



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:54 AM UTC

PDB ID : 5FVM / pdb_00005fvm
EMDB ID : EMD-3329
Title : Cryo electron microscopy of a complex of Tor and Lst8
Authors : Baretic, D.; Berndt, A.; Ohashi, Y.; Johnson, C.M.; Williams, R.L.
Deposited on : 2016-02-09
Resolution : 6.70 Å(reported)
Based on initial model : 4JSV

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

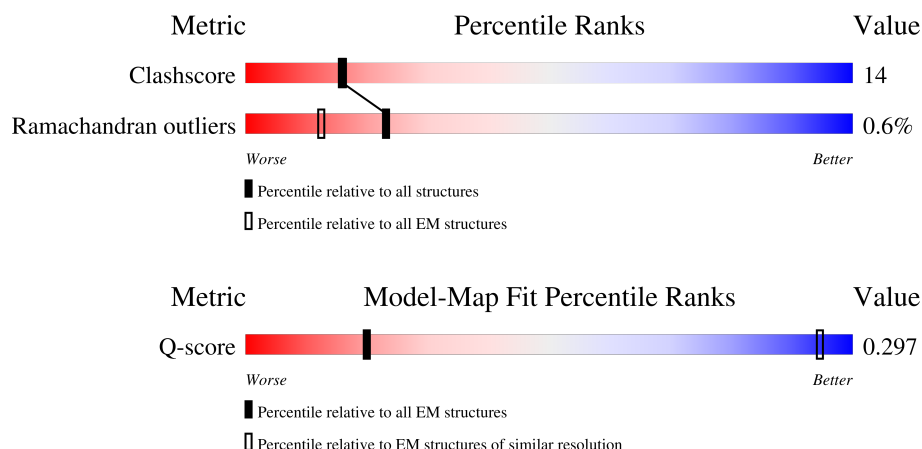
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.70 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	-
Q-score	-	25397	531 (5.60 - 6.60)

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

Mol	Chain	Length	Quality of chain
1	A	2471	 69% 15% • 14%
1	B	2471	 69% 15% • 14%
2	C	303	 71% 27% ..
2	D	303	 70% 28% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23974 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 SERINE/THREONINE-PROTEIN KINASE TOR2.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	2117	Total 10508	C 6274	N 2117	O 2117	0	0
1	B	2117	Total 10508	C 6274	N 2117	O 2117	0	0

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	GLU	-	expression tag	UNP A0A090BKR
A	-19	LEU	-	expression tag	UNP A0A090BKR
A	-18	LEU	-	expression tag	UNP A0A090BKR
A	-17	GLU	-	expression tag	UNP A0A090BKR
A	-16	GLY	-	expression tag	UNP A0A090BKR
A	-15	GLU	-	expression tag	UNP A0A090BKR
A	-14	LEU	-	expression tag	UNP A0A090BKR
A	-13	LYS	-	expression tag	UNP A0A090BKR
A	-12	THR	-	expression tag	UNP A0A090BKR
A	-11	ALA	-	expression tag	UNP A0A090BKR
A	-10	ALA	-	expression tag	UNP A0A090BKR
A	-9	LEU	-	expression tag	UNP A0A090BKR
A	-8	ALA	-	expression tag	UNP A0A090BKR
A	-7	GLN	-	expression tag	UNP A0A090BKR
A	-6	HIS	-	expression tag	UNP A0A090BKR
A	-5	ASP	-	expression tag	UNP A0A090BKR
A	-4	GLU	-	expression tag	UNP A0A090BKR
A	-3	ALA	-	expression tag	UNP A0A090BKR
A	-2	MET	-	expression tag	UNP A0A090BKR
A	-1	GLY	-	expression tag	UNP A0A090BKR
A	0	GLY	-	expression tag	UNP A0A090BKR
A	1	SER	-	expression tag	UNP A0A090BKR
A	34	ALA	THR	conflict	UNP A0A090BKR
A	44	ALA	PRO	conflict	UNP A0A090BKR
A	48	MET	ILE	conflict	UNP A0A090BKR
A	125	ASP	GLU	conflict	UNP A0A090BKR

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Chain	Residue	Modelled	Actual	Comment	Reference
A	557	ARG	THR	conflict	UNP A0A090BKR
A	998	LEU	VAL	conflict	UNP A0A090BKR
A	1063	VAL	ALA	conflict	UNP A0A090BKR
B	-20	GLU	-	expression tag	UNP A0A090BKR
B	-19	LEU	-	expression tag	UNP A0A090BKR
B	-18	LEU	-	expression tag	UNP A0A090BKR
B	-17	GLU	-	expression tag	UNP A0A090BKR
B	-16	GLY	-	expression tag	UNP A0A090BKR
B	-15	GLU	-	expression tag	UNP A0A090BKR
B	-14	LEU	-	expression tag	UNP A0A090BKR
B	-13	LYS	-	expression tag	UNP A0A090BKR
B	-12	THR	-	expression tag	UNP A0A090BKR
B	-11	ALA	-	expression tag	UNP A0A090BKR
B	-10	ALA	-	expression tag	UNP A0A090BKR
B	-9	LEU	-	expression tag	UNP A0A090BKR
B	-8	ALA	-	expression tag	UNP A0A090BKR
B	-7	GLN	-	expression tag	UNP A0A090BKR
B	-6	HIS	-	expression tag	UNP A0A090BKR
B	-5	ASP	-	expression tag	UNP A0A090BKR
B	-4	GLU	-	expression tag	UNP A0A090BKR
B	-3	ALA	-	expression tag	UNP A0A090BKR
B	-2	MET	-	expression tag	UNP A0A090BKR
B	-1	GLY	-	expression tag	UNP A0A090BKR
B	0	GLY	-	expression tag	UNP A0A090BKR
B	1	SER	-	expression tag	UNP A0A090BKR
B	34	ALA	THR	conflict	UNP A0A090BKR
B	44	ALA	PRO	conflict	UNP A0A090BKR
B	48	MET	ILE	conflict	UNP A0A090BKR
B	125	ASP	GLU	conflict	UNP A0A090BKR
B	557	ARG	THR	conflict	UNP A0A090BKR
B	998	LEU	VAL	conflict	UNP A0A090BKR
B	1063	VAL	ALA	conflict	UNP A0A090BKR

- Molecule 2 is a protein called TARGET OF RAPAMYCIN COMPLEX SUBUNIT LST8.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	299	Total	C	N	O	0	0
			1479	881	299	299		
2	D	299	Total	C	N	O	0	0
			1479	881	299	299		

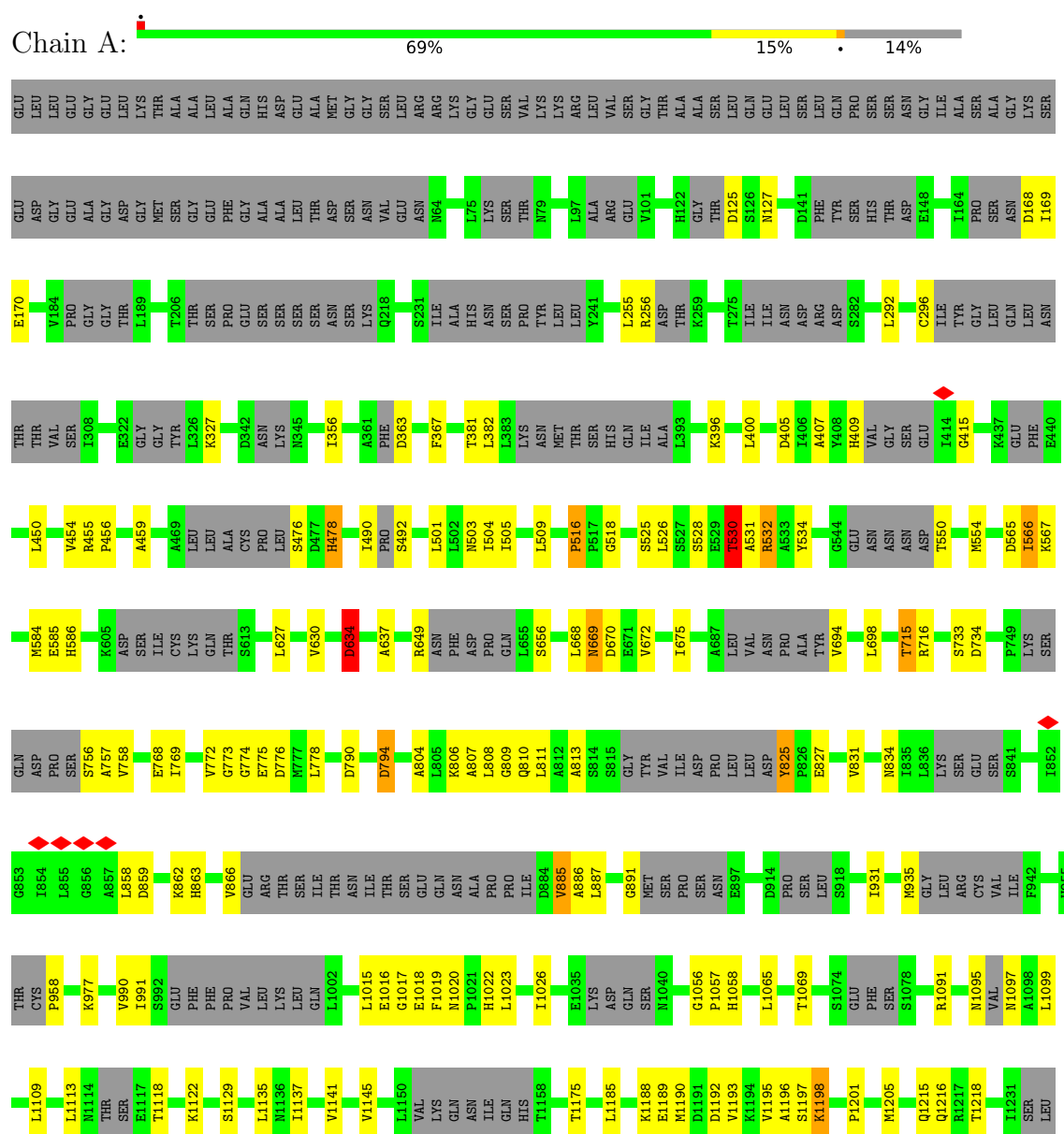
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	221	ASN	HIS	conflict	UNP A0A090BJK
D	221	ASN	HIS	conflict	UNP A0A090BJK

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: SERINE/THREONINE-PROTEIN KINASE TOR2





Frequency	Percentage
Daily	69%
Sometimes	15%
Never	14%



K567	P749	S841	F942	A1098	SER	I1351	Q1567	PRO	SER	I1934	P2086	M2262	P2368
Y570	LYS	I852	H955	L1099	LEU	M1358	LYS	SER	ASN	A1937	R2087	L2263	S2369
M554	GLN	G853	THR	L1109	THR	M1569	GLU	ASN	THR	F1955	I2090	D2264	E2370
E585	ASP	G854	LYS	L1113	ILE	H1362	V1570	MET	PHE	N1960	I2091	R2265	L2371
H586	PRO	I855	CYS	M1114	ALA	Q1363	W1573	ALA	ASN	T1961	C2093	G2268	K2269
K605	SER	G856	SER	THR	GLN	H1373	W1579	GLN	GLY	E1962	S2094	V2270	L2372
A757	ASP	A857	S766	SER	SER	H1377	R1580	SER	ALA	F1965	Q2100	V2271	L2377
V758	ASP	L858	A757	PRO	VAL	H1378	R1580	PRO	ALA	A1966	Q2101	C2278	E2380
E768	ILE	D859	V758	ASN	GLN	D1379	V1583	ASN	GLY	L1783	I2109	A2281	M2385
I769	CYS	K862	I769	LYS	THR	M1401	K1584	SER	THR	L1793	I2109	A2282	E2386
V772	GLN	H863	I769	THR	THR	A1405	K1585	SER	THR	V1794	N2113	A2405	I2405
G773	THR	V866	V772	GLN	THR	Q1405	P1586	VAL	THR	Q1795	N2113	K2285	K2406
G774	THR	GLU	G773	VAL	THR	GLY	K1587	SER	THR	H1796	L2121	E2286	D2407
E775	THR	ARG	E775	LEU	THR	GLU	Q1588	SER	THR	R1797	L2121	K2287	K2408
D776	THR	THR	D776	LEU	THR	GLU	D1589	SER	THR	H1797	T2124	E2288	L2409
W777	SER	ILE	W777	LEU	THR	ASP	M1590	SER	THR	Q1813	L2125	P2289	T2410
L778	SER	ILE	L778	GLN	THR	VAL	W1593	SER	THR	S1815	L2125	E2290	G2411
V630	THR	ASN	V630	L1002	THR	E1412	I1594	THR	THR	S1816	N2128	T2297	N2412
D634	THR	ASN	D634	L1015	THR	S1420	I1594	THR	THR	E1842	D2129	T2297	E2419
A637	THR	THR	A637	E1016	THR	S1420	I1599	THR	THR	E1846	P2130	Y2302	L2420
R649	GLU	SER	R649	F1019	GLU	L1424	S1603	THR	THR	L1846	F2133	Y2302	S2421
ASN	GLN	GLU	ASN	N1020	GLN	S1441	E1618	THR	THR	I1849	Y2142	V2306	D2424
PHE	GLN	GLU	PHE	ASN	GLN	S1441	GLU	THR	THR	W1835	Y2142	S2307	Q2425
ASP	GLN	GLU	ASP	ASN	GLN	LEU	GLY	THR	THR	W1836	I2145	G2308	G2425
PRO	GLN	GLU	PRO	ALA	GLN	E1444	ASP	THR	THR	W1837	L2163	G2311	G2426
L655	GLN	GLU	L655	ALA	GLN	P1451	PRO	THR	THR	W1838	L2164	I2315	D2427
S656	GLN	GLU	S656	ALA	GLN	P1452	ASN	THR	THR	W1839	S2160	M2322	S2435
L668	GLN	GLU	L668	ALA	GLN	P1453	ASN	THR	THR	W1840	H2170	D2326	V2436
N669	GLN	GLU	N669	ALA	GLN	P1454	ASN	THR	THR	W1841	A2173	K2328	E2437
D670	GLN	GLU	D670	ALA	GLN	P1455	ASN	THR	THR	W1842	S2174	D2341	Q2441
E671	GLN	GLU	E671	ALA	GLN	P1456	ASN	THR	THR	W1843	L2035	P2342	Y2443
V672	GLN	GLU	V672	ALA	GLN	L1460	ARG	THR	THR	W1844	D2039	N2345	T2444
I675	GLN	GLU	I675	ALA	GLN	K1474	P1632	THR	THR	W1845	L2040	V2346	G2445
A687	GLN	GLU	A687	ALA	GLN	S1477	P1633	THR	THR	W1846	A2056	N2345	S2448
LEU	GLN	GLU	LEU	ALA	GLN	S1477	V1636	THR	THR	W1847	V2057	V2346	PHE
VAL	GLN	GLU	VAL	ALA	GLN	A1481	M1643	THR	THR	W1848	G2058	L2240	TRP
ASN	GLN	GLU	ASN	ALA	GLN	A1481	M1643	THR	THR	W1849	G2059	S2224	
PRO	GLN	GLU	PRO	ALA	GLN	L1515	G1647	THR	THR	W1890	R2069	R2225	
ALA	GLN	GLU	ALA	ALA	GLN	VAL	Q1648	THR	THR	W1891	T2070	R2226	
TYR	GLN	GLU	TYR	ALA	GLN	ASN	Q1649	THR	THR	W1902	T2071	S2227	
V694	GLN	GLU	V694	ALA	GLN	ASN	Q1650	THR	THR	W1912	H2072	E2228	
L698	GLN	GLU	L698	ALA	GLN	ASN	E1651	THR	THR	D1913	P2075	G2248	
T715	GLN	GLU	T715	ALA	GLN	ASN	A1652	THR	THR	D1913	V2076	L2251	
R716	GLN	GLU	R716	ALA	GLN	ASN	A1652	THR	THR	D1913	P2076	G2252	
L835	GLN	GLU	L835	ALA	GLN	ASN	A1664	THR	THR	R1916	V2076	L2251	
I836	GLN	GLU	I836	ALA	GLN	ASN	A1664	THR	THR	R1916	V2076	L2251	
LYS	GLN	GLU	LYS	ALA	GLN	ASN	A1668	THR	THR	R1917	V2079	G2257	
SER	GLN	GLU	SER	ALA	GLN	ASN	L1668	THR	THR	R1917	L2080	L2261	
GLU	GLN	GLU	GLU	ALA	GLN	ASN	L1669	THR	THR	R1918	L2080	L2261	
VAL	GLN	GLU	VAL	ALA	GLN	ASN	L1669	THR	THR	R1918	L2080	L2261	
ILE	GLN	GLU	ILE	ALA	GLN	ASN	L1669	THR	THR	R1918	L2080	L2261	

