



Full wwPDB EM Validation Report ⓘ

Aug 18, 2026 – 06:27 PM JST

PDB ID : 23FD / pdb_000023fd
EMDB ID : EMD-68920
Title : Cryo-EM structure of human ATR-ATRIP complex with ATPgammaS, Chk1 and TopBp1
Authors : Wang, L.; Wang, M.; Zhao, L.; Rao, Q.; Wu, H.; Ma, B.; Wang, J.; Zheng, J.; Li, Y.; Xu, Y.; Guo, J.; Cheng, J.; Qiao, S.
Deposited on : 2026-02-04
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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) : 2.50

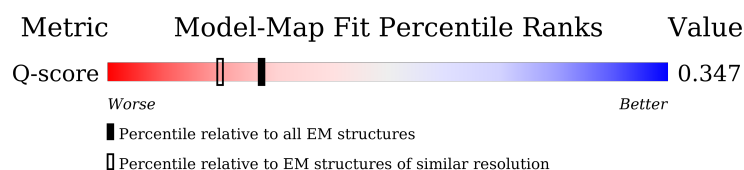
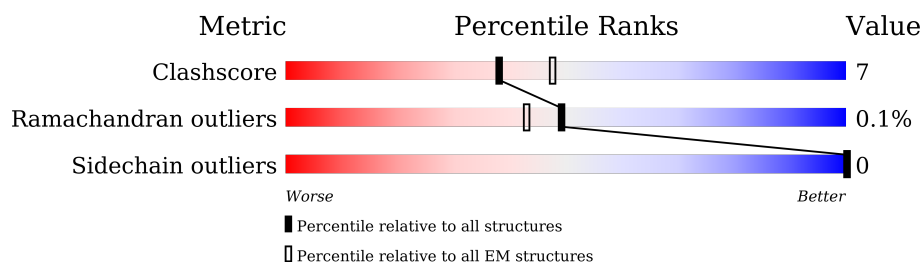
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	2644	
1	B	2644	
2	C	791	
2	D	791	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	14	 43% 7% 50%
3	F	14	 43% 57%
4	G	545	 10% 89%
4	H	545	 10% 89%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 46339 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 ATR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2486	Total	C	N	O	S	0	0
			19929	12792	3383	3614	140		
1	B	2480	Total	C	N	O	S	0	0
			19896	12774	3375	3607	140		

- Molecule 2 is a protein called ATR-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	361	Total	C	N	O	S	0	0
			2779	1776	484	494	25		
2	D	361	Total	C	N	O	S	0	0
			2779	1776	484	494	25		

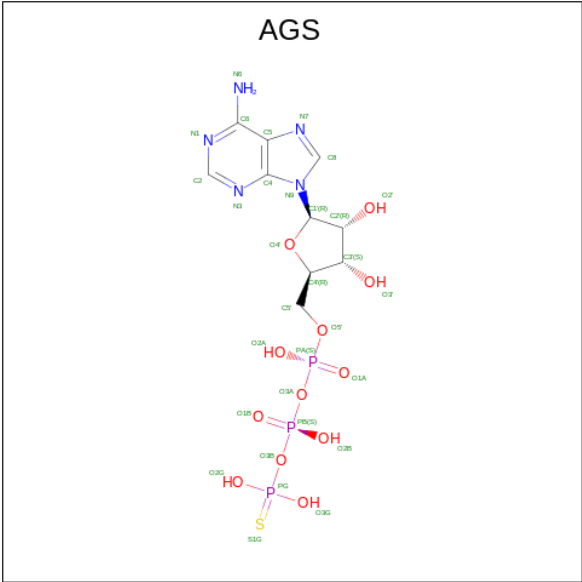
- Molecule 3 is a protein called Serine/threonine-protein kinase Chk1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	7	Total	C	N	O	0	0
			51	31	8	12		
3	F	6	Total	C	N	O	0	0
			39	22	7	10		

- Molecule 4 is a protein called DNA topoisomerase 2-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	62	Total	C	N	O	S	0	0
			405	245	78	81	1		
4	H	60	Total	C	N	O		0	0
			393	239	76	78			

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	S
			31	10	5	12	3	1
5	B	1	Total	C	N	O	P	S
			31	10	5	12	3	1

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	A	2	Total	Mg	0
			2	2	
6	B	2	Total	Mg	0
			2	2	

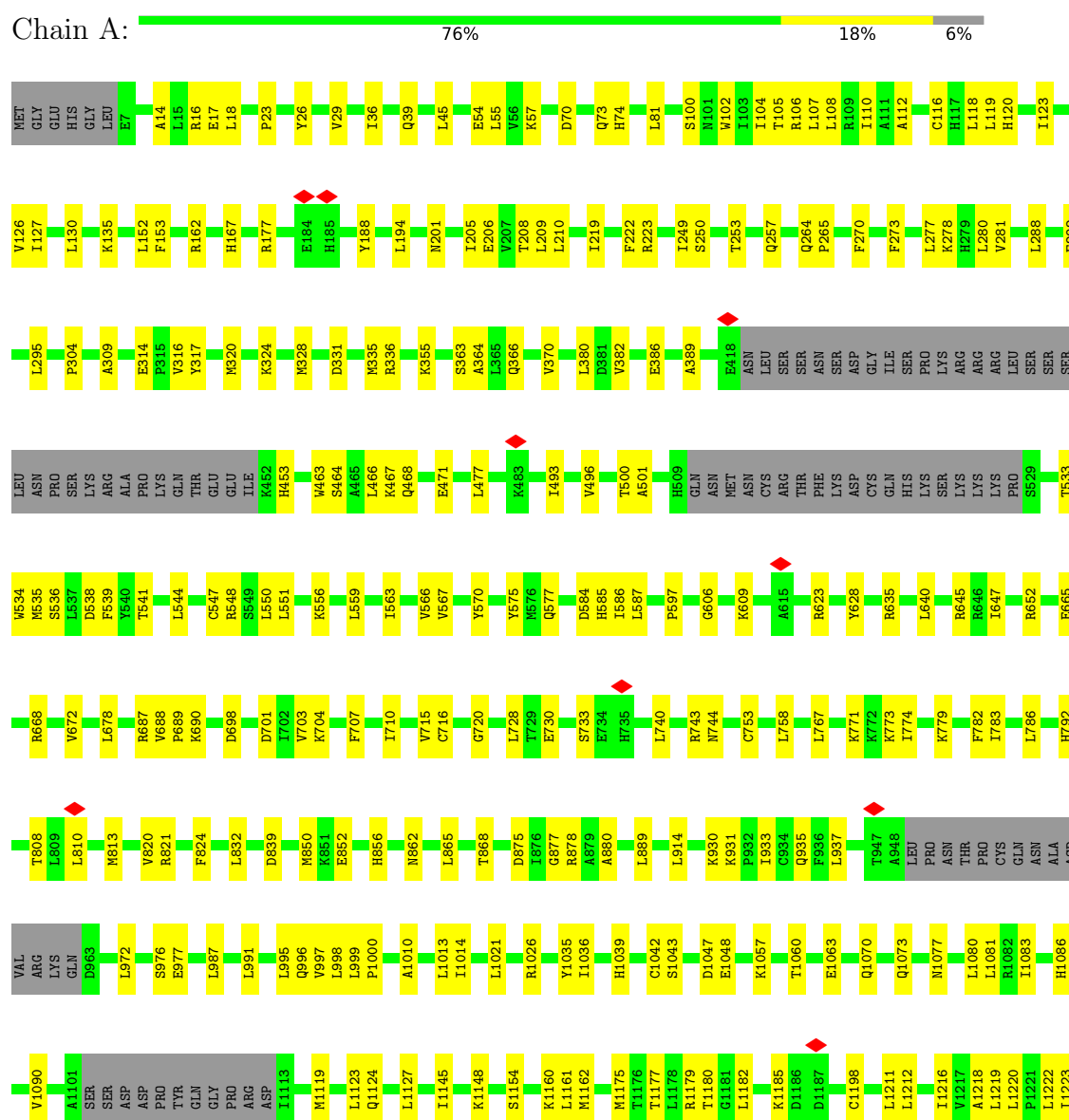
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

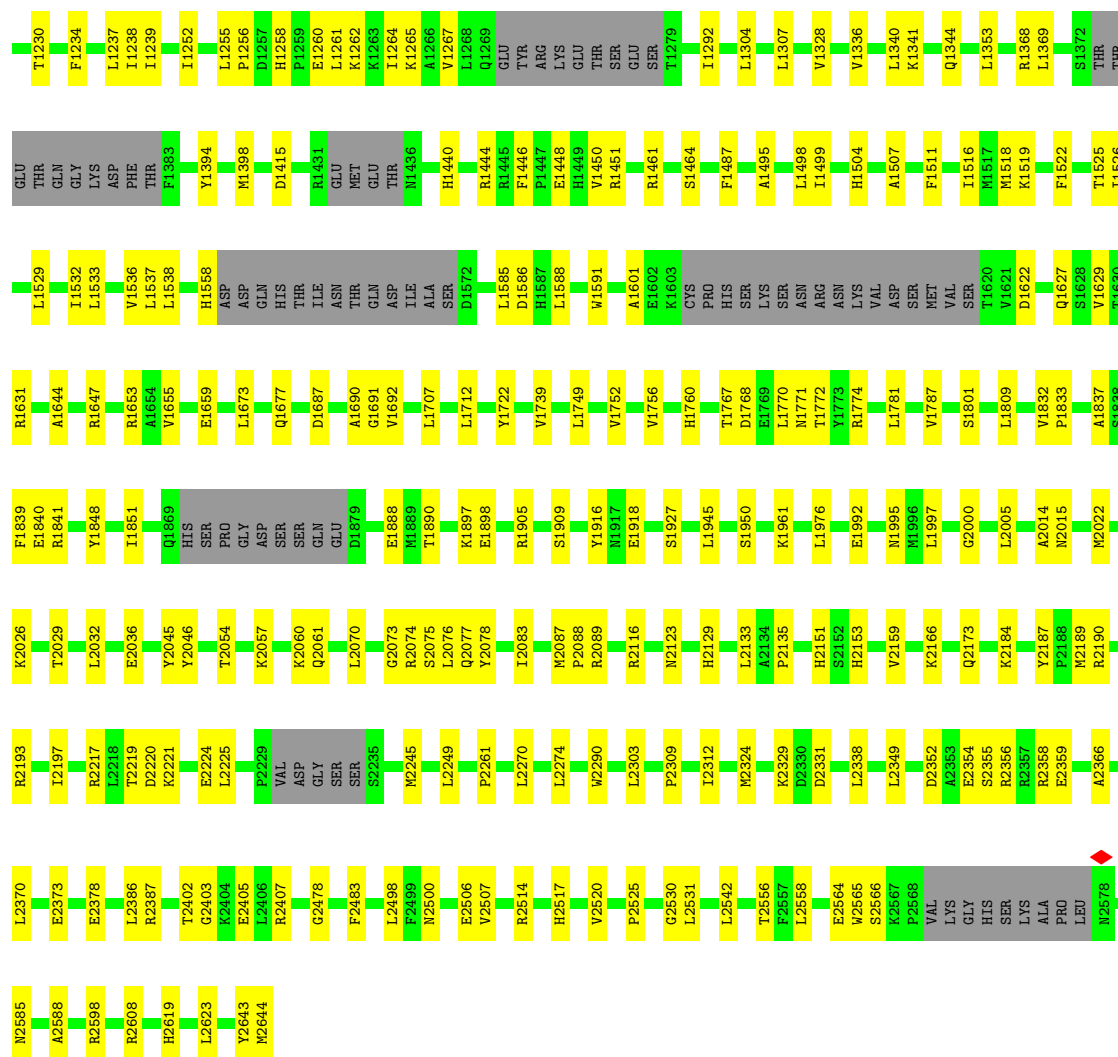
Mol	Chain	Residues	Atoms		AltConf
7	C	1	Total	Zn	0
			1	1	
7	D	1	Total	Zn	0
			1	1	

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.

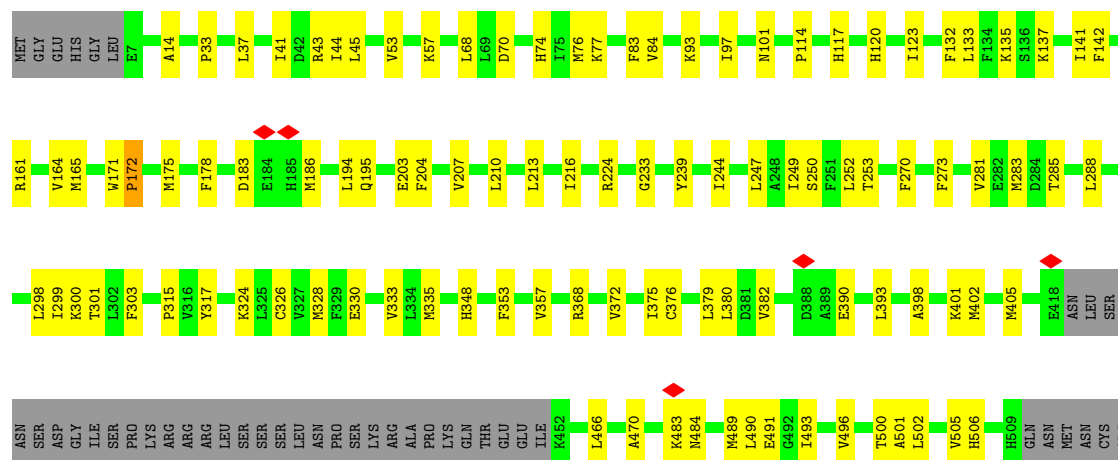
- Molecule 1: Serine/threonine-protein kinase ATR





• Molecule 1: Serine/threonine-protein kinase ATR

Chain B: 76% 18% 6%



R2514	L2377	L2169	K2022	R1846	R1647	M1553	GLN	L1191	K1057	L896	D739	I624
L2515	E2378	A2175	K2023	V1852	S1660	L1556	GLY	W1196	PHE	L897	L740	
H2517	L2386	N2176	Y2024	R1853	S1660	H1558	ASP	T1060	LYS	Y628	F741	
V2520	L2390	W2177	K2026	M1856	E1664	H1558	PHE	L1203	ASP	G905	C742	
N2521	L2393	M2178	T2029	M1856	Q1677	ASP	THR	L1212	THR	Y908	R743	
M2523	L2393	M2179	T2029	L1860	V1689	ASP	GLN	L1216	S1066	T911	K746	
T2528	M2401	Y2187	L2032	E1861	A1689	HIS	S1390	I1216	L1075	V915	Q750	
E2529	T2402	R2190	A2043	H1862	G1691	ILE	L1397	A1218	L1079	A948	A760	
G2403	G2404	R2193	Y2046	H1862	G1691	ASN	L1397	L1219	L1080	LEU	S761	
M2540	E2405	K2205	D2063	K1865	R1696	THR	T1401	T1230	I1083	ASN	L767	
T2556	L2406	R2217	R2066	Q1869	I1706	GLN	E1423	F1234	G1084	THR	L770	
P2568	R2407			HIS	L1715	ALA	L1424	H1086	E1085	PRO	L70	
VAL	M2410	R2217	R2066	PRO	L1715	SER	R1431	D1247	H1086	CYS	K771	
LYS	K2413	P2229	H2071	GLY	Y1722	D1572	GLU	D1257	A1101	GLN	K772	
GLY	S2414	VAL	LYS	ASP	D1723	L1585	MET	H1258	SER	ASN	P777	
HIS	A2415	ASP	G2073	SER	A1725	L1588	THR	P1259	ASP	ALA	L780	
SER	K2420	GLY	N2080	GLN	H1737	L1588	N1436	K1262	ASP	VAL	L780	
LYS	K2422	SER	Y2084	GLU	G1738	K1600	N1436	R1272	PRO	ARG	L783	
ALA	L2422	S2235	Y2084	D1679	G1738	ALA	L1442	GLY	PRO	LYS	L786	
LEU	M2239	M2239	P2088	M1889	S1742	LYS	V1450	GLN	ARG	GLN	L786	
M2578	E2426	F2427	E2105	I1900	N1762	CYS	L1454	THR	ARG	R968	L789	
N2585	L2428	F2427	E2105	L1900	R1763	PRO	L1454	SER	ASP	T974	C790	
A2588	R2431	K2244	R2112	L1903	T1767	HIS	K1463	GLU	I1113		F675	
L2614	H2432	M2245	Q2113	L1907	D1768	LYS	Q1466	SER	I1114		L678	
	P2433	L2249	Q2114	L1908	E1769	SER	E1769	THR	S1115		L679	
	P2434	L2259	N2115	M1919	L1770	ASN	W1471	L1281	P1116		Q801	
Y2622	L2435	L2259	R2116	M1919	N1771	ARG	W1471	L1281	E1117		V802	
	F2436	P2271	K2124	L1944	T1772	ASN	G1484	L1118	L1118		K303	
M2636	W2439	N2279	T2127	L1944	Y1773	LYS	G1484	S1288			N811	
Y2643	F2440	N2279	E2128	E1949	R1774	VAL	W1490	I1292	M1150		V821	
M2644	D2446	A2294	H2129	L1952	E1776	SER	Y1497	N1296	L999		V822	
		S2305	P2135	E1958	W1779	MET	L1498	V1299	A1004		S825	
	W2450	P2309	Y2136	E1958	D1785	SER	K1501	V1299	S880		F707	
	R2454	P2309	L2139	W1962	D1785	V1621	D1505	K1317	S1011		S834	
	T2470	K2315	L2139	S1965	W1800	Y1621	L1506	K1173	I710		L710	
		M2325	F2142	L1976	S1801	Y1623	A1507	M1174	L711		E838	
	L2481	K2326	L2145	L1976	L1804	D1625	S1508	M1175	G712		G712	
	F2483	K2327	L2145	P1990	L1812	Y1626	K1509	T1176	L714		Q713	
		L2338	C2150	P1990	K1813	Q1627	I1510	T1177	S895		L714	
			H2151	N1995	R1814	K1813	I1510	L1178	M721		M721	
	L2498	K2347	H2151	M1995	R1814	S1628	I1516	R1179	S860		R861	
	V2507	Y2365	E2155	M1997	R1814	V1629	L1533	T1180	S860		R861	
	P2508	F2157	F2156	L1997	Y1820	I1636	L1533	G1181	F732		T968	
	A2366	F2157	F2156	L1997	Y1820	P1637	V1536	L1182	SER		GLU	
	E2509	V2367	V2156	V2006	Q1830	T1640	E1547	F1184	HIS		D883	
								K1185	GLY		C1042	
									HIS		P886	
											V738	

