER		SER			S1021	K959	G998	L704	A760	
E1522	ARG		ARG				E961	K999	Q705	Q705	
I1523	LYS		LYS				K962	K900	N706	Q705	
M1524	ARG		ARG				K963	L901	E707	E707	
A1525	ASN		ASN				G964	Y902	T708	T708	
S1526	GLN		GLN				I965	L903	F709	F709	
S1527	LEU		LEU				K966	S904	W710	W710	
T1528	THR		THR				K967	Y905	N711	N711	
L1529	ASN		ASN				R968	C907	K712	K712	
G1530							F972	S908	N713	N713	
Q1531							N973	M909	K714	K714	
I1531							E974	L910	F715	F715	
Y1532							D975	N911	S716	S716	
K1533							G976	Y912	K717	K717	
D1534							S977	R913	K718	K718	
M1535							L978	H915	K719	K719	
F1536							A979	Q916	W720	W720	
E1537							E980				



• Molecule 2: DNA polymerase epsilon subunit B



MET	PHE	GLY	SER	GLY	ASN	VAL	LEU	PRO	PRO	VAL	LYS	ILE	GLN	PRO	PRO	LEU	LEU	ARG	ARG	ALA	TYR	TYR	VAL	LEU	SER	ARG	LYS	TYR	GLY	LEU	SER	ILE	LYS	SER	ASP	GLY	LEU	SER	ALA	GLU	PHE	VAL	GLY	THR	ASN	ILE	GLY	ALA	ASN	TRP	ARG	GLN	GLY	PRO	ALA	THR	ILE
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● Molecule 4: DNA polymerase epsilon subunit D



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N25
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F33
R43
E44
V45
P46
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Q48
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L54
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R65
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V95
D100
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P110
D113
D116
E117
Y118
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Q124
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	187298	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.223	Depositor
Minimum map value	-0.112	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	263.424, 263.424, 263.424	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.029, 1.029, 1.029	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	3/15201 (0.0%)	1.10	125/20663 (0.6%)
2	2	0.44	0/3286	1.19	34/4467 (0.8%)
3	3	0.37	0/660	1.01	5/891 (0.6%)
4	4	0.55	1/839 (0.1%)	1.24	12/1132 (1.1%)
All	All	0.46	4/19986 (0.0%)	1.12	176/27153 (0.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1161	PRO	N-CD	-8.78	1.35	1.47
1	A	1515	LYS	C-N	8.25	1.41	1.33
4	4	110	PRO	N-CD	-7.32	1.37	1.47
1	A	490	HIS	C-N	6.62	1.42	1.34

