



Full wwPDB EM Validation Report ⓘ

May 2, 2026 – 12:44 PM EDT

PDB ID : 9YNF / pdb_00009ynf
EMDB ID : EMD-73176
Title : Motor domain of human dynein-1 in post1 state
Authors : Yang, J.; Rao, Q.; Chai, P.; Zhang, K.
Deposited on : 2025-10-10
Resolution : 3.92 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.49

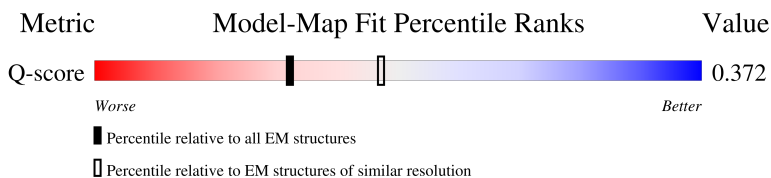
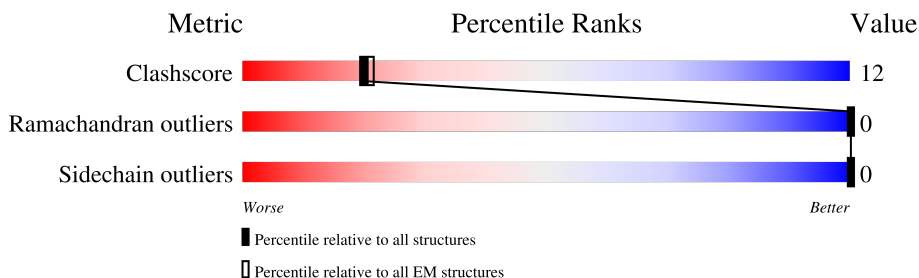
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.92 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	7862 (3.42 - 4.42)

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	4646	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24588 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 Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3038	24471	15586	4225	4538	122	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



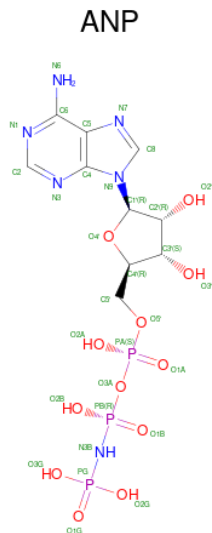
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
2	A	1	27	10	5	10	2	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 31	C 10	N 6	O 12	P 3	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

E2248	Y2086	E1984	W1838	Y1738	I1611	H1495	L1399	VAL	TRP	ARG	GLU	ALA	ASN	GLU	ASN	PHE
G2278	L2090	H1985	R1843	W1741	Y1618	K1496	V1400	ALA	GLU	PHE	PHE	LEU	LYS	LEU	LYS	ASN
H2282	L2093	S1986	F1844	Q1748	R1621	V1497	I1401	LEU	THR	GLN	THR	GLU	ASP	GLN	GLN	PHE
V2283	L2097	N1987	Q1860	L1749	F1626	S1503	L1403	LEU	LYS	PRO	PRO	ILE	ARG	VAL	VAL	LYS
I2287	K2115	T1997	M1861	V1750	P1627	V1504	K1404	GLU	VAL	SER	TRP	LYS	ASP	GLU	ILE	GLY
Q2299	R2118	C1999	N1863	L1751	E1635	M1507	A1407	D1328	THR	TRP	TRP	GLY	ASP	VAL	GLN	ASP
W2300	V2122	V2006	Y1872	A1754	L1638	L1514	D1410	V1332	ASN	ILE	ASN	VAL	ALA	ASN	GLY	LEU
D2306	W2129	K2007	Q1876	I1756	F1615	F1516	R1411	E1335	ARG	PRO	PRO	LEU	THR	PRO	VAL	ILE
V2307	G2125	S2009	D1877	A1757	Q1651	E1517	K1414	L1336	GLU	ILE	GLU	GLU	ASP	GLU	ARG	GLU
W2311	E2129	P2010	K1878	W1758	A1659	E1515	M1417	L1337	GLU	GLY	GLU	ASN	ASN	ILE	LEU	GLY
V2312	E2133	D2011	L1879	E1763	G1660	S1522	V1422	K1338	ALA	GLY	GLU	GLY	GLU	GLU	ALA	LYS
L2315	E2157	A2013	T1882	A1765	V1661	W1523	N1423	V1339	GLN	GLY	TRP	THR	THR	GLY	ALA	ILE
K2323	L2157	F2014	T1885	L1766	I1664	E1524	V1424	E1341	ALA	GLY	GLY	ASP	ASP	GLY	LEU	ASP
L2324	L2141	T2016	C1888	M1769	I1665	D1525	V1426	D1344	THR	PHE	ALA	VAL	VAL	ARG	GLU	GLY
R2332	L2149	M2017	G1770	G1771	V1673	L1527	S1427	K1347	GLY	ILE	ILE	VAL	VAL	GLN	LEU	THR
L2335	V2150	G2021	F1905	A1776	G1675	I1530	E1428	P1350	LYS	ARG	MET	ASP	GLY	GLU	LEU	THR
P2336	L2156	ALA	E1914	P1777	I1676	M1531	L1429	V1354	PHE	ARG	ALA	VAL	VAL	GLU	LEU	CYS
P2337	L2157	GLY	E1917	W1785	S1677	A1532	L1431	Q1355	THR	LYS	ARG	GLY	GLY	GLU	GLY	MET
M2338	L2157	ARG	K1917	V1785	G1678	L1533	G1432	P1356	PHE	LYS	ASP	THR	GLN	TRP	GLN	TYR
V2339	L2161	S2026	L1923	L1789	R1679	F1534	I1434	R1357	ILE	SER	ILE	GLY	LYS	LYS	ALA	TYR
R2340	L2161	D2030	E1923	L1789	G1680	Q1541	W1435	R1360	LYS	ALA	ALA	VAL	VAL	VAL	ASP	LYS
I2341	R2172	F1926	F1926	A1776	G1681	I1559	D1438	Q1361	ASP	ILE	ILE	GLN	VAL	VAL	THR	THR
M2342	G2173	V1927	V1927	P1777	I1682	L1560	L1439	Q1362	ARG	GLN	GLN	TRP	LEU	LEU	ALA	PHE
V2345	L2179	D1933	D1933	W1785	K1687	L1561	Q1440	L1363	GLU	GLN	GLN	LYS	GLY	VAL	GLU	GLY
A2354	M2189	E1934	E1934	Q1800	V1690	E1564	K1441	L1367	CYS	ALA	ALA	ASN	TYR	PRO	ASP	ILE
R2358	G2200	F1938	F1938	L1803	T1698	E1564	M1457	A1375	LYS	LYS	LYS	LEU	ILE	ARG	MET	LEU
W2363	L2208	R1804	R1804	R1803	Y1701	L1571	E1460	Q1378	GLU	LYS	GLY	GLN	GLN	GLN	ASP	ASN
F2364	G2209	R1806	R1806	R1806	L1702	E1564	E1461	Y1380	ALA	LYS	VAL	TRP	TRP	PRO	ALA	LYS
L2369	L2210	G1949	G1949	H1810	M1709	K1580	K1464	A1383	GLU	GLN	VAL	GLN	GLN	VAL	VAL	VAL
S2370	T2214	Q1950	Q1950	L1811	T1712	K1581	V1469	S1382	LEU	GLY	GLU	GLY	GLY	SER	ASP	ASP
M2373	M2222	V1951	V1951	T1812	L1713	V1582	W1470	E1384	THR	ASP	VAL	VAL	ASN	GLY	HIS	LYS
I2374	S2228	G1952	G1952	T1813	A1714	S1583	V1473	F1385	ASP	ARG	GLU	LEU	ILE	LEU	LEU	ASN
M2377	G2229	W1954	W1954	L1815	K1715	K1584	Y1473	V1386	THR	ALA	VAL	VAL	TYR	PRO	ASN	PRO
L2382	S2231	R1962	R1962	Q1818	E1719	M1589	E1474	Q1387	GLY	VAL	GLU	ARG	ASN	GLY	GLY	HIS
P2386	M2232	L1963	L1963	E1719	S1720	D1590	E1474	R1388	LEU	GLY	LEU	GLY	ARG	LEU	GLY	GLY
L2387	M2233	E1964	E1964	V1721	V1721	V1591	L1475	K1391	THR	ARG	GLY	GLY	GLY	THR	PRO	THR
Q2395	M2234	I2069	I2069	W1724	E1725	L1592	V1478	G1392	GLY	THR	THR	THR	GLY	GLY	LYS	LYS
R2396	R2235	M1967	M1967	V1725	E1725	H1593	Y1393	L1394	SER	ARG	ARG	LEU	ILE	GLY	ILE	ASN
R2397	K2239	V1975	V1975	A1833	D1734	I1594	L1486	K1395	GLY	THR	THR	LEU	ASP	GLY	LYS	LYS
		I1978	I1978	A1833	T1737	L1604	R1488	I1396	GLU	LEU	LEU	LEU	ASN	LYS	ASN	PRO
		F1836	F1836	E1837	T1737	L1608	F1494	M1398	VAL	THR	THR	THR	LYS	PHE	VAL	ILE
		E1837	E1837	E1837	T1737	L1608	F1494	M1398	ARG	ASP	ASP	ASP	GLN	THR	VAL	HIS





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	326895	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.624	Depositor
Minimum map value	-1.305	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	444.416, 444.416, 444.416	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.736, 1.736, 1.736	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP, MG, ANP

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	0.13	0/24989	0.34	0/33856

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2597	PRO	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	24471	0	24528	609	0
2	A	54	0	24	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	12	6	0
4	A	31	0	13	4	0
5	A	1	0	0	0	0
All	All	24588	0	24577	609	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 12.