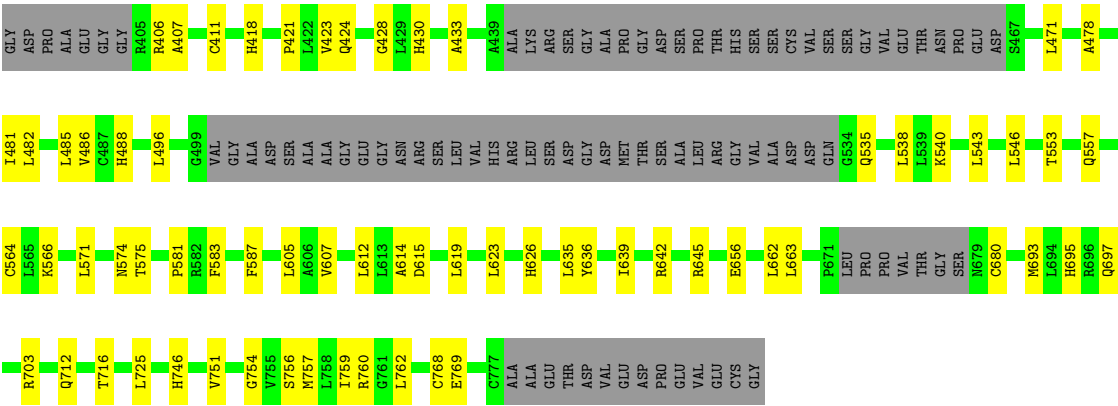
• Molecule 2: ATR-interacting protein

Response	Percentage
Yes	37%
No	9%
Don't know	54%

- Molecule 2: ATR-interacting protein

Category	Percentage
Very bad	36%
Bad	9%
Good	54%

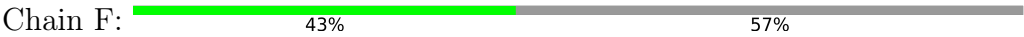




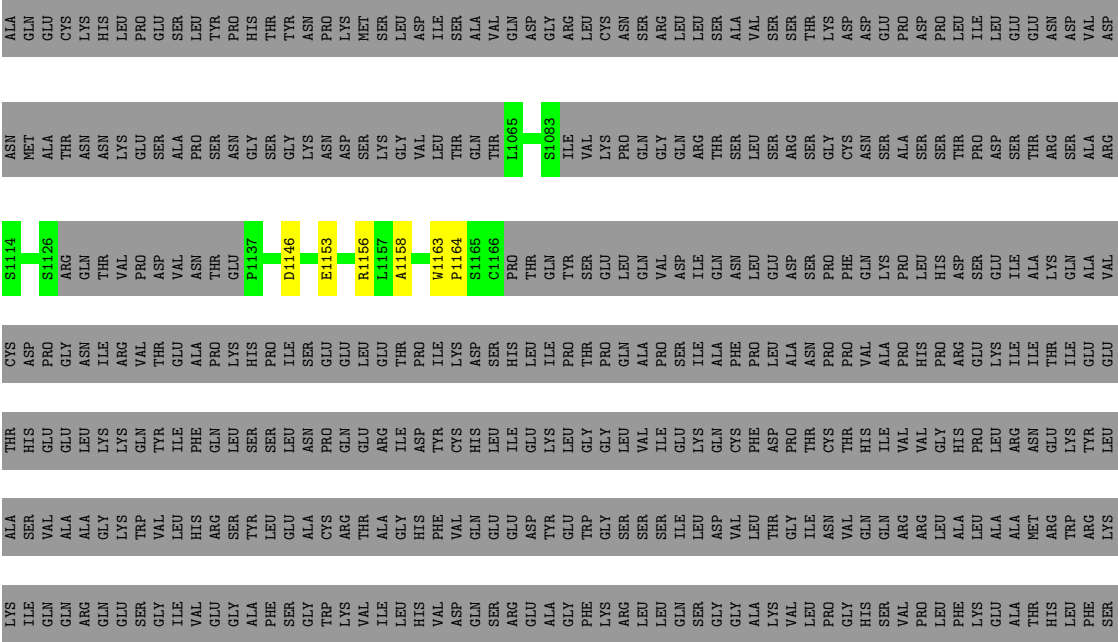
• Molecule 3: Serine/threonine-protein kinase Chk1



• Molecule 3: Serine/threonine-protein kinase Chk1



• Molecule 4: DNA topoisomerase 2-binding protein 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70253	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.905	Depositor
Minimum map value	-0.622	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	401.76, 401.76, 401.76	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.93, 0.93, 0.93	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, AGS, MG

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	0.28	0/20341	0.56	2/27488 (0.0%)
1	B	0.25	0/20306	0.56	0/27439
2	C	0.29	0/2826	0.60	0/3837
2	D	0.26	0/2826	0.57	0/3837
3	E	0.11	0/52	0.28	0/70
3	F	0.15	0/39	0.50	0/52
4	G	0.16	0/409	0.44	0/559
4	H	0.22	0/397	0.53	0/543
All	All	0.26	0/47196	0.56	2/63825 (0.0%)

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	B	0	1
2	C	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	ARG	CB-CG-CD	5.55	124.08	111.30
1	A	1601	ALA	CB-CA-C	-5.30	110.45	116.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	171	TRP	Peptide
2	C	319	GLN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	19929	0	20229	311	0
1	B	19896	0	20201	294	0
2	C	2779	0	2872	49	0
2	D	2779	0	2872	46	0
3	E	51	0	40	1	0
3	F	39	0	31	0	0
4	G	405	0	297	4	0
4	H	393	0	287	7	0
5	A	31	0	12	0	0
5	B	31	0	12	1	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
All	All	46339	0	46853	688	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 7.