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1310	ILE	N-CA-C	-11.10	102.91	111.90
4	4	28	ILE	N-CA-C	-10.89	103.08	111.90
1	A	1552	ILE	N-CA-C	-10.35	102.97	112.90
1	A	1721	ILE	N-CA-C	-10.01	103.29	112.90
2	2	385	ILE	N-CA-C	-9.61	103.32	112.83
4	4	44	GLU	N-CA-C	9.60	123.02	111.02
1	A	1903	LYS	N-CA-C	9.50	122.90	111.02
1	A	958	SER	N-CA-C	9.08	121.57	110.41
2	2	405	ASN	N-CA-C	8.89	121.31	110.91
2	2	403	GLY	N-CA-C	8.39	133.07	113.18
2	2	334	SER	CA-C-O	-8.35	108.57	120.51
1	A	808	GLU	N-CA-C	-8.29	103.30	113.50
1	A	1884	TYR	CA-CB-CG	8.27	128.78	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1944	PHE	N-CA-C	8.21	120.31	111.36
1	A	1826	LYS	CA-C-N	8.16	137.12	121.54
1	A	1826	LYS	C-N-CA	8.16	137.12	121.54
2	2	493	SER	N-CA-C	7.67	122.68	113.16
1	A	2105	ASP	N-CA-C	7.65	121.80	111.24
2	2	534	TYR	CA-C-N	7.57	136.00	121.54
2	2	534	TYR	C-N-CA	7.57	136.00	121.54
1	A	2211	ASP	N-CA-C	7.49	119.44	111.28
3	3	55	VAL	N-CA-C	-7.40	101.92	112.35
2	2	403	GLY	CA-C-N	7.37	135.62	121.54
2	2	403	GLY	C-N-CA	7.37	135.62	121.54
1	A	1909	LEU	N-CA-C	7.33	119.78	110.33
1	A	2049	ASN	N-CA-C	7.29	123.52	113.16
1	A	1432	THR	N-CA-C	-7.28	100.25	110.29
1	A	947	ASP	N-CA-C	7.22	119.37	109.11
1	A	2131	VAL	N-CA-C	-7.21	106.11	113.10
1	A	1933	TYR	CA-CB-CG	7.14	126.75	113.90
1	A	1894	MET	CA-C-N	7.08	135.07	121.54
1	A	1894	MET	C-N-CA	7.08	135.07	121.54
2	2	225	THR	N-CA-C	-6.98	103.14	113.61
1	A	489	VAL	N-CA-C	6.96	119.58	112.90
1	A	1506	GLY	CA-C-N	6.96	133.97	123.05
1	A	1506	GLY	C-N-CA	6.96	133.97	123.05
1	A	1434	HIS	N-CA-C	6.89	120.57	111.75
2	2	299	GLU	N-CA-C	6.88	117.36	108.34
1	A	1386	ASN	N-CA-C	6.76	124.75	109.81
1	A	1879	TYR	N-CA-C	6.75	118.64	111.28
2	2	666	HIS	N-CA-C	-6.74	99.49	108.19
1	A	507	THR	N-CA-C	-6.73	103.75	112.23
2	2	662	GLY	N-CA-C	6.71	129.09	113.18
2	2	603	VAL	N-CA-C	-6.69	105.81	112.17
4	4	94	ASP	N-CA-C	-6.69	106.06	114.56
1	A	1444	SER	N-CA-C	-6.67	105.27	113.41
1	A	1047	CYS	N-CA-C	6.58	119.05	110.43
1	A	121	PHE	N-CA-C	6.57	119.15	109.69
1	A	889	GLU	N-CA-C	6.55	121.64	112.93
1	A	347	PHE	N-CA-C	6.48	121.25	107.70
1	A	876	THR	N-CA-C	6.47	118.33	111.28
1	A	1703	ASN	CA-C-N	6.46	134.87	121.94
1	A	1703	ASN	C-N-CA	6.46	134.87	121.94
1	A	316	ASP	N-CA-C	6.44	120.06	111.30
1	A	1703	ASN	N-CA-C	6.44	116.78	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1494	ILE	N-CA-C	-6.43	100.51	109.45
1	A	985	GLU	CA-C-N	6.37	133.71	121.54
1	A	985	GLU	C-N-CA	6.37	133.71	121.54
1	A	1271	GLY	CA-C-N	6.35	133.66	121.54
1	A	1271	GLY	C-N-CA	6.35	133.66	121.54
1	A	1365	THR	N-CA-C	-6.35	104.84	112.59
1	A	419	HIS	N-CA-C	6.32	120.00	110.64
1	A	1285	ARG	N-CA-C	-6.27	105.46	113.23
1	A	1881	TYR	CA-CB-CG	6.26	125.17	113.90
1	A	1942	LYS	N-CA-C	-6.23	104.02	111.69
1	A	1694	PRO	CA-C-N	6.23	137.00	121.80
1	A	1694	PRO	C-N-CA	6.23	137.00	121.80
1	A	1118	ILE	N-CA-C	-6.22	104.78	110.82
1	A	1910	ILE	N-CA-C	-6.22	99.75	108.27
1	A	161	GLU	N-CA-C	6.21	118.86	111.71
1	A	844	MET	N-CA-C	-6.18	104.44	112.23
1	A	1143	TRP	N-CA-C	-6.18	105.57	113.23
1	A	1929	GLU	N-CA-C	6.15	119.88	111.39
1	A	1658	ILE	N-CA-C	-6.14	104.16	109.19
1	A	588	LEU	N-CA-C	6.12	121.07	112.75
2	2	475	LEU	CA-C-N	6.10	129.07	120.28
2	2	475	LEU	C-N-CA	6.10	129.07	120.28
1	A	1803	LEU	CA-C-N	6.10	133.19	121.54
1	A	1803	LEU	C-N-CA	6.10	133.19	121.54
1	A	384	TRP	N-CA-C	6.05	123.17	109.81
1	A	643	SER	CA-C-N	6.02	129.16	120.79
1	A	643	SER	C-N-CA	6.02	129.16	120.79
1	A	1663	LEU	CA-C-N	6.02	133.03	121.54
1	A	1663	LEU	C-N-CA	6.02	133.03	121.54
1	A	423	PHE	N-CA-C	-6.01	105.98	113.38
1	A	176	THR	N-CA-C	-5.99	104.49	112.94
2	2	336	GLY	N-CA-C	-5.97	99.03	113.18
1	A	207	ARG	N-CA-C	5.96	121.62	113.16
1	A	1736	VAL	N-CA-C	5.95	116.97	108.93
1	A	1099	ASN	CA-CB-CG	5.91	118.51	112.60
1	A	1463	PHE	N-CA-C	5.91	117.66	109.15
1	A	417	CYS	N-CA-C	5.90	120.76	113.50
1	A	1941	LEU	N-CA-C	-5.84	106.80	114.04
1	A	1695	LEU	N-CA-C	5.80	122.62	109.81
2	2	629	THR	N-CA-C	-5.79	106.35	113.41
1	A	1178	ASP	N-CA-C	5.78	123.12	110.80
2	2	474	ASN	N-CA-C	-5.78	106.86	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2133	CYS	N-CA-C	-5.77	100.84	109.96
1	A	1668	MET	N-CA-C	-5.77	102.92	111.81
2	2	634	PRO	N-CA-C	-5.76	101.17	110.74
2	2	459	LYS	N-CA-C	-5.74	104.64	111.69
3	3	66	SER	N-CA-C	-5.73	106.93	114.04
1	A	1713	MET	CA-C-N	5.71	130.93	122.82
1	A	1713	MET	C-N-CA	5.71	130.93	122.82
1	A	1302	GLU	N-CA-C	-5.71	106.67	113.97
1	A	1098	PHE	CA-C-N	5.70	130.45	122.08
1	A	1098	PHE	C-N-CA	5.70	130.45	122.08
1	A	1721	ILE	CB-CA-C	5.69	118.26	111.20
1	A	2210	PHE	N-CA-C	5.62	119.09	111.17
2	2	333	TYR	CA-C-N	5.60	132.24	121.54
2	2	333	TYR	C-N-CA	5.60	132.24	121.54
1	A	398	MET	N-CA-C	5.59	117.38	111.28
2	2	495	VAL	N-CA-C	-5.59	106.34	113.22
1	A	528	ASN	N-CA-C	5.57	119.08	111.39
4	4	32	LEU	N-CA-C	5.49	117.63	108.02
1	A	429	ASP	N-CA-C	5.45	120.77	112.54
4	4	95	VAL	N-CA-C	-5.45	106.38	111.45
1	A	1141	ILE	N-CA-C	5.45	117.47	109.63
1	A	1613	VAL	N-CA-C	5.45	116.12	108.17
3	3	91	ILE	N-CA-C	-5.44	106.53	113.22
1	A	1322	TRP	CA-CB-CG	5.40	123.87	113.60
1	A	404	PHE	N-CA-C	5.38	117.69	109.62
1	A	1711	TRP	CA-C-N	5.37	128.61	120.77
1	A	1711	TRP	C-N-CA	5.37	128.61	120.77
1	A	2111	CYS	N-CA-C	-5.37	106.40	113.17
1	A	1593	GLN	N-CA-C	5.36	117.73	110.06
1	A	905	TYR	N-CA-C	5.32	119.48	112.35
3	3	54	LEU	N-CA-C	-5.31	106.48	113.17
1	A	2165	SER	N-CA-C	5.29	116.85	111.14
1	A	196	SER	N-CA-C	-5.28	106.68	113.23
1	A	1600	LEU	N-CA-C	-5.28	106.89	113.38
1	A	1712	ILE	N-CA-C	5.28	116.06	108.93
1	A	1722	ASN	N-CA-C	5.28	117.62	111.02
1	A	1431	ILE	N-CA-C	5.27	116.77	109.29
1	A	416	TYR	N-CA-C	5.26	118.86	112.23
1	A	315	ILE	CA-C-N	5.24	129.85	122.46
1	A	315	ILE	C-N-CA	5.24	129.85	122.46
2	2	509	PRO	CA-C-N	5.22	128.96	120.60
2	2	509	PRO	C-N-CA	5.22	128.96	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1733	ASP	N-CA-C	-5.21	104.09	110.61
2	2	506	ASP	N-CA-C	-5.21	103.62	110.39
4	4	85	GLN	CA-C-N	5.21	129.95	122.40
4	4	85	GLN	C-N-CA	5.21	129.95	122.40
1	A	1712	ILE	CA-C-N	5.20	131.47	121.54
1	A	1712	ILE	C-N-CA	5.20	131.47	121.54
1	A	1714	ASN	N-CA-C	5.19	118.49	111.17
2	2	635	ILE	N-CA-C	5.19	113.09	108.63
4	4	29	GLN	N-CA-C	-5.18	107.34	113.97
1	A	1876	GLU	N-CA-C	5.17	122.49	114.64
1	A	1479	GLY	N-CA-C	-5.16	100.96	113.18
1	A	850	THR	N-CA-C	5.15	117.29	111.11
2	2	653	TYR	N-CA-C	-5.14	105.76	113.89
2	2	341	VAL	N-CA-C	5.14	114.69	106.88
1	A	1493	SER	N-CA-C	-5.13	106.87	113.23
1	A	1925	ILE	N-CA-C	-5.13	106.05	113.07
1	A	1478	SER	N-CA-C	5.11	118.52	107.49
4	4	81	ILE	N-CA-C	-5.10	106.94	113.22
1	A	397	ASP	CA-C-N	5.10	127.11	120.28
1	A	397	ASP	C-N-CA	5.10	127.11	120.28
1	A	1661	CYS	N-CA-C	-5.08	106.92	114.64
1	A	794	ASN	N-CA-C	5.07	116.50	111.07
1	A	1116	ILE	N-CA-C	5.07	118.43	112.35
3	3	17	VAL	N-CA-C	-5.06	105.61	110.72
4	4	51	LYS	CA-C-N	5.06	130.12	122.68
4	4	51	LYS	C-N-CA	5.06	130.12	122.68
4	4	53	LEU	N-CA-C	5.05	117.56	111.40
1	A	849	ILE	N-CA-C	-5.05	105.92	110.82
2	2	451	ASN	N-CA-C	-5.04	107.51	113.97
1	A	644	MET	N-CA-C	5.04	117.17	111.02
2	2	299	GLU	CA-C-N	5.04	134.10	121.80
2	2	299	GLU	C-N-CA	5.04	134.10	121.80
2	2	220	THR	N-CA-C	-5.02	107.00	113.23
1	A	2137	PHE	CA-C-N	5.02	132.90	122.41
1	A	2137	PHE	C-N-CA	5.02	132.90	122.41
1	A	967	LYS	N-CA-C	5.00	118.50	111.90
1	A	1937	SER	N-CA-C	5.00	116.98	110.43

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	14886	0	13968	185	0
2	2	3225	0	3134	42	0
3	3	652	0	664	4	0
4	4	829	0	842	10	0
5	A	1	0	0	0	0
All	All	19593	0	18608	231	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 6.