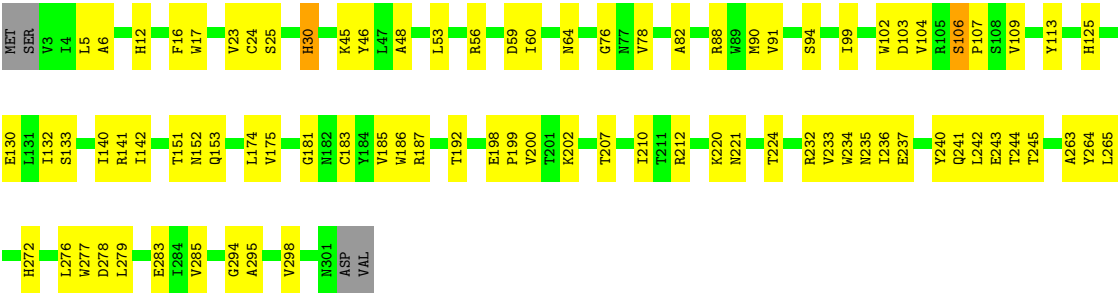
- Molecule 2: TARGET OF RAPAMYCIN COMPLEX SUBUNIT LST8

Chain C:

71%

27%

..



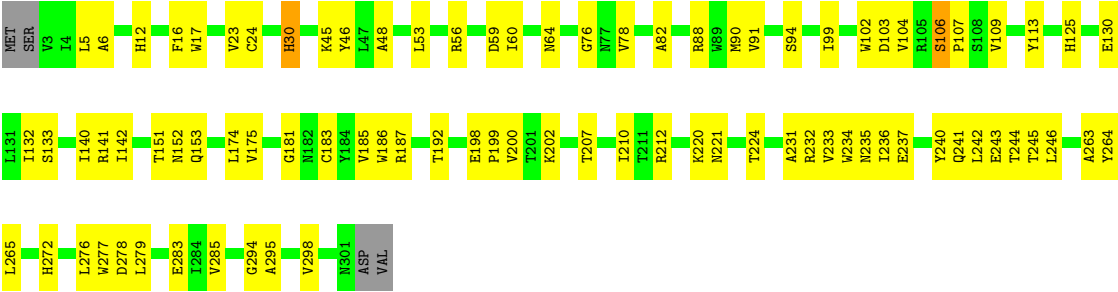
● Molecule 2: TARGET OF RAPAMYCIN COMPLEX SUBUNIT LST8

Chain D:

70%

28%

..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	28877	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE (GCTF)	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105263	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.282	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.044	Depositor
Map size ($\text{\AA}$)	425.6, 425.6, 425.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.33, 1.33, 1.33	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	0.70	0/10457	1.33	112/14512 (0.8%)
1	B	0.70	0/10457	1.34	114/14512 (0.8%)
2	C	0.47	0/1478	1.48	6/2058 (0.3%)
2	D	0.47	0/1478	1.48	6/2058 (0.3%)
All	All	0.67	0/23870	1.36	238/33140 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	19
1	B	0	19
2	C	0	3
2	D	0	3
All	All	0	44

There are no bond length outliers.