All (609) 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:3194:LEU:HD22	1:A:3500:MET:HE3	1.57	0.87
1:A:2603:MET:HE2	4:A:4703:ANP:H5'2	1.60	0.82
1:A:2387:LEU:HB3	1:A:2467:ARG:HH21	1.44	0.80
1:A:3817:SER:HB3	1:A:4349:LEU:HD21	1.63	0.80
1:A:2386:PRO:HA	1:A:2416:GLN:HE22	1.47	0.79
1:A:1361:GLN:NE2	1:A:1362:ASN:OD1	2.18	0.77
1:A:1938:PHE:HB2	1:A:1967:MET:HE3	1.67	0.77
1:A:1391:LYS:HA	1:A:1394:MET:HE3	1.67	0.77
1:A:2910:VAL:HG21	1:A:3105:VAL:HG22	1.67	0.77
1:A:4168:ARG:HA	1:A:4171:LYS:HE3	1.70	0.74
1:A:3724:VAL:HG11	1:A:3797:VAL:HG21	1.69	0.74
1:A:4107:MET:HE1	1:A:4137:ASN:HD21	1.53	0.74
1:A:3870:ARG:NH2	1:A:4034:GLU:OE1	2.22	0.73
1:A:2065:LEU:HD11	1:A:2133:GLU:HB3	1.69	0.73
1:A:3884:ALA:HB1	1:A:4009:VAL:HG11	1.68	0.72
1:A:3664:LEU:HB3	1:A:3669:ILE:HD13	1.72	0.72
1:A:2963:VAL:HG22	1:A:2998:ASN:HB3	1.73	0.71
1:A:3818:LEU:HD23	1:A:4346:MET:HE1	1.73	0.70
1:A:2179:ARG:HD3	1:A:2208:LEU:HD11	1.72	0.70
1:A:2684:ARG:NH1	1:A:2688:GLU:OE1	2.25	0.70
1:A:1698:ILE:HD13	1:A:1701:TRP:HE1	1.55	0.70
1:A:1509:LEU:HD22	1:A:3608:LYS:HG2	1.73	0.70
1:A:4088:VAL:HG13	1:A:4118:PRO:HA	1.74	0.70
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.74	0.69
1:A:1396:ILE:HB	1:A:1439:LEU:HD12	1.73	0.69
1:A:4176:ARG:NH1	1:A:4220:ASP:OD1	2.26	0.68
1:A:2337:PRO:O	1:A:2340:ARG:NH1	2.26	0.68
1:A:3902:ASP:OD1	1:A:3903:ALA:N	2.26	0.68
1:A:4437:VAL:HG21	1:A:4444:GLN:HG3	1.76	0.68
1:A:2729:ARG:NH2	3:A:4702:ATP:O2A	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2229:GLY:O	1:A:2233:ALA:HB2	1.94	0.68
1:A:2200:GLY:HA2	1:A:2373:MET:HE3	1.77	0.67
1:A:2306:ASP:HA	1:A:2345:VAL:HG23	1.76	0.67
1:A:2312:VAL:HA	1:A:2315:LEU:HD23	1.76	0.67
1:A:2448:ASP:OD2	1:A:2725:HIS:NE2	2.28	0.66
1:A:2943:LYS:NZ	2:A:4704:ADP:O2B	2.25	0.66
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.77	0.66
1:A:3597:THR:O	1:A:3601:MET:HG2	1.96	0.66
1:A:1561:LEU:HB3	1:A:1564:GLU:HB2	1.78	0.66
1:A:2287:ILE:HD12	1:A:2299:GLN:HG3	1.78	0.66
1:A:4412:PHE:HE1	1:A:4516:VAL:HG23	1.61	0.65
1:A:1751:VAL:HG11	1:A:1878:LYS:HE3	1.79	0.65
1:A:3824:LEU:HD11	1:A:4130:ILE:HD12	1.78	0.65
1:A:3208:ILE:O	1:A:3212:VAL:HG23	1.96	0.64
1:A:2768:PRO:HB2	1:A:2858:PHE:HE1	1.63	0.64
1:A:2054:LEU:HD21	1:A:2097:LEU:HD12	1.80	0.64
1:A:3585:ARG:HB2	1:A:3697:THR:HG23	1.78	0.64
1:A:3005:LEU:HD12	1:A:3085:LEU:HD11	1.79	0.64
1:A:2138:ILE:HG23	1:A:2161:LEU:HD21	1.79	0.64
1:A:3113:MET:O	1:A:3140:ARG:NH1	2.30	0.64
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.80	0.64
1:A:2918:HIS:O	1:A:2922:ILE:HG12	1.97	0.64
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.31	0.63
1:A:3100:GLU:HG3	1:A:3130:TYR:HE1	1.63	0.63
1:A:3193:GLU:O	1:A:3196:GLU:HG3	1.99	0.63
1:A:2965:ARG:H	1:A:3620:ARG:HH21	1.45	0.63
1:A:3471:LYS:HE3	1:A:3474:ARG:HH22	1.64	0.63
1:A:1946:VAL:HG13	1:A:2006:VAL:HG21	1.80	0.62
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.81	0.62
1:A:4165:PRO:HG2	1:A:4168:ARG:HB2	1.80	0.62
1:A:4395:LEU:HD21	1:A:4486:ILE:HG23	1.80	0.62
1:A:2942:GLY:HA2	2:A:4704:ADP:H5'2	1.81	0.62
1:A:2078:GLU:N	1:A:2078:GLU:OE2	2.32	0.62
1:A:2804:ARG:HD3	1:A:2929:PRO:HG2	1.81	0.62
1:A:1350:PRO:HA	1:A:1430:THR:HA	1.80	0.62
1:A:2299:GLN:HB2	1:A:2339:VAL:HG22	1.81	0.62
1:A:4185:TRP:O	1:A:4189:ILE:HG12	1.99	0.62
1:A:1356:PRO:HB3	1:A:1401:ILE:HG12	1.82	0.61
1:A:2413:LEU:HA	1:A:2416:GLN:HE21	1.64	0.61
1:A:2505:ASP:HB3	1:A:2733:VAL:HG13	1.81	0.61
1:A:2993:ILE:HG22	1:A:3065:VAL:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4431:LEU:HA	1:A:4434:VAL:HG12	1.82	0.61
1:A:3172:THR:HG21	1:A:3694:SER:HB2	1.80	0.61
1:A:2232:MET:HA	1:A:2235:ARG:HB2	1.83	0.61
1:A:4239:PRO:HB2	1:A:4242:ALA:HB3	1.83	0.61
1:A:4407:ASP:OD2	1:A:4410:PHE:N	2.33	0.61
1:A:4496:ALA:HB2	1:A:4504:LEU:HD21	1.83	0.61
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.83	0.60
1:A:4100:HIS:O	1:A:4133:LYS:NZ	2.33	0.60
1:A:2603:MET:HE1	4:A:4703:ANP:N9	2.16	0.60
1:A:4178:ARG:HH21	1:A:4300:ILE:HG22	1.66	0.60
1:A:4199:LEU:HD23	1:A:4330:VAL:HG11	1.81	0.60
1:A:1964:GLU:OE1	1:A:1964:GLU:N	2.33	0.60
1:A:4042:LEU:HD13	1:A:4139:LEU:HD23	1.83	0.60
1:A:1514:LYS:HG3	1:A:1515:VAL:HG13	1.82	0.60
1:A:3925:GLN:OE1	1:A:3925:GLN:N	2.28	0.60
1:A:3474:ARG:HE	1:A:3764:ASP:HB3	1.65	0.60
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.83	0.60
1:A:4243:LEU:O	1:A:4247:MET:HG2	2.02	0.60
1:A:2590:PRO:HB3	1:A:2708:PHE:HB2	1.84	0.60
1:A:3476:THR:O	1:A:3480:LYS:HG3	2.02	0.60
1:A:2307:VAL:HG12	1:A:2345:VAL:HG21	1.84	0.59
1:A:2115:LYS:HE3	1:A:2122:VAL:HG12	1.84	0.59
1:A:4569:THR:HG22	1:A:4583:THR:HG21	1.84	0.59
1:A:4176:ARG:NH2	1:A:4224:ASP:OD1	2.36	0.59
1:A:1469:VAL:O	1:A:1473:TYR:HB2	2.02	0.59
1:A:2925:ILE:HG21	1:A:2933:LEU:HB2	1.85	0.59
1:A:4205:TYR:OH	1:A:4257:ASP:OD1	2.18	0.59
1:A:2836:ARG:HG2	1:A:3091:LEU:HB2	1.85	0.59
1:A:3495:THR:O	1:A:3499:GLN:NE2	2.36	0.59
1:A:3923:ARG:HD3	1:A:3929:VAL:HG12	1.84	0.59
1:A:1665:ILE:N	1:A:1675:GLY:O	2.36	0.58
1:A:2446:ILE:HG23	1:A:2447:MET:HG3	1.85	0.58
1:A:3200:HIS:CE1	1:A:3747:LYS:HD3	2.38	0.58
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.85	0.58
1:A:2030:ASP:HA	1:A:2033:LYS:HG3	1.85	0.58
1:A:1474:GLU:OE1	1:A:1474:GLU:N	2.36	0.58
1:A:2369:LEU:HD21	1:A:2374:ILE:HD11	1.86	0.58
1:A:2387:LEU:HB2	1:A:2412:MET:HE2	1.85	0.58
1:A:4105:TRP:CZ3	1:A:4109:LEU:HD12	2.39	0.58
1:A:2569:VAL:HG11	1:A:2747:ILE:HA	1.84	0.58
1:A:2603:MET:HE1	4:A:4703:ANP:C4	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3885:MET:HB3	1:A:4343:MET:HE1	1.86	0.57
1:A:1810:HIS:NE2	1:A:1876:GLN:O	2.37	0.57
1:A:1825:LEU:HD22	1:A:1830:ILE:HD11	1.87	0.57
1:A:1975:VAL:HA	1:A:1978:ILE:HG22	1.86	0.57
1:A:2703:LEU:HD22	1:A:2706:ILE:HD12	1.85	0.57
1:A:2923:ASP:OD2	1:A:2927:ARG:NH2	2.37	0.57
1:A:1409:LYS:HD2	1:A:1410:ASP:N	2.19	0.57
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	1.86	0.57
1:A:4012:ASN:HB3	1:A:4013:LEU:HD12	1.86	0.57
1:A:2046:ARG:HA	1:A:2049:ILE:HG22	1.85	0.57
1:A:1792:LEU:HB3	1:A:1812:ILE:HD11	1.86	0.57
1:A:2889:LEU:HD21	1:A:2920:LEU:HD21	1.87	0.56
1:A:3499:GLN:HA	1:A:3502:THR:HG22	1.86	0.56
1:A:3750:LEU:HD12	1:A:3753:LEU:HD11	1.87	0.56
1:A:4176:ARG:HH12	1:A:4220:ASP:HA	1.70	0.56
1:A:1571:ILE:HG21	1:A:1608:LEU:HD21	1.88	0.56
1:A:1635:GLU:OE1	1:A:1635:GLU:N	2.35	0.56
1:A:1679:ARG:NH1	1:A:1680:GLU:OE2	2.38	0.56
1:A:3757:LYS:HE2	1:A:3759:ARG:HH21	1.71	0.56
1:A:4454:GLU:OE2	1:A:4461:PRO:HG3	2.05	0.56
1:A:2382:LEU:HD22	1:A:2420:ALA:HB2	1.86	0.56
1:A:2563:ALA:O	1:A:2804:ARG:NH2	2.38	0.56
1:A:4385:SER:O	1:A:4389:HIS:ND1	2.38	0.56
1:A:3883:PHE:HD1	1:A:3886:LEU:HD12	1.71	0.56
1:A:4100:HIS:NE2	1:A:4129:GLU:OE2	2.39	0.56
1:A:3741:ARG:NH1	1:A:3776:GLU:OE1	2.37	0.56
1:A:4423:LEU:HD22	1:A:4482:PHE:CE1	2.40	0.56
1:A:1582:VAL:HG23	1:A:1591:VAL:HG11	1.88	0.56
1:A:4084:ILE:O	1:A:4088:VAL:HG23	2.05	0.56
1:A:2554:GLN:OE1	1:A:2753:ARG:NH2	2.38	0.56
1:A:2324:LEU:HD11	1:A:2332:ARG:HB3	1.89	0.55
1:A:2595:GLY:O	1:A:2714:PRO:HD3	2.06	0.55
1:A:1800:GLN:OE1	1:A:1804:ARG:NH1	2.38	0.55
1:A:3219:ARG:NH1	1:A:3472:VAL:HA	2.21	0.55
1:A:3196:GLU:HA	1:A:3199:MET:HG3	1.87	0.55
1:A:3888:ALA:HB1	1:A:4012:ASN:HD22	1.72	0.55
1:A:4215:ALA:HB1	1:A:4247:MET:HE1	1.87	0.55
1:A:2229:GLY:O	1:A:2233:ALA:CB	2.53	0.55
1:A:2872:LEU:HD23	1:A:2889:LEU:HD23	1.88	0.55
1:A:1337:SER:O	1:A:1341:GLU:HG2	2.06	0.55
1:A:2796:PRO:HB2	4:A:4703:ANP:HI'	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3205:LEU:O	1:A:3209:LYS:HG2	2.07	0.55
1:A:4178:ARG:HH11	1:A:4296:MET:HE1	1.72	0.55
1:A:1952:GLY:HA2	1:A:2012:MET:HB3	1.88	0.55
1:A:3705:ARG:NH2	1:A:4349:LEU:O	2.39	0.54
1:A:4443:LYS:HD2	1:A:4444:GLN:N	2.22	0.54
1:A:1431:LEU:HD12	1:A:1434:ILE:HB	1.89	0.54
1:A:2488:ARG:O	1:A:2492:ARG:HG2	2.06	0.54
1:A:2635:PHE:HE1	1:A:2661:LEU:HD11	1.71	0.54
1:A:2571:THR:HG22	1:A:2574:THR:HG23	1.89	0.54
1:A:3068:MET:HE1	1:A:3081:THR:HG21	1.88	0.54
1:A:1812:ILE:HG21	1:A:2056:SER:HA	1.89	0.54
1:A:2492:ARG:HD2	1:A:2545:TRP:CZ2	2.43	0.54
1:A:2930:GLN:NE2	1:A:3013:ALA:O	2.40	0.54
1:A:3167:ARG:NH2	1:A:3684:PRO:O	2.34	0.54
1:A:4314:ASP:OD1	1:A:4315:THR:N	2.40	0.54
1:A:3110:THR:O	1:A:3140:ARG:NH2	2.39	0.54
1:A:4457:LYS:HE3	1:A:4457:LYS:HA	1.90	0.54
1:A:4518:GLU:OE2	1:A:4518:GLU:N	2.39	0.54
1:A:1985:HIS:CD2	1:A:1997:ILE:HD12	2.42	0.53
1:A:4244:LYS:HA	1:A:4269:LEU:HD12	1.89	0.53
1:A:4284:LEU:HG	1:A:4296:MET:HB2	1.91	0.53
1:A:4402:VAL:O	1:A:4406:LYS:HG3	2.07	0.53
1:A:4434:VAL:HA	1:A:4437:VAL:HG12	1.90	0.53
1:A:1397:ASN:O	1:A:1401:ILE:HG13	2.08	0.53
1:A:2888:GLU:OE1	1:A:2888:GLU:N	2.29	0.53
1:A:4071:ILE:HG13	1:A:4099:VAL:HG12	1.91	0.53
1:A:1461:GLU:HG3	1:A:3659:ARG:HD3	1.91	0.53
1:A:1417:MET:HE3	1:A:1417:MET:HA	1.90	0.53
1:A:2748:TYR:CZ	1:A:2799:MET:HB3	2.44	0.53
1:A:2813:LEU:HD21	1:A:2816:LEU:HG	1.91	0.53
1:A:4454:GLU:HA	1:A:4457:LYS:HG2	1.89	0.53
1:A:4517:PRO:O	1:A:4521:ILE:HG12	2.08	0.53
1:A:2973:ASP:HA	1:A:2976:LEU:HD12	1.91	0.53
1:A:4010:SER:HB2	1:A:4015:GLU:HA	1.90	0.53
1:A:2898:LYS:HA	1:A:2901:TYR:HD1	1.73	0.52
1:A:3128:VAL:HG23	1:A:3145:ASN:HD21	1.74	0.52
1:A:3957:PHE:HZ	1:A:3996:PHE:CE1	2.27	0.52
1:A:1888:CYS:HB2	1:A:2041:MET:HE3	1.91	0.52
1:A:4448:LEU:HD13	1:A:4451:LEU:HD23	1.91	0.52
1:A:3931:GLN:O	1:A:3935:VAL:HG23	2.09	0.52
1:A:1426:VAL:HA	1:A:1429:LEU:HG	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4206:GLU:OE2	1:A:4255:ARG:NH1	2.43	0.52
1:A:4399:LYS:HE2	1:A:4497:ALA:HA	1.92	0.52
1:A:2927:ARG:HG3	1:A:2928:GLN:HE21	1.75	0.52
1:A:3663:THR:OG1	1:A:3668:ASP:OD1	2.28	0.52
1:A:1664:ILE:HG22	1:A:1676:ILE:HG22	1.92	0.52
1:A:2756:LEU:HD12	1:A:2766:ALA:HB2	1.92	0.52
1:A:1590:ASP:O	1:A:1594:ILE:HG13	2.09	0.52
1:A:1555:ALA:O	1:A:1559:HIS:ND1	2.35	0.51
1:A:1789:LEU:HD21	1:A:1815:LEU:HB3	1.92	0.51
1:A:2422:ILE:HD12	1:A:2487:GLU:HG2	1.92	0.51
1:A:2944:THR:OG1	2:A:4704:ADP:O2A	2.26	0.51
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.92	0.51
1:A:2510:MET:HE3	1:A:2510:MET:HA	1.91	0.51
1:A:1475:LEU:HD11	1:A:1534:PHE:HZ	1.75	0.51
1:A:2600:GLY:HA2	1:A:2603:MET:HE3	1.92	0.51
1:A:3705:ARG:HH22	1:A:4350:GLU:HA	1.75	0.51
1:A:3825:TYR:CZ	1:A:3875:MET:HG3	2.46	0.51
1:A:1721:VAL:O	1:A:1725:GLU:HG2	2.10	0.51
1:A:1497:VAL:HG13	1:A:1531:MET:HE1	1.92	0.51
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.93	0.51
1:A:4488:GLN:O	1:A:4492:ILE:HG12	2.10	0.51
1:A:2093:LEU:HD23	1:A:2097:LEU:HD23	1.93	0.51
1:A:4107:MET:HE3	1:A:4107:MET:HA	1.93	0.51
1:A:1843:ARG:NH2	1:A:1861:MET:O	2.44	0.51
1:A:2125:GLY:O	1:A:2129:GLU:HG2	2.11	0.51
1:A:4235:PRO:HB3	1:A:4278:PHE:CD2	2.45	0.51
1:A:1398:MET:HG3	1:A:1399:LEU:HD12	1.94	0.51
1:A:3133:LEU:HD12	1:A:3134:PRO:HD2	1.92	0.51
1:A:3591:ASP:HB2	1:A:3701:PHE:HB2	1.93	0.51
1:A:2397:ARG:NH2	1:A:2406:GLU:OE2	2.44	0.50
1:A:2443:LEU:HD11	1:A:2510:MET:HB3	1.93	0.50
1:A:4179:LEU:HD12	1:A:4223:LEU:HD22	1.93	0.50
1:A:4348:MET:HE1	1:A:4453:ASN:HA	1.93	0.50
1:A:2283:VAL:O	1:A:2287:ILE:HG12	2.11	0.50
1:A:4564:LYS:HG3	1:A:4646:GLU:HB2	1.93	0.50
1:A:1407:ALA:HA	1:A:1457:MET:HE3	1.92	0.50
1:A:2465:ALA:HB2	1:A:2493:TYR:CD2	2.46	0.50
1:A:2755:MET:HE1	1:A:2807:PHE:HA	1.92	0.50
1:A:3514:ILE:HD11	1:A:3579:MET:HA	1.92	0.50
1:A:2943:LYS:HG2	1:A:3094:PHE:HD2	1.77	0.50
1:A:2053:MET:O	1:A:2056:SER:OG	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2248:GLU:N	1:A:2248:GLU:OE1	2.45	0.50
1:A:2395:GLN:HB2	1:A:2396:ARG:HH21	1.75	0.50
1:A:2465:ALA:HB2	1:A:2493:TYR:HD2	1.77	0.50
1:A:2377:ASN:HB2	3:A:4702:ATP:H2	1.77	0.50
1:A:2493:TYR:HD1	1:A:2539:VAL:HB	1.75	0.50
1:A:2964:HIS:HB2	1:A:3620:ARG:HH22	1.77	0.50
1:A:2090:LEU:HD23	2:A:4701:ADP:C8	2.47	0.49
1:A:2418:ASP:O	1:A:2422:ILE:HG12	2.11	0.49
1:A:2115:LYS:HG2	1:A:2118:ARG:HH12	1.77	0.49
1:A:2658:TRP:CE3	1:A:2705:ARG:HA	2.47	0.49
1:A:3835:ILE:HD12	1:A:3870:ARG:HD2	1.94	0.49
1:A:4288:VAL:HG21	1:A:4294:ILE:HG13	1.95	0.49
1:A:2838:VAL:HG22	1:A:3093:TRP:CD2	2.48	0.49
1:A:4462:ARG:HA	1:A:4462:ARG:NE	2.28	0.49
1:A:1793:ALA:HB1	1:A:2060:ARG:HH12	1.77	0.49
1:A:2150:VAL:HG12	1:A:2363:TRP:CE2	2.46	0.49
1:A:2571:THR:H	1:A:2574:THR:HG1	1.55	0.49
1:A:2228:SER:N	3:A:4702:ATP:O2B	2.31	0.49
1:A:2409:ALA:H	1:A:2413:LEU:HD23	1.77	0.49
1:A:3508:LEU:HD23	1:A:3536:LEU:HD21	1.93	0.49
1:A:4505:LYS:HG3	1:A:4527:TYR:CZ	2.48	0.49
1:A:1375:ALA:HA	1:A:1378:ARG:HB2	1.94	0.49
1:A:2723:LEU:HB2	1:A:2728:LEU:HD21	1.95	0.49
1:A:3966:PRO:HG3	1:A:3997:ARG:HE	1.78	0.49
1:A:4206:GLU:N	1:A:4206:GLU:OE1	2.42	0.49
1:A:4387:TRP:NE1	1:A:4479:VAL:HG21	2.28	0.49
1:A:1917:LYS:HG3	1:A:1927:VAL:HG11	1.95	0.49
1:A:2503:SER:HB2	1:A:2511:ARG:HG2	1.94	0.49
1:A:3869:ASN:O	1:A:3873:ARG:HG2	2.12	0.49
1:A:1905:PHE:HB3	1:A:2018:MET:HB3	1.95	0.48
1:A:2377:ASN:HB2	3:A:4702:ATP:C2	2.48	0.48
1:A:2789:GLN:HE21	1:A:2838:VAL:HG21	1.77	0.48
1:A:3593:SER:OG	1:A:3595:GLN:HG3	2.13	0.48
1:A:1360:ARG:NH1	1:A:2902:GLU:HG3	2.27	0.48
1:A:1411:ARG:HA	1:A:1414:LYS:HB3	1.95	0.48
1:A:3886:LEU:O	1:A:3890:ILE:HG12	2.14	0.48
1:A:1664:ILE:HA	1:A:1676:ILE:HA	1.95	0.48
1:A:1709:MET:HE3	1:A:1713:LEU:HD12	1.94	0.48
1:A:2222:MET:HE1	1:A:2342:MET:HG2	1.94	0.48
1:A:3567:LEU:HB2	1:A:3599:PHE:CD1	2.48	0.48
1:A:3999:ASP:OD1	1:A:4000:ARG:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1478:VAL:HG21	1:A:1488:ARG:HH21	1.78	0.48
1:A:2491:GLN:HB3	1:A:2524:VAL:HG21	1.95	0.48
1:A:2964:HIS:HA	1:A:3665:GLY:HA2	1.95	0.48
1:A:2012:MET:HE1	1:A:2014:ILE:HD11	1.94	0.48
1:A:4080:ALA:O	1:A:4084:ILE:HG12	2.14	0.48
1:A:3194:LEU:HD23	1:A:3194:LEU:O	2.13	0.48
1:A:3649:LEU:HB2	1:A:3695:ARG:HG3	1.96	0.48
1:A:1478:VAL:HG21	1:A:1488:ARG:HE	1.79	0.48
1:A:1748:GLN:HE22	1:A:1872:TYR:HA	1.78	0.48
1:A:1765:ALA:O	1:A:1769:MET:HG2	2.14	0.48
1:A:2485:GLN:HA	1:A:2488:ARG:HE	1.78	0.48
1:A:2499:LEU:O	1:A:2503:SER:OG	2.22	0.48
1:A:2472:TYR:CG	1:A:2541:ILE:HG21	2.49	0.48
1:A:3856:LEU:O	1:A:3859:ILE:HG22	2.14	0.48
1:A:1344:ASP:OD1	1:A:1347:LYS:NZ	2.34	0.47
1:A:2370:SER:N	1:A:2373:MET:SD	2.85	0.47
1:A:4481:ASP:O	1:A:4484:GLU:HG2	2.14	0.47
1:A:1863:ASN:O	1:A:1863:ASN:ND2	2.46	0.47
1:A:2554:GLN:HE22	1:A:2746:GLN:HE21	1.62	0.47
1:A:3888:ALA:HA	1:A:4013:LEU:HD11	1.95	0.47
1:A:2964:HIS:CE1	1:A:2967:TYR:HA	2.49	0.47
1:A:4444:GLN:HE22	1:A:4452:ILE:HG21	1.79	0.47
1:A:2082:SER:HA	1:A:2086:TYR:CD2	2.48	0.47
1:A:3003:GLY:HA2	1:A:3006:GLU:OE2	2.15	0.47
1:A:1523:TRP:HA	1:A:1526:LYS:HE3	1.95	0.47
1:A:1830:ILE:HG21	1:A:1837:GLU:OE2	2.14	0.47
1:A:1844:PHE:CD2	1:A:1859:ILE:HG12	2.50	0.47
1:A:1949:CYS:HB3	1:A:2008:VAL:HA	1.97	0.47
1:A:2901:TYR:OH	1:A:2909:LEU:O	2.33	0.47
1:A:4297:PRO:HB3	1:A:4308:TRP:CD1	2.50	0.47
1:A:4443:LYS:HD2	1:A:4444:GLN:H	1.79	0.47
1:A:2936:ILE:HG23	1:A:3093:TRP:HE3	1.78	0.47
1:A:1769:MET:HE1	1:A:1777:PRO:HD2	1.95	0.47
1:A:2685:GLN:O	1:A:2685:GLN:NE2	2.45	0.47
1:A:2996:GLU:HA	1:A:2999:VAL:HG22	1.95	0.47
1:A:4460:LEU:HD21	1:A:4473:MET:HG3	1.97	0.47
1:A:2597:PRO:HG3	1:A:2793:ILE:HD11	1.97	0.47
1:A:2757:ARG:HA	1:A:2763:ARG:HH22	1.80	0.47
1:A:4267:THR:HG21	1:A:4636:TYR:HD2	1.80	0.47
1:A:2751:PHE:O	1:A:2755:MET:HG2	2.15	0.47
1:A:3662:ILE:HG21	1:A:3671:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3948:ILE:O	1:A:3952:GLN:HG3	2.15	0.47
1:A:1984:GLU:OE1	1:A:1987:ASN:ND2	2.48	0.47
1:A:4264:LEU:O	1:A:4267:THR:OG1	2.29	0.47
1:A:1527:LEU:HA	1:A:1530:ILE:HG22	1.97	0.46
1:A:2080:LEU:HD23	1:A:2156:LEU:HD23	1.97	0.46
1:A:2554:GLN:NE2	1:A:2746:GLN:HE21	2.12	0.46
1:A:2972:PHE:CE2	1:A:2976:LEU:HD11	2.50	0.46
1:A:4437:VAL:HG21	1:A:4444:GLN:CG	2.45	0.46
1:A:1933:ASP:HB3	1:A:1962:ARG:NH2	2.30	0.46
1:A:3113:MET:HE2	1:A:3184:ALA:HA	1.96	0.46
1:A:3511:ALA:HA	1:A:3514:ILE:HG22	1.98	0.46
1:A:3882:THR:O	1:A:3886:LEU:HG	2.16	0.46
1:A:2896:ARG:HA	1:A:2899:VAL:HG12	1.96	0.46
1:A:4485:ARG:HG2	1:A:4513:GLY:HA2	1.96	0.46
1:A:1749:LEU:HD23	1:A:1749:LEU:HA	1.81	0.46
1:A:1981:ALA:HB2	1:A:1999:CYS:HB2	1.97	0.46
1:A:4482:PHE:O	1:A:4486:ILE:HD12	2.14	0.46
1:A:1384:GLU:O	1:A:1388:ARG:HG3	2.16	0.46
1:A:1428:GLU:OE1	1:A:1428:GLU:N	2.49	0.46
1:A:1734:ASP:HB3	1:A:1737:THR:OG1	2.16	0.46
1:A:2875:ASN:HB3	1:A:2881:TYR:HA	1.97	0.46
1:A:2049:ILE:HD12	2:A:4701:ADP:C6	2.50	0.46
1:A:3838:ASN:ND2	1:A:4034:GLU:OE1	2.48	0.46
1:A:1329:LEU:HA	1:A:1332:VAL:HG12	1.96	0.46
1:A:1914:GLU:CD	2:A:4701:ADP:H3'	2.40	0.46
1:A:2924:ARG:O	1:A:2928:GLN:HG2	2.15	0.46
1:A:4263:ARG:HD2	1:A:4636:TYR:CZ	2.51	0.46
1:A:2189:MET:HE3	1:A:2239:LYS:HD3	1.97	0.46
1:A:2413:LEU:HA	1:A:2416:GLN:NE2	2.31	0.46
1:A:2759:ILE:HG21	1:A:2762:LEU:HD12	1.97	0.46
1:A:4103:PRO:HD3	1:A:4133:LYS:NZ	2.31	0.46
1:A:1409:LYS:HD2	1:A:1410:ASP:H	1.80	0.46
1:A:1417:MET:SD	1:A:1423:ASN:HB3	2.55	0.46
1:A:2427:PHE:HD1	1:A:2433:VAL:HG11	1.82	0.45
1:A:2922:ILE:HD13	1:A:2933:LEU:HD23	1.98	0.45
1:A:3478:LEU:HB2	1:A:3767:ILE:HD11	1.98	0.45
1:A:2569:VAL:HB	1:A:2747:ILE:HG23	1.96	0.45
1:A:2729:ARG:NH1	3:A:4702:ATP:O2G	2.41	0.45
1:A:3167:ARG:CZ	1:A:3685:THR:HA	2.46	0.45
1:A:3588:LEU:HD11	1:A:3638:VAL:HG21	1.99	0.45
1:A:3810:SER:OG	1:A:3890:ILE:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3997:ARG:HH12	1:A:4329:ARG:NH2	2.14	0.45
1:A:4271:ARG:HG3	1:A:4633:ARG:HH22	1.81	0.45
1:A:1470:TRP:HB3	1:A:1589:MET:CE	2.47	0.45
1:A:2644:THR:HG22	1:A:2646:ASN:H	1.81	0.45
1:A:2686:MET:SD	1:A:2703:LEU:HD11	2.56	0.45
1:A:4153:VAL:HG13	1:A:4188:ALA:HB1	1.98	0.45
1:A:4407:ASP:O	1:A:4411:ARG:HG3	2.16	0.45
1:A:1715:LYS:O	1:A:1719:GLU:HG3	2.16	0.45
1:A:2354:ALA:O	1:A:2358:ARG:HG3	2.16	0.45
1:A:4451:LEU:O	1:A:4454:GLU:HG3	2.17	0.45
1:A:2049:ILE:HD13	1:A:2090:LEU:HD21	1.98	0.45
1:A:3990:LEU:HA	1:A:4004:MET:HG2	1.97	0.45
1:A:2804:ARG:O	1:A:2808:GLU:HG2	2.17	0.45
1:A:3199:MET:SD	1:A:3200:HIS:N	2.90	0.45
1:A:4186:PHE:O	1:A:4190:ILE:HG12	2.17	0.45
1:A:4481:ASP:O	1:A:4485:ARG:HG3	2.17	0.45
1:A:1470:TRP:HB3	1:A:1589:MET:HE3	1.97	0.45
1:A:2614:ASP:C	1:A:2615:MET:HE2	2.41	0.45
1:A:2278:GLY:O	1:A:2282:HIS:HB3	2.17	0.45
1:A:2726:ARG:NH1	3:A:4702:ATP:O1G	2.50	0.45
1:A:3510:SER:OG	1:A:3553:LEU:HD21	2.17	0.45
1:A:1438:ASP:HB3	1:A:1441:LYS:HB3	1.99	0.45
1:A:2594:CYS:O	1:A:2735:TYR:HA	2.17	0.45
1:A:2609:LEU:HD22	1:A:2615:MET:HG3	1.99	0.45
1:A:3621:LYS:O	1:A:3624:GLU:HG3	2.16	0.45
1:A:1356:PRO:HD3	1:A:1404:LYS:HD2	1.99	0.44
1:A:1470:TRP:HE1	1:A:1527:LEU:HD11	1.81	0.44
1:A:2172:ARG:NH1	1:A:2173:GLY:H	2.15	0.44
1:A:3151:HIS:HD1	1:A:3516:TYR:HH	1.58	0.44
1:A:3762:ASP:OD1	1:A:3763:ASP:N	2.45	0.44
1:A:1407:ALA:HB1	1:A:1453:ALA:HB1	1.99	0.44
1:A:2923:ASP:OD1	1:A:2954:ASN:ND2	2.37	0.44
1:A:4276:ARG:HD2	1:A:4276:ARG:N	2.33	0.44
1:A:1753:SER:HA	1:A:1756:ILE:HG12	2.00	0.44
1:A:2016:ILE:HG12	1:A:2036:PHE:CE2	2.52	0.44
1:A:1763:GLU:OE2	1:A:1838:TRP:NE1	2.40	0.44
1:A:2370:SER:O	1:A:2373:MET:HB2	2.16	0.44
1:A:3597:THR:O	1:A:3600:ILE:HG22	2.17	0.44
1:A:3655:ARG:HA	1:A:3660:VAL:HA	1.99	0.44
1:A:4452:ILE:O	1:A:4456:VAL:HG23	2.18	0.44
1:A:1393:TYR:HE1	1:A:1435:TRP:CD2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1618:TYR:HA	1:A:1621:ARG:HE	1.82	0.44
1:A:1738:TYR:HE2	1:A:1792:LEU:HD21	1.82	0.44
1:A:1882:THR:HG22	1:A:1885:THR:HG23	1.98	0.44
1:A:2584:TRP:CZ3	1:A:2732:PRO:HB2	2.53	0.44
1:A:3017:VAL:HG22	1:A:3020:LEU:HD23	1.99	0.44
1:A:3851:ASP:O	1:A:3855:ARG:HG3	2.17	0.44
1:A:3881:ILE:HD13	1:A:4006:HIS:ND1	2.33	0.44
1:A:4302:ARG:O	1:A:4306:VAL:HG23	2.17	0.44
1:A:4379:THR:O	1:A:4383:THR:HG23	2.18	0.44
1:A:4563:LEU:HD12	1:A:4588:THR:HG21	1.99	0.44
1:A:3033:CYS:SG	1:A:3054:PHE:HB2	2.58	0.44
1:A:4065:GLN:CD	1:A:4092:ARG:HE	2.26	0.44
1:A:4266:ASN:O	1:A:4270:GLU:HG2	2.18	0.44
1:A:4482:PHE:CE1	1:A:4486:ILE:HD11	2.53	0.44
1:A:2420:ALA:HA	1:A:2423:MET:HG2	2.00	0.44
1:A:2994:MET:HB3	1:A:2998:ASN:OD1	2.18	0.44
1:A:3200:HIS:HE1	1:A:3747:LYS:HD3	1.82	0.44
1:A:1985:HIS:ND1	1:A:2010:PRO:HB3	2.33	0.43
1:A:2054:LEU:HA	1:A:2054:LEU:HD23	1.57	0.43
1:A:2427:PHE:CD1	1:A:2433:VAL:HG11	2.53	0.43
1:A:2671:MET:SD	1:A:2675:GLY:HA2	2.58	0.43
1:A:3109:PHE:HD2	1:A:3180:ILE:HG21	1.83	0.43
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	2.00	0.43
1:A:4395:LEU:HD12	1:A:4421:ALA:HA	2.01	0.43
1:A:1651:GLN:HE22	1:A:1664:ILE:HG12	1.81	0.43
1:A:3147:CYS:HB3	1:A:3179:PHE:HE2	1.83	0.43
1:A:3835:ILE:HD11	1:A:3866:VAL:HG12	2.00	0.43
1:A:4150:PRO:HD2	1:A:4159:ARG:HH21	1.82	0.43
1:A:1432:GLY:HA2	1:A:1435:TRP:CE3	2.54	0.43
1:A:2485:GLN:HG3	1:A:2488:ARG:HH21	1.82	0.43
1:A:2571:THR:O	1:A:2575:VAL:HG22	2.18	0.43
1:A:2813:LEU:HD11	1:A:2816:LEU:HD21	2.00	0.43
1:A:4297:PRO:HD3	1:A:4308:TRP:CE2	2.54	0.43
1:A:2435:LYS:NZ	1:A:2521:ILE:HB	2.32	0.43
1:A:2672:ASP:N	1:A:2672:ASP:OD1	2.51	0.43
1:A:3139:HIS:O	1:A:3143:ILE:HG12	2.17	0.43
1:A:3885:MET:CG	1:A:4343:MET:HE1	2.48	0.43
1:A:4424:LEU:HD12	1:A:4486:ILE:HG12	2.00	0.43
1:A:1335:GLU:O	1:A:1339:VAL:HG13	2.18	0.43
1:A:3788:ASP:OD1	1:A:3789:ILE:N	2.51	0.43
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1378:ARG:HG2	1:A:1383:TYR:CZ	2.54	0.43
1:A:1687:LYS:HG2	1:A:1712:THR:HG23	2.01	0.43
1:A:1785:VAL:O	1:A:1789:LEU:HD23	2.18	0.43
1:A:4175:GLU:HG2	1:A:4278:PHE:CE2	2.54	0.43
1:A:4192:GLU:OE1	1:A:4192:GLU:HA	2.18	0.43
1:A:1332:VAL:HG11	1:A:1380:TYR:CE2	2.54	0.43
1:A:3574:THR:O	1:A:3578:ILE:HG12	2.19	0.43
1:A:2527:PRO:HD3	1:A:2545:TRP:CE2	2.54	0.43
1:A:3101:ALA:O	1:A:3105:VAL:HG23	2.18	0.43
1:A:1678:SER:OG	1:A:1679:ARG:N	2.52	0.42
1:A:1769:MET:HB3	1:A:1831:ASP:HB2	2.00	0.42
1:A:2435:LYS:O	1:A:2438:GLU:HG3	2.18	0.42
1:A:2793:ILE:O	1:A:2836:ARG:NH2	2.41	0.42
1:A:2981:ARG:O	1:A:2985:CYS:HB3	2.18	0.42
1:A:4043:MET:HB2	1:A:4127:THR:HA	2.01	0.42
1:A:1387:GLN:O	1:A:1391:LYS:HG3	2.18	0.42
1:A:1678:SER:OG	1:A:1680:GLU:OE1	2.32	0.42
1:A:3007:ARG:CZ	1:A:3020:LEU:HD21	2.49	0.42
1:A:3779:GLU:HG2	1:A:3783:LYS:HE3	1.99	0.42
1:A:3893:LYS:HE2	1:A:3893:LYS:HB3	1.74	0.42
1:A:3945:LYS:HA	1:A:3945:LYS:HD2	1.82	0.42
1:A:3983:ILE:HD12	1:A:4012:ASN:OD1	2.19	0.42
1:A:1354:VAL:HG23	1:A:1404:LYS:HE3	2.00	0.42
1:A:1503:SER:O	1:A:1507:MET:HG2	2.19	0.42
1:A:2925:ILE:HG13	1:A:2933:LEU:HD22	2.00	0.42
1:A:2968:THR:HG22	1:A:2970:GLU:H	1.84	0.42
1:A:3684:PRO:HB3	1:A:3702:THR:HG21	2.01	0.42
1:A:1404:LYS:HE2	1:A:1404:LYS:HB2	1.79	0.42
1:A:1494:PHE:HA	1:A:1497:VAL:HG12	2.02	0.42
1:A:1836:PHE:CD2	1:A:4242:ALA:HA	2.55	0.42
1:A:2464:GLN:OE1	1:A:2467:ARG:NH1	2.52	0.42
1:A:2772:ALA:HA	1:A:2857:HIS:CE1	2.54	0.42
1:A:2934:LEU:HD21	1:A:3068:MET:SD	2.59	0.42
1:A:3756:VAL:C	1:A:3757:LYS:HD3	2.44	0.42
1:A:1758:TRP:CD2	1:A:1818:GLN:HG2	2.54	0.42
1:A:1766:LEU:HD13	1:A:1833:ALA:HA	2.02	0.42
1:A:2324:LEU:HD21	1:A:2332:ARG:HD3	2.01	0.42
1:A:1533:LEU:HD13	1:A:1592:LEU:HD13	2.01	0.42
1:A:2239:LYS:HE2	1:A:2239:LYS:HB3	1.88	0.42
1:A:2402:GLU:O	1:A:2402:GLU:HG3	2.19	0.42
1:A:2863:ARG:O	1:A:2863:ARG:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3839:VAL:HG13	1:A:3840:LEU:HD22	2.01	0.42
1:A:4404:ASN:HB3	1:A:4410:PHE:CE2	2.54	0.42
1:A:1398:MET:O	1:A:1402:GLU:OE1	2.38	0.42
1:A:1417:MET:HE1	1:A:1423:ASN:HB3	2.02	0.42
1:A:2840:ASP:HA	1:A:2843:ARG:HD2	2.01	0.42
1:A:3158:ASN:HD21	1:A:3171:ILE:HG12	1.83	0.42
1:A:3554:SER:OG	1:A:3558:GLU:OE1	2.38	0.42
1:A:1504:VAL:O	1:A:1507:MET:HB2	2.19	0.42
1:A:1882:THR:HG23	1:A:1885:THR:H	1.85	0.42
1:A:1397:ASN:C	1:A:1397:ASN:HD22	2.26	0.42
1:A:1423:ASN:OD1	1:A:1424:TRP:N	2.49	0.42
1:A:1661:VAL:HG13	1:A:1676:ILE:HB	2.02	0.42
1:A:2049:ILE:HG21	1:A:2090:LEU:HD11	2.01	0.42
1:A:2093:LEU:O	1:A:2097:LEU:HD23	2.20	0.42
1:A:2517:TYR:O	1:A:2521:ILE:HG12	2.19	0.42
1:A:2765:TYR:C	1:A:2768:PRO:HD2	2.45	0.42
1:A:2777:TYR:CB	1:A:2799:MET:HE1	2.50	0.42
1:A:3003:GLY:HA2	1:A:3006:GLU:CD	2.44	0.42
1:A:3628:ARG:HD3	1:A:3669:ILE:HG23	2.02	0.42
1:A:4107:MET:HE1	1:A:4137:ASN:ND2	2.27	0.42
1:A:1439:LEU:HD23	1:A:1439:LEU:HA	1.89	0.42
1:A:1755:GLN:HG2	1:A:1814:GLU:OE2	2.20	0.42
1:A:2478:ASP:OD1	1:A:2479:PHE:N	2.52	0.42
1:A:2493:TYR:CD1	1:A:2539:VAL:HB	2.54	0.42
1:A:2927:ARG:HG3	1:A:2928:GLN:NE2	2.35	0.42
1:A:4348:MET:CE	1:A:4453:ASN:HA	2.50	0.42
1:A:4474:THR:OG1	1:A:4477:GLN:HG3	2.20	0.42
1:A:2934:LEU:HB2	1:A:3089:CYS:SG	2.59	0.41
1:A:4549:GLN:HE22	1:A:4587:LEU:HB2	1.85	0.41
1:A:1496:LYS:HE2	1:A:1496:LYS:HB2	1.92	0.41
1:A:1626:PHE:CZ	1:A:1702:LEU:HB3	2.55	0.41
1:A:1741:TRP:CH2	1:A:1750:VAL:HG23	2.55	0.41
1:A:2648:VAL:HG11	1:A:2694:ARG:NH2	2.35	0.41
1:A:2903:GLU:OE1	1:A:2903:GLU:N	2.48	0.41
1:A:3017:VAL:O	1:A:3017:VAL:HG13	2.21	0.41
1:A:4336:GLY:O	1:A:4340:ILE:HG12	2.20	0.41
1:A:4375:ALA:O	1:A:4379:THR:HG23	2.20	0.41
1:A:1580:LYS:O	1:A:1584:LYS:HG2	2.20	0.41
1:A:2033:LYS:HE2	1:A:2033:LYS:HB3	1.94	0.41
1:A:2527:PRO:HG3	1:A:2545:TRP:CG	2.56	0.41
1:A:2747:ILE:O	1:A:2750:THR:OG1	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2777:TYR:CG	1:A:2799:MET:HE1	2.55	0.41
1:A:4031:VAL:HA	1:A:4035:VAL:HG12	2.02	0.41
1:A:4105:TRP:O	1:A:4108:GLN:HG3	2.20	0.41
1:A:4303:GLU:O	1:A:4307:GLN:NE2	2.53	0.41
1:A:1486:LEU:HD12	1:A:1541:GLN:HG3	2.02	0.41
1:A:1879:LEU:HD12	2:A:4701:ADP:C6	2.56	0.41
1:A:2335:LEU:HD12	1:A:2336:PRO:HD2	2.02	0.41
1:A:2437:LEU:HD22	1:A:2455:LEU:HD21	2.03	0.41
1:A:2451:ARG:O	1:A:2455:LEU:HD23	2.20	0.41
1:A:2467:ARG:NH1	1:A:2587:GLU:OE2	2.38	0.41
1:A:3488:ARG:NH2	1:A:3489:TRP:HE1	2.18	0.41
1:A:4554:ASP:OD1	1:A:4555:ALA:N	2.53	0.41
1:A:1363:LEU:O	1:A:1367:LEU:HG	2.20	0.41
1:A:2054:LEU:CD2	1:A:2097:LEU:HD12	2.49	0.41
1:A:2210:LEU:O	1:A:2214:THR:HG23	2.21	0.41
1:A:2396:ARG:HD3	1:A:2399:LYS:HE2	2.03	0.41
1:A:2965:ARG:HG3	1:A:2966:LYS:HD3	2.00	0.41
1:A:3172:THR:HG23	1:A:3174:ARG:HB2	2.02	0.41
1:A:3825:TYR:CE1	1:A:3875:MET:HG3	2.55	0.41
1:A:4105:TRP:HZ3	1:A:4109:LEU:HD12	1.83	0.41
1:A:3781:THR:O	1:A:3785:GLU:HG2	2.21	0.41
1:A:3984:GLY:HA2	1:A:3987:ILE:HG22	2.03	0.41
1:A:1422:VAL:HG13	1:A:1422:VAL:O	2.20	0.41
1:A:1550:ILE:HD12	1:A:1638:LEU:HD22	2.02	0.41
1:A:2300:TRP:CD1	1:A:2340:ARG:HB2	2.55	0.41
1:A:2844:ARG:HG2	1:A:2844:ARG:HH11	1.86	0.41
1:A:3498:ASN:O	1:A:3501:SER:OG	2.22	0.41
1:A:3804:LEU:HD13	1:A:3860:THR:HG22	2.01	0.41
1:A:1391:LYS:HA	1:A:1394:MET:HG2	2.03	0.41
1:A:1521:LEU:O	1:A:1524:GLU:HG3	2.21	0.41
1:A:1571:ILE:HG23	1:A:1604:LEU:HD22	2.01	0.41
1:A:1673:VAL:HB	1:A:1690:VAL:HG23	2.03	0.41
1:A:1682:GLU:OE1	1:A:1803:LEU:HD11	2.20	0.41
1:A:2879:LYS:HE3	1:A:2879:LYS:HB3	1.90	0.41
1:A:4071:ILE:HD11	1:A:4096:LEU:HD22	2.02	0.41
1:A:1357:ARG:CZ	1:A:2903:GLU:HB3	2.51	0.41
1:A:1923:LEU:HD12	1:A:1954:TRP:CZ2	2.56	0.41
1:A:1985:HIS:HD2	1:A:1997:ILE:HD12	1.86	0.41
1:A:2323:LYS:HE2	1:A:2323:LYS:HB3	1.85	0.41
1:A:3169:MET:HE3	1:A:3169:MET:HA	2.03	0.41
1:A:3210:GLU:HA	1:A:3213:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3654:ARG:O	1:A:3660:VAL:HA	2.21	0.41
1:A:3856:LEU:HA	1:A:3859:ILE:HG22	2.03	0.41
1:A:3886:LEU:HD11	1:A:4346:MET:SD	2.61	0.41
1:A:4149:PRO:HA	1:A:4150:PRO:HD3	1.97	0.41
1:A:4387:TRP:O	1:A:4391:ILE:HG12	2.20	0.41
1:A:4603:SER:O	1:A:4603:SER:OG	2.36	0.41
1:A:1517:GLU:O	1:A:1521:LEU:HD23	2.20	0.41
1:A:2307:VAL:HA	1:A:2311:TRP:HZ2	1.84	0.41
1:A:2447:MET:HE2	1:A:2447:MET:HB3	1.90	0.41
1:A:2599:SER:H	1:A:2601:LYS:HZ3	1.68	0.41
1:A:3138:SER:HB3	1:A:3141:GLU:HG3	2.03	0.41
1:A:3194:LEU:O	1:A:3198:GLN:HG2	2.21	0.41
1:A:4388:LEU:HD22	1:A:4428:ARG:NH1	2.36	0.41
1:A:1497:VAL:HG23	1:A:1527:LEU:HD12	2.02	0.40
1:A:1608:LEU:O	1:A:1611:ILE:HG22	2.20	0.40
1:A:1776:ALA:HB3	1:A:1777:PRO:HD3	2.03	0.40
1:A:2138:ILE:HA	1:A:2141:VAL:HG12	2.02	0.40
1:A:2230:LYS:HG2	1:A:2364:PHE:CD2	2.56	0.40
1:A:3051:TYR:O	1:A:3055:THR:HG23	2.21	0.40
1:A:3554:SER:OG	1:A:3555:ASN:N	2.54	0.40
1:A:3749:LEU:HD22	1:A:3773:LEU:HD22	2.02	0.40
1:A:3755:GLU:C	1:A:3759:ARG:HH22	2.27	0.40
1:A:4301:ARG:HG3	1:A:4301:ARG:HH11	1.86	0.40
1:A:1382:SER:O	1:A:1386:VAL:HG22	2.20	0.40
1:A:1460:GLU:HG2	1:A:1464:LYS:HE3	2.03	0.40
1:A:2519:ARG:HH21	1:A:2526:LEU:HB3	1.86	0.40
1:A:3813:PHE:O	1:A:3816:GLU:HG3	2.22	0.40
1:A:3930:GLU:OE1	1:A:3930:GLU:N	2.37	0.40
1:A:4077:PHE:HB3	1:A:4105:TRP:NE1	2.36	0.40
1:A:4422:LYS:HD2	1:A:4423:LEU:N	2.36	0.40
1:A:4453:ASN:O	1:A:4457:LYS:HG2	2.21	0.40
1:A:4504:LEU:O	1:A:4507:ILE:HG22	2.21	0.40
1:A:1978:ILE:HD13	1:A:2014:ILE:HD11	2.04	0.40
1:A:3585:ARG:NH2	1:A:3697:THR:HG22	2.36	0.40
1:A:4055:VAL:HG11	1:A:4095:MET:SD	2.61	0.40
1:A:4107:MET:O	1:A:4111:LYS:HE2	2.22	0.40
1:A:1698:ILE:O	1:A:1702:LEU:HD23	2.21	0.40
1:A:1806:ARG:NH2	1:A:1877:ASP:OD1	2.54	0.40
1:A:2411:PRO:O	1:A:2415:ILE:HG12	2.21	0.40
1:A:2799:MET:HB2	1:A:2799:MET:HE2	1.76	0.40
1:A:3045:ASP:HA	1:A:3050:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4019:SER:O	1:A:4022:GLU:HG3	2.21	0.40
1:A:4412:PHE:CZ	1:A:4514:LEU:HD13	2.57	0.40
1:A:1347:LYS:HG2	1:A:1432:GLY:HA2	2.04	0.40
1:A:1432:GLY:HA2	1:A:1435:TRP:HE3	1.86	0.40
1:A:1659:ALA:HA	1:A:1926:PHE:CE1	2.57	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	3028/4646 (65%)	2937 (97%)	91 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2703/4125 (66%)	2703 (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 (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1361	GLN
1	A	1397	ASN
1	A	2416	GLN
1	A	2554	GLN
1	A	2964	HIS
1	A	3135	GLN
1	A	3145	ASN
1	A	3188	HIS
1	A	3197	GLN
1	A	3200	HIS
1	A	3214	GLN
1	A	3498	ASN
1	A	3499	GLN
1	A	3526	GLN
1	A	3837	HIS
1	A	3854	GLN
1	A	3931	GLN
1	A	4078	ASN
1	A	4098	ASN
1	A	4156	ASN
1	A	4174	ASN
1	A	4397	HIS
1	A	4508	HIS
1	A	4526	GLN
1	A	4532	ASN
1	A	4549	GLN
1	A	4595	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
4	ANP	A	4703	-	33,33,33	2.34	6 (18%)	45,52,52	1.44	6 (13%)
2	ADP	A	4704	-	28,29,29	1.41	4 (14%)	43,45,45	1.82	9 (20%)
3	ATP	A	4702	5	32,33,33	0.42	0	48,52,52	0.32	0
2	ADP	A	4701	-	28,29,29	1.42	5 (17%)	43,45,45	1.79	9 (20%)