All (688) 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:1340:LEU:HB3	1:A:1839:PHE:CE1	1.79	1.17
1:A:1340:LEU:HB3	1:A:1839:PHE:HE1	1.12	1.04
1:A:127:ILE:HD12	1:A:130:LEU:HD12	1.46	0.95
1:A:1340:LEU:CB	1:A:1839:PHE:CE1	2.50	0.93
1:A:1340:LEU:CB	1:A:1839:PHE:HE1	1.86	0.82
1:A:1182:LEU:HA	1:A:1185:LYS:HE3	1.67	0.77
1:A:1499:ILE:HD12	1:A:1511:PHE:HB3	1.67	0.75
1:B:2393:LEU:HD11	1:B:2439:TRP:HB2	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:630:CYS:HB3	2:C:633:LEU:HD23	1.73	0.71
1:A:991:LEU:O	1:A:995:LEU:HB2	1.91	0.70
1:A:104:ILE:HG12	1:A:127:ILE:HD11	1.72	0.70
1:B:1171:ARG:HH21	1:B:1203:LEU:HD11	1.57	0.70
1:A:2261:PRO:HG2	1:A:2324:MET:HE1	1.76	0.68
1:B:43:ARG:HG3	1:B:44:ILE:HG13	1.75	0.68
2:C:310:SER:O	2:C:314:ASN:ND2	2.26	0.68
1:B:1767:THR:O	1:B:1771:ASN:HB2	1.93	0.68
1:A:1756:VAL:HG11	1:A:1774:ARG:HB3	1.76	0.67
1:B:1557:LYS:HA	1:B:1647:ARG:HH22	1.58	0.67
2:C:702:ARG:HH22	2:C:758:LEU:HB2	1.59	0.67
1:B:1853:ARG:HA	1:B:1856:MET:HE2	1.75	0.67
1:B:1860:LEU:HA	1:B:1907:LEU:HD21	1.77	0.66
1:A:687:ARG:NH1	1:A:688:VAL:O	2.30	0.65
1:A:1219:LEU:HD12	1:A:1230:THR:HG23	1.77	0.65
1:B:1390:SER:HB2	1:B:1442:LEU:HD13	1.78	0.65
1:A:852:GLU:O	1:A:856:HIS:ND1	2.26	0.65
2:C:566:LYS:HB2	2:C:605:LEU:HD13	1.78	0.65
1:A:2015:ASN:HD22	1:B:2622:TYR:HB2	1.61	0.64
1:A:1340:LEU:HB2	1:A:1839:PHE:CZ	2.32	0.64
1:B:1113:ILE:HG21	1:B:1118:LEU:HD23	1.79	0.64
1:B:1949:GLU:O	1:B:1952:LEU:HB2	1.97	0.64
1:A:335:MET:HE3	1:A:382:VAL:HG23	1.80	0.64
1:A:740:LEU:HD22	1:A:743:ARG:HG3	1.80	0.64
1:B:783:ILE:HA	1:B:786:LEU:HD13	1.80	0.63
2:D:482:LEU:HA	2:D:485:LEU:HD12	1.80	0.63
1:B:1281:LEU:HD13	1:B:1317:LYS:HE2	1.79	0.63
1:A:324:LYS:HG3	1:A:328:MET:HE3	1.80	0.63
1:A:2083:ILE:HG21	1:A:2270:LEU:HD13	1.81	0.62
1:A:70:ASP:O	1:A:74:HIS:ND1	2.32	0.62
1:B:70:ASP:O	1:B:74:HIS:ND1	2.30	0.62
1:A:1258:HIS:O	1:A:1262:LYS:N	2.32	0.62
1:B:859:ILE:O	1:B:861:ARG:NH1	2.32	0.62
2:C:320:PRO:HB3	2:C:326:SER:HA	1.82	0.62
1:B:1463:LYS:HB2	4:G:1146:ASP:HB2	1.82	0.62
1:B:84:VAL:HG13	1:B:137:LYS:HD2	1.80	0.61
1:B:687:ARG:HH21	1:B:690:LYS:HD2	1.64	0.61
1:A:2217:ARG:HB3	1:A:2249:LEU:HD11	1.82	0.61
1:B:905:GLY:HA2	2:D:746:HIS:HB3	1.82	0.61
2:D:486:VAL:HG21	2:D:571:LEU:HD22	1.83	0.61
1:A:467:LYS:HG2	1:A:535:MET:HE1	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1737:HIS:HE1	1:B:1769:GLU:HB3	1.65	0.61
1:B:1812:LYS:O	1:B:1814:ARG:NH1	2.34	0.61
1:A:18:LEU:HD23	1:A:29:VAL:HG12	1.83	0.61
1:A:331:ASP:OD1	1:A:336:ARG:NH2	2.31	0.61
1:A:937:LEU:HD11	1:A:998:LEU:HD11	1.82	0.61
1:A:2187:TYR:HB2	1:A:2190:ARG:HD2	1.82	0.61
1:B:299:ILE:HG22	1:B:348:HIS:HD2	1.65	0.61
1:B:2136:TYR:O	1:B:2139:LEU:HB3	2.01	0.61
1:A:257:GLN:HB3	2:C:714:ARG:HH12	1.65	0.60
1:B:1423:GLU:OE1	1:B:1509:LYS:NZ	2.34	0.60
1:B:2401:MET:HB2	1:B:2431:ARG:HG2	1.84	0.60
1:B:707:PHE:O	1:B:711:LEU:HB2	2.02	0.60
1:B:183:ASP:HB3	1:B:186:MET:HB2	1.83	0.60
2:D:642:ARG:HH21	2:D:693:MET:HE1	1.67	0.60
1:B:1172:VAL:HA	1:B:1175:MET:HE2	1.84	0.60
1:B:1677:GLN:OE1	1:B:1696:ARG:NH2	2.34	0.60
1:B:2139:LEU:HA	1:B:2142:PHE:HB2	1.83	0.60
1:B:2187:TYR:HB2	1:B:2190:ARG:HD3	1.84	0.60
1:B:2338:LEU:HD22	1:B:2498:LEU:HD11	1.84	0.60
1:B:506:HIS:NE2	1:B:575:TYR:OH	2.35	0.59
2:D:430:HIS:O	2:D:433:ALA:HB3	2.02	0.59
1:B:767:LEU:HA	1:B:770:LEU:HD23	1.83	0.59
2:D:308:GLN:NE2	2:D:411:CYS:SG	2.75	0.59
1:B:2413:LYS:HD3	1:B:2507:VAL:HG22	1.84	0.59
1:B:537:LEU:HA	1:B:540:TYR:HD2	1.68	0.59
1:B:2407:ARG:HA	1:B:2410:MET:HE3	1.83	0.59
1:A:464:SER:O	1:A:468:GLN:NE2	2.36	0.59
1:B:1856:MET:HB3	1:B:1903:LEU:HD23	1.85	0.59
2:C:432:GLN:O	2:C:436:ASP:N	2.35	0.59
2:D:423:VAL:HG23	2:D:478:ALA:HB1	1.85	0.59
1:B:1691:GLY:HA3	1:B:2530:GLY:HA2	1.84	0.59
1:A:153:PHE:HE1	1:A:209:LEU:HB3	1.68	0.59
1:B:672:VAL:HG21	1:B:703:VAL:HG13	1.86	0.58
1:A:1010:ALA:HA	1:A:1013:LEU:HD12	1.85	0.58
1:A:774:ILE:O	1:A:779:LYS:NZ	2.36	0.58
1:A:1216:ILE:HG21	1:A:1252:ILE:HG13	1.86	0.58
1:A:1292:ILE:HG12	1:A:1304:LEU:HD22	1.85	0.58
1:A:2022:MET:HG2	1:A:2046:TYR:HE1	1.69	0.58
1:A:1961:LYS:HG3	1:A:2005:LEU:HD21	1.86	0.58
1:B:707:PHE:HA	1:B:710:ILE:HG12	1.85	0.58
2:C:639:ILE:HD11	2:C:659:VAL:HG21	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2367:VAL:HG13	1:B:2377:ILE:HG12	1.85	0.58
2:D:754:GLY:HA2	2:D:757:MET:HE2	1.84	0.58
2:D:759:ILE:HA	2:D:762:LEU:HD23	1.84	0.58
1:B:645:ARG:NE	1:B:680:GLN:OE1	2.36	0.58
1:B:1182:LEU:HA	1:B:1185:LYS:HE3	1.85	0.57
1:A:556:LYS:HA	1:A:559:LEU:HB2	1.86	0.57
1:B:164:VAL:HG21	1:B:239:TYR:HB3	1.85	0.57
1:B:1079:LEU:HD12	1:B:1080:LEU:HG	1.86	0.57
1:A:1127:LEU:HD22	1:A:1162:MET:HE2	1.85	0.57
1:A:1179:ARG:HA	1:A:1182:LEU:HD12	1.85	0.57
1:B:790:CYS:HB3	1:B:834:SER:HB3	1.87	0.57
2:C:566:LYS:HA	2:C:569:VAL:HG12	1.86	0.57
1:A:316:VAL:HG11	2:C:314:ASN:HB3	1.85	0.57
1:B:596:LEU:HD13	1:B:624:ILE:HG13	1.87	0.57
1:A:672:VAL:HG21	1:A:703:VAL:HG13	1.87	0.57
1:A:250:SER:O	1:A:253:THR:OG1	2.21	0.57
2:D:316:LEU:HD22	2:D:481:ILE:HG23	1.86	0.57
1:B:772:LYS:NZ	1:B:811:ASN:O	2.38	0.57
1:B:1484:GLY:HA2	1:B:1490:TRP:HB2	1.87	0.57
1:A:567:VAL:HA	1:A:570:TYR:HD2	1.70	0.57
1:B:759:LYS:HD3	1:B:761:SER:H	1.70	0.57
1:B:1401:THR:HG21	1:B:1450:VAL:HG12	1.85	0.57
1:B:1171:ARG:NH1	1:B:1175:MET:SD	2.78	0.56
1:A:875:ASP:OD1	1:A:878:ARG:NH1	2.38	0.56
1:A:1655:VAL:O	1:A:1659:GLU:HG2	2.06	0.56
1:A:813:MET:HE2	1:A:824:PHE:HE2	1.70	0.56
1:B:233:GLY:HA3	1:B:252:LEU:HD21	1.87	0.56
2:C:583:PHE:O	2:C:586:VAL:HB	2.05	0.56
1:A:2135:PRO:HG3	1:A:2166:LYS:HE3	1.87	0.56
1:B:1498:LEU:HD22	1:B:1536:VAL:HG11	1.87	0.56
1:B:2585:ASN:HB3	1:B:2588:ALA:HB2	1.87	0.56
1:A:1446:PHE:O	1:A:1451:ARG:NH2	2.39	0.56
1:B:1553:MET:SD	1:B:1557:LYS:NZ	2.79	0.56
1:B:2073:GLY:HA3	1:B:2129:HIS:CE1	2.41	0.55
4:H:1153:GLU:OE1	4:H:1156:ARG:NH2	2.39	0.55
1:A:1890:THR:OG1	1:A:1897:LYS:NZ	2.39	0.55
1:B:1800:TRP:CH2	1:B:1853:ARG:HB3	2.41	0.55
2:C:600:LEU:HD22	2:C:651:GLN:HB3	1.88	0.55
1:A:931:LYS:O	1:A:935:GLN:NE2	2.40	0.55
1:A:1673:LEU:HD22	1:A:1692:VAL:HG13	1.89	0.55
1:A:23:PRO:HA	1:A:26:TYR:HB3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1360:GLU:OE2	1:B:1862:HIS:NE2	2.32	0.55
1:A:2116:ARG:HH22	1:A:2153:HIS:HE2	1.55	0.55
1:A:2329:LYS:HA	1:A:2373:GLU:HG2	1.89	0.55
1:A:707:PHE:HA	1:A:710:ILE:HG12	1.89	0.55
1:B:357:VAL:O	1:B:368:ARG:NH2	2.40	0.55
1:A:2054:THR:OG1	1:A:2061:GLN:NE2	2.36	0.55
1:B:204:PHE:HA	1:B:207:VAL:HG12	1.89	0.55
1:A:108:LEU:HD22	1:A:205:ILE:HD11	1.88	0.54
1:B:556:LYS:HA	1:B:559:LEU:HB2	1.88	0.54
1:B:1057:LYS:HE3	1:B:1063:GLU:HA	1.88	0.54
1:B:705:LYS:HE2	1:B:777:PRO:HB2	1.89	0.54
1:A:500:THR:HG21	1:A:535:MET:HG2	1.89	0.54
1:A:1258:HIS:HB3	1:A:1261:LEU:HB2	1.89	0.54
1:A:1945:LEU:O	1:B:1724:ARG:NH1	2.41	0.54
1:B:1466:GLN:HB2	1:B:1516:ILE:HD11	1.88	0.54
2:D:756:SER:O	2:D:760:ARG:NH1	2.41	0.54
1:A:116:CYS:O	1:A:120:HIS:N	2.38	0.54
1:A:355:LYS:NZ	1:A:730:GLU:OE2	2.41	0.54
1:B:303:PHE:O	1:B:348:HIS:NE2	2.40	0.54
2:D:768:CYS:SG	2:D:769:GLU:N	2.80	0.54
1:A:2184:LYS:NZ	1:A:2220:ASP:OD1	2.41	0.54
1:B:1997:LEU:HA	1:B:2032:LEU:HD11	1.89	0.54
1:A:1026:ARG:NH1	1:A:1060:THR:O	2.39	0.53
1:B:594:LEU:HD12	1:B:643:PHE:HZ	1.72	0.53
1:B:224:ARG:NE	2:D:615:ASP:OD2	2.33	0.53
1:A:1495:ALA:O	1:A:1499:ILE:HG12	2.09	0.53
1:A:584:ASP:OD1	1:A:585:HIS:N	2.41	0.53
2:D:626:HIS:HA	2:D:680:CYS:HB2	1.90	0.53
1:B:132:PHE:O	1:B:135:LYS:HB3	2.09	0.53
1:B:1505:ASP:OD1	1:B:1506:LEU:N	2.42	0.53
1:A:1440:HIS:HB3	1:A:1444:ARG:HH12	1.72	0.53
1:A:1627:GLN:HB3	1:A:1631:ARG:HH21	1.74	0.53
1:B:1324:ASP:OD2	1:B:2279:ASN:ND2	2.41	0.53
2:C:685:GLU:OE1	2:C:688:ARG:NH1	2.42	0.53
1:A:1787:VAL:HG12	1:A:1809:LEU:HD22	1.90	0.53
1:A:1175:MET:HE1	1:A:1211:LEU:HB3	1.91	0.53
1:A:1772:THR:OG1	1:A:1801:SER:OG	2.26	0.53
1:B:402:MET:HA	1:B:405:MET:HG3	1.90	0.53
1:B:675:PHE:HA	1:B:678:LEU:HD13	1.90	0.53
4:H:1146:ASP:OD1	4:H:1147:ASP:N	2.43	0.53
1:A:931:LYS:HB2	1:A:935:GLN:HE22	1.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2151:HIS:O	1:A:2193:ARG:NH2	2.42	0.52
1:B:175:MET:HE1	1:B:178:PHE:HB2	1.91	0.52
1:A:635:ARG:HD3	1:A:740:LEU:HD12	1.91	0.52
1:A:875:ASP:HA	1:A:878:ARG:HG2	1.91	0.52
1:B:376:CYS:HA	1:B:379:LEU:HD12	1.90	0.52
1:A:2585:ASN:HB3	1:A:2588:ALA:HB2	1.91	0.52
1:A:1767:THR:O	1:A:1771:ASN:N	2.43	0.52
1:B:372:VAL:HA	1:B:375:ILE:HG22	1.91	0.52
1:A:1220:LEU:HD23	1:A:1223:ILE:HD12	1.91	0.52
1:B:547:CYS:HG	1:B:570:TYR:HH	1.54	0.52
1:B:1004:ALA:HA	1:B:1040:LEU:HD11	1.90	0.52
1:B:213:LEU:HA	1:B:216:ILE:HG22	1.90	0.52
1:A:2352:ASP:HB3	1:A:2355:SER:HB2	1.92	0.52
1:B:547:CYS:SG	1:B:570:TYR:OH	2.65	0.52
2:C:633:LEU:HD22	2:C:682:CYS:HB3	1.92	0.52
1:A:2608:ARG:NH1	1:B:2016:PHE:O	2.43	0.52
1:A:107:LEU:HD12	1:A:123:ILE:HG12	1.91	0.52
1:A:701:ASP:OD1	1:A:701:ASP:N	2.42	0.52
1:A:2219:THR:HG23	1:A:2370:LEU:HD22	1.92	0.52
1:B:897:LEU:HD11	1:B:974:THR:HG23	1.91	0.52
1:B:1585:LEU:HD13	1:B:1588:LEU:HD21	1.92	0.52
2:D:312:LEU:HD23	2:D:389:VAL:HG21	1.92	0.52
1:B:172:PRO:HB3	1:B:195:GLN:HB2	1.92	0.51
1:B:1990:PRO:HB2	1:B:1995:ASN:HD22	1.74	0.51
1:A:26:TYR:HA	1:A:29:VAL:HB	1.93	0.51
1:B:1556:LEU:O	1:B:1647:ARG:NH2	2.43	0.51
1:A:501:ALA:HB1	1:A:575:TYR:HD2	1.76	0.51
1:B:759:LYS:NZ	1:B:801:ASP:OD2	2.43	0.51
1:A:14:ALA:HA	1:A:17:GLU:HG2	1.92	0.51
1:A:977:GLU:OE2	2:C:746:HIS:NE2	2.35	0.51
1:B:1247:ASP:OD1	1:B:1247:ASP:N	2.44	0.51
1:B:1259:PRO:HA	1:B:1262:LYS:HG2	1.93	0.51
2:D:406:ARG:NH1	2:D:575:THR:O	2.43	0.51
1:B:161:ARG:HG2	1:B:165:MET:HE1	1.92	0.51
1:B:1501:LYS:NZ	1:B:1547:GLU:OE1	2.35	0.51
1:B:2063:ASP:OD1	1:B:2066:ARG:NH2	2.42	0.51
1:B:2407:ARG:NH2	3:E:314:TYR:OH	2.42	0.51
2:C:319:GLN:HG3	2:C:320:PRO:HD3	1.92	0.51
1:A:1498:LEU:HB3	1:A:1536:VAL:HG21	1.92	0.51
1:A:2517:HIS:HA	1:A:2520:VAL:HG22	1.93	0.51
1:B:76:MET:HB3	1:B:83:PHE:HE2	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:482:LEU:HD11	2:C:538:LEU:HD21	1.92	0.51
1:A:105:THR:HG23	1:A:194:LEU:HB2	1.91	0.51
1:A:1262:LYS:HA	1:A:1265:LYS:HZ2	1.76	0.51
1:B:1773:TYR:HA	1:B:1776:GLU:OE1	2.11	0.51
2:D:695:HIS:HA	2:D:751:VAL:HG11	1.93	0.51
1:A:1677:GLN:HG2	1:A:1707:LEU:HD23	1.93	0.51
2:C:318:LYS:NZ	2:C:320:PRO:O	2.43	0.51
1:B:993:ARG:O	1:B:996:GLN:NE2	2.44	0.51
1:B:1776:GLU:OE2	1:B:1801:SER:OG	2.24	0.51
2:C:642:ARG:NH2	2:C:656:GLU:OE2	2.43	0.51
2:D:581:PRO:HA	2:D:619:LEU:HD11	1.92	0.51
1:B:799:GLU:OE1	1:B:803:LYS:NZ	2.38	0.50
2:C:420:LEU:HD11	2:C:492:VAL:HG22	1.92	0.50
1:B:224:ARG:NH2	2:D:612:LEU:O	2.44	0.50
1:B:390:GLU:O	1:B:393:LEU:HB2	2.11	0.50
1:B:628:TYR:OH	1:B:636:CYS:SG	2.66	0.50
1:B:1800:TRP:CE3	1:B:1830:GLN:HG2	2.46	0.50
2:C:392:ASN:OD1	2:C:393:GLU:N	2.44	0.50
2:D:329:LEU:HD12	2:D:481:ILE:HD12	1.93	0.50
2:D:381:LEU:HG	2:D:418:HIS:HB3	1.94	0.50
1:A:606:GLY:HA2	1:A:609:LYS:HE2	1.92	0.50
1:B:1026:ARG:NE	1:B:1060:THR:O	2.44	0.50
1:B:1976:LEU:HD22	1:B:2006:VAL:HG23	1.94	0.50
1:A:102:TRP:HE1	1:A:106:ARG:HE	1.59	0.50
1:A:1073:GLN:O	1:A:1077:ASN:ND2	2.45	0.50
1:A:1677:GLN:HB2	1:A:1692:VAL:HG11	1.94	0.50
1:B:555:GLN:HE22	1:B:557:LEU:HB2	1.75	0.50
1:B:2142:PHE:HA	1:B:2145:LEU:HD12	1.92	0.50
1:B:2509:GLU:HA	1:B:2636:MET:HE1	1.94	0.50
1:A:1909:SER:HA	1:A:1916:TYR:HE2	1.76	0.50
2:C:702:ARG:HB3	2:C:703:ARG:HH11	1.76	0.50
1:A:563:ILE:HA	1:A:566:VAL:HG12	1.92	0.50
1:A:1119:MET:HE1	1:A:1161:LEU:HD21	1.93	0.50
1:A:1292:ILE:HD11	1:A:1307:LEU:HD22	1.93	0.50
1:A:2356:ARG:NH1	1:A:2359:GLU:OE2	2.45	0.50
1:A:2366:ALA:H	1:A:2378:GLU:HB3	1.77	0.50
1:A:493:ILE:HA	1:A:496:VAL:HG12	1.94	0.50
1:A:1304:LEU:HB3	1:A:1353:LEU:HB3	1.92	0.50
1:A:1767:THR:HA	1:A:1770:LEU:HB2	1.93	0.50
1:A:2386:LEU:HD13	1:A:2483:PHE:HE2	1.77	0.50
1:B:142:PHE:HZ	1:B:216:ILE:HD11	1.75	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2113:VAL:O	1:B:2116:ARG:HB3	2.12	0.50
1:A:1042:CYS:HB2	1:A:1086:HIS:CG	2.47	0.49
1:A:1415:ASP:HB3	4:H:1143:ILE:HD11	1.92	0.49
1:B:556:LYS:HD3	1:B:559:LEU:HD12	1.94	0.49
1:B:570:TYR:CZ	1:B:593:MET:HE1	2.46	0.49
1:B:2365:TYR:HB2	1:B:2378:GLU:HB3	1.94	0.49
1:A:277:LEU:HD12	1:A:280:LEU:HD12	1.94	0.49
1:A:2088:PRO:HB3	1:A:2556:THR:HG21	1.94	0.49
1:A:26:TYR:OH	1:A:81:LEU:O	2.29	0.49
1:A:39:GLN:HG3	1:A:188:TYR:CE2	2.47	0.49
1:A:1690:ALA:HB2	1:A:1712:LEU:HD11	1.94	0.49
1:B:250:SER:O	1:B:253:THR:OG1	2.21	0.49
1:A:782:PHE:O	1:A:786:LEU:HB2	2.12	0.49
2:D:636:TYR:HA	2:D:639:ILE:HG22	1.93	0.49
1:A:930:LYS:HG2	1:A:997:VAL:HG21	1.94	0.49
1:B:2116:ARG:NH1	1:B:2155:GLU:OE2	2.45	0.49
1:A:678:LEU:HB3	1:A:689:PRO:HG2	1.95	0.49
1:B:324:LYS:HG3	1:B:328:MET:HE2	1.95	0.49
1:B:2112:ARG:O	1:B:2116:ARG:N	2.39	0.49
2:C:483:GLN:NE2	2:C:563:GLN:OE1	2.41	0.49
4:G:1153:GLU:OE2	4:G:1156:ARG:NH2	2.43	0.49
1:A:1997:LEU:HA	1:A:2032:LEU:HD11	1.95	0.49
1:B:1800:TRP:HE1	1:B:1804:LEU:HD22	1.78	0.49
2:D:642:ARG:O	2:D:645:ARG:NH2	2.44	0.49
1:A:55:LEU:HD11	1:A:119:LEU:HD13	1.95	0.49
1:B:656:TYR:CE2	1:B:678:LEU:HD11	2.48	0.49
1:A:999:LEU:HB3	1:A:1036:ILE:HD11	1.95	0.49
1:A:2036:GLU:HG3	1:A:2075:SER:HB2	1.95	0.49
1:A:821:ARG:HB3	1:A:868:THR:HG21	1.94	0.49
1:A:832:LEU:HD13	1:A:880:ALA:HB2	1.94	0.49
1:A:779:LYS:HD3	1:A:820:VAL:HG21	1.95	0.48
1:B:617:LEU:HG	1:B:620:LEU:HD22	1.95	0.48
1:B:783:ILE:HD12	1:B:786:LEU:HD13	1.95	0.48
1:A:810:LEU:HA	1:A:813:MET:HE3	1.94	0.48
1:A:1234:PHE:HA	1:A:1237:LEU:HD12	1.94	0.48
1:A:127:ILE:CD1	1:A:130:LEU:HD12	2.32	0.48
1:B:1820:TYR:OH	1:B:1865:LYS:NZ	2.43	0.48
1:B:2520:VAL:HG13	1:B:2528:THR:HG23	1.94	0.48
1:A:1440:HIS:HB3	1:A:1444:ARG:NH1	2.28	0.48
1:A:281:VAL:HG11	1:A:336:ARG:HH21	1.78	0.48
1:A:715:VAL:HG13	1:A:758:LEU:HD13	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:LEU:HD23	1:A:813:MET:HE1	1.95	0.48
1:A:1518:MET:HE3	1:A:1525:THR:HA	1.95	0.48
1:A:779:LYS:O	1:A:783:ILE:HG12	2.14	0.48
2:C:381:LEU:HD23	2:C:421:PRO:HG2	1.96	0.48
2:D:662:LEU:HD23	2:D:663:LEU:HD23	1.94	0.48
1:B:1178:LEU:HD13	1:B:1196:TRP:HH2	1.78	0.48
1:A:1529:LEU:HA	1:A:1532:ILE:HD12	1.96	0.47
1:B:491:GLU:HG3	1:B:565:LYS:HG3	1.96	0.47
1:A:771:LYS:HE3	1:A:773:LYS:HE2	1.96	0.47
1:B:1034:LYS:HA	1:B:1075:LEU:HD23	1.96	0.47
2:D:566:LYS:HG3	2:D:605:LEU:HD21	1.97	0.47
1:A:1487:PHE:HZ	1:A:1526:ILE:HD11	1.79	0.47
1:B:1834:LEU:O	1:B:1846:ARG:NH2	2.41	0.47
1:B:2217:ARG:HB3	1:B:2249:LEU:HD21	1.96	0.47
1:A:2517:HIS:NE2	1:A:2643:TYR:O	2.47	0.47
1:B:786:LEU:HA	1:B:789:LEU:HB2	1.97	0.47
1:B:1216:ILE:HA	1:B:1219:LEU:HG	1.95	0.47
1:A:996:GLN:HB2	1:A:1035:TYR:CD2	2.49	0.47
1:A:2057:LYS:HE2	1:A:2060:LYS:HG3	1.95	0.47
1:B:577:GLN:HE22	1:B:581:SER:HA	1.79	0.47
1:B:1175:MET:HA	1:B:1178:LEU:HG	1.96	0.47
1:B:1768:ASP:OD1	1:B:1768:ASP:N	2.43	0.47
1:A:112:ALA:O	1:A:201:ASN:ND2	2.40	0.47
1:A:1219:LEU:HD13	1:A:1222:LEU:HD12	1.97	0.47
1:A:1341:LYS:NZ	1:A:1839:PHE:CD2	2.80	0.47
1:A:2087:MET:HE2	1:A:2087:MET:HB2	1.82	0.47
1:B:41:ILE:HD12	1:B:45:LEU:HD12	1.97	0.47
1:B:298:LEU:HA	1:B:301:THR:HG22	1.97	0.47
1:B:380:LEU:HD21	1:B:466:LEU:HG	1.97	0.47
1:B:566:VAL:HA	1:B:569:ILE:HD12	1.95	0.47
1:B:1949:GLU:HB2	1:B:1952:LEU:HD13	1.96	0.47
1:B:2043:ALA:HB2	1:B:2071:HIS:HB2	1.96	0.47
1:B:2080:ASN:HD22	1:B:2271:PRO:HD2	1.80	0.47
1:A:1768:ASP:OD1	1:A:1768:ASP:N	2.47	0.47
2:D:607:VAL:HG22	2:D:635:LEU:HD11	1.96	0.47
1:A:277:LEU:HG	1:A:328:MET:HE1	1.97	0.47
1:B:739:ASP:OD2	1:B:743:ARG:NH1	2.48	0.47
1:B:1623:TYR:HA	1:B:1626:TYR:CZ	2.49	0.47
1:B:175:MET:HG2	1:B:194:LEU:H	1.80	0.47
2:C:424:GLN:O	2:C:428:GLY:N	2.44	0.47
2:D:543:LEU:HD23	2:D:546:LEU:HD21	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1533:LEU:HD22	1:A:1588:LEU:HD11	1.97	0.46
1:A:1760:HIS:CE1	1:A:1767:THR:HG21	2.49	0.46
1:A:2073:GLY:HA3	1:A:2129:HIS:CE1	2.50	0.46
1:A:1262:LYS:HA	1:A:1265:LYS:HG2	1.97	0.46
1:B:505:VAL:HA	1:B:579:ASN:HD22	1.80	0.46
1:B:1450:VAL:O	1:B:1454:LEU:HG	2.14	0.46
1:B:2239:MET:HG2	1:B:2243:PHE:HB2	1.97	0.46
2:C:653:LEU:HD21	2:C:715:ARG:HB3	1.95	0.46
1:B:2517:HIS:NE2	1:B:2643:TYR:O	2.45	0.46
1:A:1160:LYS:NZ	1:A:1198:CYS:SG	2.74	0.46
1:A:2387:ARG:HB2	1:A:2478:GLY:HA3	1.97	0.46
1:B:2084:TYR:OH	1:B:2347:LYS:NZ	2.45	0.46
1:A:270:PHE:CD2	1:A:317:TYR:HB3	2.49	0.46
1:B:577:GLN:HE22	1:B:582:PHE:H	1.62	0.46
1:B:1296:ASN:HB3	1:B:1299:VAL:HG22	1.98	0.46
1:A:1848:TYR:HA	1:A:1851:ILE:HD12	1.96	0.46
1:B:281:VAL:HG22	1:B:333:VAL:HG23	1.98	0.46
1:B:570:TYR:HA	1:B:573:LEU:HD12	1.96	0.46
1:B:1626:TYR:HA	1:B:1629:VAL:HG12	1.97	0.46
1:B:1785:ASP:OD1	1:B:1785:ASP:N	2.48	0.46
1:A:278:LYS:HA	1:A:328:MET:HE2	1.97	0.46
1:A:698:ASP:OD1	1:A:698:ASP:N	2.47	0.46
1:B:1637:PRO:O	1:B:1640:THR:OG1	2.28	0.46
1:A:1238:ILE:HG13	1:A:1239:ILE:HG13	1.97	0.46
1:B:2515:LEU:HD11	1:B:2523:MET:HE1	1.98	0.46
2:C:755:VAL:O	2:C:759:ILE:HG12	2.16	0.46
2:C:759:ILE:HA	2:C:762:LEU:HD23	1.97	0.46
1:A:1010:ALA:O	1:A:1014:ILE:HG12	2.15	0.46
1:A:2403:GLY:O	1:A:2407:ARG:NE	2.49	0.46
1:A:2564:GLU:O	1:A:2566:SER:N	2.49	0.46