All (238) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	106	SER	CA-C-N	31.32	158.99	119.84
2	D	106	SER	C-N-CA	31.32	158.99	119.84
2	C	106	SER	CA-C-N	31.30	158.97	119.84
2	C	106	SER	C-N-CA	31.30	158.97	119.84
1	B	2341	ASP	CA-C-N	27.94	154.77	119.84
1	B	2341	ASP	C-N-CA	27.94	154.77	119.84
1	A	2341	ASP	CA-C-N	27.92	154.74	119.84
1	A	2341	ASP	C-N-CA	27.92	154.74	119.84
1	A	2129	ASP	CA-C-N	19.89	144.70	119.84
1	A	2129	ASP	C-N-CA	19.89	144.70	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2129	ASP	CA-C-N	19.87	144.67	119.84
1	B	2129	ASP	C-N-CA	19.87	144.67	119.84
1	B	825	TYR	CA-C-N	-17.62	103.86	121.65
1	B	825	TYR	C-N-CA	-17.62	103.86	121.65
1	A	825	TYR	CA-C-N	-17.59	103.88	121.65
1	A	825	TYR	C-N-CA	-17.59	103.88	121.65
1	B	1736	THR	N-CA-C	11.90	123.44	108.45
1	A	1736	THR	N-CA-C	11.85	123.38	108.45
1	B	2363	LEU	CA-C-N	-11.36	105.64	119.84
1	B	2363	LEU	C-N-CA	-11.36	105.64	119.84
1	A	2363	LEU	CA-C-N	-11.29	105.73	119.84
1	A	2363	LEU	C-N-CA	-11.29	105.73	119.84
1	A	1742	HIS	N-CA-C	-10.23	99.68	111.03
1	B	1742	HIS	N-CA-C	-10.21	99.70	111.03
1	B	2085	ARG	CA-C-N	8.90	130.97	119.84
1	B	2085	ARG	C-N-CA	8.90	130.97	119.84
1	B	2360	GLY	N-CA-C	8.83	122.04	112.33
1	A	2360	GLY	N-CA-C	8.79	122.00	112.33
1	B	1747	ALA	N-CA-C	-8.65	101.43	111.03
1	A	1747	ALA	N-CA-C	-8.62	101.46	111.03
1	A	2011	ILE	N-CA-C	8.34	118.37	110.53
1	B	2011	ILE	N-CA-C	8.32	118.35	110.53
1	A	530	THR	CA-C-N	8.20	136.47	121.70
1	A	530	THR	C-N-CA	8.20	136.47	121.70
1	B	634	ASP	CA-C-N	8.20	128.98	119.47
1	B	634	ASP	C-N-CA	8.20	128.98	119.47
1	A	634	ASP	CA-C-N	8.17	128.95	119.47
1	A	634	ASP	C-N-CA	8.17	128.95	119.47
1	B	530	THR	CA-C-N	8.16	136.40	121.70
1	B	530	THR	C-N-CA	8.16	136.40	121.70
1	B	415	GLY	CA-C-N	8.03	127.67	119.56
1	B	415	GLY	C-N-CA	8.03	127.67	119.56
1	A	415	GLY	CA-C-N	8.00	127.64	119.56
1	A	415	GLY	C-N-CA	8.00	127.64	119.56
1	B	1795	GLN	N-CA-C	-7.71	103.87	113.28
1	A	1795	GLN	N-CA-C	-7.71	103.87	113.28
1	A	2228	GLU	N-CA-C	-7.62	103.99	113.28
1	B	2228	GLU	N-CA-C	-7.60	104.01	113.28
1	B	455	ARG	CA-C-N	7.50	128.18	119.47
1	B	455	ARG	C-N-CA	7.50	128.18	119.47
1	A	455	ARG	CA-C-N	7.50	128.17	119.47
1	A	455	ARG	C-N-CA	7.50	128.17	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	SER	N-CA-C	7.48	119.06	108.00
1	A	1175	THR	CB-CA-C	-7.46	107.96	116.54
1	A	885	VAL	N-CA-C	-7.43	103.04	110.62
1	B	525	SER	N-CA-C	7.43	119.00	108.00
1	B	1175	THR	CB-CA-C	-7.43	108.00	116.54
1	B	1276	GLN	N-CA-C	-7.43	103.27	111.36
1	B	885	VAL	N-CA-C	-7.40	103.07	110.62
1	A	1276	GLN	N-CA-C	-7.39	103.30	111.36
1	A	1718	GLU	CB-CA-C	-7.28	108.17	116.54
1	B	1718	GLU	CB-CA-C	-7.25	108.20	116.54
2	D	64	ASN	CA-C-N	-7.16	112.38	119.90
2	D	64	ASN	C-N-CA	-7.16	112.38	119.90
1	A	2180	ILE	N-CA-C	-7.15	103.28	113.07
1	B	2180	ILE	N-CA-C	-7.14	103.28	113.07
2	C	64	ASN	CA-C-N	-7.13	112.41	119.90
2	C	64	ASN	C-N-CA	-7.13	112.41	119.90
1	B	478	HIS	N-CA-C	-6.99	103.71	111.82
1	B	1198	LYS	CB-CA-C	-6.94	107.79	117.23
1	A	1198	LYS	CB-CA-C	-6.92	107.82	117.23
1	A	532	ARG	N-CA-C	-6.91	102.86	112.12
1	A	1363	GLN	N-CA-C	-6.88	104.62	113.16
1	B	1363	GLN	N-CA-C	-6.88	104.64	113.16
1	B	532	ARG	N-CA-C	-6.87	102.92	112.12
1	B	630	VAL	N-CA-C	-6.79	104.04	110.42
1	B	794	ASP	N-CA-C	6.79	117.45	107.88
1	A	2367	ASN	CA-C-N	6.78	128.32	119.84
1	A	2367	ASN	C-N-CA	6.78	128.32	119.84
1	A	794	ASP	N-CA-C	6.77	117.43	107.88
1	A	478	HIS	N-CA-C	-6.76	103.71	112.23
1	B	2367	ASN	CA-C-N	6.75	128.28	119.84
1	B	2367	ASN	C-N-CA	6.75	128.28	119.84
1	A	630	VAL	N-CA-C	-6.75	104.08	110.42
1	B	2145	ILE	CA-C-N	-6.69	113.41	120.03
1	B	2145	ILE	C-N-CA	-6.69	113.41	120.03
1	B	525	SER	CB-CA-C	-6.65	107.03	116.34
1	A	525	SER	CB-CA-C	-6.65	107.03	116.34
1	A	2145	ILE	CA-C-N	-6.64	113.45	120.03
1	A	2145	ILE	C-N-CA	-6.64	113.45	120.03
1	A	1189	GLU	N-CA-C	6.63	117.82	108.00
1	B	1189	GLU	N-CA-C	6.60	117.77	108.00
1	A	670	ASP	N-CA-C	6.49	118.24	110.19
1	A	1856	ILE	CA-C-N	-6.49	112.22	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1856	ILE	C-N-CA	-6.49	112.22	118.97
1	B	1745	ALA	N-CA-C	-6.48	104.86	112.89
1	B	1856	ILE	CA-C-N	-6.47	112.24	118.97
1	B	1856	ILE	C-N-CA	-6.47	112.24	118.97
1	A	1745	ALA	N-CA-C	-6.46	104.88	112.89
1	B	516	PRO	CA-C-N	6.46	127.91	119.84
1	B	516	PRO	C-N-CA	6.46	127.91	119.84
1	B	670	ASP	N-CA-C	6.45	118.18	110.19
1	A	516	PRO	CA-C-N	6.42	127.87	119.84
1	A	516	PRO	C-N-CA	6.42	127.87	119.84
1	A	1185	LEU	CA-C-N	6.38	127.82	119.84
1	A	1185	LEU	C-N-CA	6.38	127.82	119.84
1	B	1751	VAL	N-CA-C	-6.38	104.04	111.00
1	A	1919	SER	CA-C-N	6.38	126.87	119.47
1	A	1919	SER	C-N-CA	6.38	126.87	119.47
1	B	1919	SER	CA-C-N	6.38	126.87	119.47
1	B	1919	SER	C-N-CA	6.38	126.87	119.47
1	A	1751	VAL	N-CA-C	-6.37	104.06	111.00
1	B	1185	LEU	CA-C-N	6.37	127.80	119.84
1	B	1185	LEU	C-N-CA	6.37	127.80	119.84
1	B	2288	TYR	CA-C-N	6.35	127.78	119.84
1	B	2288	TYR	C-N-CA	6.35	127.78	119.84
1	A	2288	TYR	CA-C-N	6.32	127.75	119.84
1	A	2288	TYR	C-N-CA	6.32	127.75	119.84
1	B	1019	PHE	N-CA-C	-6.29	104.35	111.14
1	A	1631	ALA	CA-C-N	-6.29	113.91	120.38
1	A	1631	ALA	C-N-CA	-6.29	113.91	120.38
1	A	1190	MET	N-CA-C	6.28	116.53	108.24
1	B	1190	MET	N-CA-C	6.28	116.52	108.24
1	B	1631	ALA	CA-C-N	-6.28	113.92	120.38
1	B	1631	ALA	C-N-CA	-6.28	113.92	120.38
1	A	1019	PHE	N-CA-C	-6.27	104.37	111.14
1	A	1633	PRO	CA-C-N	-6.26	112.55	119.19
1	A	1633	PRO	C-N-CA	-6.26	112.55	119.19
2	D	106	SER	N-CA-C	-6.26	103.66	112.17
2	C	106	SER	N-CA-C	-6.24	103.69	112.17
1	B	2071	THR	N-CA-C	-6.22	105.44	113.16
1	B	1633	PRO	CA-C-N	-6.22	112.60	119.19
1	B	1633	PRO	C-N-CA	-6.22	112.60	119.19
1	A	2071	THR	N-CA-C	-6.20	105.47	113.16
1	A	1718	GLU	N-CA-C	6.13	117.63	108.31
1	B	1198	LYS	N-CA-C	6.13	118.91	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1198	LYS	N-CA-C	6.11	118.88	108.67
1	B	1718	GLU	N-CA-C	6.10	117.59	108.31
1	A	733	SER	CB-CA-C	-6.10	109.53	116.54
1	B	733	SER	CB-CA-C	-6.10	109.53	116.54
1	A	1481	ALA	N-CA-C	-6.05	104.60	111.14
1	B	1481	ALA	N-CA-C	-6.05	104.60	111.14
1	B	734	ASP	CB-CA-C	-6.04	109.63	116.63
1	A	734	ASP	CB-CA-C	-5.99	109.69	116.63
1	B	858	LEU	CB-CA-C	-5.94	109.15	117.23
1	A	858	LEU	CB-CA-C	-5.94	109.15	117.23
1	A	1632	PRO	CA-C-N	5.83	126.39	120.38
1	A	1632	PRO	C-N-CA	5.83	126.39	120.38
1	A	1189	GLU	CB-CA-C	-5.81	108.21	116.34
1	A	2142	TYR	CA-C-N	-5.80	113.96	119.76
1	A	2142	TYR	C-N-CA	-5.80	113.96	119.76
1	B	2142	TYR	CA-C-N	-5.80	113.96	119.76
1	B	2142	TYR	C-N-CA	-5.80	113.96	119.76
1	B	1961	THR	CB-CA-C	-5.80	109.34	117.23
1	A	1961	THR	CB-CA-C	-5.76	109.39	117.23
1	B	1189	GLU	CB-CA-C	-5.76	108.28	116.34
1	B	1632	PRO	CA-C-N	5.75	126.31	120.38
1	B	1632	PRO	C-N-CA	5.75	126.31	120.38
1	A	1015	LEU	CA-C-N	-5.74	114.96	123.11
1	A	1015	LEU	C-N-CA	-5.74	114.96	123.11
1	B	1015	LEU	CA-C-N	-5.72	114.99	123.11
1	B	1015	LEU	C-N-CA	-5.72	114.99	123.11
1	B	1651	GLU	N-CA-C	-5.69	104.99	111.14
1	A	1651	GLU	N-CA-C	-5.66	105.02	111.14
1	A	2362	ASP	N-CA-C	5.66	118.18	111.33
1	B	2362	ASP	N-CA-C	5.60	118.11	111.33
1	B	1345	GLU	CA-C-N	5.59	128.84	120.96
1	B	1345	GLU	C-N-CA	5.59	128.84	120.96
1	A	1345	GLU	CA-C-N	5.55	128.78	120.96
1	A	1345	GLU	C-N-CA	5.55	128.78	120.96
1	A	1188	LYS	N-CA-C	5.54	115.69	107.88
1	B	1188	LYS	N-CA-C	5.51	115.65	107.88
1	B	2174	SER	N-CA-C	-5.50	106.35	113.16
1	A	2121	LEU	N-CA-C	-5.48	105.39	111.36
1	B	2121	LEU	N-CA-C	-5.48	105.39	111.36
1	A	1522	ARG	CB-CA-C	-5.46	109.81	117.23
1	A	2174	SER	N-CA-C	-5.46	106.39	113.16
1	B	1522	ARG	CB-CA-C	-5.46	109.81	117.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1379	ASP	CB-CA-C	-5.42	110.31	116.54
1	B	1379	ASP	CB-CA-C	-5.39	110.34	116.54
1	B	570	TYR	CB-CA-C	-5.38	109.91	117.23
1	A	1056	GLY	CA-C-N	-5.37	114.72	120.03
1	A	1056	GLY	C-N-CA	-5.37	114.72	120.03
1	B	1960	ASN	N-CA-C	-5.37	105.07	111.03
1	A	1317	SER	CB-CA-C	-5.34	108.86	116.34
1	A	1960	ASN	N-CA-C	-5.34	105.10	111.03
1	B	1317	SER	CB-CA-C	-5.33	108.87	116.34
1	B	1056	GLY	CA-C-N	-5.33	114.75	120.03
1	B	1056	GLY	C-N-CA	-5.33	114.75	120.03
1	A	977	LYS	N-CA-C	-5.31	103.02	110.50
1	B	2173	ALA	N-CA-C	-5.30	106.79	113.20
1	B	977	LYS	N-CA-C	-5.29	103.04	110.50
1	A	356	ILE	CA-C-N	5.28	124.91	119.05
1	A	356	ILE	C-N-CA	5.28	124.91	119.05
1	A	2173	ALA	N-CA-C	-5.26	106.83	113.20
1	B	356	ILE	CA-C-N	5.26	124.89	119.05
1	B	356	ILE	C-N-CA	5.26	124.89	119.05
1	A	1333	LYS	N-CA-C	-5.25	105.73	111.82
1	B	1333	LYS	N-CA-C	-5.25	105.73	111.82
1	B	2297	THR	N-CA-C	-5.25	102.28	110.10
1	A	2297	THR	N-CA-C	-5.21	102.33	110.10
1	B	669	ASN	N-CA-C	5.19	125.53	111.00
1	A	669	ASN	N-CA-C	5.17	125.48	111.00
2	C	30	HIS	N-CA-C	-5.17	106.93	113.18
1	A	958	PRO	CA-C-N	5.17	124.83	119.56
1	A	958	PRO	C-N-CA	5.17	124.83	119.56
1	B	1474	LYS	CA-C-N	5.14	124.32	118.97
1	B	1474	LYS	C-N-CA	5.14	124.32	118.97
1	B	1197	SER	N-CA-C	5.14	114.62	107.73
1	B	2268	GLY	N-CA-C	5.14	119.06	112.18
1	A	2268	GLY	N-CA-C	5.13	119.05	112.18
1	B	2410	THR	N-CA-C	5.12	123.53	113.29
1	A	1197	SER	N-CA-C	5.12	114.59	107.73
1	A	2350	LEU	CA-C-N	5.11	125.40	119.47
1	A	2350	LEU	C-N-CA	5.11	125.40	119.47
1	A	2219	VAL	N-CA-C	-5.11	105.44	111.00
1	B	2219	VAL	N-CA-C	-5.10	105.44	111.00
1	B	2350	LEU	CA-C-N	5.10	125.39	119.47
1	B	2350	LEU	C-N-CA	5.10	125.39	119.47
2	D	30	HIS	N-CA-C	-5.09	106.90	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2410	THR	N-CA-C	5.08	123.46	113.29
1	A	1320	THR	N-CA-C	-5.08	107.03	113.18
1	A	2350	LEU	N-CA-C	-5.08	105.69	112.55
1	A	1474	LYS	CA-C-N	5.08	124.25	118.97
1	A	1474	LYS	C-N-CA	5.08	124.25	118.97
1	B	958	PRO	CA-C-N	5.07	124.74	119.56
1	B	958	PRO	C-N-CA	5.07	124.74	119.56
1	B	1320	THR	N-CA-C	-5.07	107.04	113.18
1	B	327	LYS	CB-CA-C	-5.07	110.33	117.23
1	A	327	LYS	CB-CA-C	-5.07	110.34	117.23
1	B	1816	SER	CB-CA-C	-5.06	110.72	116.54
1	B	2350	LEU	N-CA-C	-5.06	105.72	112.55
1	A	1816	SER	CB-CA-C	-5.06	110.72	116.54
1	B	2072	HIS	CB-CA-C	-5.06	110.76	116.63
1	A	1349	SER	N-CA-C	-5.05	105.42	111.03
1	A	1985	ILE	N-CA-C	-5.01	104.72	111.44
1	B	1985	ILE	N-CA-C	-5.01	104.72	111.44
1	A	2072	HIS	CB-CA-C	-5.01	110.82	116.63

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1016	GLU	Peptide
1	A	1192	ASP	Peptide
1	A	1198	LYS	Peptide
1	A	1522	ARG	Peptide
1	A	1713	PRO	Peptide
1	A	1735	LYS	Peptide
1	A	2010	ASP	Peptide
1	A	2341	ASP	Peptide
1	A	2342	PRO	Peptide
1	A	2359	THR	Peptide
1	A	509	LEU	Peptide
1	A	530	THR	Peptide
1	A	566	ILE	Peptide
1	A	567	LYS	Peptide
1	A	627	LEU	Peptide
1	A	634	ASP	Peptide
1	A	668	LEU	Peptide
1	A	669	ASN	Peptide
1	A	715	THR	Peptide

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Mol	Chain	Res	Type	Group
1	B	1016	GLU	Peptide
1	B	1192	ASP	Peptide
1	B	1198	LYS	Peptide
1	B	1522	ARG	Peptide
1	B	1713	PRO	Peptide
1	B	1735	LYS	Peptide
1	B	2010	ASP	Peptide
1	B	2341	ASP	Peptide
1	B	2342	PRO	Peptide
1	B	2359	THR	Peptide
1	B	509	LEU	Peptide
1	B	530	THR	Peptide
1	B	566	ILE	Peptide
1	B	567	LYS	Peptide
1	B	627	LEU	Peptide
1	B	634	ASP	Peptide
1	B	668	LEU	Peptide
1	B	669	ASN	Peptide
1	B	715	THR	Peptide
2	C	106	SER	Peptide
2	C	192	THR	Peptide
2	C	295	ALA	Peptide
2	D	106	SER	Peptide
2	D	192	THR	Peptide
2	D	295	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10508	0	4629	194	0
1	B	10508	0	4629	197	0
2	C	1479	0	673	54	0
2	D	1479	0	673	54	0
All	All	23974	0	10604	499	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 14.