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
4	ANP	A	4703	-	-	7/18/38/38	0/3/3/3
2	ADP	A	4704	-	-	4/16/32/32	0/3/3/3
3	ATP	A	4702	5	-	7/22/38/38	0/3/3/3
2	ADP	A	4701	-	-	4/16/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4703	ANP	PB-O3A	9.14	1.70	1.59
4	A	4703	ANP	PG-N3B	6.20	1.79	1.63
4	A	4703	ANP	PG-O1G	4.80	1.53	1.46
2	A	4704	ADP	C5-C4	4.65	1.47	1.39
2	A	4701	ADP	C5-C4	4.65	1.47	1.39
4	A	4703	ANP	PB-O1B	2.78	1.50	1.46
2	A	4704	ADP	C5-C6	2.70	1.48	1.41
2	A	4701	ADP	C5-C6	2.63	1.48	1.41
2	A	4704	ADP	C5-N7	-2.36	1.34	1.39
2	A	4701	ADP	C5-N7	-2.36	1.34	1.39
2	A	4704	ADP	C8-N7	2.30	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4701	ADP	C8-N7	2.26	1.36	1.31
4	A	4703	ANP	PB-O2B	-2.16	1.51	1.56
4	A	4703	ANP	PA-O3A	2.08	1.61	1.59
2	A	4701	ADP	PA-O3A	2.03	1.61	1.59