1:B:335:MET:HE2	1:B:382:VAL:HA	1.98	0.46
1:B:1715:LEU:HD12	1:B:1742:SER:HA	1.98	0.46
1:A:304:PRO:HD2	1:A:309:ALA:HB1	1.97	0.46
1:A:1185:LYS:HZ2	1:A:1222:LEU:HD11	1.81	0.46
1:A:2076:LEU:HD13	1:A:2087:MET:HE2	1.97	0.46
1:A:1070:GLN:HE22	4:H:1154:ARG:HA	1.81	0.45
1:B:76:MET:HE1	1:B:133:LEU:HD23	1.98	0.45
2:C:695:HIS:HA	2:C:751:VAL:HG21	1.98	0.45
1:B:1737:HIS:CE1	1:B:1769:GLU:HB3	2.48	0.45
1:A:2619:HIS:O	1:A:2623:LEU:HG	2.17	0.45
1:B:353:PHE:O	1:B:368:ARG:NH2	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:710:ILE:O	1:B:714:LEU:CB	2.65	0.45
1:B:2177:TRP:NE1	1:B:2259:LEU:O	2.49	0.45
1:A:991:LEU:HB2	1:A:1021:LEU:HD21	1.98	0.45
1:A:1145:ILE:HA	1:A:1148:LYS:HD2	1.99	0.45
1:B:2175:ALA:O	1:B:2179:MET:HG2	2.16	0.45
2:C:421:PRO:O	2:C:424:GLN:HB2	2.16	0.45
1:A:17:GLU:HG3	1:A:29:VAL:HG13	1.98	0.45
1:A:1083:ILE:HA	1:A:1090:VAL:HG11	1.98	0.45
1:A:1691:GLY:HA3	1:A:2530:GLY:HA2	1.98	0.45
1:A:2402:THR:OG1	1:A:2405:GLU:OE1	2.33	0.45
1:A:2514:ARG:NH2	1:A:2644:MET:OXT	2.50	0.45
1:B:1471:TRP:HB3	1:B:1497:TYR:HD1	1.81	0.45
1:B:2024:LYS:HA	1:B:2024:LYS:HD3	1.68	0.45
1:B:2390:LEU:HD21	1:B:2436:PHE:HD1	1.81	0.45
2:C:698:TRP:CH2	2:C:702:ARG:HG2	2.52	0.45
1:A:316:VAL:O	1:A:320:MET:HG3	2.17	0.45
1:A:1992:GLU:HB2	1:A:1995:ASN:HB2	1.99	0.45
1:B:999:LEU:HD13	1:B:1014:ILE:HD13	1.97	0.45
1:B:1533:LEU:HA	1:B:1536:VAL:HG12	1.99	0.45
1:A:976:SER:HA	1:A:987:LEU:HD13	1.98	0.45
1:A:1255:LEU:HD12	1:A:1256:PRO:HD2	1.99	0.45
1:B:2026:LYS:HA	1:B:2029:THR:HG22	1.99	0.45
2:D:424:GLN:O	2:D:428:GLY:N	2.46	0.45
1:A:767:LEU:HG	1:A:808:THR:HG21	1.99	0.45
1:A:1239:ILE:HG12	1:A:1267:VAL:HG11	1.97	0.45
1:B:1776:GLU:HA	1:B:1779:TRP:CD1	2.52	0.45
1:A:264:GLN:NE2	2:C:487:CYS:SG	2.74	0.45
1:A:1212:LEU:O	1:A:1216:ILE:HG12	2.16	0.45
1:A:1918:GLU:HG3	1:A:1950:SER:HB3	1.99	0.45
1:B:2446:ASP:O	1:B:2450:TRP:N	2.46	0.45
2:D:553:THR:HA	2:D:557:GLN:HB2	1.99	0.45
1:A:1771:ASN:OD1	1:A:1774:ARG:NE	2.46	0.45
1:A:1898:GLU:OE1	1:A:1927:SER:OG	2.35	0.45
1:B:2325:MET:HE3	1:B:2327:LYS:HB2	1.98	0.45
1:B:2422:LYS:O	1:B:2426:GLU:HB2	2.17	0.45
2:C:578:ASP:N	2:C:578:ASP:OD1	2.50	0.45
2:D:712:GLN:O	2:D:716:THR:OG1	2.30	0.45
1:A:1081:LEU:O	1:A:1154:SER:OG	2.31	0.44
1:A:1340:LEU:CB	1:A:1839:PHE:CZ	2.89	0.44
1:B:285:THR:HA	1:B:288:LEU:HD12	1.99	0.44
1:B:1722:TYR:CZ	1:B:1738:GLY:HA3	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:LEU:HD11	1:A:493:ILE:HD13	1.98	0.44
1:A:1328:VAL:HG13	1:A:1368:ARG:HB3	1.99	0.44
1:B:995:LEU:HA	1:B:998:LEU:HG	1.99	0.44
2:D:656:GLU:HG2	2:D:697:GLN:HE22	1.82	0.44
1:A:1585:LEU:HD23	1:A:1588:LEU:HD12	1.98	0.44
1:B:538:ASP:OD1	1:B:538:ASP:N	2.48	0.44
1:B:649:LEU:HA	1:B:652:ARG:CZ	2.46	0.44
1:B:1944:LEU:HD13	1:B:1958:GLU:HG3	1.99	0.44
1:B:2440:PHE:HE2	1:B:2454:ARG:HA	1.81	0.44
2:D:312:LEU:HD13	2:D:488:HIS:HB2	1.99	0.44
1:A:466:LEU:HD22	1:A:496:VAL:HG23	1.98	0.44
1:A:536:SER:OG	1:A:538:ASP:OD1	2.35	0.44
1:A:1504:HIS:HB3	1:A:1507:ALA:HB3	1.99	0.44
1:A:1781:LEU:HA	1:A:1781:LEU:HD23	1.80	0.44
1:B:565:LYS:HA	1:B:565:LYS:HD2	1.75	0.44
1:B:1660:SER:O	1:B:1664:GLU:HB2	2.18	0.44
1:A:453:HIS:HE1	1:A:533:THR:HG23	1.82	0.44
1:A:2077:GLN:HB3	1:A:2133:LEU:HD23	1.99	0.44
1:B:908:TYR:HD1	1:B:981:VAL:HG13	1.82	0.44
1:B:1085:GLU:H	1:B:1150:MET:HE1	1.83	0.44
1:B:1288:SER:O	1:B:1292:ILE:HG12	2.18	0.44
2:D:725:LEU:HD12	2:D:725:LEU:HA	1.89	0.44
1:A:100:SER:O	1:A:104:ILE:HG13	2.17	0.44
1:A:1659:GLU:OE1	1:A:2525:PRO:HD2	2.18	0.44
1:A:2123:ASN:HB3	1:A:2159:VAL:HG21	2.00	0.44
1:B:300:LYS:HD3	1:B:348:HIS:CD2	2.52	0.44
1:B:1011:SER:HA	1:B:1014:ILE:HG22	2.00	0.44
1:B:1397:LEU:HD23	1:B:1397:LEU:HA	1.68	0.44
1:A:1177:THR:O	1:A:1180:THR:OG1	2.30	0.44
1:B:502:LEU:HD11	1:B:741:PHE:CE2	2.53	0.44
1:B:1083:ILE:HG23	1:B:1157:SER:HB2	1.99	0.44
1:B:1173:LYS:O	1:B:1176:THR:OG1	2.34	0.44
2:D:486:VAL:O	2:D:574:ASN:ND2	2.50	0.44
1:B:2124:LYS:O	1:B:2127:THR:HB	2.18	0.44
1:A:551:LEU:O	1:A:623:ARG:NH2	2.51	0.43
1:A:1558:HIS:O	1:A:1647:ARG:NH1	2.51	0.43
1:B:44:ILE:HD12	1:B:68:LEU:HD11	2.00	0.43
1:B:1625:ASP:O	1:B:1628:SER:OG	2.27	0.43
1:B:2245:MET:SD	1:B:2245:MET:N	2.88	0.43
1:A:1536:VAL:HG12	1:A:1537:LEU:HD22	2.00	0.43
1:B:484:ASN:ND2	1:B:489:MET:SD	2.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1182:LEU:HD11	1:B:1218:ALA:HB1	2.00	0.43
1:B:1397:LEU:HD21	1:B:1424:LEU:HD13	2.00	0.43
1:B:2415:ALA:HB3	1:B:2420:LYS:HE3	2.00	0.43
1:B:2481:ILE:HD12	1:B:2514:ARG:HD3	2.00	0.43
2:C:496:LEU:HD21	2:C:538:LEU:HD23	1.99	0.43
1:A:162:ARG:HH21	1:A:167:HIS:HB3	1.83	0.43
1:A:2500:ASN:HD21	1:A:2598:ARG:HH22	1.65	0.43
1:B:249:ILE:O	1:B:253:THR:HG23	2.19	0.43
1:B:398:ALA:O	1:B:401:LYS:HB3	2.19	0.43
1:B:1063:GLU:OE2	1:B:1066:SER:N	2.50	0.43
1:B:1622:ASP:OD1	1:B:1622:ASP:N	2.51	0.43
1:B:1767:THR:O	1:B:1771:ASN:CB	2.64	0.43
1:B:2470:ILE:HD11	1:B:2540:MET:HE1	1.99	0.43
1:A:36:ILE:HA	1:A:39:GLN:OE1	2.17	0.43
1:A:152:LEU:HA	1:A:177:ARG:HG3	2.00	0.43
1:A:1591:TRP:HZ3	1:A:1629:VAL:HG11	1.84	0.43
1:B:577:GLN:NE2	1:B:581:SER:HA	2.34	0.43
1:B:1762:ASN:OD1	1:B:1763:ARG:N	2.52	0.43
2:C:434:LEU:HA	2:C:437:LEU:HG	2.01	0.43
1:A:471:GLU:HG3	1:A:539:PHE:HE2	1.82	0.43
1:A:541:THR:HG22	1:A:586:ILE:HD11	2.00	0.43
1:A:1832:VAL:HB	1:A:1833:PRO:HD3	2.00	0.43
1:A:2189:MET:HE2	1:A:2193:ARG:NH1	2.33	0.43
1:B:74:HIS:HA	1:B:77:LYS:HG2	2.00	0.43
1:A:1464:SER:HA	4:H:1143:ILE:HA	2.00	0.43
1:B:490:LEU:HD23	1:B:493:ILE:HD11	2.00	0.43
1:B:1677:GLN:HE21	1:B:1689:VAL:HG13	1.83	0.43
1:B:1771:ASN:HA	1:B:1774:ARG:HG2	2.01	0.43
1:A:273:PHE:HE1	1:A:295:LEU:HD11	1.82	0.43
1:A:1840:GLU:O	1:A:1841:ARG:C	2.62	0.43
1:A:2026:LYS:HA	1:A:2029:THR:HG22	2.00	0.43
1:B:326:CYS:O	1:B:330:GLU:HB2	2.18	0.43
1:B:1507:ALA:HA	1:B:1510:ILE:HG22	2.00	0.43
2:C:764:ASP:OD1	2:C:764:ASP:N	2.50	0.43
2:D:614:ALA:HB2	2:D:623:LEU:HD11	2.00	0.43
1:A:839:ASP:OD1	1:A:839:ASP:N	2.52	0.43
1:B:14:ALA:HB1	1:B:33:PRO:HB3	2.00	0.43
1:B:270:PHE:CD2	1:B:317:TYR:HB3	2.54	0.43
1:B:1800:TRP:HE3	1:B:1830:GLN:HG2	1.83	0.43
1:A:135:LYS:HG2	1:A:219:ILE:HD11	2.00	0.43
1:A:463:TRP:CZ2	1:A:534:TRP:HB3	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:VAL:HG12	1:B:57:LYS:HE3	2.00	0.43
1:B:315:PRO:HG2	2:D:318:LYS:HD2	2.01	0.43
2:C:434:LEU:HD13	2:C:437:LEU:HD21	2.00	0.43
1:A:1124:GLN:HA	1:A:1127:LEU:HB3	2.01	0.43
1:A:1522:PHE:O	1:A:1525:THR:OG1	2.28	0.43
1:A:2354:GLU:OE1	1:A:2358:ARG:NH1	2.43	0.43
1:B:2386:LEU:HD13	1:B:2483:PHE:HE2	1.84	0.43
1:A:1070:GLN:OE1	4:H:1154:ARG:NE	2.51	0.42
1:A:1344:GLN:HE22	1:A:1837:ALA:HA	1.83	0.42
1:B:1908:LEU:HD13	1:B:1919:MET:HB3	2.01	0.42
1:B:2436:PHE:HD2	1:B:2522:GLY:HA3	1.84	0.42
1:A:547:CYS:HA	1:A:550:LEU:HG	2.02	0.42
1:A:1083:ILE:HG13	1:A:1090:VAL:HG11	2.00	0.42
1:A:1212:LEU:HD11	1:A:1238:ILE:HG22	2.01	0.42
1:A:1722:TYR:HB3	1:A:1739:VAL:HG23	2.01	0.42
1:A:2221:LYS:HA	1:A:2221:LYS:HD3	1.88	0.42
1:B:97:ILE:O	1:B:101:ASN:HB2	2.19	0.42
1:B:675:PHE:HZ	1:B:713:GLN:HG2	1.85	0.42
1:B:1230:THR:HG22	1:B:1234:PHE:CZ	2.55	0.42
1:B:2088:PRO:HB3	1:B:2556:THR:HG21	2.02	0.42
1:A:730:GLU:OE1	1:A:733:SER:N	2.53	0.42
1:A:1000:PRO:HB3	1:A:1039:HIS:HB3	2.01	0.42
1:B:559:LEU:HA	1:B:562:THR:HB	2.00	0.42
1:B:612:THR:HG23	1:B:648:PHE:HZ	1.85	0.42
1:B:665:GLU:HA	1:B:668:ARG:HG2	2.02	0.42
1:B:2433:PRO:HA	1:B:2434:PRO:HD3	1.91	0.42
2:C:426:PHE:HD2	2:C:474:PHE:HB3	1.84	0.42
1:A:1336:VAL:HG11	1:A:1369:LEU:HD13	2.02	0.42
1:B:721:MET:HE3	1:B:750:GLN:HG3	2.01	0.42
1:B:1636:ILE:HA	1:B:1637:PRO:HD3	1.86	0.42
1:A:118:LEU:HG	1:A:119:LEU:HD12	2.02	0.42
1:A:1057:LYS:HE2	1:A:1063:GLU:HA	2.02	0.42
1:A:1749:LEU:HA	1:A:1752:VAL:HG12	2.01	0.42
1:B:210:LEU:HD23	1:B:247:LEU:HB3	2.02	0.42
1:B:1039:HIS:O	1:B:1043:SER:OG	2.31	0.42
2:C:427:ILE:HD11	2:C:478:ALA:HB3	2.02	0.42
1:A:222:PHE:HB3	2:C:665:LYS:HE2	2.00	0.42
1:A:363:SER:OG	1:A:364:ALA:N	2.51	0.42
1:A:1446:PHE:HB3	1:A:1450:VAL:HG23	2.01	0.42
1:A:2077:GLN:HG3	1:A:2078:TYR:CD1	2.55	0.42
2:C:428:GLY:O	2:C:431:CYS:HB3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:PRO:HG3	1:A:628:TYR:CE2	2.55	0.42
1:A:850:MET:HE2	1:A:850:MET:HB2	1.89	0.42
1:A:2000:GLY:HA3	1:A:2032:LEU:HD12	2.02	0.42
1:A:2173:GLN:HG3	1:A:2290:TRP:HZ3	1.84	0.42
1:B:390:GLU:HA	1:B:393:LEU:HD13	2.01	0.42
1:B:2112:ARG:HA	1:B:2115:MET:HB3	2.00	0.42
1:A:249:ILE:O	1:A:253:THR:HG23	2.20	0.42
1:A:264:GLN:HE22	2:C:570:LYS:NZ	2.17	0.42
1:A:463:TRP:HZ2	1:A:534:TRP:HB3	1.83	0.42
1:A:544:LEU:HB3	1:A:548:ARG:HH21	1.85	0.42
1:B:638:PHE:O	1:B:641:THR:OG1	2.33	0.42
1:B:1771:ASN:O	1:B:1775:VAL:HG23	2.20	0.42
1:A:2349:LEU:HD23	1:A:2542:LEU:HD23	2.01	0.42
1:B:76:MET:HB3	1:B:83:PHE:CE2	2.54	0.42
1:B:2169:LEU:HB3	1:B:2205:LYS:HD3	2.01	0.42
2:D:546:LEU:HB3	2:D:564:CYS:SG	2.59	0.42
1:A:577:GLN:HG3	1:A:587:LEU:HD21	2.02	0.42
1:A:1461:ARG:HH12	4:H:1148:PRO:HB3	1.85	0.42
1:A:2225:LEU:HD21	1:A:2312:ILE:HG21	2.02	0.42
1:A:2303:LEU:HB2	1:A:2309:PRO:HD2	2.02	0.42
1:B:496:VAL:O	1:B:500:THR:HG23	2.19	0.42
1:B:1138:LEU:HD22	1:B:1180:THR:HB	2.02	0.42
4:G:1158:ALA:HA	4:G:1163:TRP:HB2	2.01	0.42
1:A:73:GLN:HG2	1:A:126:VAL:HG22	2.01	0.41
1:A:889:LEU:HD21	1:A:933:ILE:HD11	2.01	0.41
1:A:1394:TYR:CD2	1:A:1398:MET:HE1	2.55	0.41
1:A:1644:ALA:HA	1:A:1647:ARG:HE	1.84	0.41
1:B:203:GLU:HA	1:B:244:ILE:HD11	2.01	0.41
1:A:716:CYS:HA	1:A:792:HIS:ND1	2.35	0.41
1:B:2105:GLU:HG2	1:B:2112:ARG:HB2	2.02	0.41
1:B:2305:SER:OG	5:B:5001:AGS:O2B	2.38	0.41
2:C:542:LEU:HB3	2:C:568:LEU:HD21	2.02	0.41
2:C:543:LEU:HD11	2:C:586:VAL:HG22	2.02	0.41
1:A:54:GLU:HA	1:A:57:LYS:HD2	2.02	0.41
1:A:205:ILE:HA	1:A:208:THR:HG22	2.03	0.41
1:A:222:PHE:HZ	2:C:668:VAL:HG21	1.85	0.41
1:A:1238:ILE:HD11	1:A:1264:ILE:HG23	2.01	0.41
1:B:652:ARG:NH1	1:B:653:THR:HG23	2.36	0.41
1:B:1115:SER:HA	1:B:1116:PRO:HD3	1.94	0.41
1:B:1852:VAL:HG13	1:B:1900:ILE:HD11	2.02	0.41
1:B:2294:ALA:O	1:B:2315:LYS:NZ	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2305:SER:HB3	1:B:2309:PRO:HD3	2.02	0.41
2:D:535:GLN:HB2	2:D:540:LYS:NZ	2.36	0.41
1:A:1047:ASP:OD1	1:A:1048:GLU:N	2.53	0.41
1:A:1516:ILE:HA	1:A:1519:LYS:HE2	2.01	0.41
1:A:1976:LEU:HD21	1:A:2005:LEU:HB3	2.02	0.41
1:B:821:ARG:HE	1:B:868:THR:HG21	1.85	0.41
1:B:822:VAL:O	1:B:825:SER:OG	2.36	0.41
1:B:838:GLU:HA	1:B:842:ILE:HD11	2.03	0.41
1:B:1190:GLU:HG2	1:B:1191:LEU:HD12	2.03	0.41
1:B:2150:CYS:SG	1:B:2190:ARG:HG3	2.60	0.41
1:A:467:LYS:HE2	1:A:467:LYS:HB3	1.94	0.41
1:A:640:LEU:HD11	1:A:652:ARG:HG2	2.03	0.41
1:A:701:ASP:HA	1:A:704:LYS:HD2	2.02	0.41
1:A:1888:GLU:HB2	1:A:2274:LEU:HD21	2.03	0.41
1:A:2193:ARG:O	1:A:2197:ILE:HD12	2.20	0.41
1:B:470:ALA:HB2	1:B:496:VAL:HG11	2.03	0.41
1:B:1026:ARG:HB3	4:G:1164:PRO:HB3	2.02	0.41
1:B:1212:LEU:O	1:B:1216:ILE:HG12	2.21	0.41
1:B:2151:HIS:O	1:B:2193:ARG:NH2	2.53	0.41
2:D:482:LEU:HD11	2:D:538:LEU:HD21	2.02	0.41
1:A:587:LEU:HD13	1:A:647:ILE:HG13	2.03	0.41
1:A:862:ASN:HB3	1:A:865:LEU:HB3	2.02	0.41
1:A:1538:LEU:HD12	1:A:1538:LEU:HA	1.94	0.41
1:A:2331:ASP:OD1	1:A:2331:ASP:N	2.46	0.41
1:B:283:MET:HE1	1:B:288:LEU:HD23	2.03	0.41
1:B:483:LYS:HB2	1:B:483:LYS:HE2	1.87	0.41
1:B:968:ARG:HE	1:B:1016:THR:HA	1.86	0.41
1:B:2428:LEU:HB3	1:B:2643:TYR:HB3	2.03	0.41
1:B:2515:LEU:HD21	1:B:2528:THR:HG21	2.02	0.41
2:D:571:LEU:HB3	2:D:583:PHE:HZ	1.84	0.41
2:D:587:PHE:HE2	2:D:619:LEU:HD23	1.86	0.41
1:A:331:ASP:O	1:A:336:ARG:NH1	2.48	0.41
1:A:877:GLY:HA3	1:A:914:LEU:HD11	2.03	0.41
1:A:1687:ASP:HB2	1:A:2531:LEU:HD23	2.01	0.41
1:A:2014:ALA:HB3	1:B:2614:LEU:HD21	2.02	0.41
1:A:2221:LYS:O	1:A:2224:GLU:HG3	2.20	0.41
1:B:37:LEU:O	1:B:41:ILE:HG12	2.21	0.41
1:B:114:PRO:O	1:B:117:HIS:ND1	2.48	0.41
1:B:273:PHE:HE1	1:B:295:LEU:HD11	1.85	0.41
2:D:381:LEU:HD23	2:D:421:PRO:HG2	2.01	0.41
1:A:206:GLU:O	1:A:210:LEU:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:GLU:HB3	1:A:389:ALA:HB2	2.02	0.41
1:A:728:LEU:HD23	1:A:744:ASN:HD22	1.85	0.41
1:A:1586:ASP:HB2	1:A:1653:ARG:HH22	1.85	0.41
1:A:2070:LEU:O	1:A:2074:ARG:HG2	2.21	0.41
1:A:2089:ARG:HA	1:A:2089:ARG:HD2	1.86	0.41
1:A:2506:GLU:HG2	1:A:2507:VAL:HG23	2.01	0.41
1:B:746:LYS:HE3	1:B:746:LYS:HB2	1.92	0.41
1:B:780:LEU:HA	1:B:783:ILE:HG22	2.02	0.41
1:B:1216:ILE:HD13	1:B:1219:LEU:HD21	2.03	0.41
1:B:1325:SER:OG	1:B:1327:THR:O	2.33	0.41
1:B:1962:TRP:O	1:B:1965:SER:OG	2.34	0.41
1:B:2135:PRO:HG3	1:B:2166:LYS:HE3	2.03	0.41
2:D:430:HIS:HA	2:D:471:LEU:HD21	2.02	0.41
1:A:45:LEU:HB3	1:A:110:ILE:HD11	2.03	0.41
1:A:366:GLN:O	1:A:370:VAL:HG23	2.20	0.41
1:A:645:ARG:NH2	1:A:720:GLY:O	2.54	0.41
1:A:972:LEU:HD12	1:A:972:LEU:HA	1.89	0.41
1:A:1119:MET:HE3	1:A:1119:MET:HB3	1.89	0.41
1:A:1123:LEU:O	1:A:1127:LEU:N	2.52	0.41
1:A:1182:LEU:HD11	1:A:1218:ALA:HB1	2.03	0.41
1:A:1905:ARG:HH12	1:A:1927:SER:HB2	1.86	0.41
1:A:2245:MET:SD	1:A:2245:MET:N	2.80	0.41
1:B:883:ASP:C	1:B:886:PRO:HD2	2.45	0.41
1:B:1706:ILE:HD11	1:B:1725:ALA:HB2	2.02	0.41
1:B:2157:PHE:CZ	1:B:2193:ARG:HD2	2.55	0.41
1:A:265:PRO:HB3	2:C:408:PHE:CE1	2.56	0.40
1:A:538:ASP:OD1	1:A:539:PHE:N	2.54	0.40
1:A:1039:HIS:O	1:A:1043:SER:OG	2.37	0.40
1:B:911:ILE:O	1:B:915:VAL:HG23	2.21	0.40
1:B:1042:CYS:HB2	1:B:1086:HIS:ND1	2.36	0.40
2:C:469:CYS:O	2:C:472:GLU:HG3	2.21	0.40
1:A:314:GLU:HB3	1:A:317:TYR:CD1	2.56	0.40
1:A:380:LEU:HD23	1:A:380:LEU:HA	1.88	0.40
1:A:690:LYS:HA	1:A:690:LYS:HD3	1.97	0.40
1:A:813:MET:HE2	1:A:824:PHE:CE2	2.54	0.40
1:A:2022:MET:HG3	1:A:2045:TYR:HE2	1.86	0.40
1:B:93:LYS:HB3	1:B:141:ILE:HD11	2.03	0.40
1:B:120:HIS:HA	1:B:123:ILE:HD12	2.03	0.40
1:B:2404:LYS:O	1:B:2407:ARG:HG2	2.21	0.40
2:D:406:ARG:NH1	2:D:407:ALA:H	2.19	0.40
1:A:223:ARG:HD3	1:A:223:ARG:HA	1.83	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:CYS:HB3	1:A:792:HIS:HE2	1.86	0.40
1:A:1080:LEU:HD11	1:A:1123:LEU:HD21	2.02	0.40
1:A:1222:LEU:HD23	1:A:1222:LEU:HA	1.94	0.40
1:A:1622:ASP:N	1:A:1622:ASP:OD1	2.54	0.40
1:A:2558:LEU:HD23	1:A:2558:LEU:HA	1.95	0.40
1:B:1365:ASP:N	1:B:1889:MET:O	2.52	0.40
1:B:2022:MET:HG3	1:B:2046:TYR:HE1	1.87	0.40
1:B:2403:GLY:HA2	1:B:2406:LEU:HD13	2.03	0.40
2:C:584:GLN:OE1	2:C:622:GLN:NE2	2.54	0.40
2:D:703:ARG:HA	2:D:703:ARG:CZ	2.51	0.40
1:A:1260:GLU:O	1:A:1264:ILE:HD12	2.21	0.40
1:A:1448:GLU:HA	1:A:1451:ARG:HG2	2.03	0.40
1:A:2338:LEU:HD22	1:A:2498:LEU:HD11	2.03	0.40
1:B:501:ALA:HB1	1:B:575:TYR:HD2	1.86	0.40
1:B:635:ARG:HA	1:B:740:LEU:HD11	2.03	0.40
1:B:638:PHE:CE2	1:B:642:LEU:HD11	2.56	0.40
1:A:288:LEU:O	1:A:292:GLU:HB2	2.21	0.40
1:A:547:CYS:O	1:A:551:LEU:HG	2.20	0.40
1:A:665:GLU:OE2	1:A:668:ARG:NH1	2.40	0.40
1:B:576:MET:HE3	1:B:576:MET:HB2	1.87	0.40
1:B:896:LEU:HD21	1:B:981:VAL:HG21	2.04	0.40
1:B:1178:LEU:HD13	1:B:1196:TRP:CH2	2.56	0.40
2:C:725:LEU:HD23	2:C:725:LEU:HA	1.89	0.40
2:D:496:LEU:HD23	2:D:496:LEU:HA	1.96	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	2460/2644 (93%)	2370 (96%)	89 (4%)	1 (0%)	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	2452/2644 (93%)	2372 (97%)	78 (3%)	2 (0%)	48	79
2	C	349/791 (44%)	337 (97%)	12 (3%)	0	100	100
2	D	349/791 (44%)	341 (98%)	8 (2%)	0	100	100
3	E	5/14 (36%)	5 (100%)	0	0	100	100
3	F	4/14 (29%)	3 (75%)	1 (25%)	0	100	100
4	G	56/545 (10%)	55 (98%)	1 (2%)	0	100	100
4	H	54/545 (10%)	50 (93%)	4 (7%)	0	100	100
All	All	5729/7988 (72%)	5533 (97%)	193 (3%)	3 (0%)	49	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2565	TRP
1	B	614	ALA
1	B	172	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2216/2363 (94%)	2216 (100%)	0	100	100
1	B	2213/2363 (94%)	2213 (100%)	0	100	100
2	C	319/678 (47%)	319 (100%)	0	100	100
2	D	319/678 (47%)	319 (100%)	0	100	100
3	E	6/13 (46%)	6 (100%)	0	100	100
3	F	5/13 (38%)	5 (100%)	0	100	100
4	G	27/482 (6%)	27 (100%)	0	100	100
4	H	25/482 (5%)	25 (100%)	0	100	100
All	All	5130/7072 (72%)	5130 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	264	GLN
1	A	453	HIS
1	A	468	GLN
1	A	633	GLN
1	A	682	GLN
1	A	787	HIS
1	A	935	GLN
1	A	966	HIS
1	A	1077	ASN
1	A	1092	ASN
1	A	1137	GLN
1	A	1344	GLN
1	A	1436	ASN
1	A	1531	HIS
1	A	1667	GLN
1	A	1970	HIS
1	A	2077	GLN
1	A	2381	ASN
1	A	2518	ASN
1	B	163	ASN
1	B	374	ASN
1	B	579	ASN
1	B	682	GLN
1	B	713	GLN
1	B	785	ASN
1	B	1088	GLN
1	B	1135	ASN
1	B	1153	ASN
1	B	1205	HIS
1	B	1241	ASN
1	B	1293	GLN
1	B	1587	HIS
1	B	1667	GLN
1	B	1830	GLN
1	B	1970	HIS
1	B	1995	ASN
1	B	2080	ASN
1	B	2129	HIS
1	B	2131	ASN
1	B	2153	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2437	HIS
1	B	2521	ASN
1	B	2591	HIS
2	C	657	GLN
2	C	732	GLN
2	D	308	GLN
2	D	432	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 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	AGS	B	5001	6	29,33,33	0.49	1 (3%)	39,52,52	0.82	1 (2%)
5	AGS	A	5001	6	29,33,33	0.48	0	39,52,52	0.88	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AGS	B	5001	6	-	5/21/38/38	0/3/3/3
5	AGS	A	5001	6	-	3/21/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	5001	AGS	PG-S1G	2.06	1.95	1.90