All (499) 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)
2:D:264:TYR:HA	2:D:278:ASP:HA	1.57	0.87
2:C:264:TYR:HA	2:C:278:ASP:HA	1.57	0.84
1:B:2407:ASP:O	1:B:2412:ASN:N	2.11	0.82
1:A:2407:ASP:O	1:A:2412:ASN:N	2.10	0.82
1:A:1955:PHE:HA	1:A:1961:THR:H	1.45	0.82
1:B:1738:TYR:O	1:B:1742:HIS:N	2.13	0.81
1:B:2405:ILE:O	1:B:2409:LEU:N	2.14	0.81
1:A:1738:TYR:O	1:A:1742:HIS:N	2.13	0.81
1:A:1989:ASN:O	1:A:1993:ARG:N	2.13	0.81
2:D:235:ASN:N	2:D:241:GLN:O	2.13	0.81
1:B:2109:ILE:O	1:B:2113:ASN:N	2.14	0.81
1:B:1955:PHE:HA	1:B:1961:THR:H	1.45	0.80
1:A:2109:ILE:O	1:A:2113:ASN:N	2.14	0.79
1:A:2405:ILE:O	1:A:2409:LEU:N	2.14	0.79
1:B:1590:MET:O	1:B:1594:ILE:N	2.16	0.78
1:B:1989:ASN:O	1:B:1993:ARG:N	2.13	0.78
1:A:1590:MET:O	1:A:1594:ILE:N	2.16	0.77
1:B:1868:GLN:O	1:B:1872:ARG:N	2.18	0.77
1:A:1756:THR:O	1:A:1760:LYS:N	2.19	0.76
2:C:235:ASN:N	2:C:241:GLN:O	2.13	0.76
1:A:1643:MET:O	1:A:1647:GLY:N	2.18	0.76
1:A:1868:GLN:O	1:A:1872:ARG:N	2.18	0.76
1:B:1118:THR:O	1:B:1122:LYS:N	2.13	0.75
1:B:1756:THR:O	1:B:1760:LYS:N	2.19	0.75
1:A:1118:THR:O	1:A:1122:LYS:N	2.13	0.74
1:B:2160:SER:HA	1:B:2265:ARG:H	1.53	0.74
1:B:1373:HIS:O	1:B:1377:HIS:N	2.20	0.74
1:B:1643:MET:O	1:B:1647:GLY:N	2.18	0.73
1:A:1741:TRP:O	1:A:1745:ALA:N	2.22	0.73
1:A:2248:GLY:O	1:A:2252:GLY:N	2.22	0.72
1:A:2160:SER:HA	1:A:2265:ARG:H	1.53	0.72
1:A:1373:HIS:O	1:A:1377:HIS:N	2.20	0.72
1:B:1741:TRP:O	1:B:1745:ALA:N	2.22	0.72
1:B:2248:GLY:O	1:B:2252:GLY:N	2.22	0.72
1:B:634:ASP:O	1:B:637:ALA:N	2.22	0.72
1:B:2130:PRO:O	1:B:2133:PHE:N	2.21	0.71
1:B:2437:GLU:O	1:B:2441:GLN:N	2.24	0.71
1:A:634:ASP:O	1:A:637:ALA:N	2.22	0.71
1:A:1736:THR:C	1:A:1738:TYR:H	1.99	0.70
1:B:2070:ILE:HA	1:B:2093:GLY:HA2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2070:ILE:HA	1:A:2093:GLY:HA2	1.74	0.70
1:A:2437:GLU:O	1:A:2441:GLN:N	2.24	0.70
1:A:1742:HIS:O	1:A:1746:LEU:N	2.25	0.70
1:A:2130:PRO:O	1:A:2133:PHE:N	2.21	0.70
1:B:1742:HIS:O	1:B:1746:LEU:N	2.25	0.69
2:C:272:HIS:HA	2:C:294:GLY:HA2	1.74	0.69
1:B:1022:HIS:O	1:B:1026:ILE:N	2.24	0.69
1:B:1736:THR:C	1:B:1738:TYR:H	1.99	0.69
2:D:272:HIS:HA	2:D:294:GLY:HA2	1.74	0.69
1:A:1755:LEU:O	1:A:1759:ILE:N	2.26	0.68
2:D:220:LYS:O	2:D:237:GLU:N	2.26	0.68
1:A:2057:VAL:O	1:A:2059:GLY:N	2.26	0.68
1:B:887:LEU:O	1:B:891:GLY:N	2.23	0.68
1:B:2057:VAL:O	1:B:2059:GLY:N	2.26	0.67
1:A:1998:ALA:O	1:A:2002:VAL:N	2.28	0.67
2:C:220:LYS:O	2:C:237:GLU:N	2.26	0.67
1:A:1252:TYR:O	1:A:1256:ALA:N	2.25	0.67
1:A:887:LEU:O	1:A:891:GLY:N	2.23	0.67
2:C:133:SER:N	2:C:141:ARG:O	2.29	0.66
2:C:142:ILE:H	2:C:152:ASN:H	1.43	0.66
2:D:133:SER:O	2:D:141:ARG:N	2.27	0.66
2:D:133:SER:N	2:D:141:ARG:O	2.29	0.66
2:C:265:LEU:N	2:C:277:TRP:O	2.28	0.66
1:A:2311:GLY:O	1:A:2315:ILE:N	2.28	0.66
2:D:5:LEU:O	2:D:17:TRP:N	2.28	0.66
2:C:5:LEU:O	2:C:17:TRP:N	2.28	0.65
1:B:694:VAL:O	1:B:698:LEU:N	2.30	0.65
1:B:1998:ALA:O	1:B:2002:VAL:N	2.28	0.65
2:C:82:ALA:O	2:C:91:VAL:N	2.28	0.65
1:A:866:VAL:O	1:A:885:VAL:N	2.29	0.65
1:B:2262:MET:O	1:B:2271:VAL:N	2.26	0.65
2:D:82:ALA:O	2:D:91:VAL:N	2.28	0.65
1:A:1420:SER:O	1:A:1424:LEU:N	2.30	0.65
2:D:236:ILE:HA	2:D:240:TYR:HA	1.78	0.65
1:A:1401:ASN:O	1:A:1405:ALA:N	2.30	0.65
2:C:236:ILE:HA	2:C:240:TYR:HA	1.78	0.65
2:D:142:ILE:H	2:D:152:ASN:H	1.43	0.65
1:A:2262:MET:O	1:A:2271:VAL:N	2.26	0.65
1:B:866:VAL:O	1:B:885:VAL:N	2.29	0.65
1:B:1755:LEU:O	1:B:1759:ILE:N	2.26	0.65
1:B:2311:GLY:O	1:B:2315:ILE:N	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1738:TYR:HA	1:B:1741:TRP:H	1.62	0.64
1:A:1738:TYR:HA	1:A:1741:TRP:H	1.62	0.64
1:B:1401:ASN:O	1:B:1405:ALA:N	2.30	0.64
1:A:694:VAL:O	1:A:698:LEU:N	2.29	0.64
1:B:1097:ASN:O	1:B:1099:LEU:N	2.29	0.64
1:B:1252:TYR:O	1:B:1256:ALA:N	2.25	0.63
1:B:1999:TYR:O	1:B:2003:LEU:N	2.32	0.63
1:A:1567:GLN:O	1:A:1569:ASN:N	2.32	0.63
2:C:133:SER:O	2:C:141:ARG:N	2.27	0.63
2:D:132:ILE:HA	2:D:142:ILE:HA	1.80	0.62
2:C:132:ILE:HA	2:C:142:ILE:HA	1.80	0.62
1:A:1999:TYR:O	1:A:2003:LEU:N	2.32	0.62
1:B:531:ALA:H	1:B:534:TYR:CB	2.12	0.62
1:A:531:ALA:H	1:A:534:TYR:CB	2.13	0.62
1:A:756:SER:O	1:A:758:VAL:N	2.32	0.62
1:B:1567:GLN:O	1:B:1569:ASN:N	2.32	0.62
1:A:1022:HIS:O	1:A:1026:ILE:N	2.24	0.62
1:A:2072:HIS:O	1:A:2092:LYS:N	2.33	0.62
1:B:1420:SER:O	1:B:1424:LEU:N	2.30	0.62
1:B:1754:SER:O	1:B:1758:ARG:N	2.33	0.62
2:D:276:LEU:O	2:D:285:VAL:N	2.27	0.62
1:A:1261:ASN:O	1:A:1265:ALA:N	2.33	0.62
2:C:263:ALA:O	2:C:279:LEU:N	2.33	0.62
2:C:276:LEU:O	2:C:285:VAL:N	2.27	0.62
1:B:756:SER:O	1:B:758:VAL:N	2.32	0.61
1:A:2251:LEU:O	1:A:2278:CYS:HA	1.99	0.61
1:B:2251:LEU:O	1:B:2278:CYS:HA	1.99	0.61
2:D:46:TYR:HA	2:D:59:ASP:HA	1.82	0.61
1:B:1753:SER:O	1:B:1757:GLN:N	2.28	0.61
2:C:46:TYR:HA	2:C:59:ASP:HA	1.83	0.61
1:B:1261:ASN:O	1:B:1265:ALA:N	2.33	0.61
2:D:263:ALA:O	2:D:279:LEU:N	2.33	0.61
1:B:2072:HIS:O	1:B:2092:LYS:N	2.33	0.61
2:D:181:GLY:HA2	2:D:210:ILE:H	1.65	0.61
1:A:1097:ASN:O	1:A:1099:LEU:N	2.29	0.61
2:D:265:LEU:N	2:D:277:TRP:O	2.28	0.61
1:A:768:GLU:O	1:A:772:VAL:N	2.34	0.60
1:B:1793:LEU:H	1:B:1794:VAL:HA	1.65	0.60
1:A:2342:PRO:O	1:A:2346:TRP:N	2.23	0.60
1:B:768:GLU:O	1:B:772:VAL:N	2.34	0.60
1:B:1961:THR:O	1:B:1965:PHE:N	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:TRP:HA	2:D:24:CYS:HA	1.83	0.60
1:A:1793:LEU:H	1:A:1794:VAL:HA	1.65	0.60
2:C:181:GLY:HA2	2:C:210:ILE:H	1.65	0.60
2:C:17:TRP:HA	2:C:24:CYS:HA	1.83	0.60
1:A:1753:SER:O	1:A:1757:GLN:N	2.28	0.60
1:A:804:ALA:O	1:A:808:LEU:N	2.27	0.60
1:A:1477:SER:O	1:A:1481:ALA:N	2.35	0.60
1:B:1728:LEU:O	1:B:1732:HIS:N	2.33	0.60
1:B:2342:PRO:O	1:B:2346:TRP:N	2.23	0.59
1:B:1477:SER:O	1:B:1481:ALA:N	2.35	0.59
2:C:232:ARG:HA	2:C:245:THR:HA	1.84	0.59
1:B:2350:LEU:O	1:B:2354:ALA:HA	2.03	0.59
1:A:866:VAL:HA	1:A:886:ALA:HB2	1.85	0.59
1:A:1091:ARG:O	1:A:1095:ASN:N	2.33	0.59
1:A:1972:HIS:O	1:A:1976:LYS:N	2.35	0.59
1:A:1754:SER:O	1:A:1758:ARG:N	2.32	0.59
2:D:232:ARG:HA	2:D:245:THR:HA	1.84	0.59
1:A:516:PRO:C	1:A:518:GLY:HA3	2.28	0.59
1:A:2350:LEU:O	1:A:2354:ALA:HA	2.03	0.59
1:B:1972:HIS:O	1:B:1976:LYS:N	2.35	0.59
1:A:1961:THR:O	1:A:1965:PHE:N	2.31	0.58
1:A:2170:HIS:O	1:A:2174:SER:N	2.37	0.58
1:B:866:VAL:HA	1:B:886:ALA:HB2	1.85	0.58
1:A:807:ALA:O	1:A:811:LEU:N	2.26	0.58
1:B:516:PRO:C	1:B:518:GLY:HA3	2.28	0.58
1:B:1632:PRO:O	1:B:1636:VAL:N	2.37	0.58
1:B:2069:ARG:O	1:B:2094:SER:N	2.36	0.58
1:B:1757:GLN:O	1:B:1761:ASP:N	2.36	0.58
1:B:1456:ALA:O	1:B:1460:LEU:N	2.25	0.58
1:B:1913:ASP:O	1:B:1917:MET:N	2.37	0.58
1:A:1590:MET:O	1:A:1593:TRP:N	2.37	0.58
1:A:1757:GLN:O	1:A:1761:ASP:N	2.36	0.58
1:A:1913:ASP:O	1:A:1917:MET:N	2.37	0.58
1:A:1141:VAL:O	1:A:1145:VAL:N	2.36	0.58
1:B:807:ALA:O	1:B:811:LEU:N	2.26	0.58
1:B:2039:ASP:HA	1:B:2076:VAL:HA	1.86	0.58
1:B:1583:VAL:CB	1:B:1584:ILE:HA	2.34	0.58
1:B:2424:ASP:O	1:B:2427:ASP:N	2.37	0.58
1:A:1583:VAL:CB	1:A:1584:ILE:HA	2.34	0.57
2:D:233:VAL:N	2:D:244:THR:O	2.22	0.57
1:B:804:ALA:O	1:B:808:LEU:N	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1590:MET:O	1:B:1593:TRP:N	2.37	0.57
1:B:2170:HIS:O	1:B:2174:SER:N	2.37	0.57
2:C:6:ALA:HB2	2:C:16:PHE:HA	1.86	0.57
1:A:363:ASP:O	1:A:367:PHE:N	2.34	0.57
1:A:672:VAL:O	1:A:675:ILE:N	2.38	0.57
2:D:6:ALA:HB2	2:D:16:PHE:HA	1.86	0.57
1:A:1109:LEU:O	1:A:1113:LEU:N	2.34	0.57
2:D:234:TRP:HA	2:D:242:LEU:HA	1.87	0.57
1:B:1141:VAL:O	1:B:1145:VAL:N	2.36	0.57
1:A:2039:ASP:HA	1:A:2076:VAL:HA	1.86	0.57
1:A:2424:ASP:O	1:A:2427:ASP:N	2.37	0.57
1:B:2160:SER:HA	1:B:2264:ASP:HA	1.87	0.57
1:B:672:VAL:O	1:B:675:ILE:N	2.38	0.56
2:C:265:LEU:O	2:C:277:TRP:N	2.38	0.56
2:D:78:VAL:HA	2:D:94:SER:HA	1.87	0.56
1:A:1728:LEU:O	1:A:1732:HIS:N	2.33	0.56
1:B:2080:ILE:H	1:B:2087:ARG:HA	1.69	0.56
1:A:2090:ILE:HA	1:A:2100:GLN:HA	1.88	0.56
1:B:1091:ARG:O	1:B:1095:ASN:N	2.33	0.56
1:B:1358:ASN:O	1:B:1362:HIS:N	2.39	0.56
1:B:2090:ILE:HA	1:B:2100:GLN:HA	1.88	0.56
2:D:265:LEU:O	2:D:277:TRP:N	2.37	0.56
1:A:2080:ILE:H	1:A:2087:ARG:HA	1.69	0.56
2:C:234:TRP:HA	2:C:242:LEU:HA	1.87	0.56
2:C:78:VAL:HA	2:C:94:SER:HA	1.88	0.56
1:A:2069:ARG:O	1:A:2094:SER:N	2.36	0.56
2:C:187:ARG:O	2:C:198:GLU:N	2.38	0.55
1:A:2160:SER:HA	1:A:2264:ASP:HA	1.87	0.55
1:B:2419:GLU:C	1:B:2421:SER:H	2.15	0.55
2:D:187:ARG:O	2:D:198:GLU:N	2.39	0.55
1:A:1358:ASN:O	1:A:1362:HIS:N	2.39	0.55
2:C:233:VAL:O	2:C:243:GLU:N	2.33	0.55
1:A:931:ILE:O	1:A:935:MET:N	2.38	0.55
1:A:1632:PRO:O	1:A:1636:VAL:N	2.37	0.55
1:B:363:ASP:O	1:B:367:PHE:N	2.34	0.55
1:A:2326:ASP:C	1:A:2328:LYS:H	2.14	0.55
1:B:2145:ILE:O	1:B:2153:LEU:N	2.28	0.55
1:B:476:SER:C	1:B:478:HIS:H	2.15	0.55
1:B:2031:LYS:O	1:B:2035:LEU:N	2.40	0.55
1:A:2031:LYS:O	1:A:2035:LEU:N	2.40	0.54
2:C:233:VAL:N	2:C:244:THR:O	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1855:VAL:O	1:B:1859:LEU:N	2.39	0.54
1:B:2326:ASP:C	1:B:2328:LYS:H	2.14	0.54
2:D:187:ARG:N	2:D:198:GLU:O	2.36	0.54
2:C:45:LYS:O	2:C:60:ILE:N	2.40	0.54
1:A:1995:LEU:O	1:A:1999:TYR:N	2.32	0.54
1:B:1109:LEU:O	1:B:1113:LEU:N	2.34	0.54
2:D:45:LYS:O	2:D:60:ILE:N	2.40	0.54
1:A:806:LYS:O	1:A:810:GLN:N	2.28	0.54
1:A:1456:ALA:O	1:A:1460:LEU:N	2.25	0.54
1:A:2124:THR:O	1:A:2128:ASN:N	2.38	0.54
2:C:82:ALA:N	2:C:91:VAL:O	2.36	0.54
1:B:1962:GLU:O	1:B:1966:ALA:N	2.41	0.53
1:A:516:PRO:O	1:A:518:GLY:HA3	2.08	0.53
1:A:2419:GLU:C	1:A:2421:SER:H	2.15	0.53
1:A:476:SER:C	1:A:478:HIS:H	2.15	0.53
1:B:1520:TYR:HA	1:B:1521:ASN:CB	2.38	0.53
1:B:1737:TRP:O	1:B:1740:ALA:N	2.28	0.53
1:B:516:PRO:O	1:B:518:GLY:HA3	2.08	0.53
1:B:1855:VAL:O	1:B:1858:GLN:N	2.42	0.53
1:A:1520:TYR:HA	1:A:1521:ASN:CB	2.38	0.53
1:A:1201:PRO:O	1:A:1205:MET:N	2.42	0.53
2:C:185:VAL:O	2:C:200:VAL:N	2.39	0.53
1:A:1097:ASN:C	1:A:1099:LEU:H	2.16	0.53
1:B:2377:ILE:O	1:B:2380:GLU:N	2.39	0.53
1:A:1912:ILE:O	1:A:1916:ARG:N	2.28	0.53
1:A:1962:GLU:O	1:A:1966:ALA:N	2.41	0.53
1:A:2285:ARG:HA	1:A:2286:GLU:CB	2.39	0.52
1:A:1855:VAL:O	1:A:1858:GLN:N	2.41	0.52
1:B:2285:ARG:HA	1:B:2286:GLU:CB	2.38	0.52
1:A:1347:SER:O	1:A:1351:ILE:N	2.37	0.52
1:B:1912:ILE:O	1:B:1916:ARG:N	2.28	0.52
1:B:1743:ASN:O	1:B:1747:ALA:N	2.43	0.52
1:B:2281:ALA:O	1:B:2285:ARG:N	2.24	0.52
1:A:1737:TRP:O	1:A:1740:ALA:N	2.28	0.52
1:B:1201:PRO:O	1:B:1205:MET:N	2.42	0.52
1:B:405:ASP:O	1:B:409:HIS:N	2.41	0.52
1:B:407:ALA:HA	1:B:450:LEU:HA	1.92	0.52
2:D:125:HIS:N	2:D:130:GLU:O	2.33	0.52
1:A:407:ALA:HA	1:A:450:LEU:HA	1.92	0.52
1:A:2377:ILE:O	1:A:2380:GLU:N	2.39	0.52
1:B:806:LYS:O	1:B:810:GLN:N	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2385:MET:HA	1:A:2386:GLU:C	2.35	0.51
2:C:90:MET:H	2:C:103:ASP:HA	1.75	0.51
2:C:99:ILE:N	2:C:113:TYR:O	2.40	0.51
1:B:1550:GLU:C	1:B:1552:ARG:H	2.17	0.51
2:C:12:HIS:O	2:C:30:HIS:N	2.44	0.51
1:A:1743:ASN:O	1:A:1747:ALA:N	2.43	0.51
2:D:90:MET:H	2:D:103:ASP:HA	1.75	0.51
1:A:1550:GLU:C	1:A:1552:ARG:H	2.17	0.51