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4704	ADP	C5-C4-N3	-5.93	118.55	126.72
2	A	4701	ADP	C5-C4-N3	-5.64	118.94	126.72
2	A	4704	ADP	N3-C4-N9	4.58	134.96	127.17
4	A	4703	ANP	O2B-PB-O1B	4.52	119.57	109.87
2	A	4701	ADP	N3-C4-N9	4.50	134.82	127.17
4	A	4703	ANP	O1G-PG-N3B	-4.04	105.82	111.77
2	A	4704	ADP	C2-N3-C4	3.73	120.93	111.83
2	A	4701	ADP	C2-N3-C4	3.64	120.72	111.83
2	A	4704	ADP	C4-C5-N7	-3.51	106.57	110.58
2	A	4701	ADP	C4-C5-N7	-3.39	106.70	110.58
2	A	4701	ADP	N3-C2-N1	-3.38	123.47	128.58
2	A	4704	ADP	N3-C2-N1	-3.16	123.80	128.58
2	A	4701	ADP	C4-N9-C8	2.66	108.53	105.74
4	A	4703	ANP	O2G-PG-O3G	2.54	114.42	107.59
2	A	4704	ADP	C5-N7-C8	2.51	107.39	103.45
2	A	4701	ADP	C5-N7-C8	2.48	107.34	103.45
2	A	4704	ADP	C3'-C2'-C1'	2.43	106.07	101.46
2	A	4704	ADP	C4-N9-C8	2.41	108.27	105.74
4	A	4703	ANP	O5'-C5'-C4'	2.14	116.28	108.99
4	A	4703	ANP	O4'-C4'-C3'	-2.11	100.97	105.15
4	A	4703	ANP	O4'-C1'-N9	2.08	112.09	108.09
2	A	4701	ADP	C2-N1-C6	2.06	122.12	118.73
2	A	4704	ADP	C6-C5-N7	2.05	136.04	132.09
2	A	4701	ADP	C6-C5-N7	2.04	136.02	132.09