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	5001	AGS	PA-O3A-PB	-4.77	116.45	132.83
5	B	5001	AGS	PA-O3A-PB	-4.52	117.31	132.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	5001	AGS	O4'-C4'-C5'-O5'
5	B	5001	AGS	C3'-C4'-C5'-O5'
5	B	5001	AGS	PG-O3B-PB-O1B
5	A	5001	AGS	PB-O3A-PA-O2A
5	A	5001	AGS	O4'-C4'-C5'-O5'
5	B	5001	AGS	PG-O3B-PB-O2B
5	B	5001	AGS	C5'-O5'-PA-O1A
5	A	5001	AGS	C3'-C4'-C5'-O5'

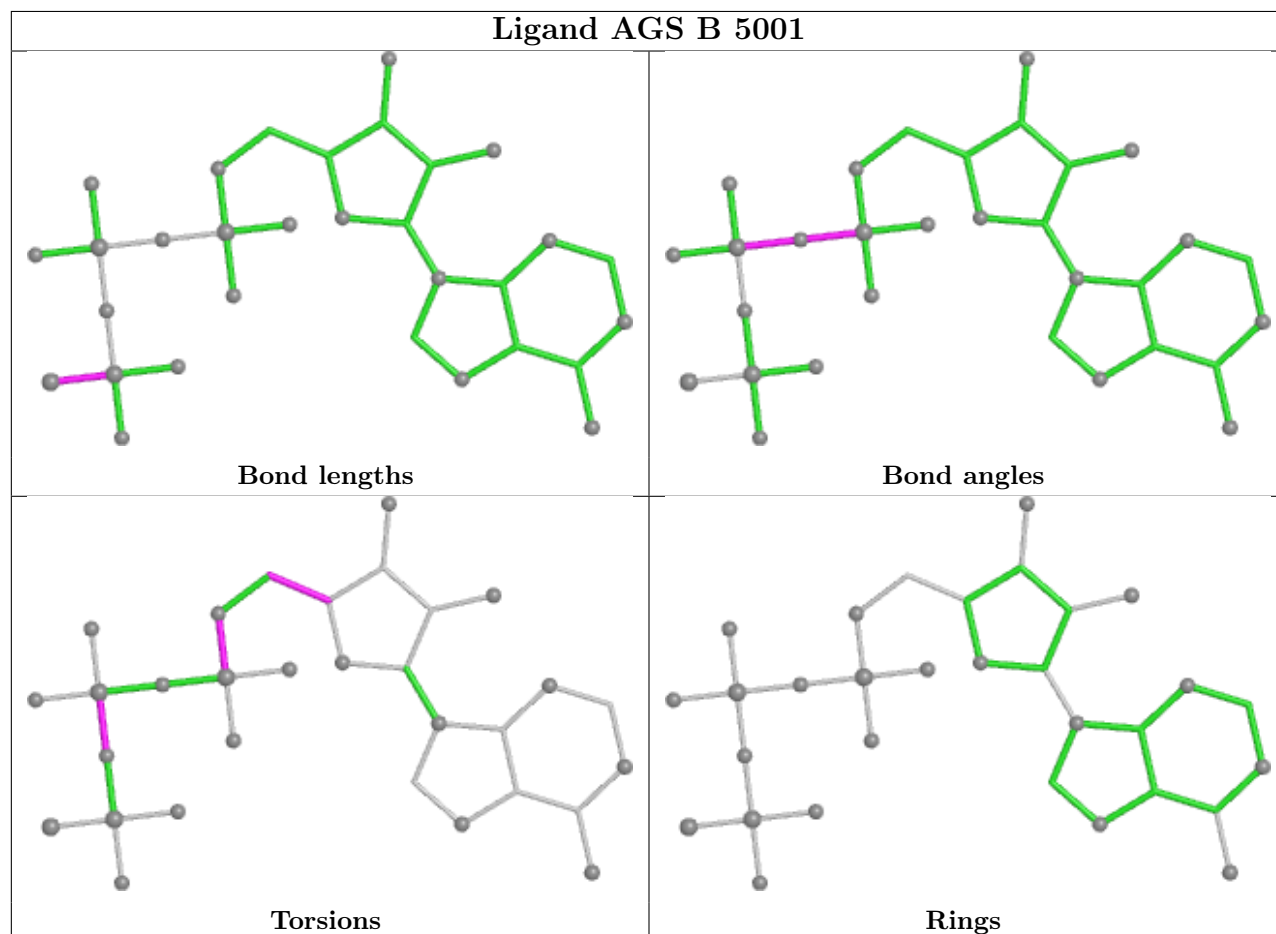
There are no ring outliers.