1:A:1855:VAL:O	1:A:1859:LEU:N	2.39	0.51
1:B:1842:GLU:O	1:B:1846:LEU:N	2.44	0.51
2:D:233:VAL:O	2:D:243:GLU:N	2.33	0.51
1:B:1097:ASN:C	1:B:1099:LEU:H	2.16	0.51
1:B:1995:LEU:O	1:B:1999:TYR:N	2.32	0.51
2:C:88:ARG:O	2:C:104:VAL:N	2.44	0.51
1:B:1889:LEU:C	1:B:1891:TYR:H	2.19	0.51
1:A:584:MET:H	1:A:586:HIS:CB	2.24	0.51
1:B:931:ILE:O	1:B:935:MET:N	2.38	0.51
1:B:1135:LEU:C	1:B:1137:ILE:H	2.19	0.51
1:A:1135:LEU:C	1:A:1137:ILE:H	2.19	0.50
1:A:1842:GLU:O	1:A:1846:LEU:N	2.44	0.50
1:B:584:MET:H	1:B:586:HIS:CB	2.24	0.50
1:B:2385:MET:HA	1:B:2386:GLU:C	2.35	0.50
2:D:186:TRP:HA	2:D:200:VAL:H	1.76	0.50
1:B:396:LYS:O	1:B:400:LEU:N	2.45	0.50
1:B:2125:LEU:O	1:B:2129:ASP:N	2.44	0.50
1:A:1889:LEU:C	1:A:1891:TYR:H	2.19	0.50
1:A:2281:ALA:O	1:A:2285:ARG:N	2.24	0.50
2:D:12:HIS:O	2:D:30:HIS:N	2.44	0.50
1:A:1215:GLN:CB	1:A:1218:THR:HA	2.42	0.50
2:C:186:TRP:HA	2:C:200:VAL:H	1.76	0.50
1:B:1215:GLN:CB	1:B:1218:THR:HA	2.42	0.50
1:A:2125:LEU:O	1:A:2129:ASP:N	2.44	0.50
1:B:1275:TYR:O	1:B:1279:LEU:N	2.41	0.50
2:C:187:ARG:N	2:C:198:GLU:O	2.36	0.50
1:B:2224:SER:O	1:B:2227:SER:N	2.41	0.49
1:B:530:THR:N	1:B:531:ALA:HB3	2.27	0.49
2:D:99:ILE:N	2:D:113:TYR:O	2.40	0.49
1:A:825:TYR:C	1:A:827:GLU:H	2.21	0.49
1:B:1347:SER:O	1:B:1351:ILE:N	2.37	0.49
1:B:1997:ASP:O	1:B:2001:TRP:N	2.40	0.49
2:D:88:ARG:O	2:D:104:VAL:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:LYS:O	1:A:400:LEU:N	2.45	0.49
1:A:530:THR:N	1:A:531:ALA:HB3	2.27	0.49
1:B:530:THR:C	1:B:532:ARG:H	2.20	0.49
1:A:381:THR:HA	1:A:382:LEU:HA	1.51	0.49
1:A:769:ILE:O	1:A:773:GLY:N	2.46	0.49
1:A:1585:LYS:O	1:A:1588:GLN:N	2.46	0.49
1:A:2145:ILE:O	1:A:2153:LEU:N	2.28	0.49
2:D:220:LYS:O	2:D:236:ILE:N	2.46	0.49
1:A:1741:TRP:HA	1:A:1744:TRP:CB	2.43	0.48
1:B:769:ILE:O	1:B:773:GLY:N	2.46	0.48
1:B:1585:LYS:O	1:B:1588:GLN:N	2.46	0.48
2:C:125:HIS:N	2:C:130:GLU:O	2.33	0.48
1:A:2354:ALA:O	1:A:2358:GLN:N	2.46	0.48
1:B:2354:ALA:O	1:B:2358:GLN:N	2.46	0.48
1:A:405:ASP:O	1:A:409:HIS:N	2.41	0.48
1:B:2257:HIS:O	1:B:2261:LEU:N	2.47	0.48
2:C:220:LYS:O	2:C:236:ILE:N	2.46	0.48
2:D:185:VAL:O	2:D:200:VAL:N	2.39	0.48
1:A:565:ASP:HA	1:A:566:ILE:HA	1.54	0.48
1:B:825:TYR:C	1:B:827:GLU:H	2.20	0.48
1:A:530:THR:C	1:A:532:ARG:H	2.20	0.48
1:A:1744:TRP:HA	1:A:1747:ALA:HB2	1.96	0.48
2:C:140:ILE:O	2:C:153:GLN:HA	2.14	0.48
1:B:125:ASP:C	1:B:127:ASN:H	2.22	0.48
1:B:1741:TRP:HA	1:B:1744:TRP:CB	2.44	0.48
1:B:2124:THR:O	1:B:2128:ASN:N	2.38	0.48
1:A:2257:HIS:O	1:A:2261:LEU:N	2.47	0.47
1:A:501:LEU:C	1:A:503:ASN:H	2.23	0.47
1:B:1065:LEU:O	1:B:1069:THR:N	2.40	0.47
1:B:1744:TRP:HA	1:B:1747:ALA:HB2	1.96	0.47
1:A:2101:TYR:HA	1:A:2154:LEU:O	2.15	0.47
1:B:1738:TYR:CA	1:B:1741:TRP:H	2.28	0.47
2:D:140:ILE:O	2:D:153:GLN:HA	2.14	0.47
1:A:1057:PRO:HA	1:A:1058:HIS:HA	1.70	0.47
1:A:1725:GLY:O	1:A:1729:LEU:N	2.31	0.47
1:A:1738:TYR:CA	1:A:1741:TRP:H	2.28	0.47
1:A:2040:LEU:N	1:A:2075:PRO:O	2.48	0.47
1:A:2443:TYR:C	1:A:2445:GLY:H	2.23	0.47
1:B:2101:TYR:HA	1:B:2154:LEU:O	2.15	0.47
1:B:2263:LEU:HA	1:B:2270:VAL:HA	1.97	0.47
1:A:773:GLY:O	1:A:776:ASP:N	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASP:C	1:A:127:ASN:H	2.22	0.47
1:A:168:ASP:C	1:A:170:GLU:H	2.23	0.47
1:A:2220:LEU:O	1:A:2224:SER:N	2.48	0.47
1:B:1793:LEU:N	1:B:1794:VAL:HA	2.28	0.46
1:B:2264:ASP:CB	1:B:2268:GLY:HA2	2.46	0.46
2:D:142:ILE:N	2:D:151:THR:HA	2.30	0.46
2:D:277:TRP:HA	2:D:283:GLU:O	2.15	0.46
1:B:2040:LEU:N	1:B:2075:PRO:O	2.48	0.46
1:B:2220:LEU:O	1:B:2224:SER:N	2.48	0.46
1:A:776:ASP:C	1:A:778:LEU:H	2.23	0.46
1:A:1215:GLN:HA	1:A:1216:GLN:C	2.41	0.46
2:D:186:TRP:HA	2:D:199:PRO:HA	1.97	0.46
1:A:456:PRO:HA	1:A:459:ALA:HB3	1.97	0.46
1:A:1339:GLU:O	1:A:1343:ILE:N	2.46	0.46
1:A:2226:SER:C	1:A:2228:GLU:H	2.23	0.46
1:B:776:ASP:C	1:B:778:LEU:H	2.23	0.46
1:B:2226:SER:C	1:B:2228:GLU:H	2.23	0.46
2:C:142:ILE:N	2:C:151:THR:HA	2.30	0.46
1:A:715:THR:CB	1:A:716:ARG:HA	2.46	0.46
1:B:2443:TYR:C	1:B:2445:GLY:H	2.23	0.46
2:C:277:TRP:HA	2:C:283:GLU:O	2.15	0.46
1:B:715:THR:CB	1:B:716:ARG:HA	2.46	0.46
1:B:1215:GLN:HA	1:B:1216:GLN:C	2.41	0.46
1:B:1215:GLN:HA	1:B:1216:GLN:O	2.16	0.46
1:A:862:LYS:O	1:A:866:VAL:N	2.49	0.45
1:B:456:PRO:HA	1:B:459:ALA:HB3	1.97	0.45
1:A:859:ASP:O	1:A:863:HIS:N	2.41	0.45
1:A:2263:LEU:HA	1:A:2270:VAL:HA	1.97	0.45
1:B:501:LEU:C	1:B:503:ASN:H	2.22	0.45
1:B:526:LEU:CB	1:B:528:SER:H	2.29	0.45
1:B:859:ASP:O	1:B:863:HIS:N	2.41	0.45
1:B:1744:TRP:HA	1:B:1747:ALA:CB	2.47	0.45
2:C:186:TRP:HA	2:C:199:PRO:HA	1.97	0.45
1:A:1744:TRP:HA	1:A:1747:ALA:CB	2.47	0.45
1:B:168:ASP:C	1:B:170:GLU:H	2.23	0.45
1:B:1020:ASN:O	1:B:1023:LEU:N	2.49	0.45
1:B:2342:PRO:O	1:B:2345:ASN:N	2.50	0.45
1:A:1020:ASN:O	1:A:1023:LEU:N	2.49	0.45
1:A:1727:TYR:O	1:A:1731:THR:N	2.37	0.45
1:A:2224:SER:O	1:A:2227:SER:N	2.41	0.45
1:A:2342:PRO:O	1:A:2345:ASN:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:THR:O	1:B:554:MET:N	2.27	0.45
1:B:2145:ILE:N	1:B:2153:LEU:O	2.50	0.45
1:A:526:LEU:CB	1:A:528:SER:H	2.29	0.45
2:C:221:ASN:HA	2:C:236:ILE:H	1.82	0.45
1:A:1579:VAL:O	1:A:1583:VAL:N	2.50	0.45
1:B:862:LYS:O	1:B:866:VAL:N	2.49	0.45
1:A:809:GLY:O	1:A:813:ALA:N	2.41	0.45
1:A:1854:GLU:C	1:A:1856:ILE:H	2.24	0.45
2:D:82:ALA:N	2:D:91:VAL:O	2.36	0.45
1:A:774:GLY:HA2	1:A:775:GLU:HA	1.52	0.45
1:A:1091:ARG:CB	1:A:1129:SER:HA	2.47	0.45
1:A:2264:ASP:CB	1:A:2268:GLY:HA2	2.46	0.45
1:B:1329:HIS:C	1:B:1331:TYR:H	2.25	0.45
1:B:1586:PRO:HA	1:B:1589:ASP:O	2.17	0.45
1:B:1725:GLY:O	1:B:1729:LEU:N	2.31	0.45
1:B:2248:GLY:O	1:B:2251:LEU:N	2.50	0.45
1:B:2435:SER:HA	1:B:2436:VAL:HA	1.80	0.44
2:C:234:TRP:HA	2:C:243:GLU:N	2.32	0.44
2:D:221:ASN:HA	2:D:236:ILE:H	1.82	0.44
2:D:234:TRP:HA	2:D:243:GLU:N	2.31	0.44
1:A:1215:GLN:HA	1:A:1216:GLN:O	2.16	0.44
1:A:2145:ILE:N	1:A:2153:LEU:O	2.50	0.44
1:B:1339:GLU:O	1:B:1343:ILE:N	2.46	0.44
1:A:504:ILE:HA	1:A:505:ILE:HA	1.50	0.44
1:B:1091:ARG:CB	1:B:1129:SER:HA	2.48	0.44
1:A:1275:TYR:O	1:A:1279:LEU:N	2.41	0.44
1:A:756:SER:O	1:A:757:ALA:N	2.51	0.44
1:A:1329:HIS:C	1:A:1331:TYR:H	2.25	0.44
1:A:1586:PRO:HA	1:A:1589:ASP:O	2.18	0.44
1:B:584:MET:HA	1:B:585:GLU:HA	1.70	0.44
1:B:1996:ASN:O	1:B:2000:GLU:N	2.40	0.44
1:A:1849:ILE:O	1:A:1852:TRP:N	2.51	0.44
2:D:181:GLY:HA3	2:D:207:THR:O	2.18	0.44
1:B:1738:TYR:C	1:B:1741:TRP:H	2.26	0.44
1:B:2072:HIS:N	1:B:2092:LYS:O	2.50	0.44
1:B:1057:PRO:HA	1:B:1058:HIS:HA	1.70	0.44
1:B:1579:VAL:O	1:B:1583:VAL:N	2.50	0.44
1:B:1794:VAL:H	1:B:1797:HIS:CB	2.31	0.43
2:C:183:CYS:C	2:C:202:LYS:HA	2.43	0.43
1:A:1017:GLY:HA2	1:A:1018:GLU:HA	1.72	0.43
1:A:1738:TYR:C	1:A:1741:TRP:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2072:HIS:N	1:A:2092:LYS:O	2.50	0.43
1:A:584:MET:HA	1:A:585:GLU:HA	1.70	0.43
1:B:381:THR:HA	1:B:382:LEU:HA	1.50	0.43
1:B:1649:GLN:O	1:B:1652:ALA:HB3	2.19	0.43
1:B:1854:GLU:C	1:B:1856:ILE:H	2.24	0.43
1:B:1599:LEU:O	1:B:1603:SER:N	2.43	0.43
2:C:174:LEU:N	2:C:186:TRP:O	2.52	0.43
2:C:265:LEU:H	2:C:277:TRP:C	2.25	0.43
1:A:1065:LEU:O	1:A:1069:THR:N	2.40	0.43
1:B:1849:ILE:O	1:B:1852:TRP:N	2.51	0.43
1:A:2248:GLY:O	1:A:2251:LEU:N	2.50	0.43
1:B:756:SER:O	1:B:757:ALA:N	2.51	0.43
2:C:181:GLY:HA3	2:C:207:THR:O	2.18	0.43
2:D:183:CYS:C	2:D:202:LYS:HA	2.43	0.43
1:A:1794:VAL:H	1:A:1797:HIS:CB	2.31	0.43
1:B:504:ILE:HA	1:B:505:ILE:HA	1.51	0.43
2:D:186:TRP:HA	2:D:200:VAL:N	2.34	0.43
1:A:292:LEU:O	1:A:296:CYS:N	2.51	0.43
1:B:292:LEU:O	1:B:296:CYS:N	2.51	0.43
1:B:2282:ALA:HB2	1:B:2290:GLU:O	2.19	0.43
2:C:16:PHE:O	2:C:25:SER:N	2.44	0.43
2:C:102:TRP:HA	2:C:109:VAL:CB	2.49	0.42
1:A:1889:LEU:C	1:A:1891:TYR:N	2.77	0.42
2:D:102:TRP:HA	2:D:109:VAL:CB	2.49	0.42
2:D:231:ALA:O	2:D:246:LEU:N	2.33	0.42
1:A:2079:VAL:HA	1:A:2087:ARG:CB	2.49	0.42
1:A:2282:ALA:HB2	1:A:2290:GLU:O	2.19	0.42
1:A:2424:ASP:O	1:A:2425:GLN:C	2.61	0.42
1:B:2262:MET:C	1:B:2271:VAL:H	2.24	0.42
1:A:1195:VAL:CB	1:A:1196:ALA:HA	2.50	0.42
2:C:53:LEU:HA	2:C:76:GLY:H	1.84	0.42
1:A:990:VAL:HA	1:A:991:ILE:HA	1.46	0.42
1:A:1451:PRO:O	1:A:1454:ALA:HB3	2.20	0.42
1:A:1649:GLN:O	1:A:1652:ALA:HB3	2.19	0.42
1:B:990:VAL:HA	1:B:991:ILE:HA	1.46	0.42
1:B:2079:VAL:HA	1:B:2087:ARG:CB	2.49	0.42
1:B:2424:ASP:O	1:B:2425:GLN:C	2.61	0.42
1:A:831:VAL:O	1:A:834:ASN:N	2.52	0.42
1:B:1889:LEU:C	1:B:1891:TYR:N	2.77	0.42
2:C:17:TRP:HA	2:C:23:VAL:O	2.20	0.42
2:D:53:LEU:HA	2:D:76:GLY:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:234:TRP:HA	2:D:243:GLU:H	1.85	0.42
1:A:550:THR:O	1:A:554:MET:N	2.27	0.42
1:A:2322:MET:O	1:A:2326:ASP:N	2.52	0.42
1:B:1195:VAL:CB	1:B:1196:ALA:HA	2.49	0.42
1:B:1744:TRP:C	1:B:1747:ALA:H	2.27	0.42
2:D:212:ARG:O	2:D:224:THR:HA	2.20	0.42
1:B:809:GLY:O	1:B:813:ALA:N	2.41	0.42
1:A:1793:LEU:N	1:A:1794:VAL:HA	2.28	0.41
1:B:126:SER:O	1:B:130:LEU:N	2.36	0.41
1:B:649:ARG:HA	1:B:656:SER:N	2.35	0.41
2:C:186:TRP:HA	2:C:200:VAL:N	2.34	0.41
1:A:790:ASP:O	1:A:794:ASP:N	2.53	0.41
1:B:1451:PRO:O	1:B:1454:ALA:HB3	2.20	0.41
1:A:2302:TYR:HA	1:A:2308:GLY:HA3	2.03	0.41
1:B:2056:ALA:O	1:B:2057:VAL:C	2.64	0.41
1:B:2326:ASP:C	1:B:2328:LYS:N	2.79	0.41
2:D:17:TRP:HA	2:D:23:VAL:O	2.20	0.41
2:D:174:LEU:N	2:D:186:TRP:O	2.52	0.41
1:A:1744:TRP:C	1:A:1747:ALA:H	2.27	0.41
1:B:790:ASP:O	1:B:794:ASP:N	2.53	0.41
2:D:48:ALA:HA	2:D:56:ARG:O	2.20	0.41
1:B:774:GLY:HA2	1:B:775:GLU:HA	1.52	0.41
1:B:2160:SER:HA	1:B:2265:ARG:N	2.27	0.41
2:C:48:ALA:HA	2:C:56:ARG:O	2.20	0.41
1:A:649:ARG:HA	1:A:656:SER:N	2.35	0.41
1:A:2160:SER:HA	1:A:2265:ARG:N	2.27	0.41
1:A:1452:LEU:O	1:A:1455:GLY:N	2.54	0.41
1:A:2435:SER:HA	1:A:2436:VAL:HA	1.80	0.41
1:B:565:ASP:HA	1:B:566:ILE:HA	1.54	0.41
1:B:1580:ARG:C	1:B:1583:VAL:H	2.29	0.41
2:C:212:ARG:O	2:C:224:THR:HA	2.20	0.41
1:A:255:LEU:HA	1:A:256:ARG:C	2.46	0.41
1:A:1580:ARG:C	1:A:1583:VAL:H	2.29	0.40
1:B:1664:ALA:O	1:B:1668:GLY:N	2.54	0.40
1:B:2322:MET:O	1:B:2326:ASP:N	2.52	0.40
2:D:183:CYS:O	2:D:202:LYS:HA	2.21	0.40
1:B:831:VAL:O	1:B:834:ASN:N	2.52	0.40
1:B:1334:ALA:O	1:B:1337:TYR:N	2.54	0.40
1:B:1885:HIS:O	1:B:1888:ALA:HB3	2.22	0.40
2:C:278:ASP:H	2:C:283:GLU:N	2.20	0.40
1:A:1550:GLU:C	1:A:1552:ARG:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1570:VAL:O	1:A:1573:TRP:N	2.55	0.40
1:A:1638:ALA:O	1:A:1641:LYS:N	2.54	0.40
1:A:2056:ALA:O	1:A:2057:VAL:C	2.64	0.40
1:B:1570:VAL:O	1:B:1573:TRP:N	2.55	0.40
1:A:1744:TRP:O	1:A:1747:ALA:HB3	2.21	0.40
1:B:1452:LEU:O	1:B:1455:GLY:N	2.54	0.40
1:B:2302:TYR:HA	1:B:2308:GLY:HA3	2.03	0.40
1:B:1934:ILE:O	1:B:1937:ALA:HB2	2.22	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	2017/2471 (82%)	1594 (79%)	411 (20%)	12 (1%)	21	59
1	B	2017/2471 (82%)	1594 (79%)	411 (20%)	12 (1%)	21	59
2	C	297/303 (98%)	253 (85%)	41 (14%)	3 (1%)	12	48
2	D	297/303 (98%)	253 (85%)	41 (14%)	3 (1%)	12	48
All	All	4628/5548 (83%)	3694 (80%)	904 (20%)	30 (1%)	23	59