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	O4'-C4'-C5'-O5'
2	A	4704	ADP	C5'-O5'-PA-O3A
3	A	4702	ATP	PB-O3B-PG-O3G
3	A	4702	ATP	C5'-O5'-PA-O3A
4	A	4703	ANP	PB-N3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
4	A	4703	ANP	PA-O3A-PB-O2B
4	A	4703	ANP	C5'-O5'-PA-O3A
4	A	4703	ANP	C4'-C5'-O5'-PA
2	A	4701	ADP	C3'-C4'-C5'-O5'
2	A	4704	ADP	C3'-C4'-C5'-O5'
2	A	4704	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'
4	A	4703	ANP	C2'-C1'-N9-C4
4	A	4703	ANP	C2'-C1'-N9-C8
3	A	4702	ATP	PB-O3B-PG-O1G
2	A	4701	ADP	PB-O3A-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O1A
4	A	4703	ANP	C5'-O5'-PA-O1A
2	A	4701	ADP	PB-O3A-PA-O1A
3	A	4702	ATP	PG-O3B-PB-O2B
3	A	4702	ATP	PB-O3A-PA-O2A

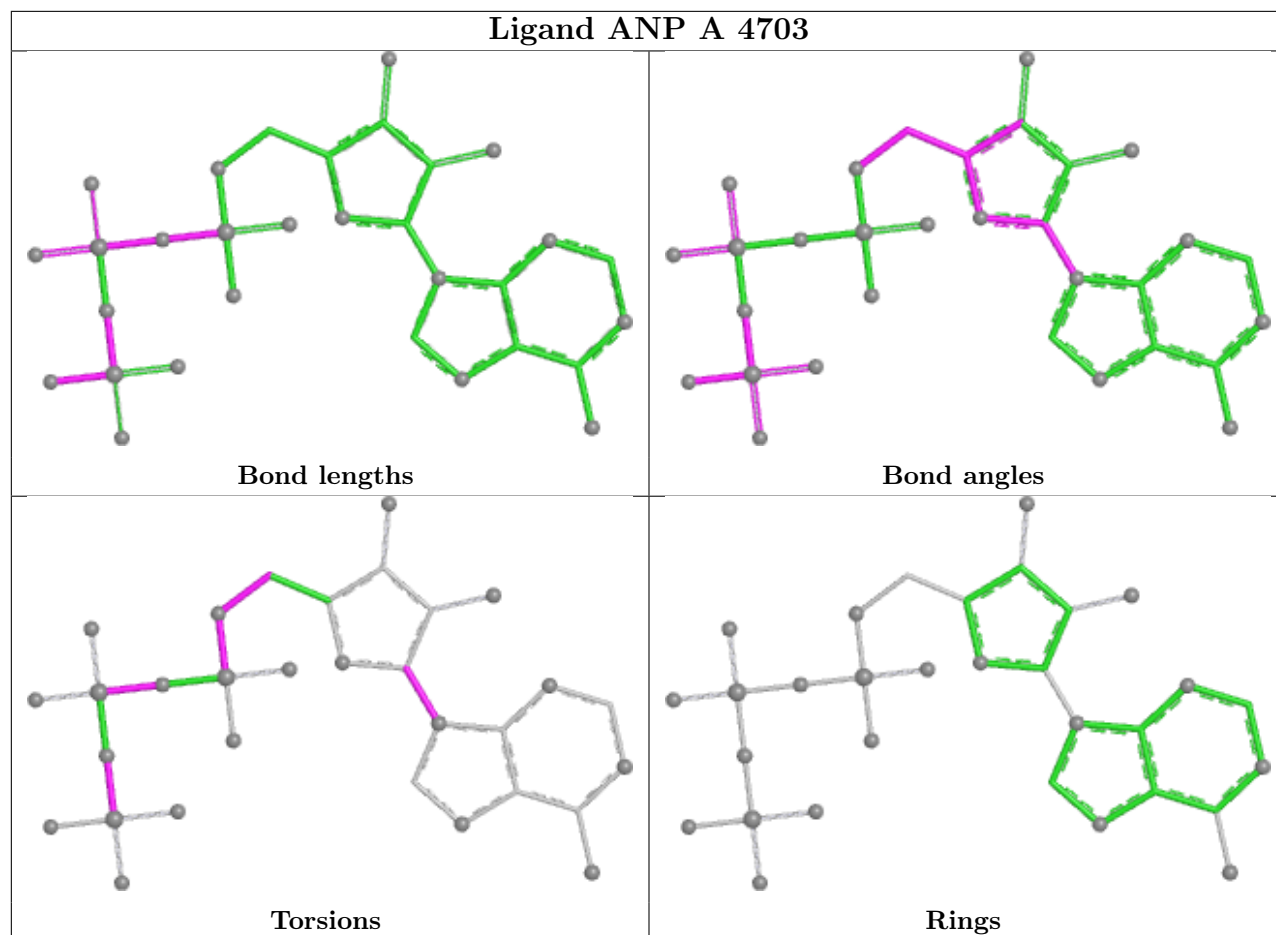
There are no ring outliers.

4 monomers are involved in 17 short contacts:

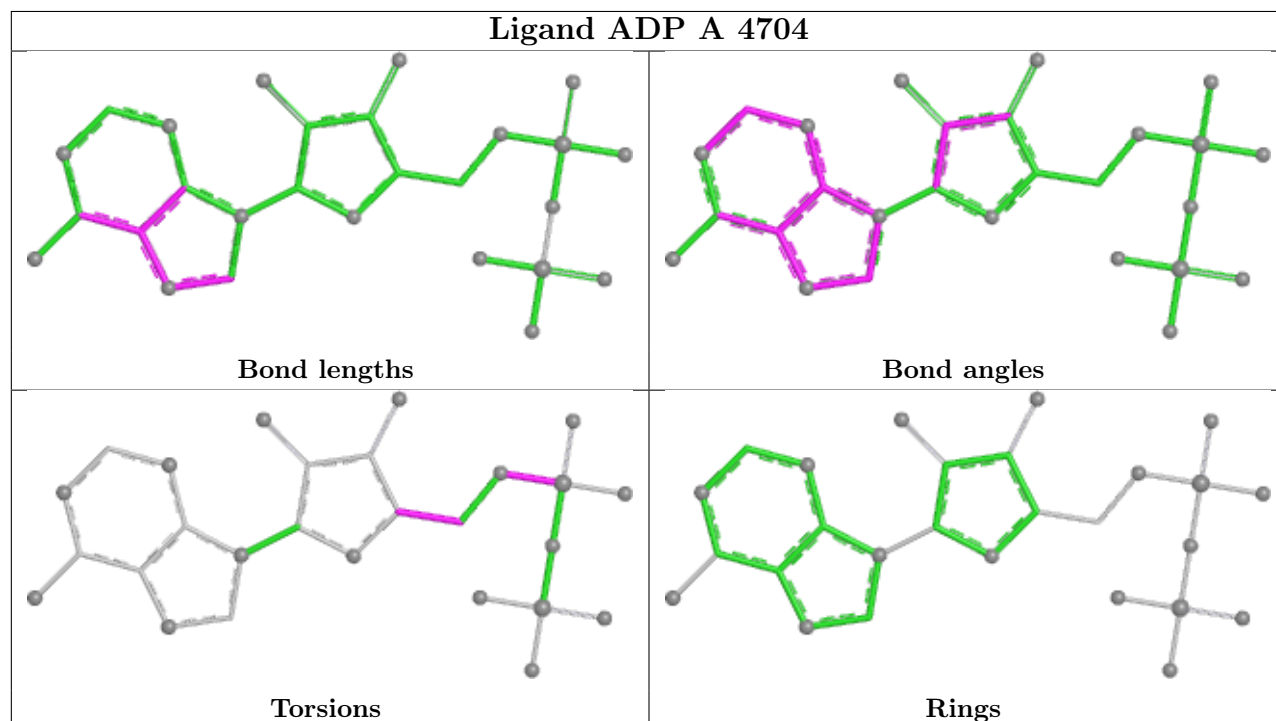
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4703	ANP	4	0
2	A	4704	ADP	3	0
3	A	4702	ATP	6	0
2	A	4701	ADP	4	0

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.