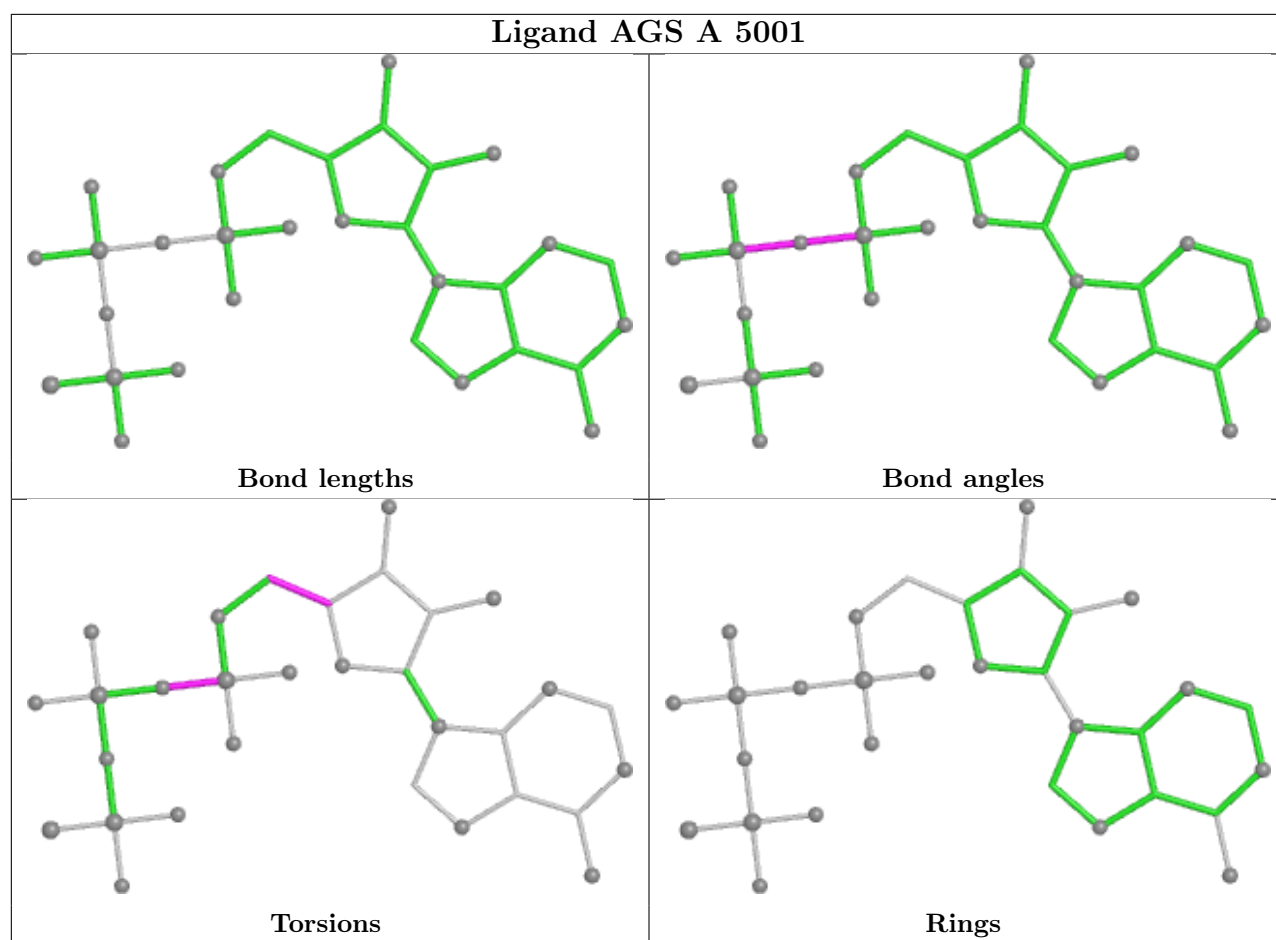
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	5001	AGS	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

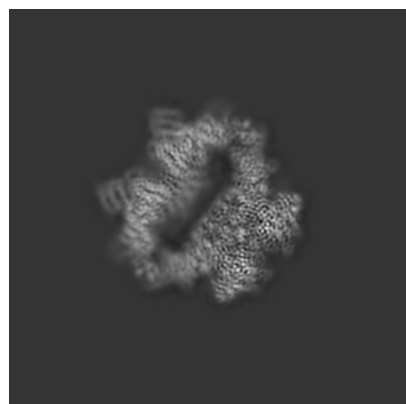
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-68920. These allow visual inspection of the internal detail of the map and identification of artifacts.

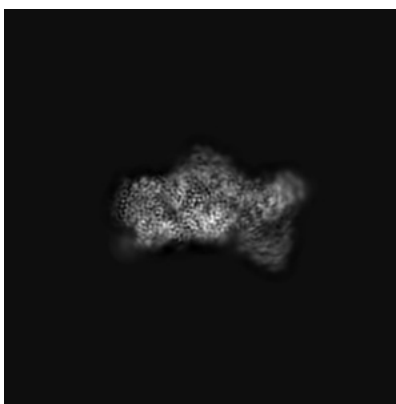
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

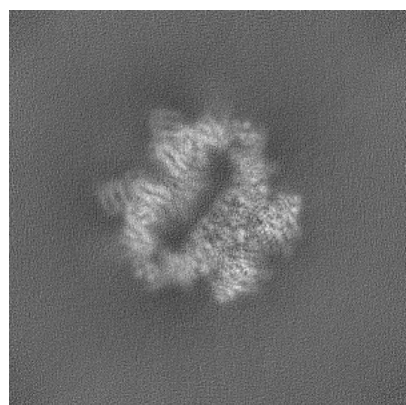


Y

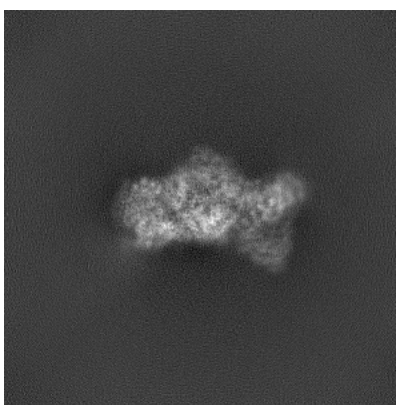


Z

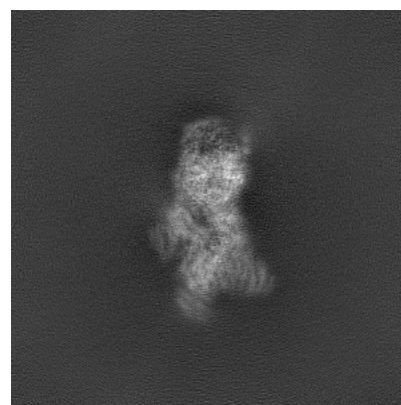
6.1.2 Raw map



X



Y

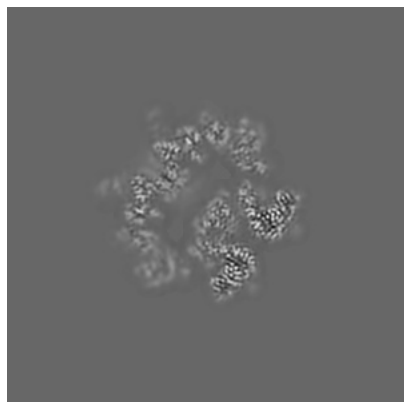


Z

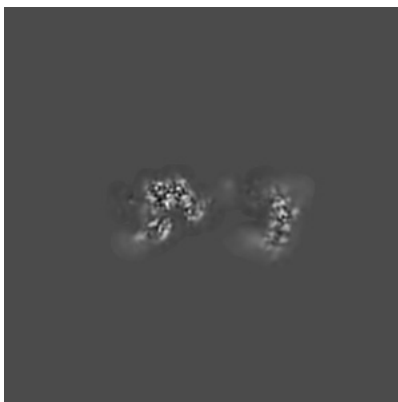
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