All (231) 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:305:VAL:HG13	1:A:1301:ARG:NH1	1.48	1.26
1:A:1115:ASP:OD1	1:A:1118:ILE:CG1	1.99	1.08
1:A:1540:LYS:HA	1:A:1543:ILE:HG22	1.32	1.05
1:A:306:ASP:OD1	1:A:1301:ARG:NH1	1.93	1.00
1:A:1115:ASP:OD1	1:A:1118:ILE:HG12	1.60	0.98
1:A:1115:ASP:CG	1:A:1118:ILE:HG12	1.90	0.97
1:A:1540:LYS:HA	1:A:1543:ILE:CG2	1.98	0.93
1:A:305:VAL:HG13	1:A:1301:ARG:HH11	1.25	0.92
2:2:497:LEU:HD22	2:2:501:GLY:HA3	1.50	0.92
1:A:1115:ASP:OD1	1:A:1118:ILE:CB	2.19	0.90
1:A:1115:ASP:CG	1:A:1118:ILE:CG1	2.44	0.90
1:A:305:VAL:CG1	1:A:1301:ARG:NH1	2.33	0.89
1:A:1115:ASP:OD2	1:A:1118:ILE:CG1	2.21	0.88
2:2:497:LEU:CD2	2:2:501:GLY:HA3	2.05	0.86
1:A:639:VAL:HG12	1:A:946:VAL:HG22	1.57	0.86
1:A:1115:ASP:OD1	1:A:1118:ILE:HB	1.74	0.86
1:A:1540:LYS:CA	1:A:1543:ILE:HG22	2.05	0.85
1:A:770:TYR:CE2	1:A:771:VAL:HG13	2.13	0.83
1:A:1115:ASP:N	1:A:1289:ARG:NH2	2.25	0.82
1:A:1115:ASP:OD2	1:A:1118:ILE:HG12	1.76	0.82
1:A:296:PRO:HD3	1:A:1301:ARG:HH22	1.44	0.81
1:A:1115:ASP:H	1:A:1289:ARG:NH2	1.77	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1582:GLU:OE2	3:3:33:VAL:CB	2.28	0.80
1:A:1641:SER:O	1:A:1645:TRP:HB2	1.82	0.78
1:A:1115:ASP:H	1:A:1289:ARG:NH1	1.83	0.77
1:A:861:ALA:O	1:A:865:VAL:HG23	1.85	0.77
1:A:1115:ASP:H	1:A:1289:ARG:HH12	1.33	0.77
1:A:305:VAL:HG13	1:A:1301:ARG:HH12	1.45	0.76
1:A:285:VAL:HG23	1:A:316:ASP:OD2	1.85	0.75
1:A:79:LEU:HG	1:A:261:VAL:HG23	1.67	0.75
1:A:1115:ASP:H	1:A:1289:ARG:CZ	2.04	0.71
1:A:285:VAL:HG13	1:A:371:PRO:HA	1.73	0.70
1:A:1303:ARG:O	1:A:1303:ARG:HG3	1.89	0.70
1:A:1118:ILE:HG21	1:A:1289:ARG:NE	2.07	0.70
1:A:1115:ASP:OD2	1:A:1118:ILE:HG13	1.90	0.69
1:A:261:VAL:HG13	1:A:497:CYS:SG	2.32	0.68
1:A:1027:LEU:O	1:A:1031:ASP:HB2	1.93	0.68
1:A:1306:LEU:CD2	1:A:1311:ARG:HH11	2.07	0.68
2:2:497:LEU:C	2:2:497:LEU:HD12	2.18	0.67
1:A:1550:VAL:HG12	1:A:1552:ILE:HG13	1.77	0.67
2:2:497:LEU:HD22	2:2:501:GLY:CA	2.25	0.66
1:A:1306:LEU:HD23	1:A:1311:ARG:HH11	1.60	0.66
1:A:770:TYR:CD2	1:A:771:VAL:HG13	2.30	0.66
1:A:1115:ASP:CG	1:A:1118:ILE:HG13	2.21	0.65
1:A:519:LEU:HD11	1:A:830:PHE:CE1	2.33	0.64
1:A:907:CYS:SG	1:A:945:GLU:HA	2.38	0.64
1:A:999:GLN:HA	1:A:1002:ILE:HG22	1.78	0.64
1:A:1484:ILE:CD1	1:A:1550:VAL:HG22	2.28	0.63
1:A:305:VAL:CG1	1:A:1301:ARG:HH11	2.06	0.61
1:A:296:PRO:CD	1:A:1301:ARG:HH22	2.13	0.60
1:A:999:GLN:HA	1:A:1002:ILE:CG2	2.31	0.59
1:A:2108:CYS:HG	1:A:2137:PHE:HE1	1.50	0.59
1:A:1484:ILE:HD12	1:A:1550:VAL:HG22	1.83	0.59
2:2:435:GLN:OE1	2:2:435:GLN:HA	2.01	0.59
1:A:519:LEU:HD11	1:A:830:PHE:HE1	1.66	0.59
1:A:1539:LYS:O	1:A:1543:ILE:HG22	2.03	0.58
2:2:654:ASN:ND2	2:2:656:CYS:SG	2.77	0.57
1:A:305:VAL:CG2	1:A:1301:ARG:HD2	2.35	0.57
1:A:1026:TRP:HA	1:A:1029:VAL:HG12	1.87	0.57
1:A:1550:VAL:HG12	1:A:1552:ILE:CG1	2.35	0.56
1:A:1002:ILE:HD11	1:A:1158:ILE:HD11	1.87	0.56
1:A:443:THR:HG21	1:A:480:ALA:HB1	1.87	0.56
1:A:659:ILE:HG21	1:A:845:GLU:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1151:GLY:O	1:A:1155:GLN:HB2	2.05	0.56
1:A:791:TRP:O	1:A:795:LEU:HB2	2.05	0.56
3:3:67:LEU:HD13	4:4:51:LYS:H	1.70	0.55
1:A:1503:LYS:HE3	1:A:1506:GLY:HA3	1.88	0.55
1:A:1736:VAL:HG11	1:A:1739:LEU:HD13	1.88	0.54
1:A:972:PHE:HA	1:A:979:ALA:H	1.72	0.54
1:A:999:GLN:CA	1:A:1002:ILE:HG22	2.38	0.54
1:A:561:LEU:HD22	1:A:871:PRO:HG2	1.90	0.53
1:A:881:CYS:SG	1:A:882:ILE:N	2.80	0.53
1:A:1414:CYS:SG	1:A:1415:THR:N	2.82	0.53
1:A:1115:ASP:N	1:A:1289:ARG:HH12	2.05	0.53
4:4:91:SER:OG	4:4:92:VAL:N	2.42	0.53
1:A:998:PHE:O	1:A:1002:ILE:HG22	2.09	0.52
2:2:286:GLY:HA3	2:2:298:LEU:CD1	2.39	0.52
1:A:305:VAL:HG22	1:A:1301:ARG:HD2	1.91	0.52
2:2:497:LEU:HD23	2:2:501:GLY:HA3	1.89	0.52
1:A:822:ALA:O	1:A:826:ILE:HG13	2.09	0.52
1:A:140:PHE:HB2	1:A:243:ARG:HB2	1.92	0.52
1:A:1303:ARG:HB2	1:A:1460:GLN:HG2	1.92	0.52
2:2:520:CYS:SG	2:2:521:LYS:N	2.83	0.52
1:A:180:HIS:HA	1:A:184:LEU:HB3	1.91	0.52
1:A:1858:ILE:HA	1:A:1867:LEU:HB3	1.92	0.52
2:2:669:ARG:HH12	2:2:687:ILE:HG13	1.74	0.52
1:A:2131:VAL:HG12	1:A:2131:VAL:O	2.09	0.52
1:A:1277:LYS:HB2	4:4:76:LEU:HD22	1.92	0.51
2:2:663:SER:OG	2:2:664:PHE:N	2.42	0.51
1:A:285:VAL:CG1	1:A:371:PRO:HA	2.39	0.51
1:A:1523:ILE:HG23	1:A:1525:ALA:H	1.75	0.51
4:4:76:LEU:HD12	4:4:77:PHE:CD2	2.45	0.51
1:A:1143:TRP:O	1:A:1147:ARG:HB2	2.10	0.51
1:A:296:PRO:HD3	1:A:1301:ARG:NH2	2.22	0.51
1:A:145:ASP:HB3	1:A:148:ARG:HB2	1.93	0.50
1:A:500:ILE:HD11	1:A:519:LEU:HD23	1.92	0.50
2:2:406:LEU:CD2	2:2:417:LEU:HD13	2.42	0.50
1:A:839:SER:HB2	1:A:842:TYR:HB2	1.93	0.50
2:2:402:LEU:HA	2:2:672:TYR:HB2	1.94	0.50
1:A:213:ASN:ND2	1:A:239:ILE:O	2.45	0.50
1:A:1303:ARG:O	1:A:1303:ARG:CG	2.57	0.50
2:2:286:GLY:HA3	2:2:298:LEU:HD11	1.93	0.50
1:A:314:MET:HA	1:A:319:GLY:HA2	1.94	0.49
1:A:261:VAL:CG1	1:A:497:CYS:SG	3.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1536:PHE:O	1:A:1540:LYS:N	2.45	0.49
1:A:958:SER:H	1:A:964:GLY:HA2	1.78	0.49
1:A:1899:ASP:OD1	1:A:1899:ASP:N	2.46	0.49
1:A:1094:SER:HA	1:A:1141:ILE:HA	1.95	0.49
1:A:562:GLU:OE2	1:A:870:ARG:NH2	2.46	0.48
1:A:348:THR:HG23	1:A:348:THR:O	2.13	0.48
2:2:178:GLN:O	2:2:180:ARG:NH1	2.46	0.48
1:A:136:ASP:OD1	1:A:136:ASP:N	2.47	0.48
1:A:552:THR:OG1	1:A:553:TYR:N	2.46	0.48
1:A:636:ILE:HB	1:A:950:TYR:HB2	1.96	0.48
2:2:669:ARG:HH12	2:2:687:ILE:CG1	2.27	0.48
3:3:87:LEU:HD11	4:4:66:GLY:HA2	1.95	0.48
1:A:415:SER:OG	1:A:416:TYR:N	2.47	0.47