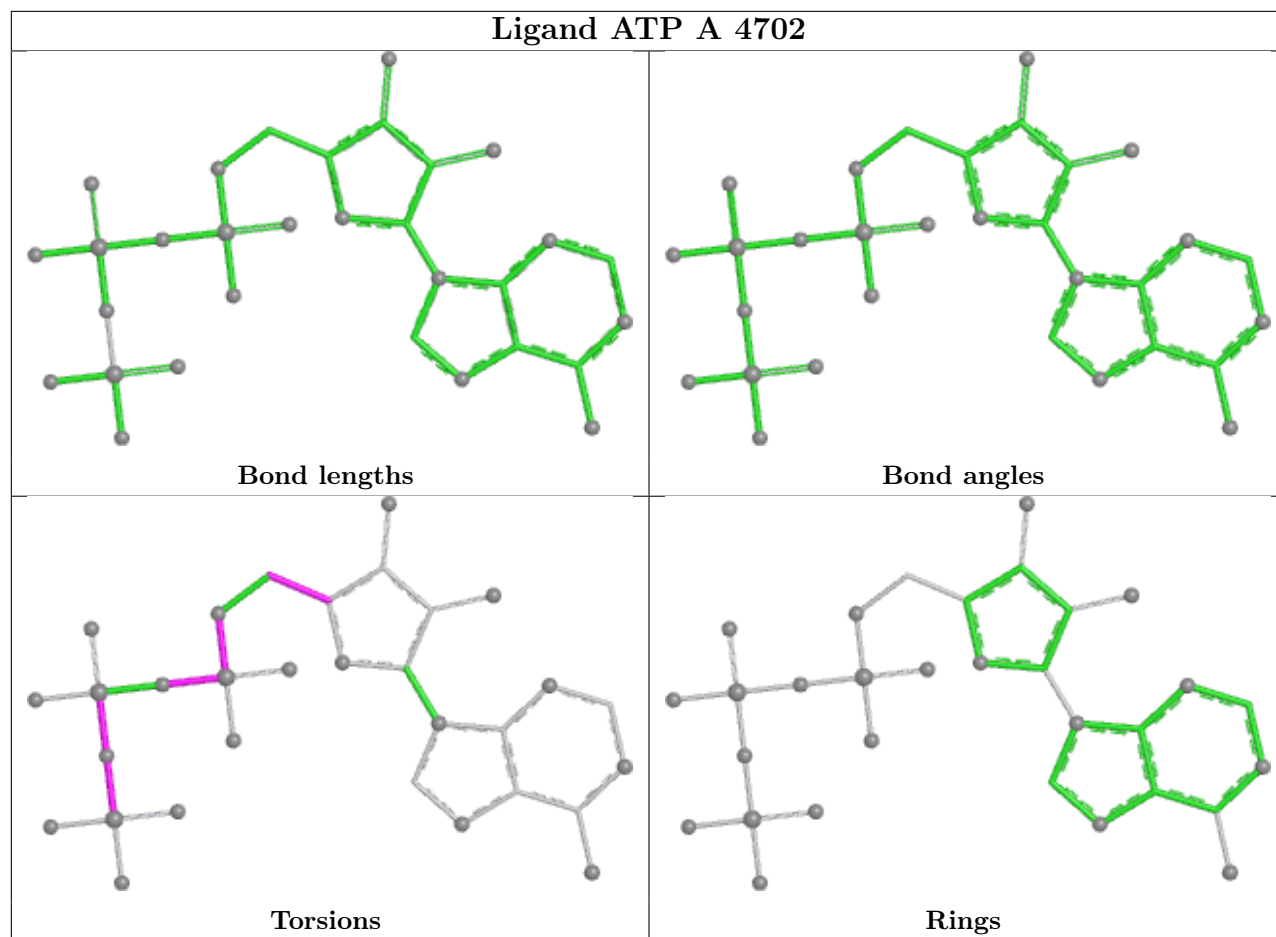
Ligand ANP A 4703



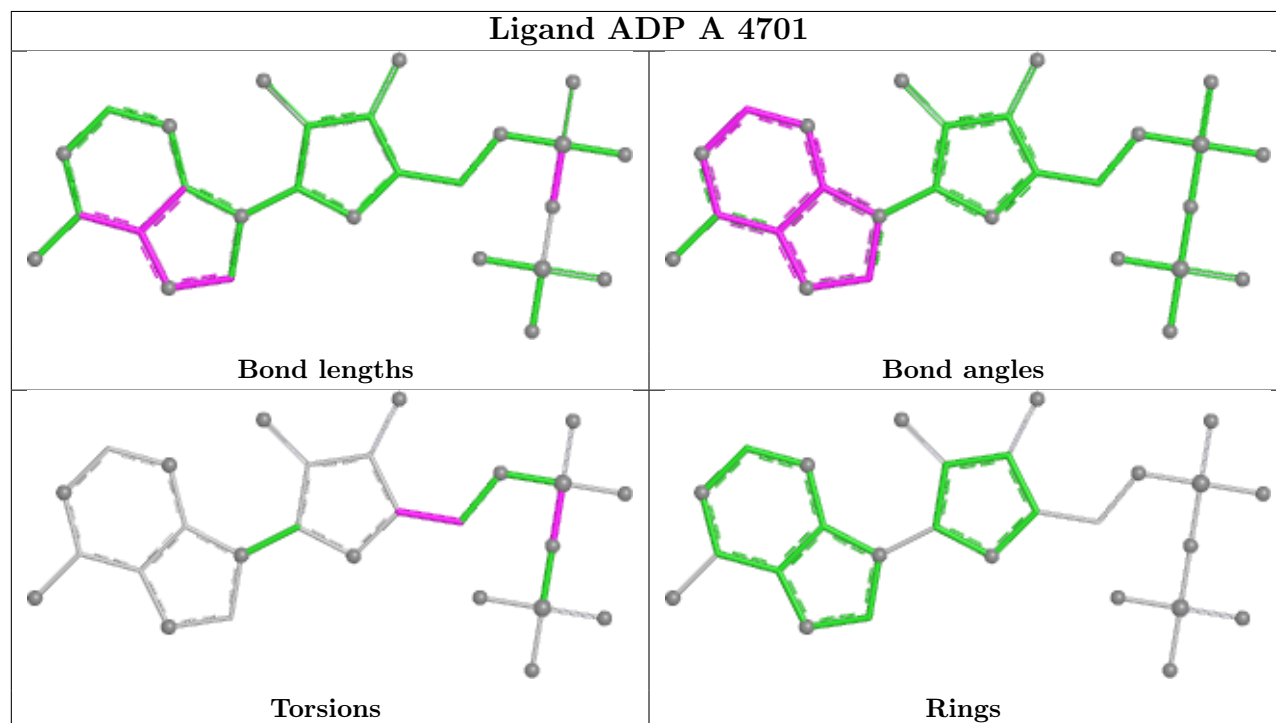
Ligand ADP A 4704



Ligand ATP A 4702



Ligand ADP A 4701



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

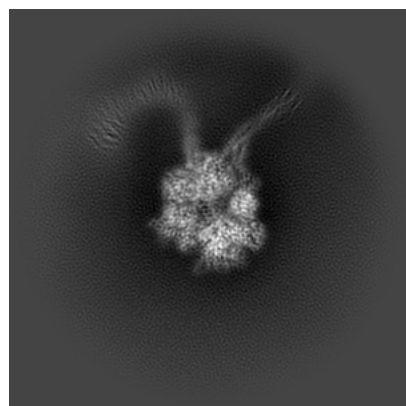
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73176. These allow visual inspection of the internal detail of the map and identification of artifacts.

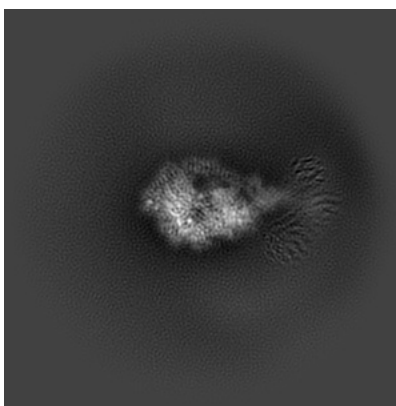
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

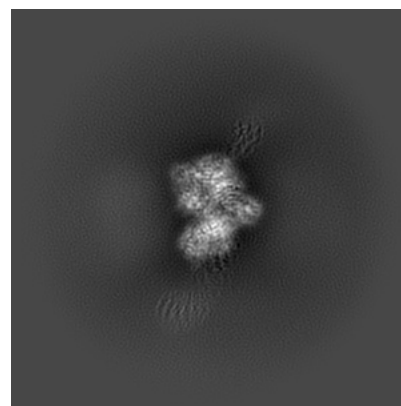
6.1.1 Primary map



X

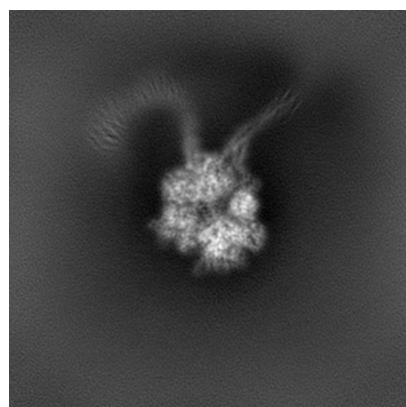


Y

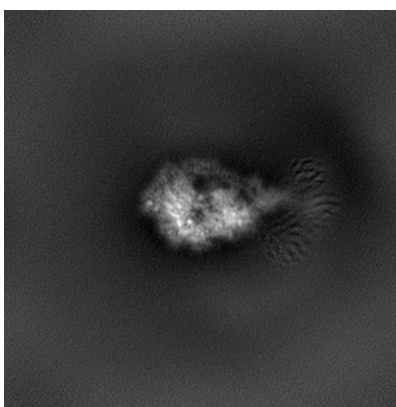


Z

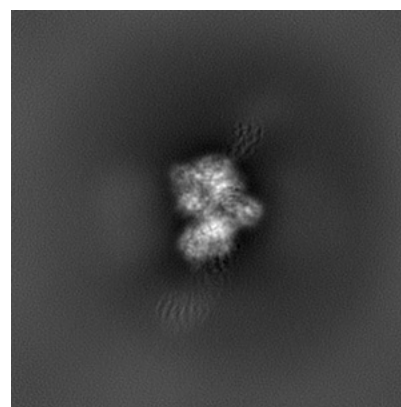
6.1.2 Raw map



X



Y

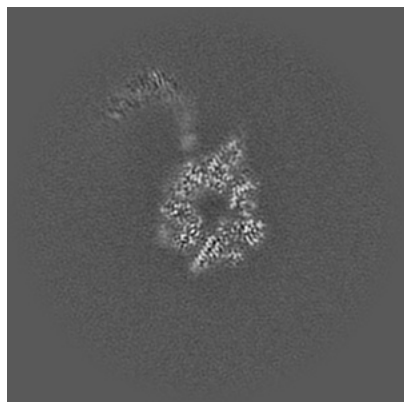


Z

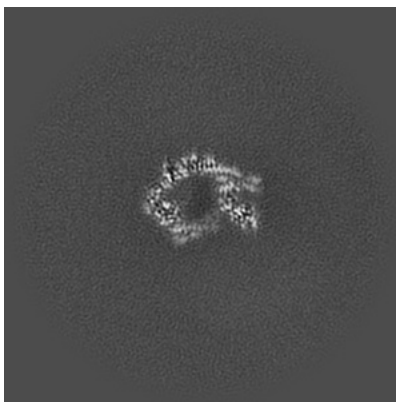
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

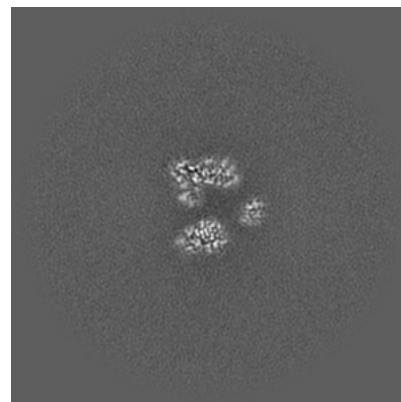
6.2.1 Primary map



X Index: 128

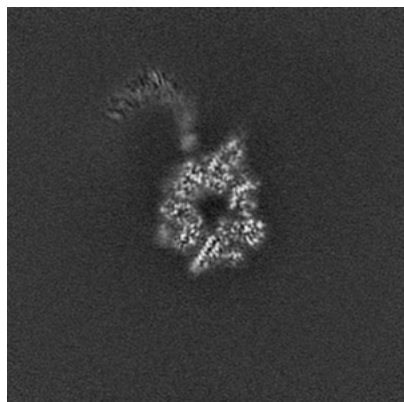


Y Index: 128

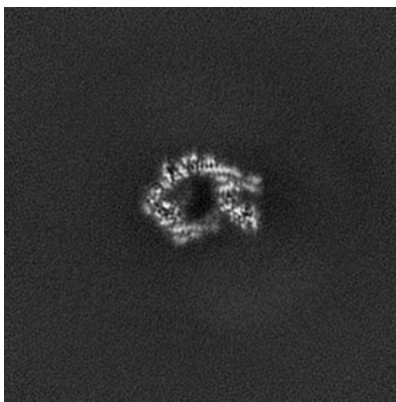


Z Index: 128

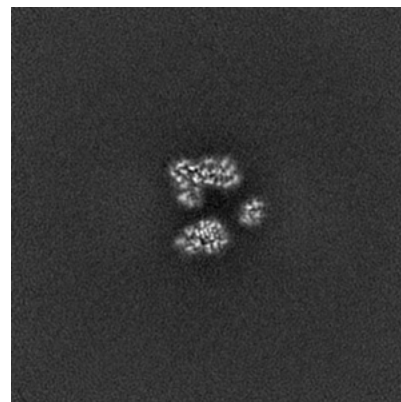
6.2.2 Raw map



X Index: 128



Y Index: 128

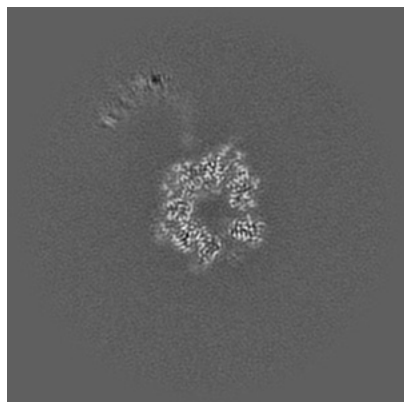


Z Index: 128

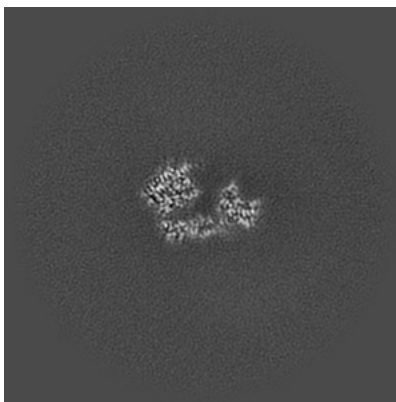
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