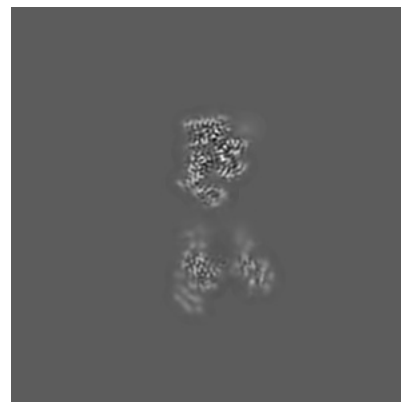
6.2.1 Primary map



X Index: 216

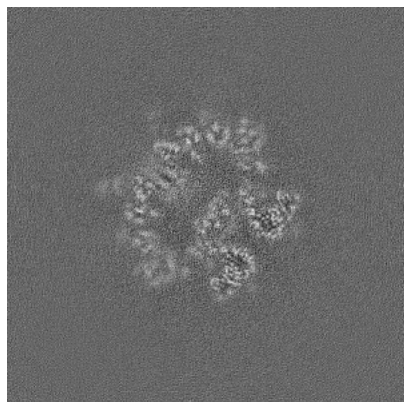


Y Index: 216

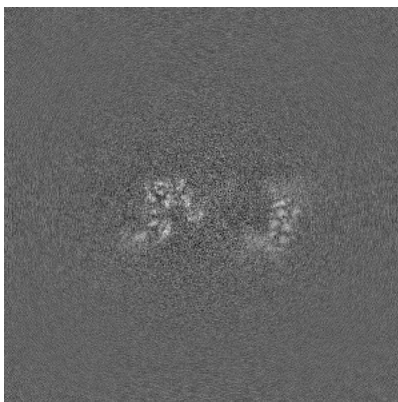


Z Index: 216

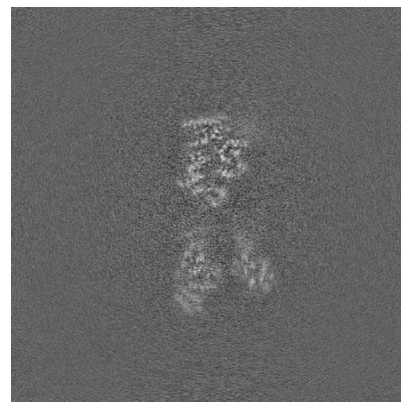
6.2.2 Raw map



X Index: 216



Y Index: 216

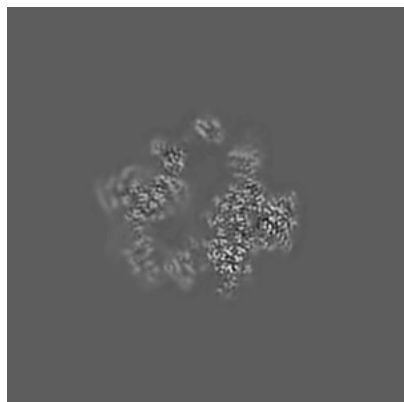


Z Index: 216

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

6.3 Largest variance slices [i](#)

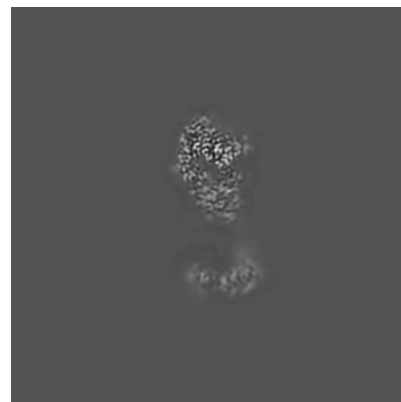
6.3.1 Primary map



X Index: 201

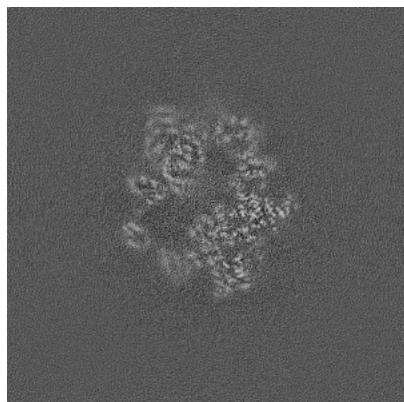


Y Index: 252

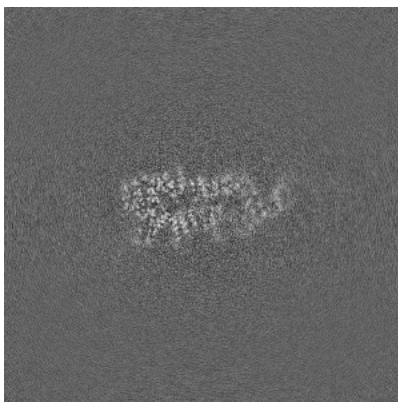


Z Index: 195

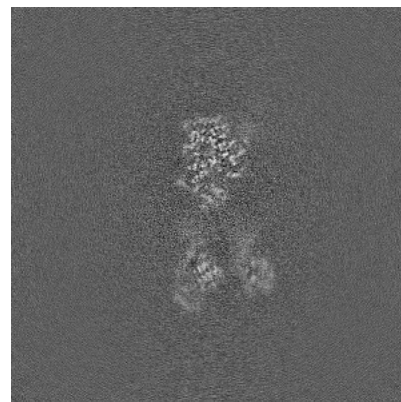
6.3.2 Raw map



X Index: 230



Y Index: 251

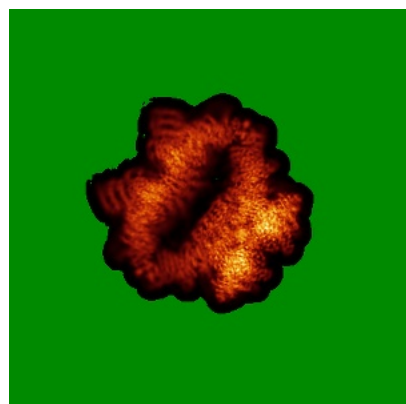


Z Index: 213

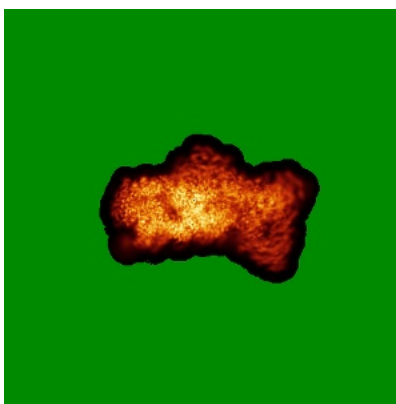
The images above show the largest variance slices of the map in three orthogonal directions.

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

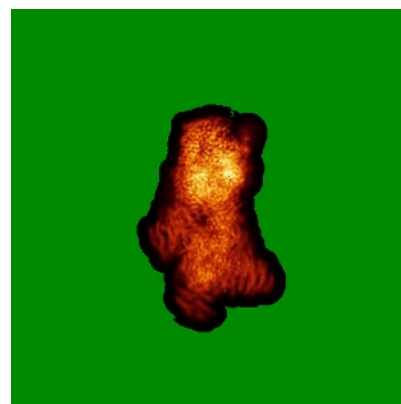
6.4.1 Primary map



X

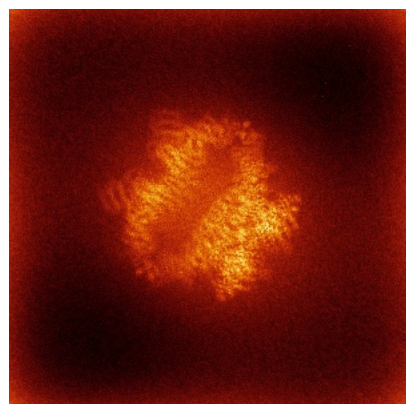


Y

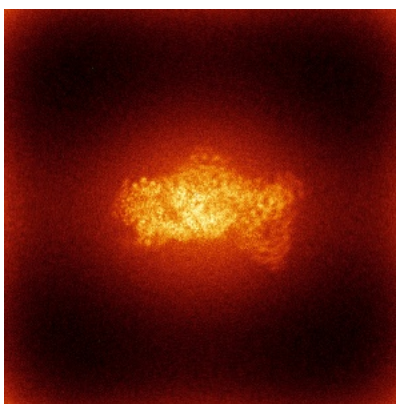


Z

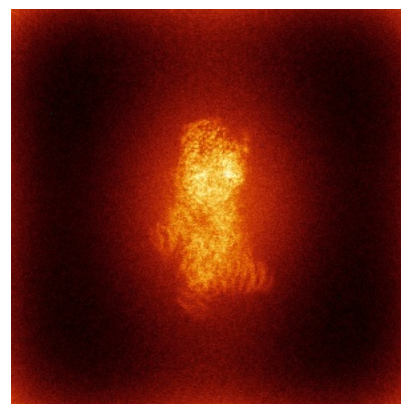
6.4.2 Raw map



X



Y

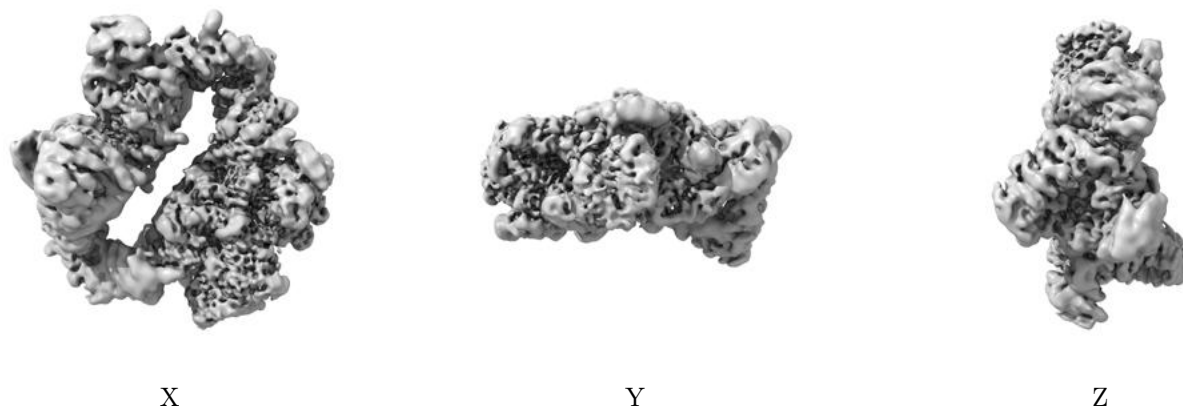


Z

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

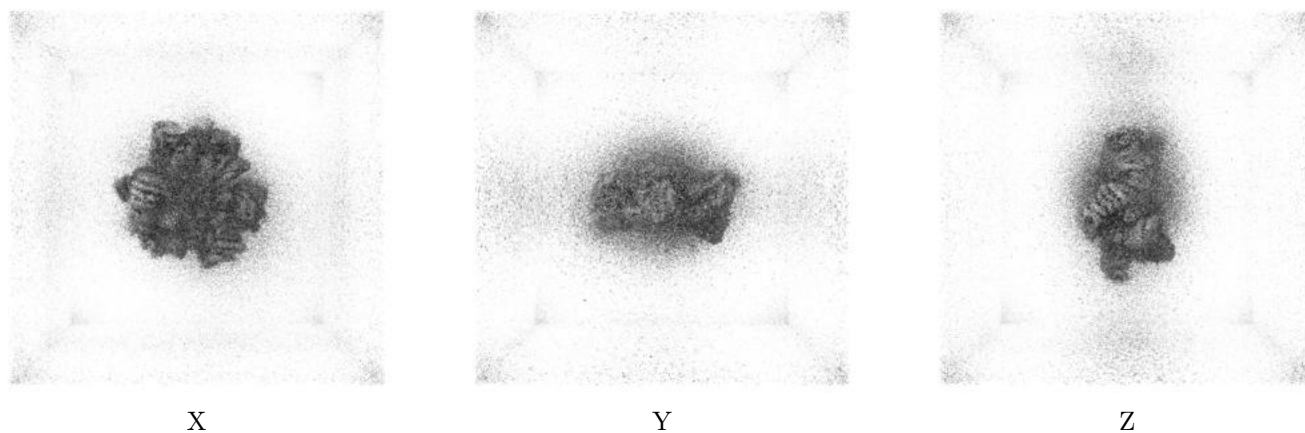
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

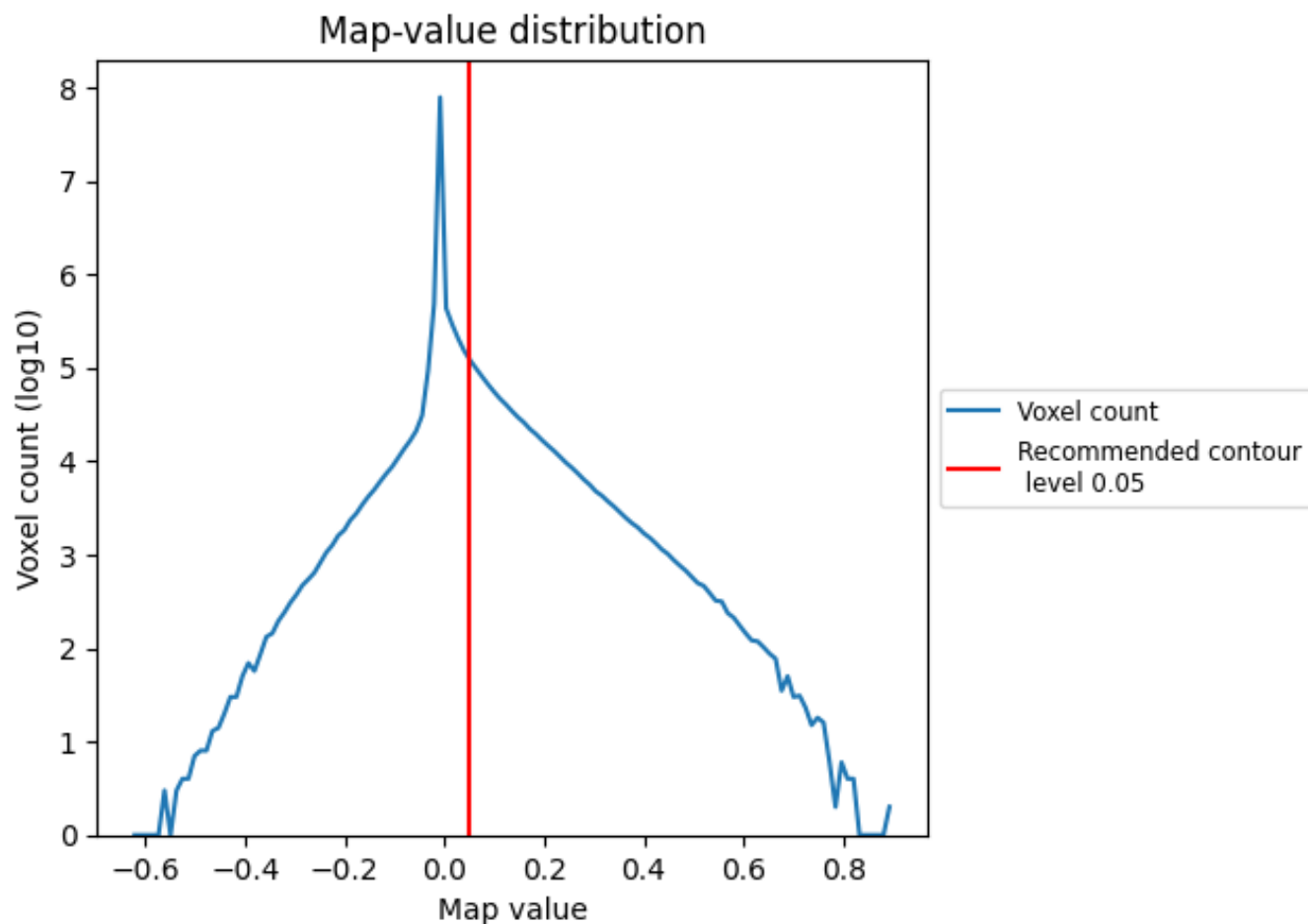
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

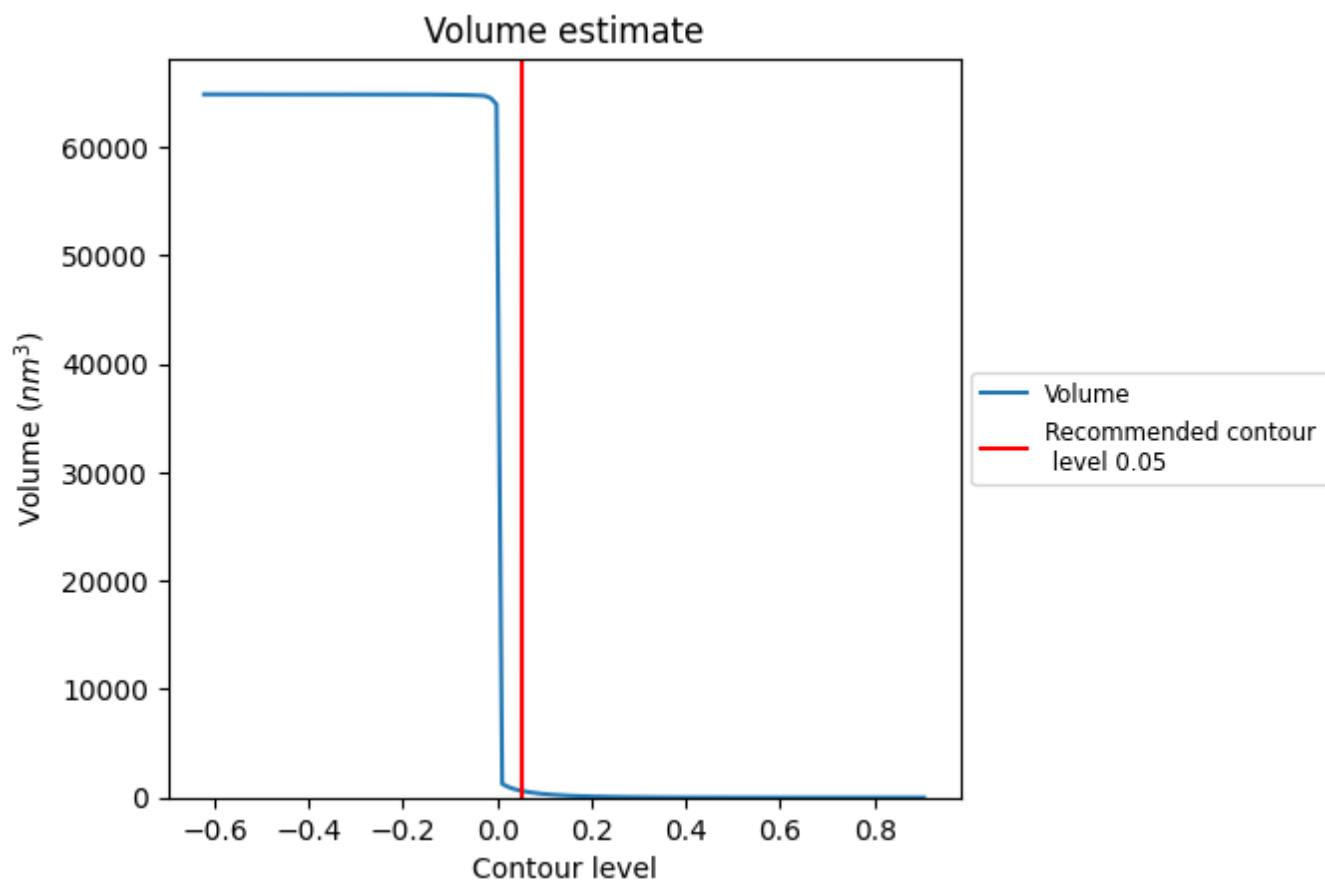
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