1:A:2172:ARG:NH2	2:2:291:ASN:O	2.47	0.47
2:2:266:MET:HG3	2:2:267:SER:N	2.29	0.47
4:4:76:LEU:CD1	4:4:77:PHE:CD2	2.97	0.47
1:A:306:ASP:CG	1:A:1301:ARG:HH12	2.17	0.47
4:4:18:SER:OG	4:4:19:TYR:N	2.45	0.47
4:4:58:ASP:OD1	4:4:58:ASP:N	2.47	0.47
1:A:376:THR:OG1	1:A:377:PHE:N	2.48	0.47
1:A:1072:ARG:NH1	1:A:1106:ALA:O	2.48	0.47
1:A:124:GLU:OE2	1:A:278:LYS:NZ	2.47	0.47
1:A:1539:LYS:HA	1:A:1542:LYS:HB2	1.96	0.47
1:A:635:LEU:HD12	1:A:949:PRO:HB3	1.97	0.47
1:A:639:VAL:HG12	1:A:946:VAL:CG2	2.37	0.47
1:A:642:ALA:O	1:A:647:ASN:ND2	2.47	0.47
1:A:730:ASP:N	1:A:730:ASP:OD1	2.47	0.47
1:A:792:LYS:O	1:A:796:SER:HB3	2.15	0.47
1:A:713:ASN:OD1	1:A:713:ASN:N	2.48	0.47
1:A:426:VAL:O	1:A:437:GLN:NE2	2.48	0.47
1:A:322:ILE:HG12	1:A:350:PHE:HB2	1.97	0.47
2:2:664:PHE:HD1	2:2:670:ALA:HA	1.80	0.47
1:A:1124:ARG:HD3	1:A:1130:PRO:HA	1.97	0.46
1:A:1724:SER:HB2	1:A:1911:TRP:H	1.80	0.46
1:A:306:ASP:O	1:A:390:ARG:NH1	2.48	0.46
1:A:1486:TYR:HB3	1:A:1502:PHE:HB3	1.98	0.46
1:A:1536:PHE:O	1:A:1540:LYS:CB	2.64	0.46
1:A:771:VAL:O	1:A:775:LYS:HB2	2.15	0.46
1:A:1048:GLU:OE2	1:A:1050:ARG:NH2	2.48	0.46
1:A:484:LEU:O	1:A:488:TYR:HB2	2.16	0.46
2:2:406:LEU:HD12	2:2:406:LEU:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:VAL:HG22	1:A:1301:ARG:CD	2.46	0.46
1:A:424:ARG:NH2	1:A:509:ARG:O	2.49	0.46
1:A:1385:ASN:HB3	1:A:1699:GLY:HA3	1.98	0.46
1:A:1490:PHE:HB2	1:A:1498:PHE:HB2	1.98	0.46
2:2:231:ARG:NH2	2:2:350:GLU:OE2	2.48	0.46
2:2:286:GLY:CA	2:2:298:LEU:HD11	2.46	0.46
1:A:1694:PRO:HD3	2:2:442:PRO:HG2	1.98	0.46
1:A:1550:VAL:HG11	1:A:1552:ILE:HD11	1.98	0.46
2:2:367:ILE:HD12	2:2:381:LYS:HE3	1.98	0.46
2:2:514:LYS:HE2	2:2:518:LYS:HE3	1.98	0.45
1:A:243:ARG:HA	1:A:533:ASN:HD21	1.82	0.45
1:A:1521:GLN:O	1:A:1627:TRP:NE1	2.46	0.45
2:2:496:SER:OG	2:2:497:LEU:N	2.50	0.45
1:A:772:ASP:O	1:A:776:SER:HB3	2.17	0.45
1:A:1081:MET:HE3	1:A:1081:MET:HB3	1.78	0.45
2:2:654:ASN:OD1	2:2:654:ASN:N	2.49	0.45
1:A:907:CYS:SG	1:A:944:PHE:O	2.74	0.45
1:A:947:ASP:OD1	1:A:947:ASP:N	2.47	0.45
1:A:994:LEU:O	1:A:998:PHE:HB2	2.17	0.45
1:A:1306:LEU:HD21	1:A:1311:ARG:HH11	1.82	0.45
1:A:1617:LEU:O	2:2:451:ASN:ND2	2.49	0.44
2:2:676:VAL:HG21	2:2:679:SER:HB3	1.99	0.44
1:A:173:GLU:HB3	1:A:529:ILE:HA	1.98	0.44
2:2:428:PRO:HB2	2:2:478:ASN:HD21	1.82	0.44
3:3:20:ILE:HB	4:4:71:VAL:HG11	1.99	0.44
2:2:554:ARG:NH1	2:2:556:GLU:O	2.51	0.44
1:A:716:SER:OG	1:A:717:LYS:N	2.50	0.44
1:A:735:ILE:O	1:A:738:ARG:NH1	2.50	0.44
1:A:1322:TRP:HA	1:A:1340:VAL:HA	1.99	0.44
1:A:372:THR:O	1:A:372:THR:HG22	2.18	0.43
1:A:1370:LYS:HA	1:A:1370:LYS:HD2	1.82	0.43
1:A:1702:GLN:HA	2:2:499:ALA:HB1	1.99	0.43
2:2:312:THR:HB	2:2:555:LEU:HD21	2.00	0.43
1:A:367:ARG:HD3	1:A:401:GLU:HB2	2.00	0.43
1:A:428:ARG:HD3	1:A:512:THR:HB	2.00	0.43
1:A:722:THR:HG22	1:A:723:PHE:N	2.33	0.43
1:A:999:GLN:C	1:A:1002:ILE:HG22	2.43	0.43
1:A:1095:SER:HB3	1:A:1142:ASP:HA	1.99	0.43
1:A:305:VAL:HG21	1:A:1301:ARG:HD2	2.00	0.43
1:A:1672:ILE:HG23	1:A:1798:TRP:HH2	1.82	0.43
2:2:355:THR:HG23	2:2:356:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:529:PRO:O	2:2:629:THR:OG1	2.37	0.43
1:A:243:ARG:HG3	1:A:530:LEU:HD21	1.99	0.43
1:A:1457:LYS:O	1:A:1461:GLN:NE2	2.52	0.43
1:A:643:SER:OG	1:A:647:ASN:ND2	2.52	0.43
2:2:174:ASN:HB2	2:2:177:GLN:HB2	2.01	0.43
2:2:355:THR:HG21	2:2:635:ILE:HG22	1.99	0.43
1:A:313:TYR:OH	1:A:365:HIS:ND1	2.39	0.43
1:A:1280:TRP:HE3	4:4:76:LEU:HD21	1.84	0.43
1:A:1532:TYR:O	1:A:1536:PHE:HB2	2.18	0.43
1:A:732:VAL:HA	1:A:735:ILE:HB	2.01	0.43
1:A:634:PRO:HB2	1:A:882:ILE:HB	2.01	0.42
1:A:924:GLN:HG2	1:A:936:THR:HB	2.01	0.42
1:A:1626:ASN:N	1:A:1626:ASN:OD1	2.51	0.42
1:A:502:LEU:HD22	1:A:506:GLU:HG3	2.00	0.42
1:A:541:ARG:NE	1:A:551:GLU:OE1	2.48	0.42
1:A:576:ILE:H	1:A:576:ILE:HG13	1.65	0.42
1:A:1724:SER:OG	1:A:1725:GLY:N	2.53	0.42
1:A:1119:LYS:O	1:A:1123:LEU:CB	2.67	0.42
1:A:2051:LEU:HA	1:A:2054:LEU:HG	2.01	0.42
1:A:1606:LEU:HB3	1:A:1607:LEU:H	1.76	0.41
1:A:573:GLU:O	1:A:870:ARG:NH1	2.50	0.41
1:A:1584:ARG:HD3	1:A:1584:ARG:HA	1.88	0.41
1:A:2065:SER:OG	1:A:2066:LYS:N	2.53	0.41
1:A:379:GLY:HA2	1:A:383:ASP:HB3	2.01	0.41
1:A:489:VAL:HG12	1:A:492:PHE:HD2	1.85	0.41
1:A:491:PRO:O	1:A:495:SER:OG	2.37	0.41
1:A:860:MET:HE2	1:A:917:LYS:HD2	2.00	0.41
1:A:2108:CYS:SG	1:A:2137:PHE:HE1	2.42	0.41
2:2:477:GLU:O	2:2:522:ASN:ND2	2.52	0.41
2:2:478:ASN:OD1	2:2:478:ASN:N	2.53	0.41
1:A:302:ASP:HB2	1:A:305:VAL:HG12	2.02	0.41
1:A:1303:ARG:NH2	1:A:1306:LEU:HD13	2.35	0.41
1:A:1934:THR:OG1	1:A:1935:ALA:N	2.51	0.41
1:A:1056:LEU:HD11	1:A:1071:ARG:HG3	2.02	0.41
1:A:1540:LYS:C	1:A:1543:ILE:HG22	2.45	0.41
1:A:2151:ARG:HA	1:A:2151:ARG:HD3	1.88	0.41
1:A:576:ILE:HG23	1:A:868:VAL:HA	2.01	0.41
1:A:992:LEU:HD12	1:A:992:LEU:HA	1.95	0.41
1:A:1051:SER:OG	1:A:1052:MET:N	2.54	0.41
2:2:305:VAL:HG12	2:2:306:GLU:N	2.36	0.41
1:A:2129:SER:OG	1:A:2130:CYS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:VAL:HG13	1:A:881:CYS:SG	2.62	0.40
2:2:437:SER:HB2	2:2:485:PRO:HA	2.01	0.40
1:A:875:ASP:OD1	1:A:875:ASP:N	2.54	0.40
2:2:327:LEU:HG	2:2:347:PRO:HD3	2.02	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	1929/2222 (87%)	1802 (93%)	127 (7%)	0	100	100
2	2	414/689 (60%)	370 (89%)	43 (10%)	1 (0%)	43	74
3	3	83/201 (41%)	80 (96%)	3 (4%)	0	100	100
4	4	105/196 (54%)	96 (91%)	9 (9%)	0	100	100
All	All	2531/3308 (76%)	2348 (93%)	182 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	434	TRP