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	ILE
1	A	454	VAL
1	A	490	ILE
1	A	1855	VAL
1	A	1890	VAL
1	A	2444	ILE
1	B	169	ILE

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Mol	Chain	Res	Type
1	B	454	VAL
1	B	490	ILE
1	B	1855	VAL
1	B	1890	VAL
1	B	2444	ILE
1	A	1583	VAL
1	B	1583	VAL
1	A	492	SER
1	A	1193	VAL
1	A	1902	VAL
1	A	2306	VAL
1	B	492	SER
1	B	1193	VAL
1	B	1902	VAL
1	B	2306	VAL
1	A	2361	ILE
1	B	2361	ILE
2	C	107	PRO
2	D	107	PRO
2	C	298	VAL
2	D	298	VAL
2	C	175	VAL
2	D	175	VAL

5.3.2 Protein sidechains [i](#)

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

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](#)

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	A	3
1	B	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1245:CYS	C	1246:SER	N	4.79
1	B	1245:CYS	C	1246:SER	N	4.79
1	A	1097:ASN	C	1098:ALA	N	4.03
1	B	1097:ASN	C	1098:ALA	N	4.03
1	A	756:SER	C	757:ALA	N	3.62
1	B	756:SER	C	757:ALA	N	3.62

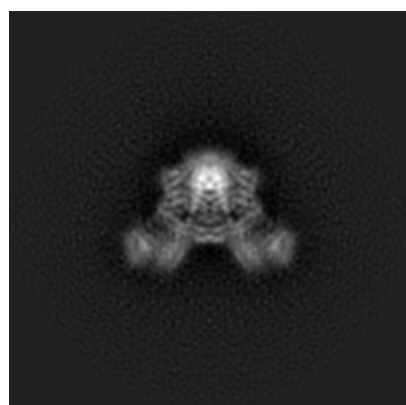
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3329. These allow visual inspection of the internal detail of the map and identification of artifacts.

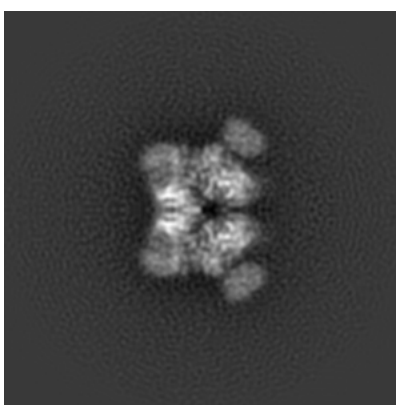
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

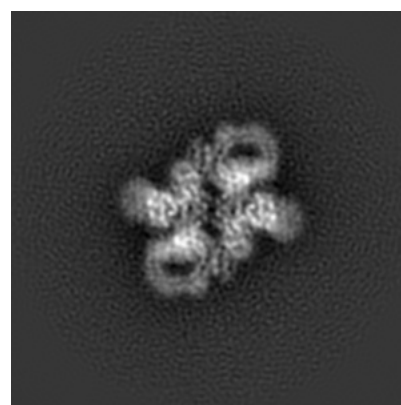
6.1.1 Primary map



X



Y

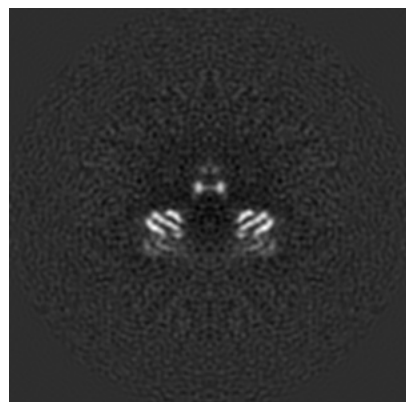


Z

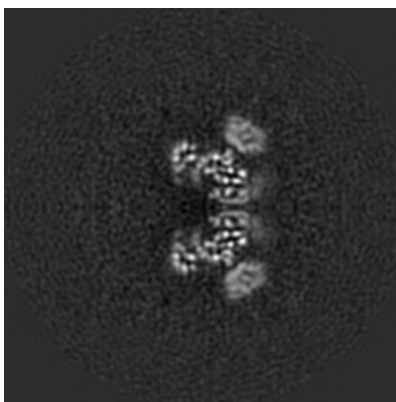
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