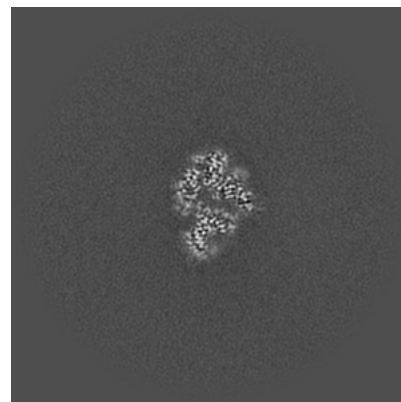
6.3.1 Primary map



X Index: 125

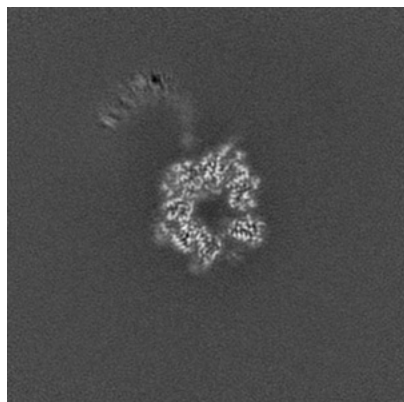


Y Index: 135

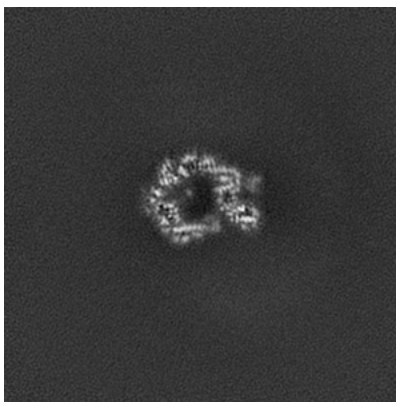


Z Index: 112

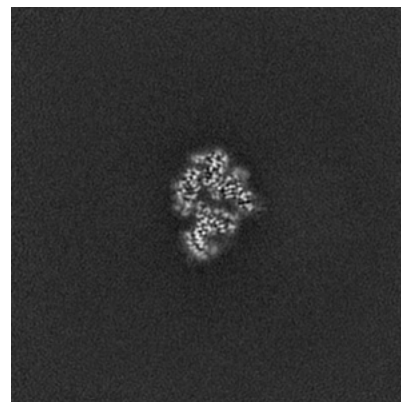
6.3.2 Raw map



X Index: 125



Y Index: 129

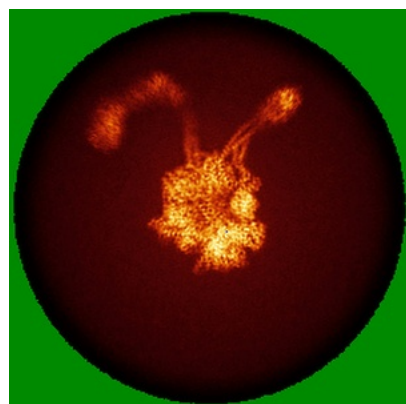


Z Index: 112

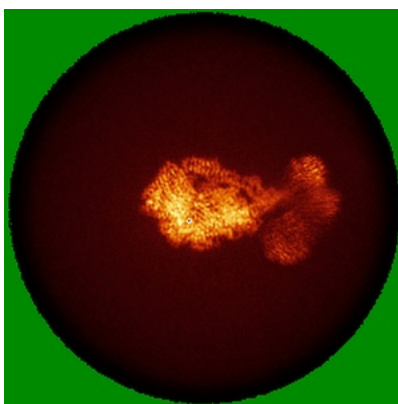
The images above show the largest variance slices of the map in three orthogonal directions.

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

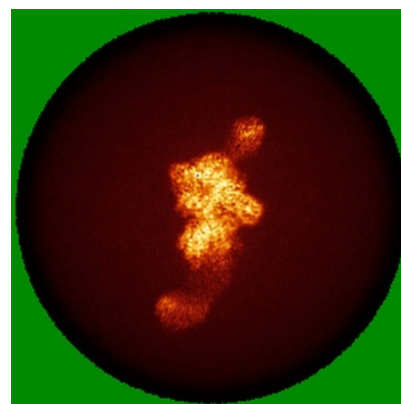
6.4.1 Primary map



X

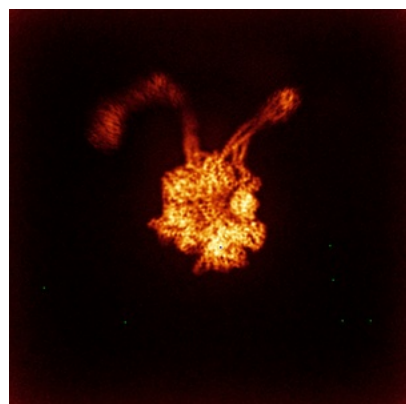


Y

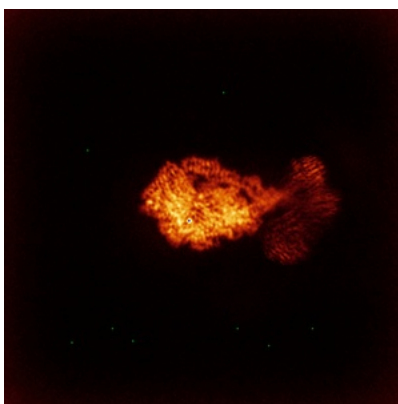


Z

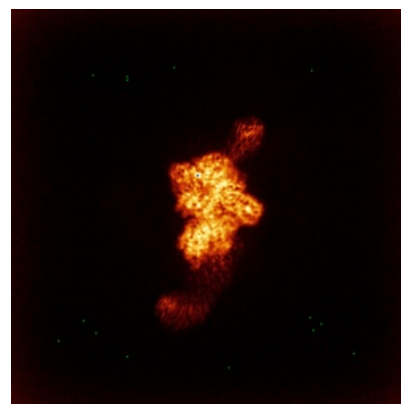
6.4.2 Raw map



X



Y

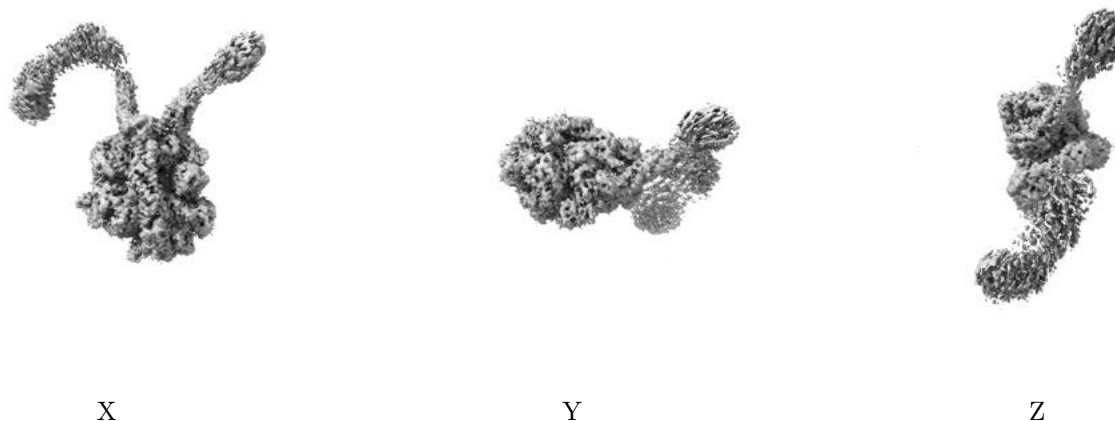


Z

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.

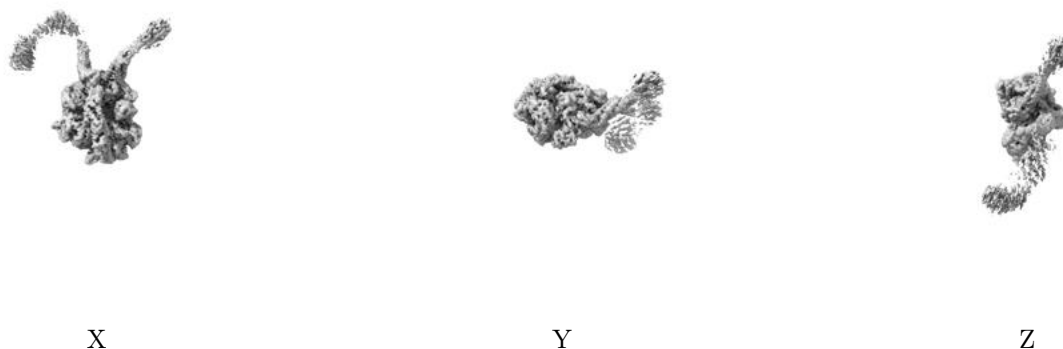
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

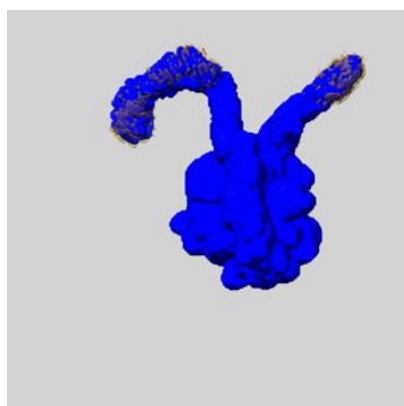
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

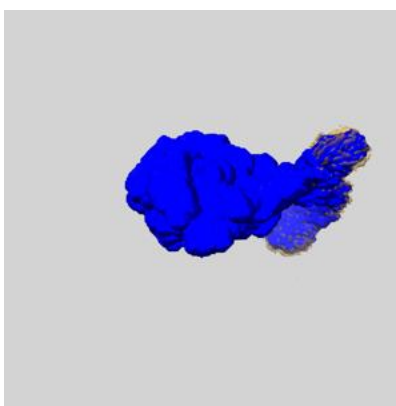
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

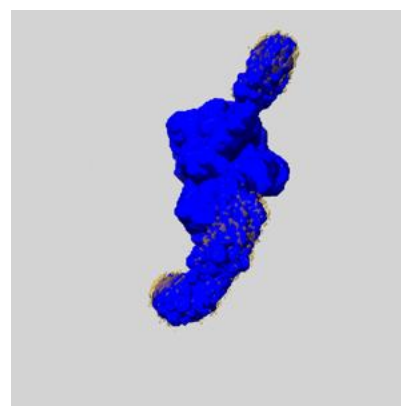
6.6.1 emd_73176_msk_1.map [i](#)



X



Y

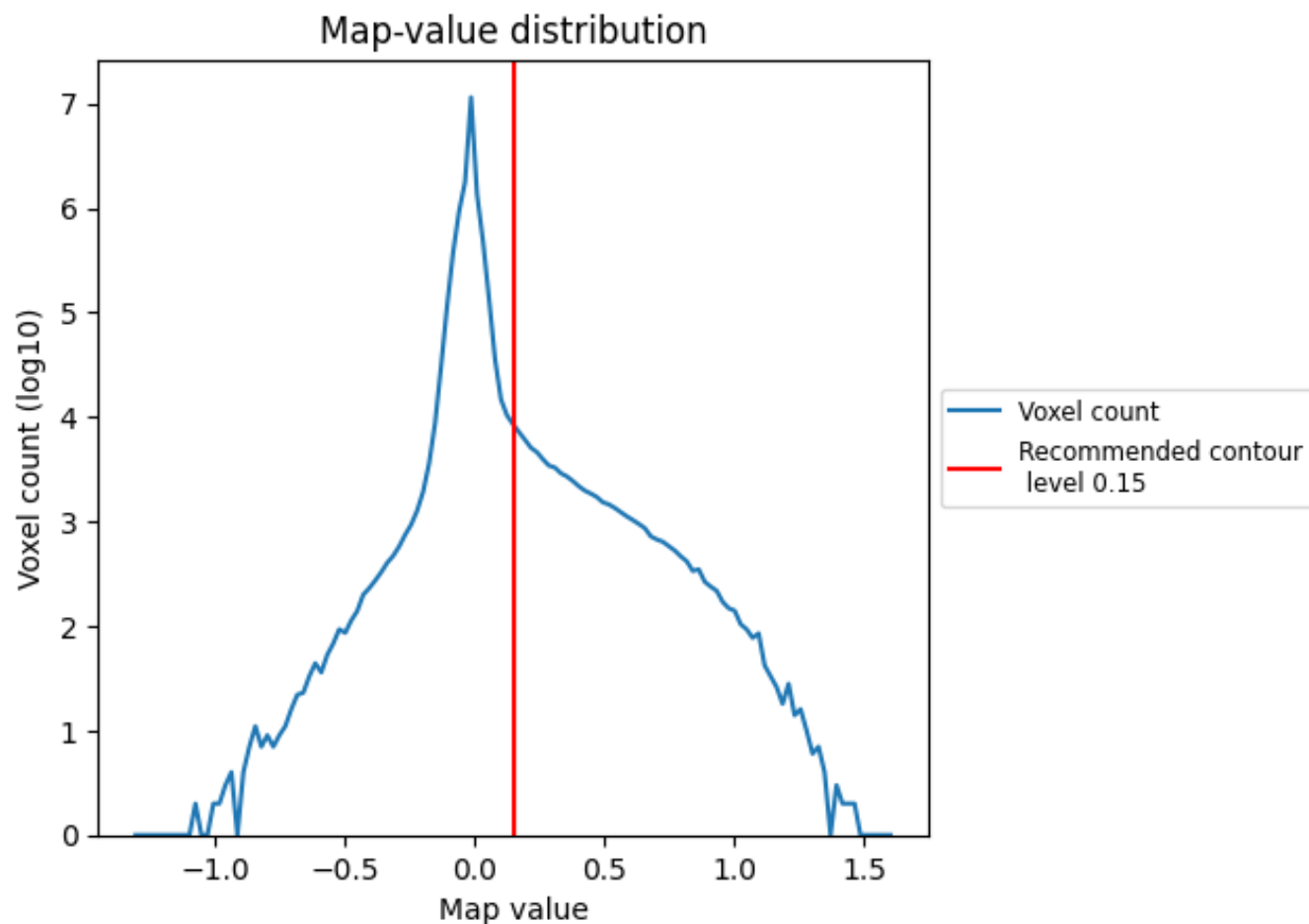


Z

7 Map analysis [i](#)

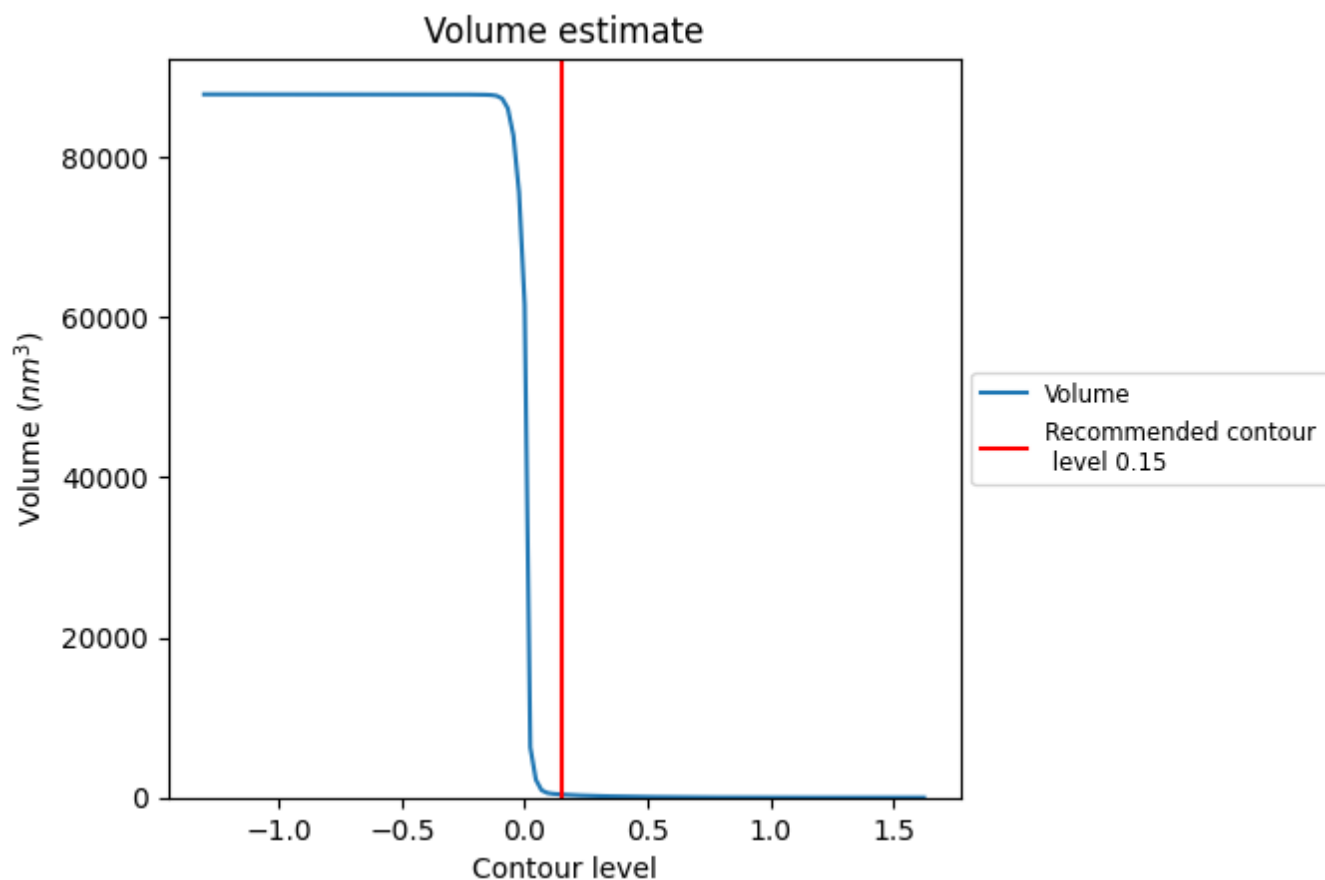
This section contains the results of statistical analysis of the map.