5.3.2 Protein sidechains [i](#)

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	1522/2014 (76%)	1522 (100%)	0	100	100
2	2	351/629 (56%)	351 (100%)	0	100	100
3	3	72/185 (39%)	71 (99%)	1 (1%)	59	71
4	4	91/173 (53%)	91 (100%)	0	100	100
All	All	2036/3001 (68%)	2035 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	43	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	351	ASN
1	A	389	ASN
1	A	437	GLN
1	A	523	GLN
1	A	533	ASN
1	A	572	ASN
1	A	631	ASN
1	A	647	ASN
1	A	706	ASN
1	A	794	ASN
1	A	940	ASN
1	A	997	ASN
1	A	1155	GLN
1	A	1169	ASN
1	A	1176	HIS
1	A	1343	ASN
1	A	1369	GLN
1	A	1386	ASN
1	A	1413	ASN
1	A	1434	HIS
1	A	1461	GLN
1	A	1618	ASN
1	A	1648	HIS
1	A	1703	ASN
1	A	1723	ASN
1	A	1789	ASN

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Mol	Chain	Res	Type
1	A	1824	ASN
1	A	1838	ASN
1	A	1916	ASN
1	A	1930	ASN
1	A	2049	ASN
1	A	2199	ASN
2	2	184	ASN
2	2	189	GLN
2	2	216	GLN
2	2	289	ASN
2	2	388	HIS
2	2	451	ASN
2	2	517	ASN
2	2	537	GLN
2	2	628	HIS
3	3	47	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

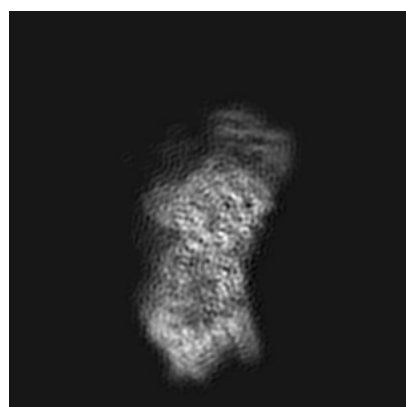
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21701. These allow visual inspection of the internal detail of the map and identification of artifacts.

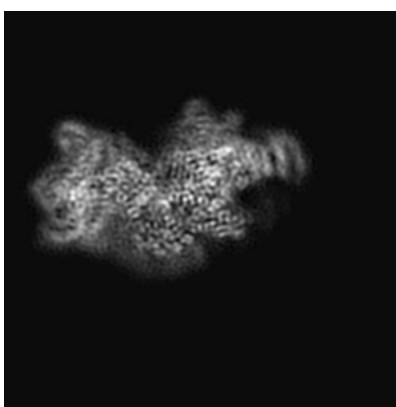
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

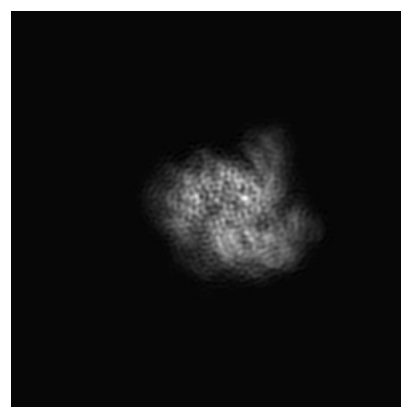
6.1.1 Primary map



X



Y



Z

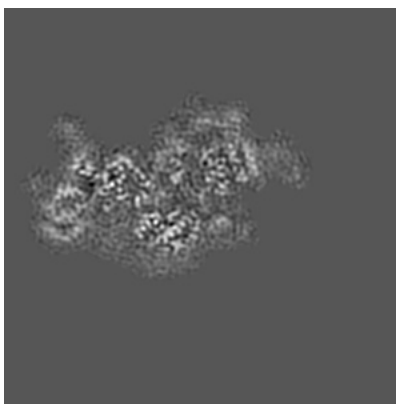
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

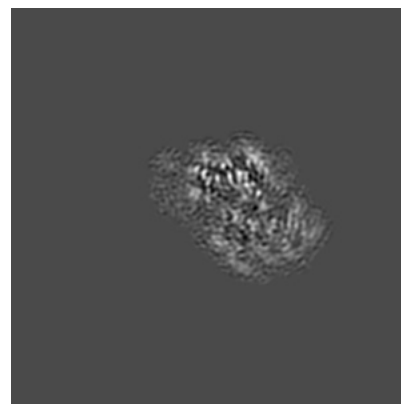
6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

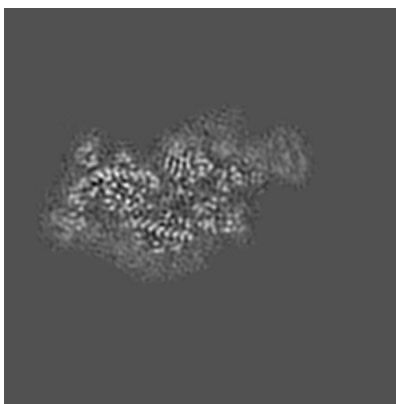
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