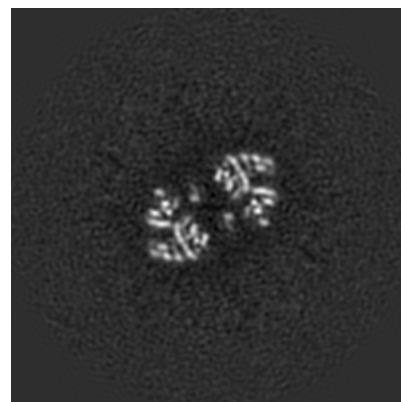
6.2.1 Primary map



X Index: 160



Y Index: 160

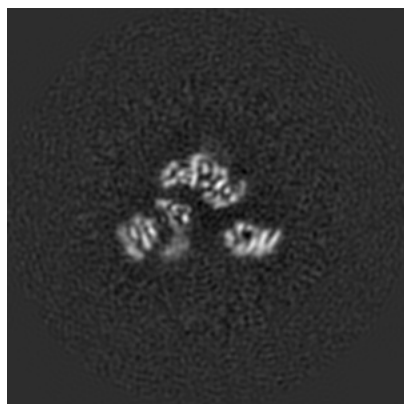


Z Index: 160

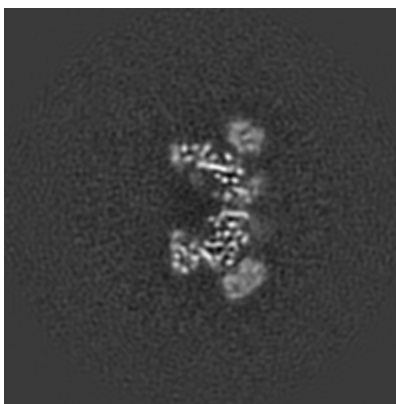
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

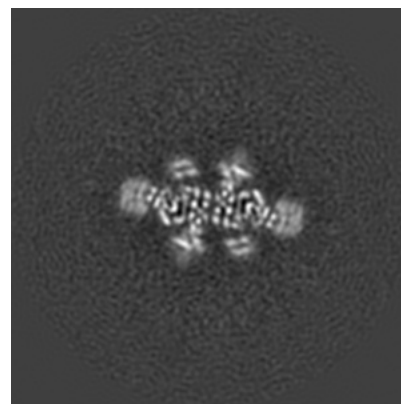
6.3.1 Primary map



X Index: 149



Y Index: 163

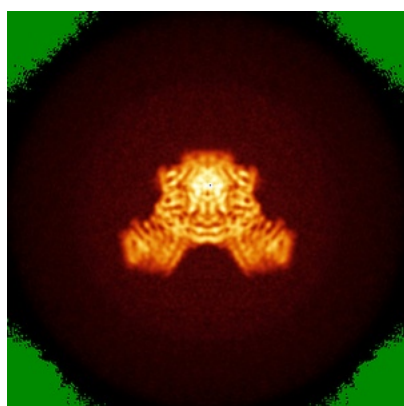


Z Index: 181

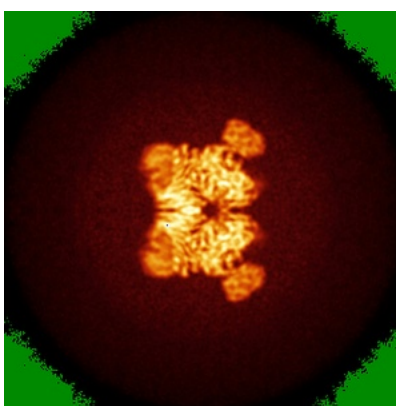
The images above show the largest variance slices of the map in three orthogonal directions.

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

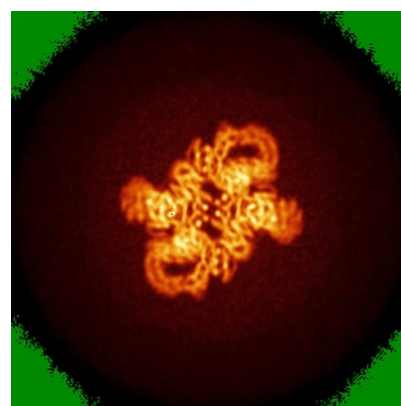
6.4.1 Primary map



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

This section was not generated.

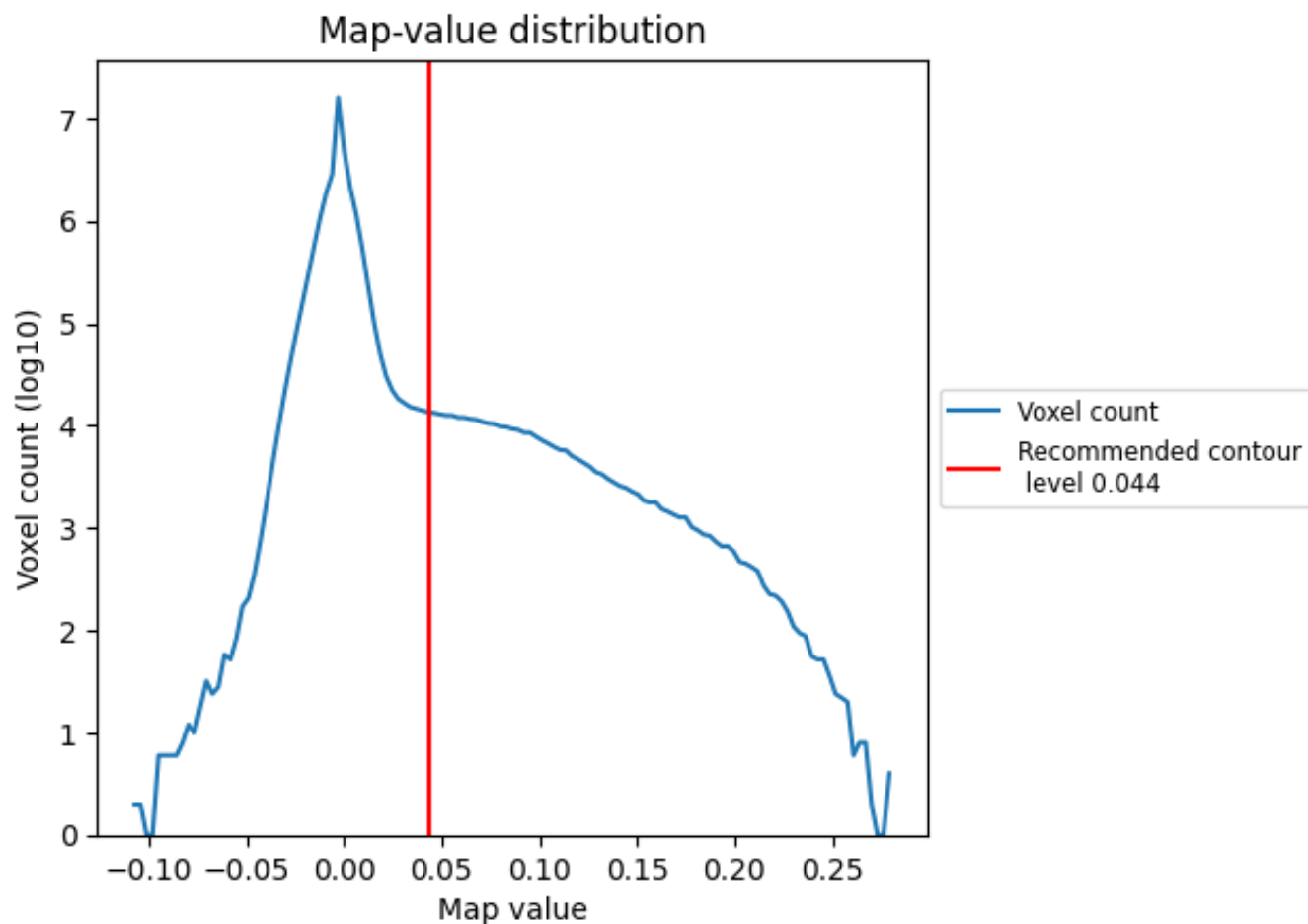
6.6 Mask visualisation

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

7 Map analysis [i](#)

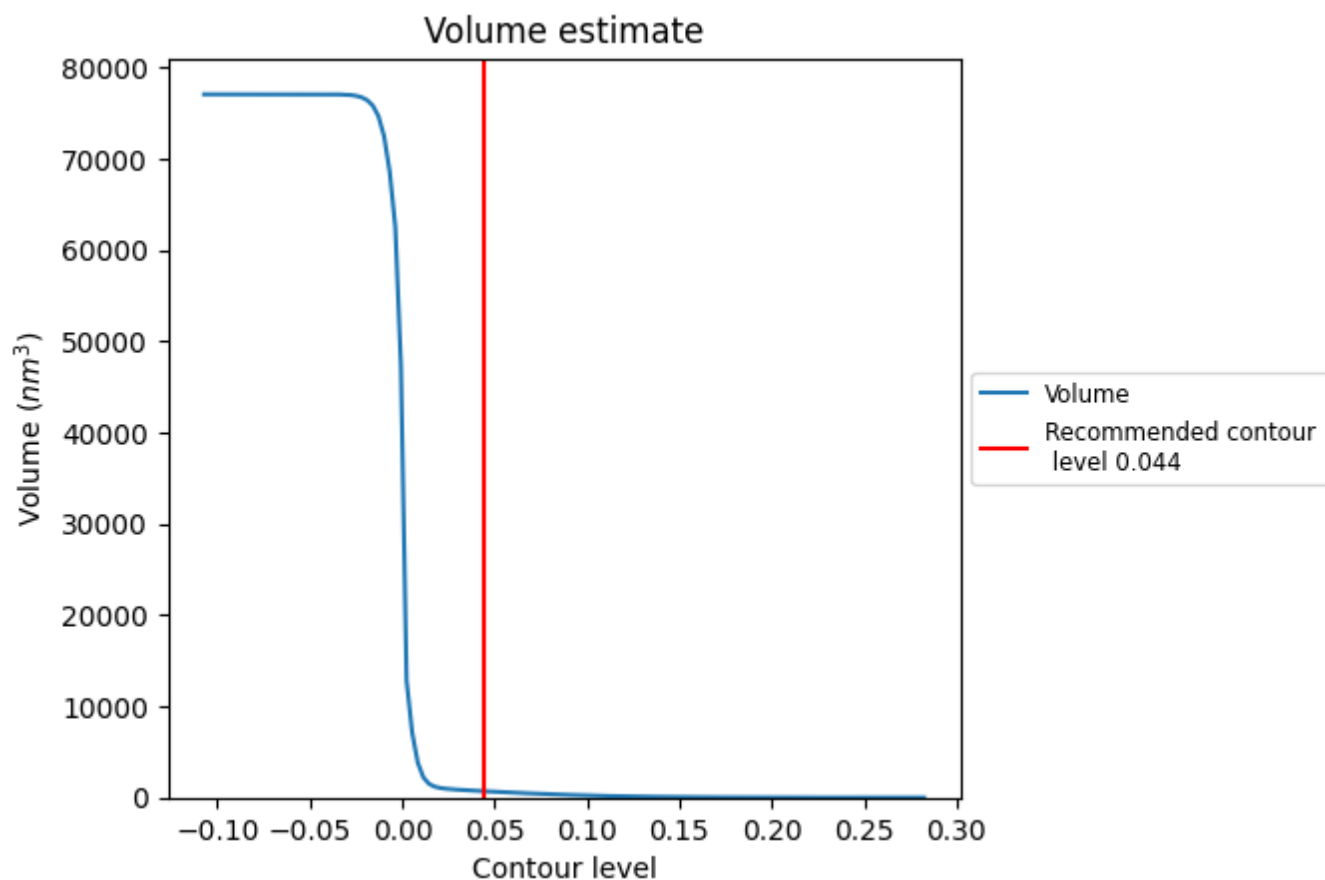
This section contains the results of statistical analysis of the map.

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.

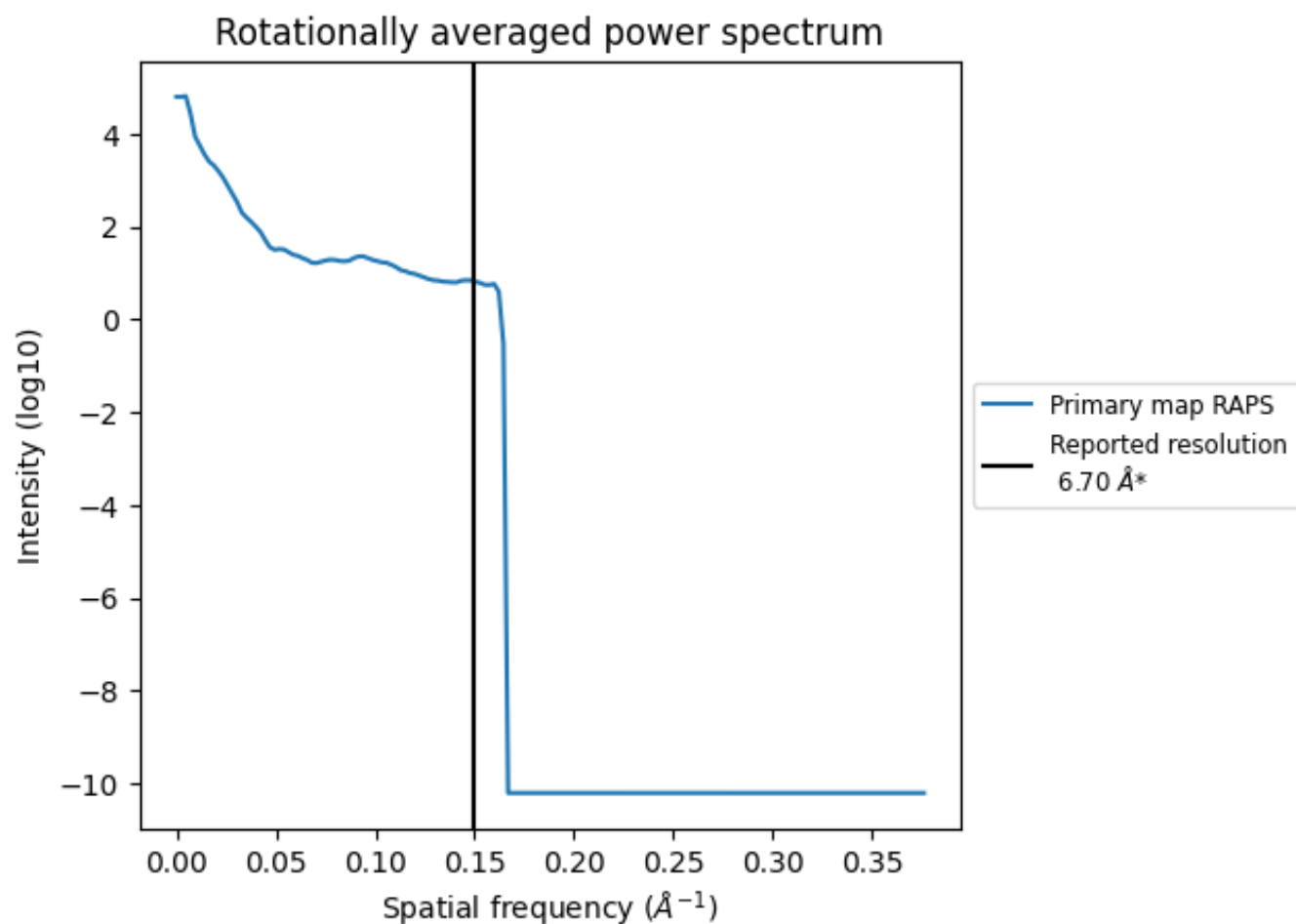
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 699 nm³; this corresponds to an approximate mass of 631 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 ⓘ