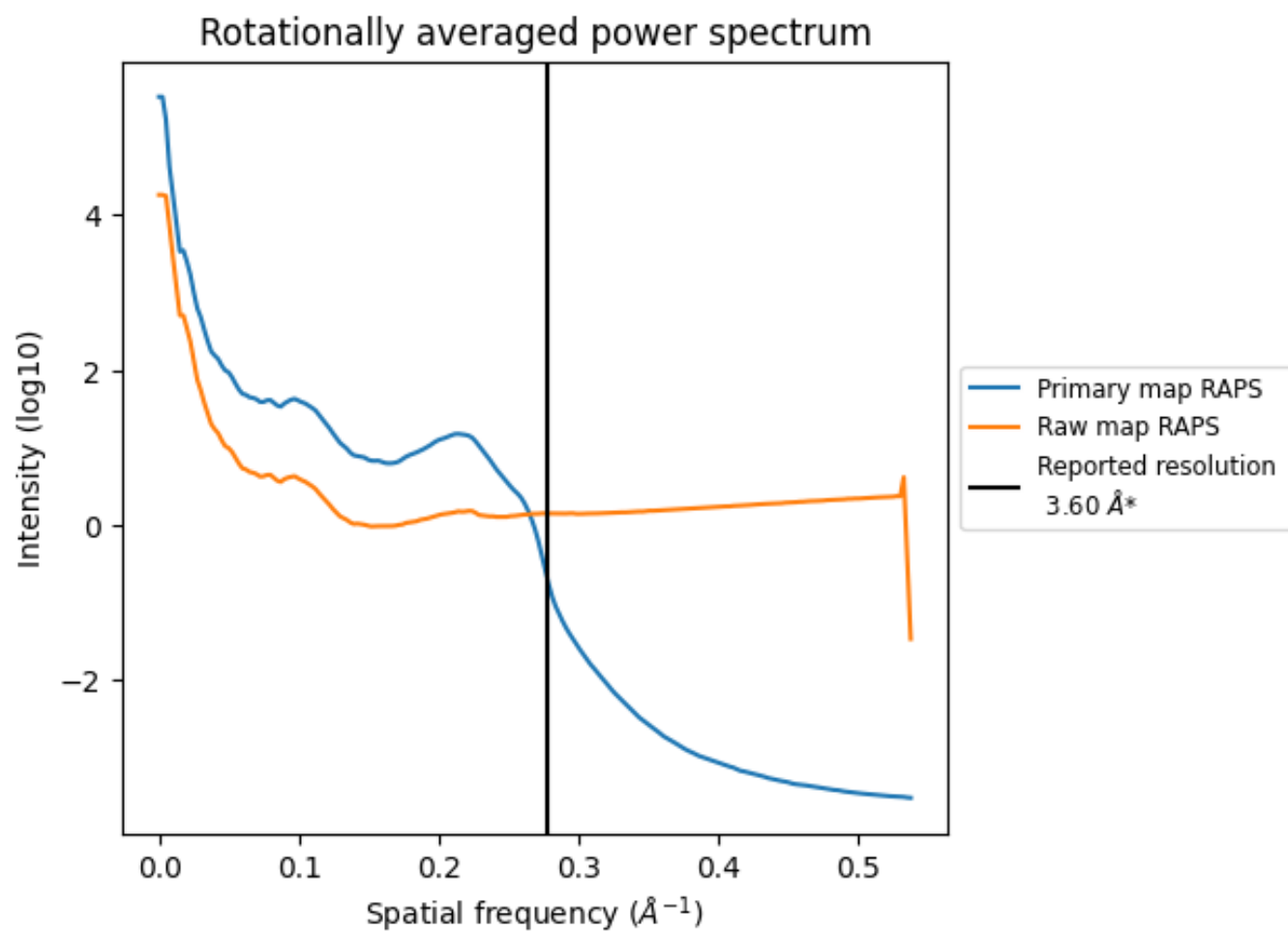
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 635 nm³; this corresponds to an approximate mass of 573 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 ⓘ

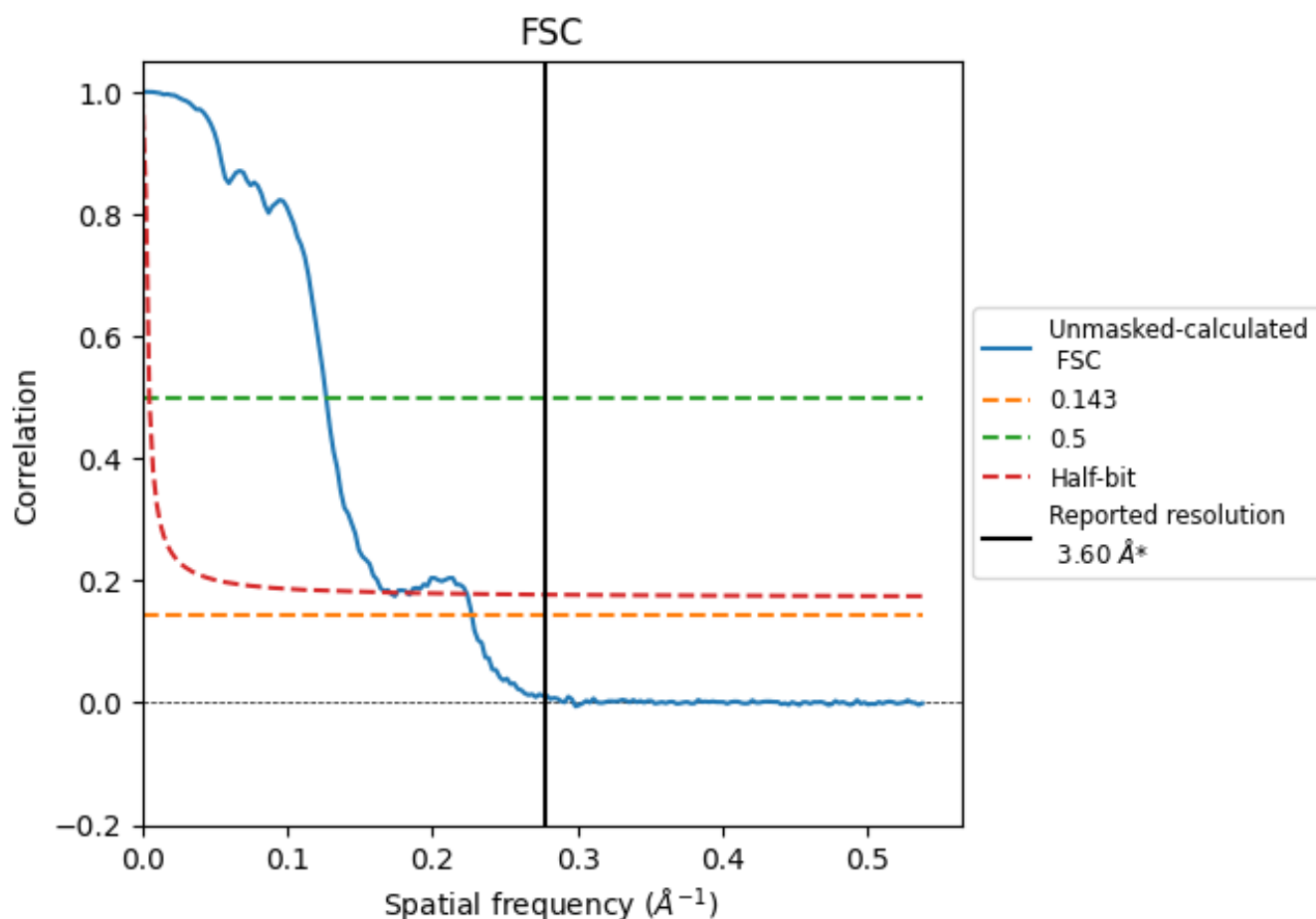


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

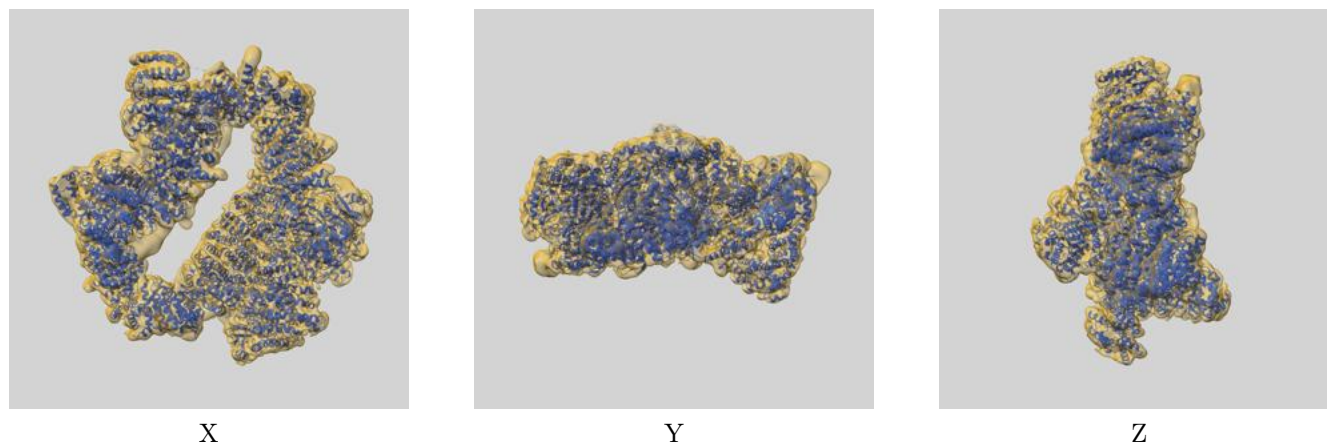
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.40	7.89	5.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.40 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

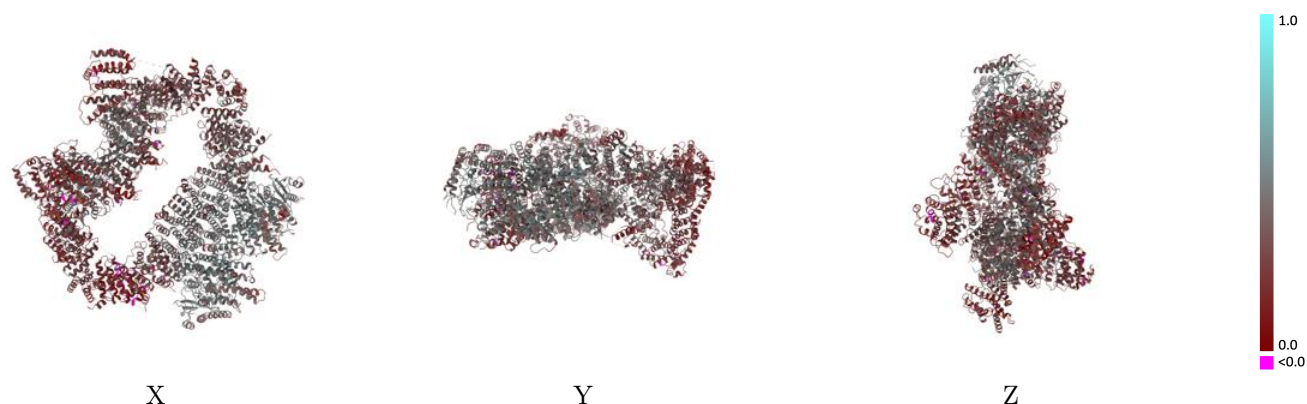
This section contains information regarding the fit between EMDB map EMD-68920 and PDB model 23FD. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



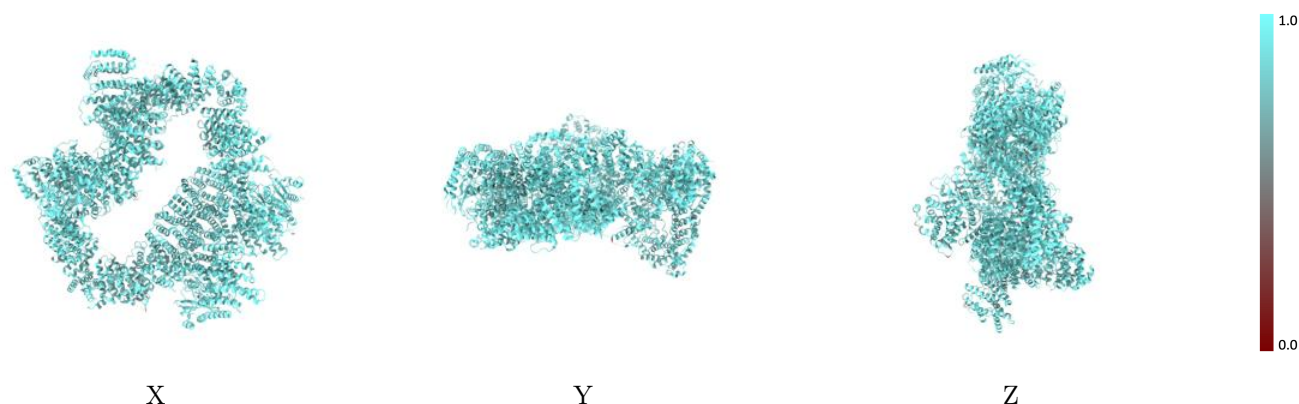
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



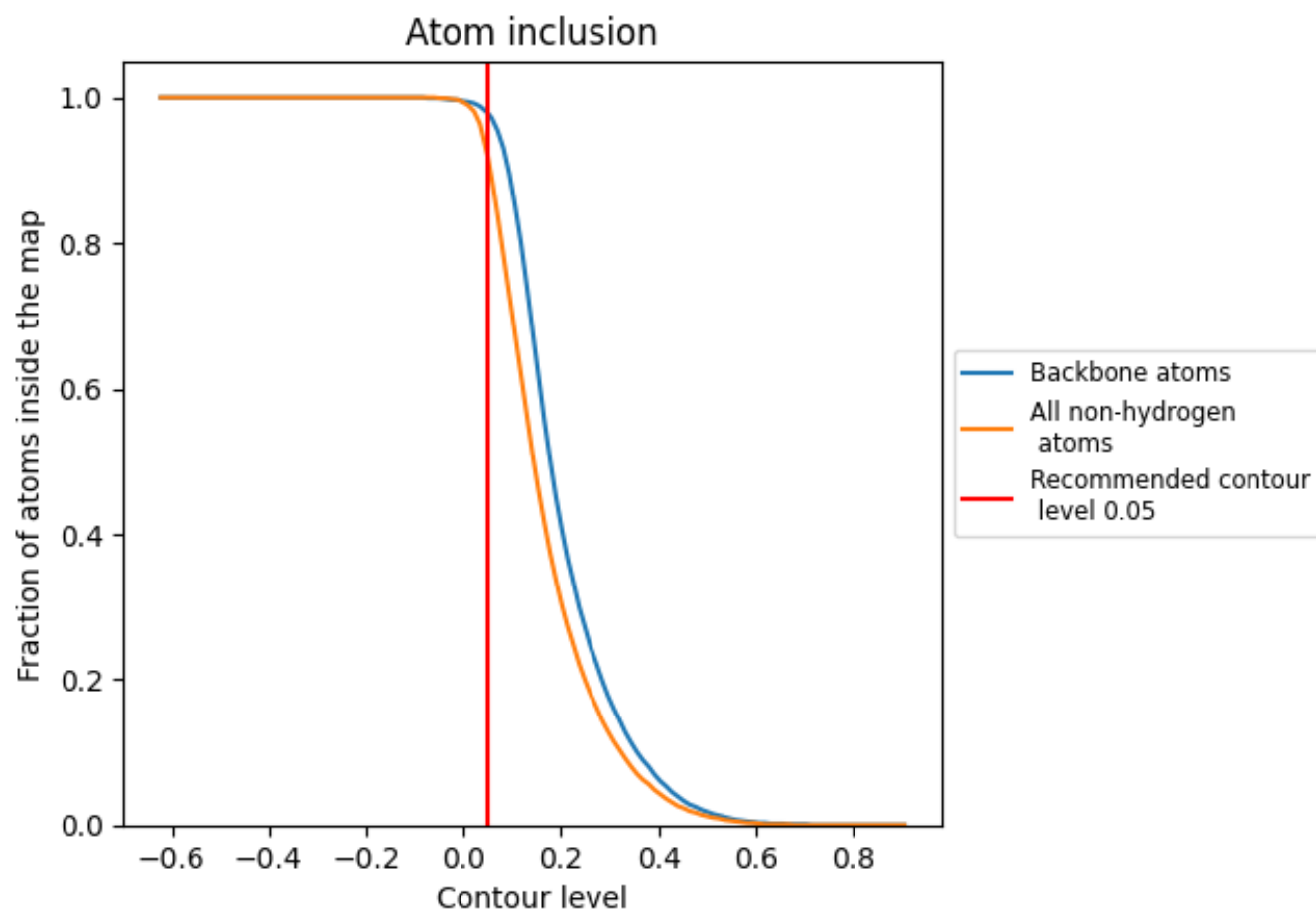
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 92% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9200	0.3470
A	0.9200	0.3630
B	0.9140	0.3320
C	0.9450	0.3670
D	0.9470	0.3590
E	0.8000	0.3010
F	0.7950	0.3120
G	0.8990	0.2190
H	0.9430	0.2650

1.0

0.0

<0.0