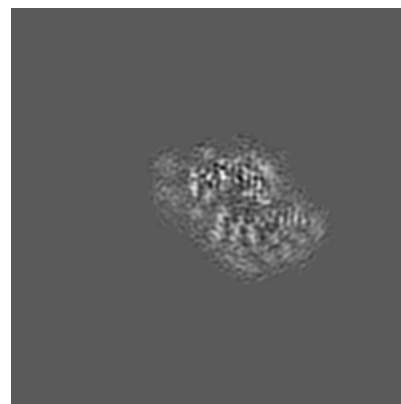
6.3.1 Primary map



X Index: 150



Y Index: 136

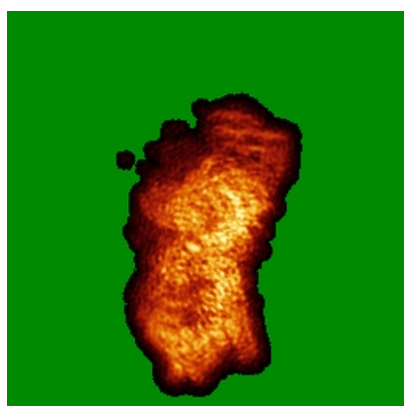


Z Index: 125

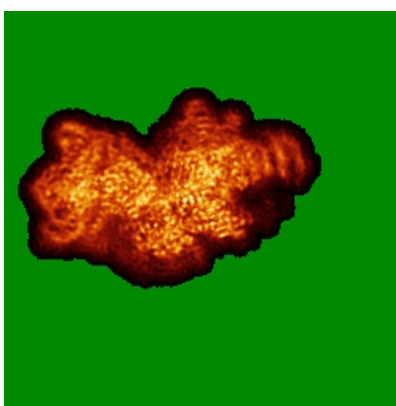
The images above show the largest variance slices of the map in three orthogonal directions.

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

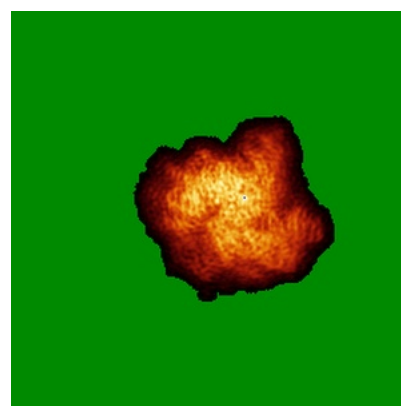
6.4.1 Primary map



X



Y

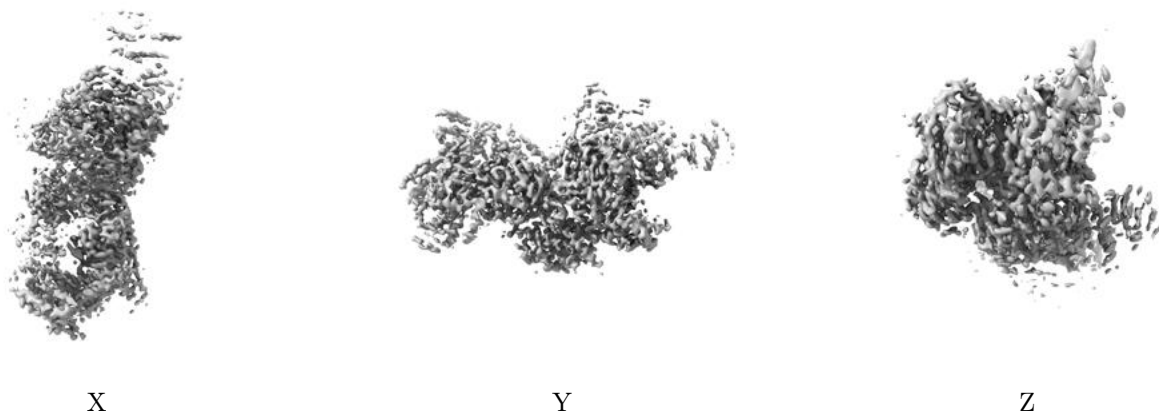


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

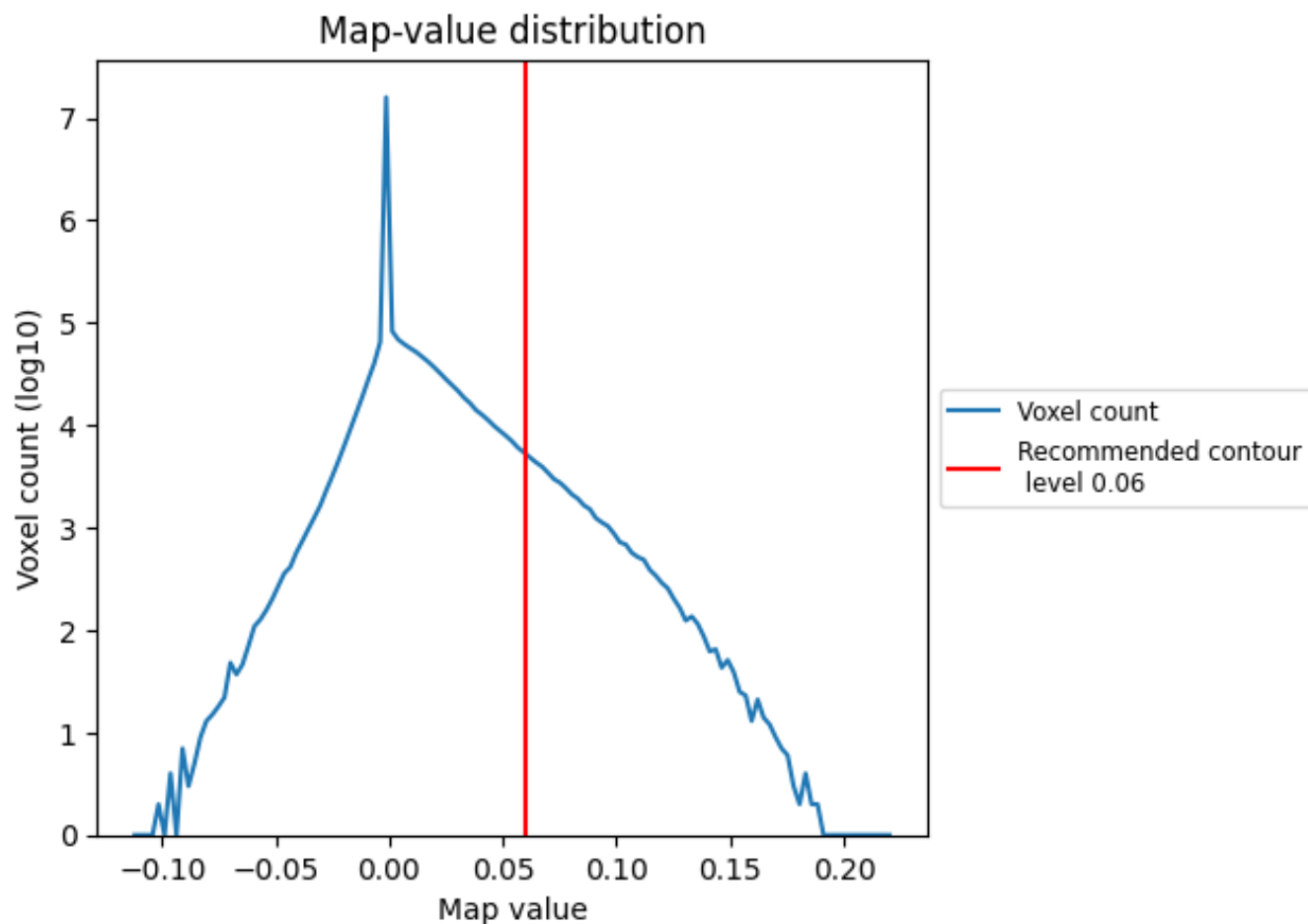
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