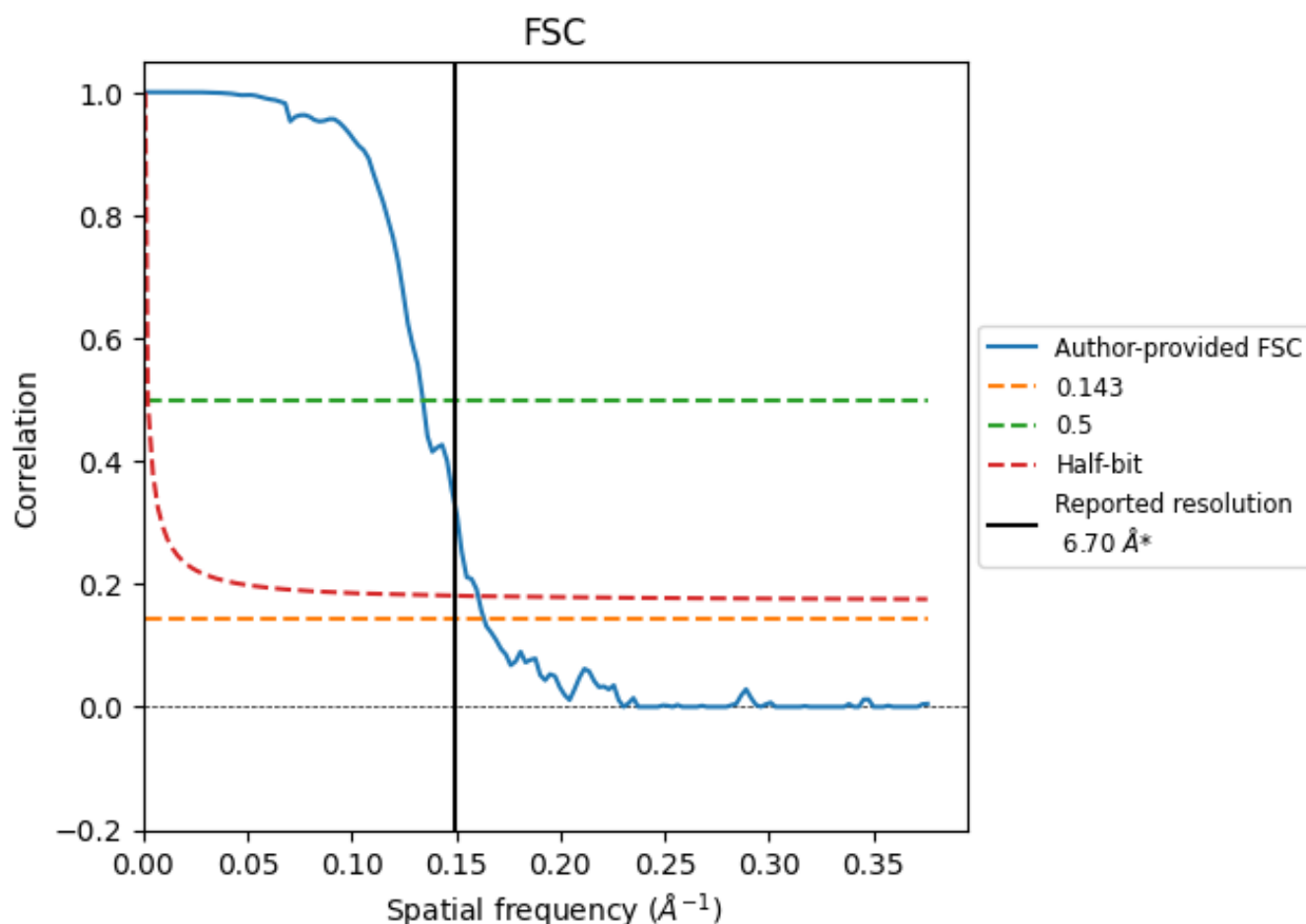


*Reported resolution corresponds to spatial frequency of 0.149 Å⁻¹

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 0.149 Å⁻¹

8.2 Resolution estimates [i](#)

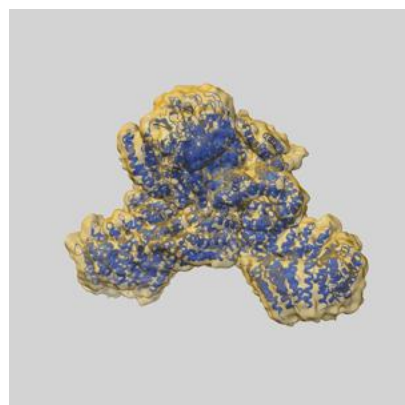
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	6.12	7.46	6.23
Unmasked-calculated*	-	-	-

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

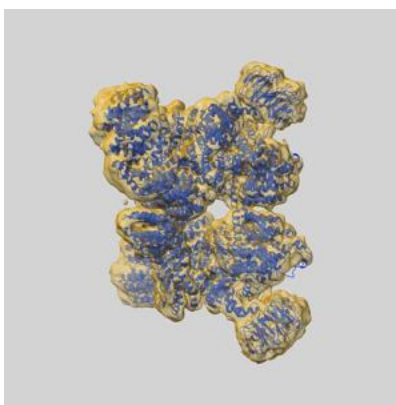
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3329 and PDB model 5FVM. Per-residue inclusion information can be found in section [3](#) on page [6](#).

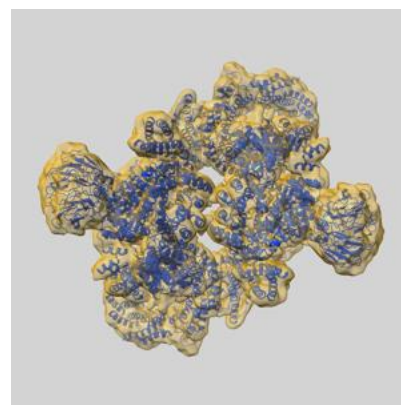
9.1 Map-model overlay [i](#)



X



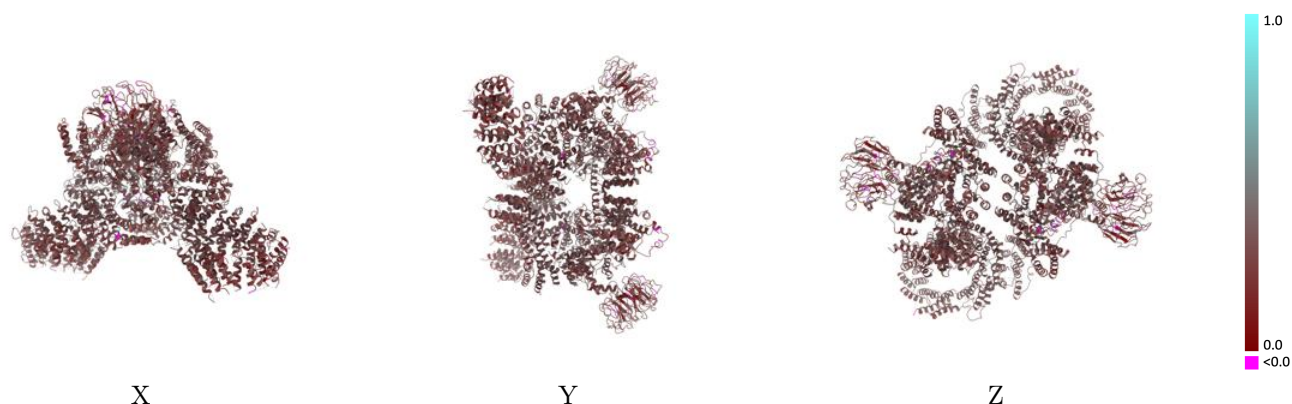
Y



Z

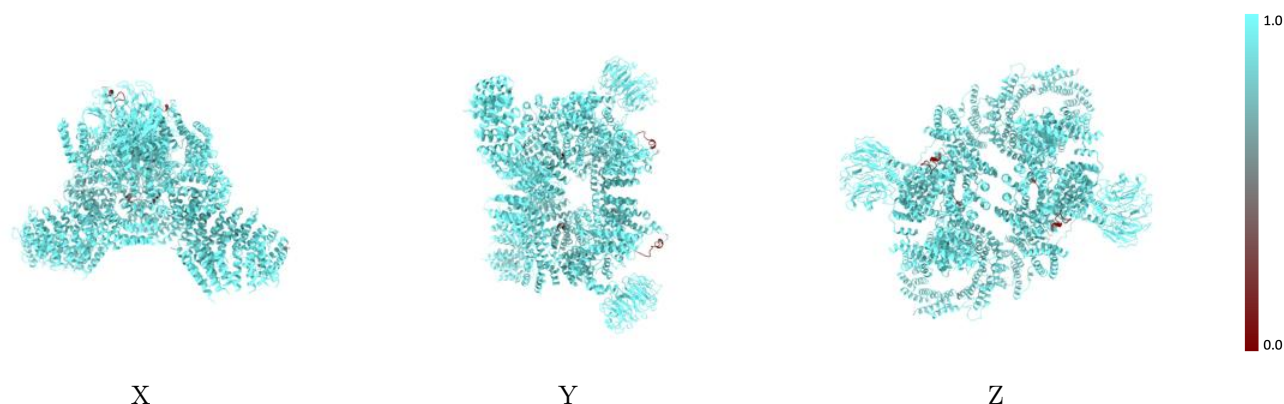
The images above show the 3D surface view of the map at the recommended contour level 0.044 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



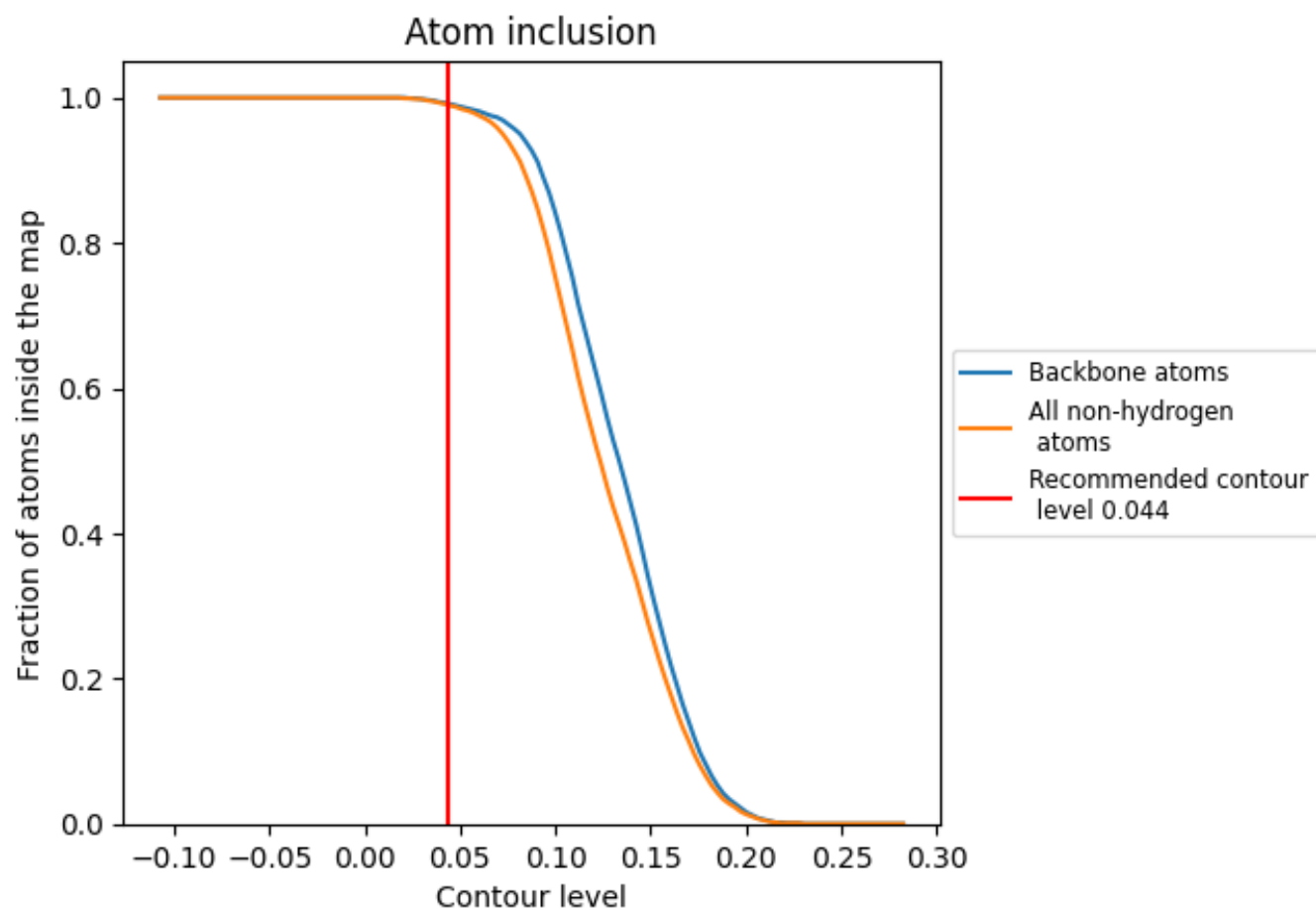
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.044).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.044) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9900	0.2970
A	0.9890	0.3030
B	0.9890	0.3020
C	1.0000	0.2560
D	1.0000	0.2580