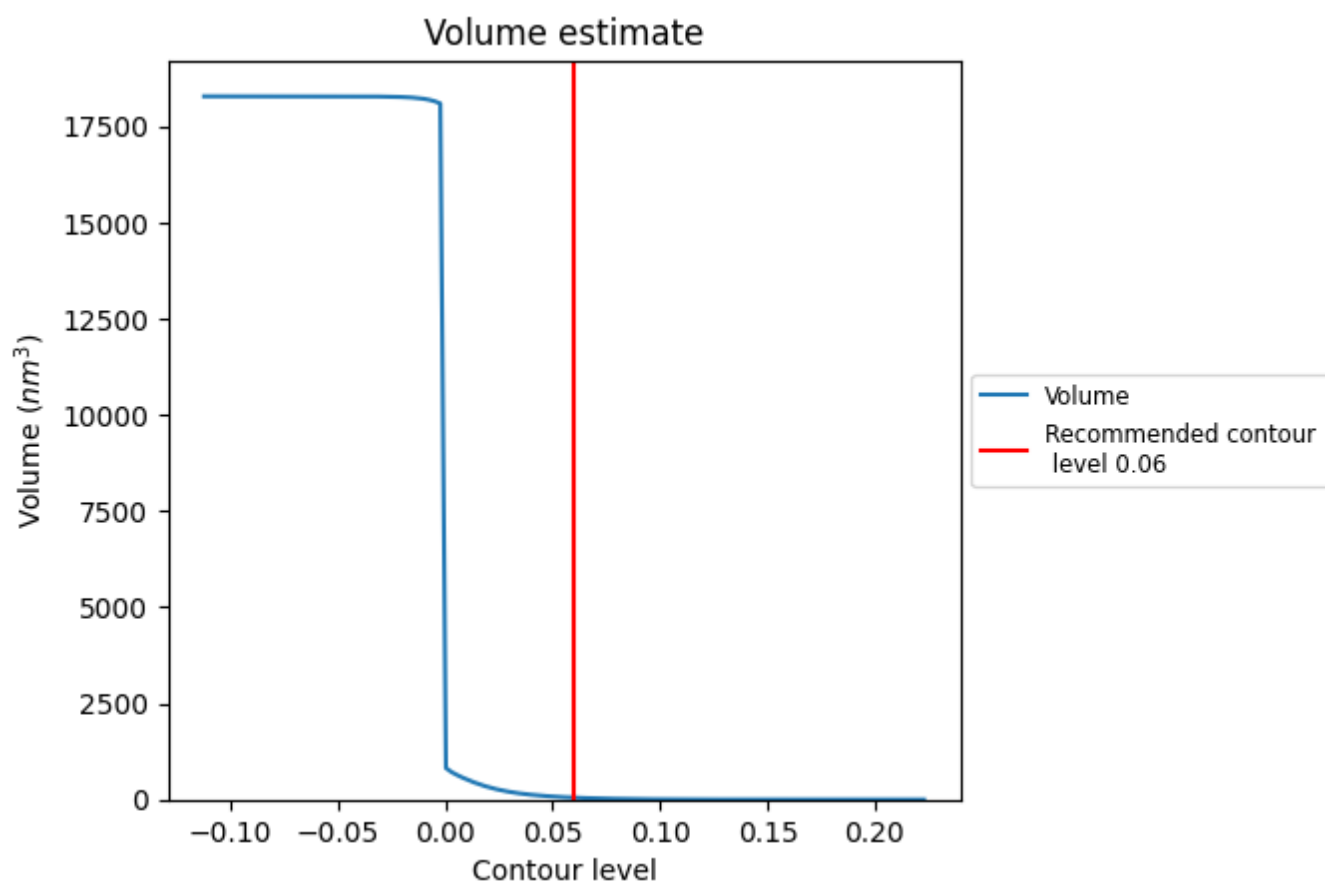
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

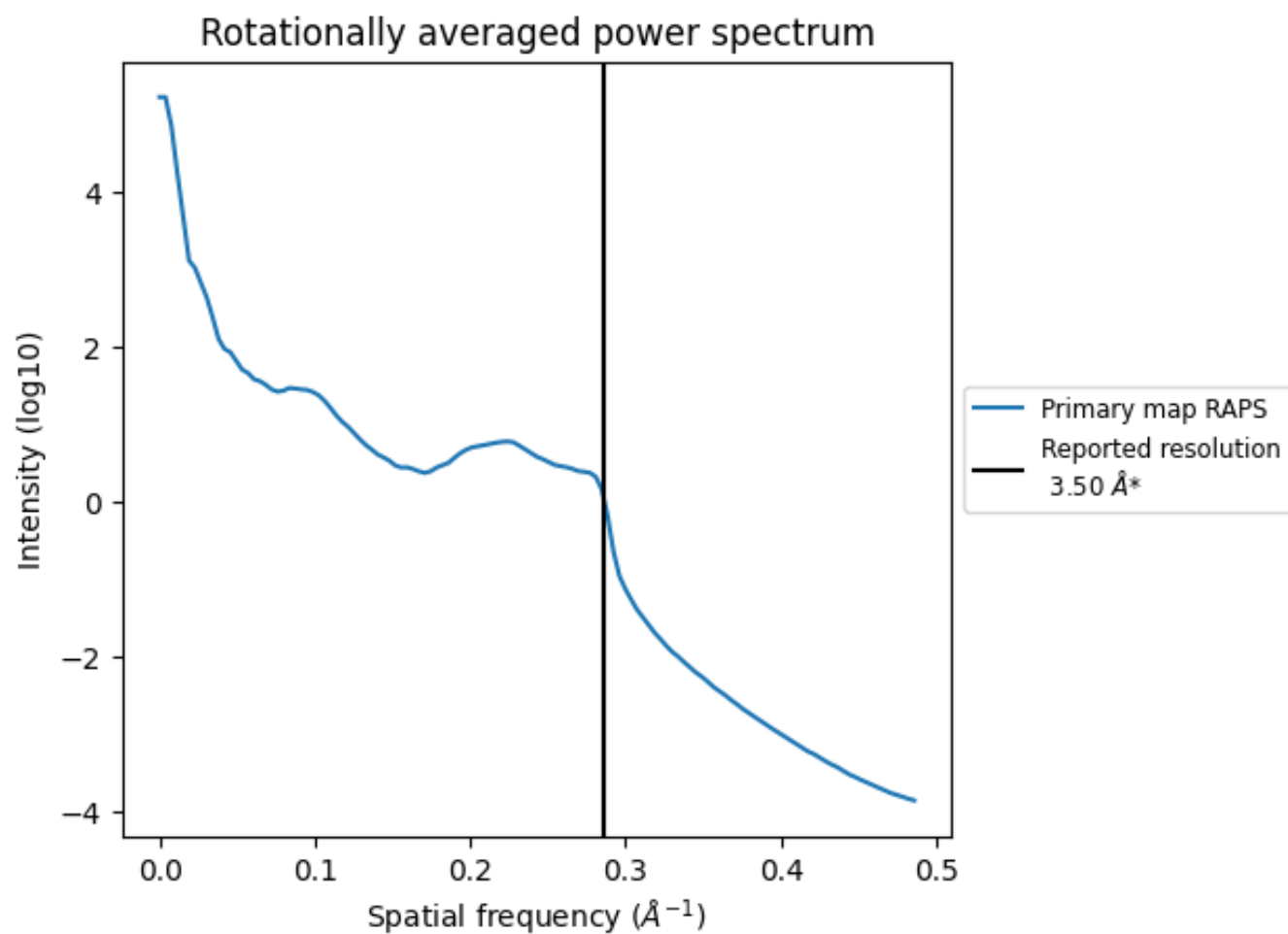
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 50 nm³; this corresponds to an approximate mass of 45 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 0.286 Å⁻¹

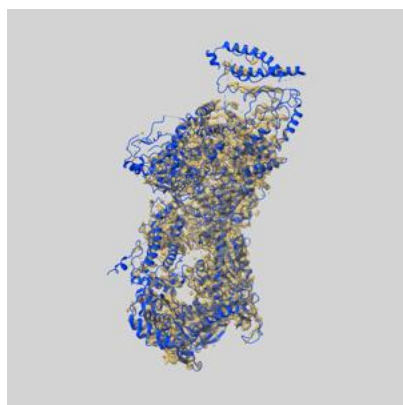
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

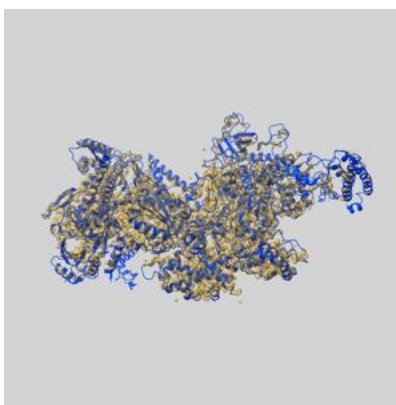
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21701 and PDB model 6WJV. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

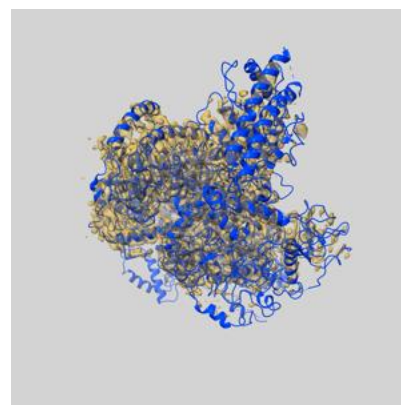
9.1 Map-model overlay [i](#)



X



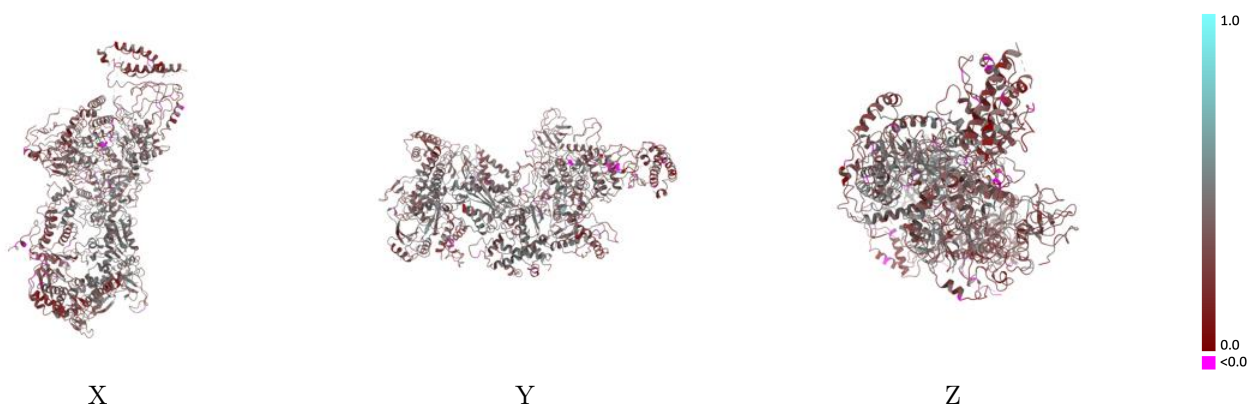
Y



Z

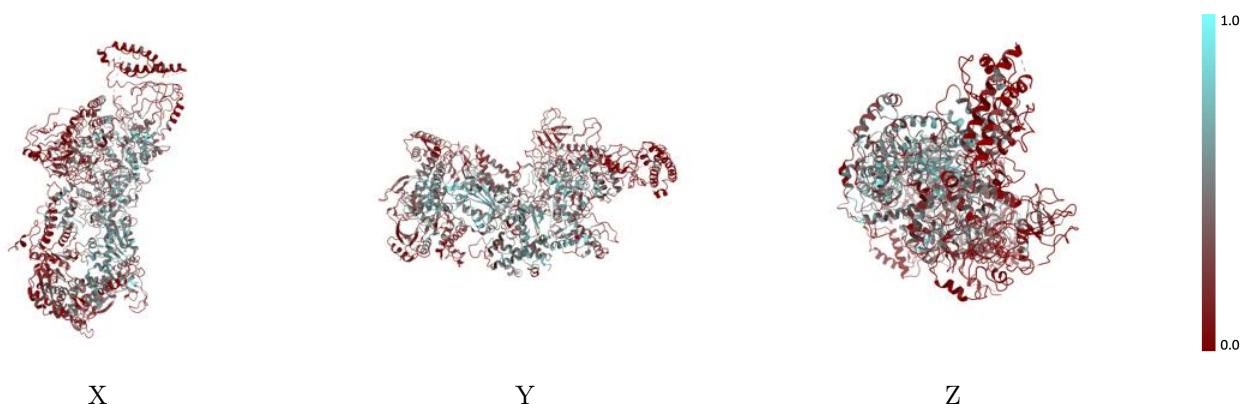
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



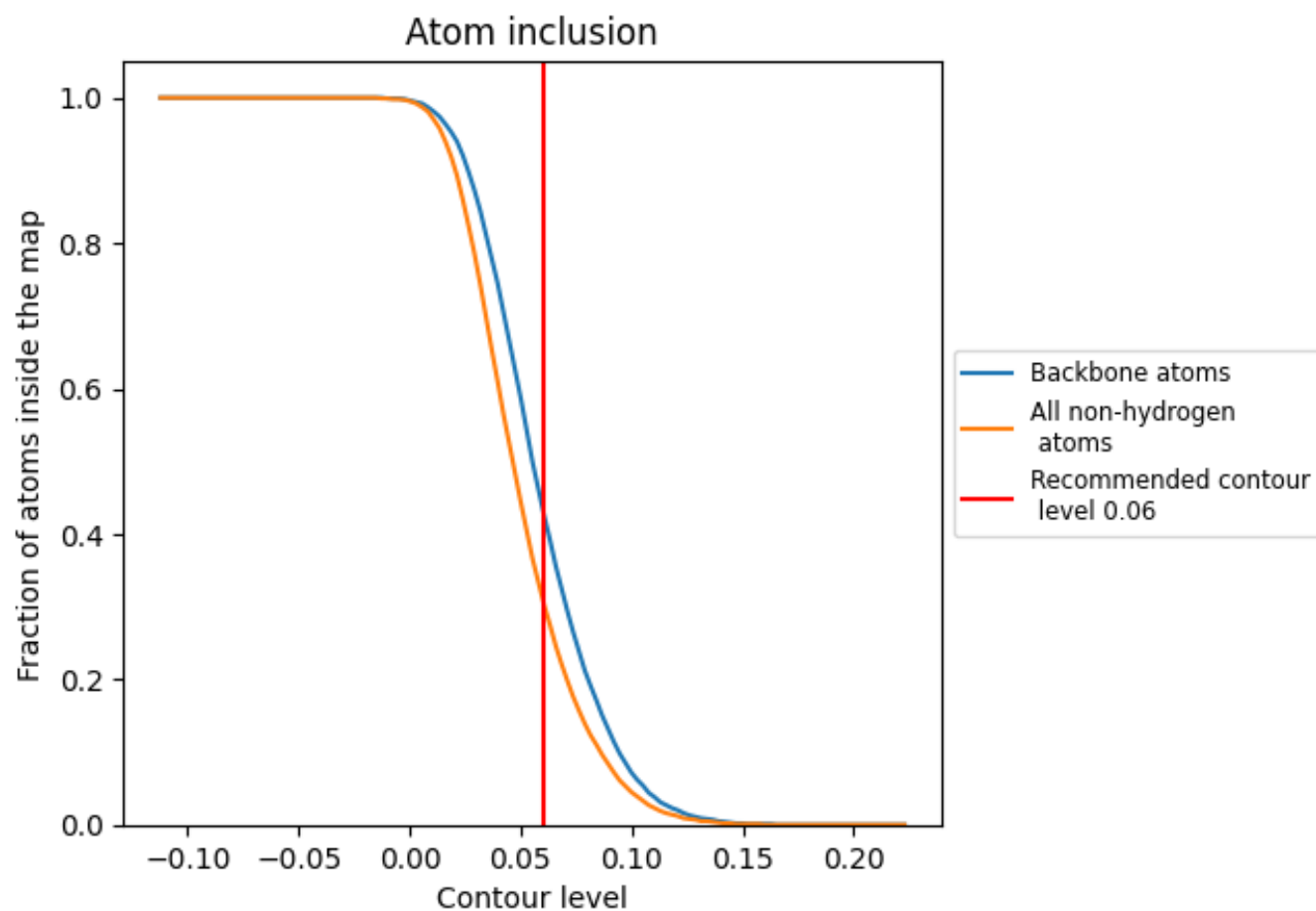
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 43% of all backbone atoms, 31% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3090	0.3490
2	0.2000	0.3340
3	0.4410	0.3700
4	0.4350	0.3910
A	0.3190	0.3490