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.

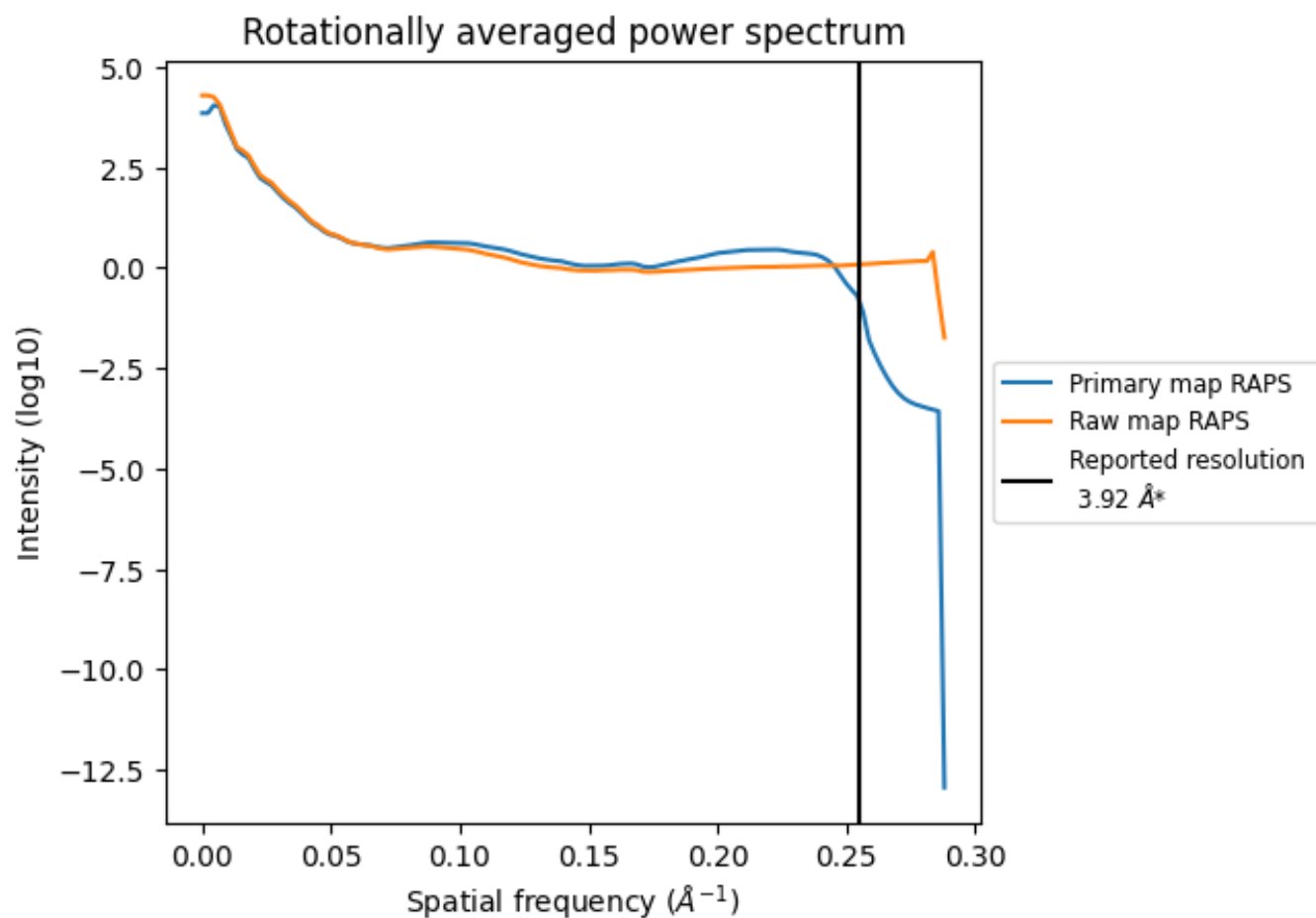
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 383 nm³; this corresponds to an approximate mass of 346 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 ⓘ

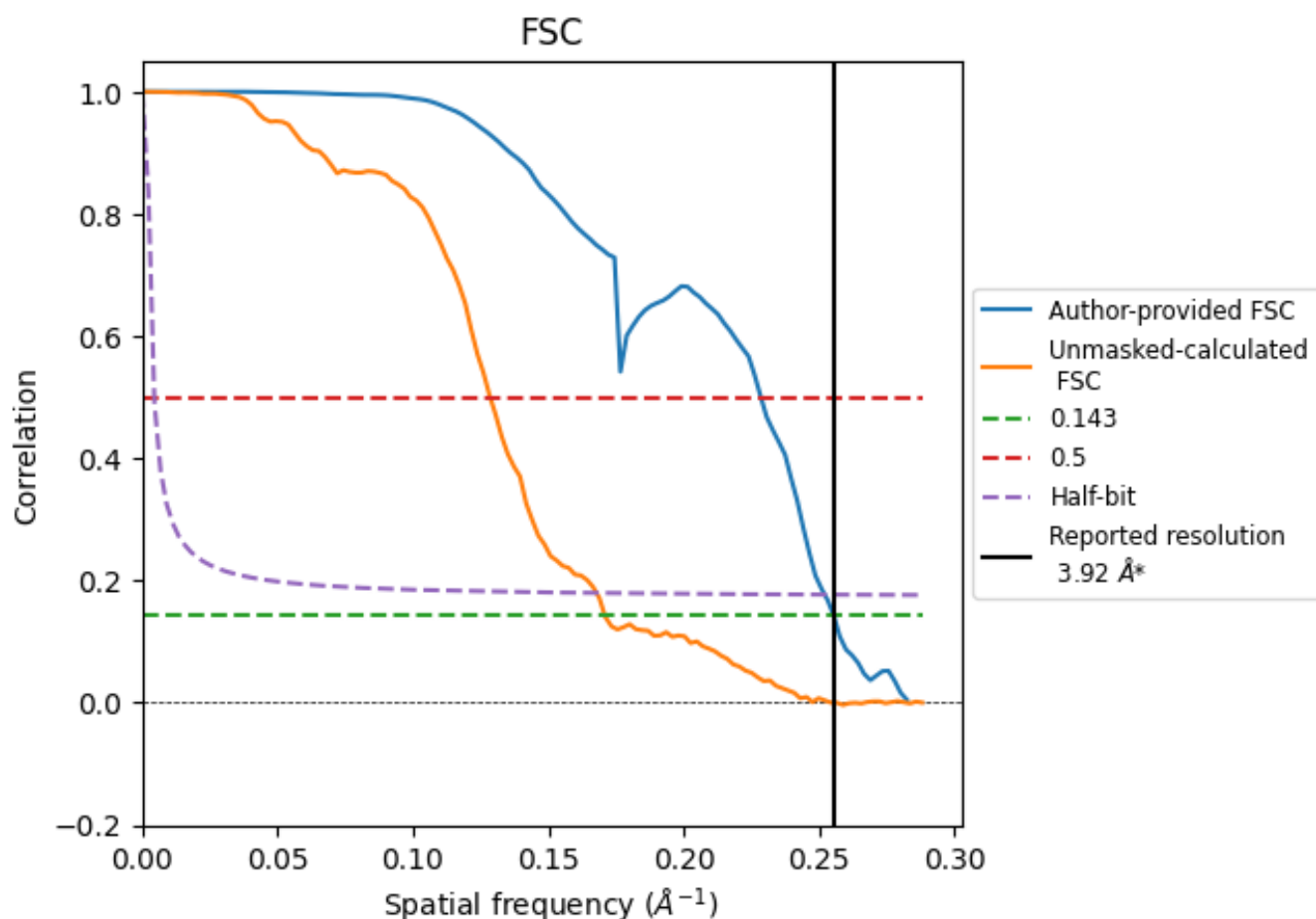


*Reported resolution corresponds to spatial frequency of 0.255 Å⁻¹

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 0.255 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

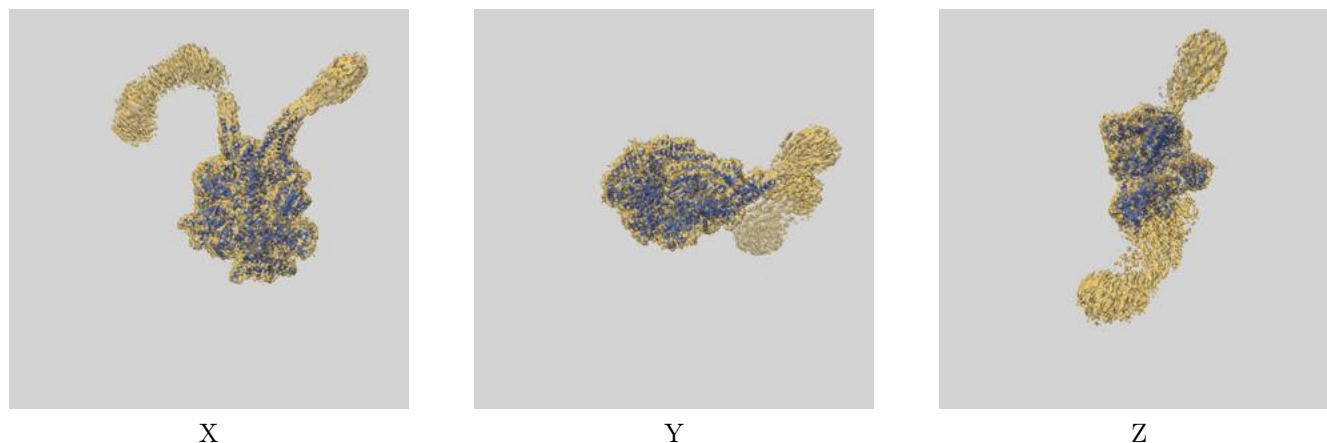
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.92	-	-
Author-provided FSC curve	3.92	4.38	3.97
Unmasked-calculated*	5.85	7.79	5.96

*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 5.85 differs from the reported value 3.92 by more than 10 %

9 Map-model fit [i](#)

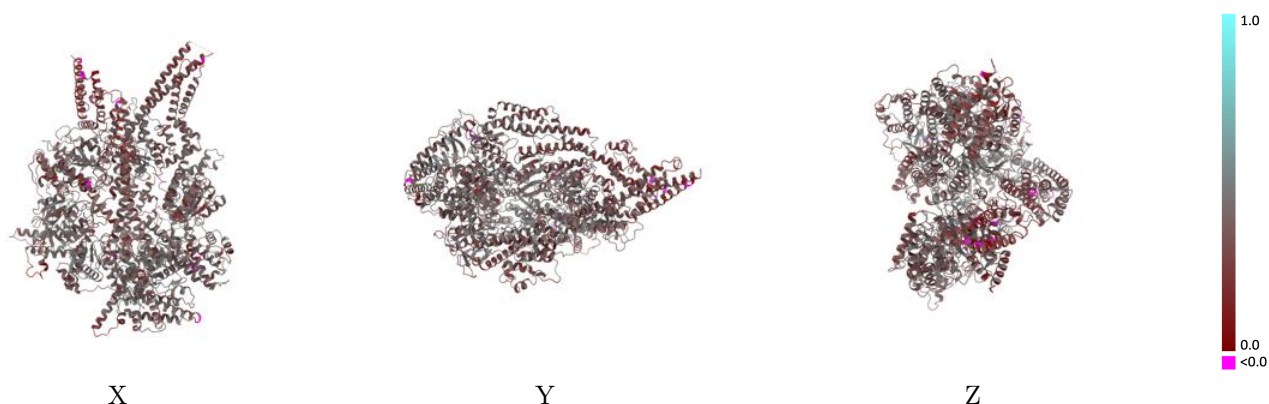
This section contains information regarding the fit between EMDB map EMD-73176 and PDB model 9YNF. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



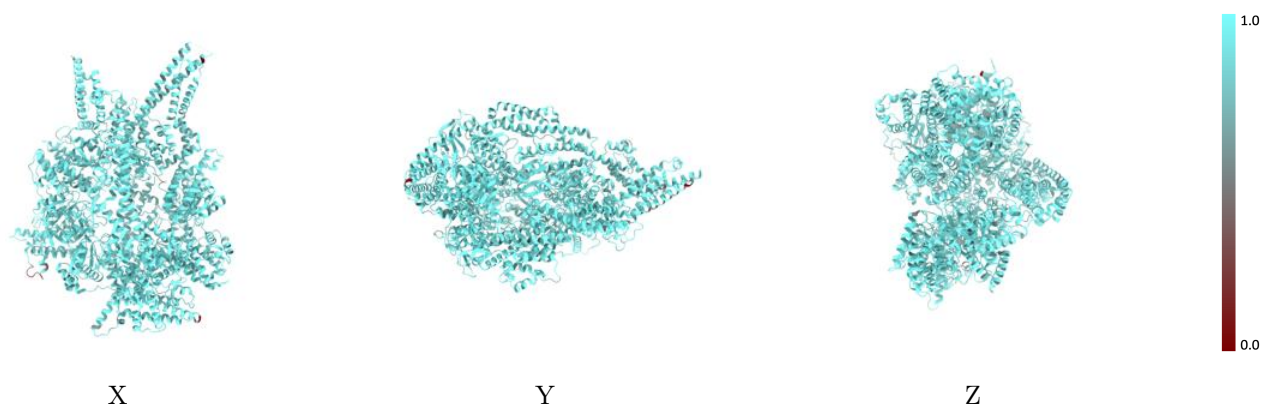
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



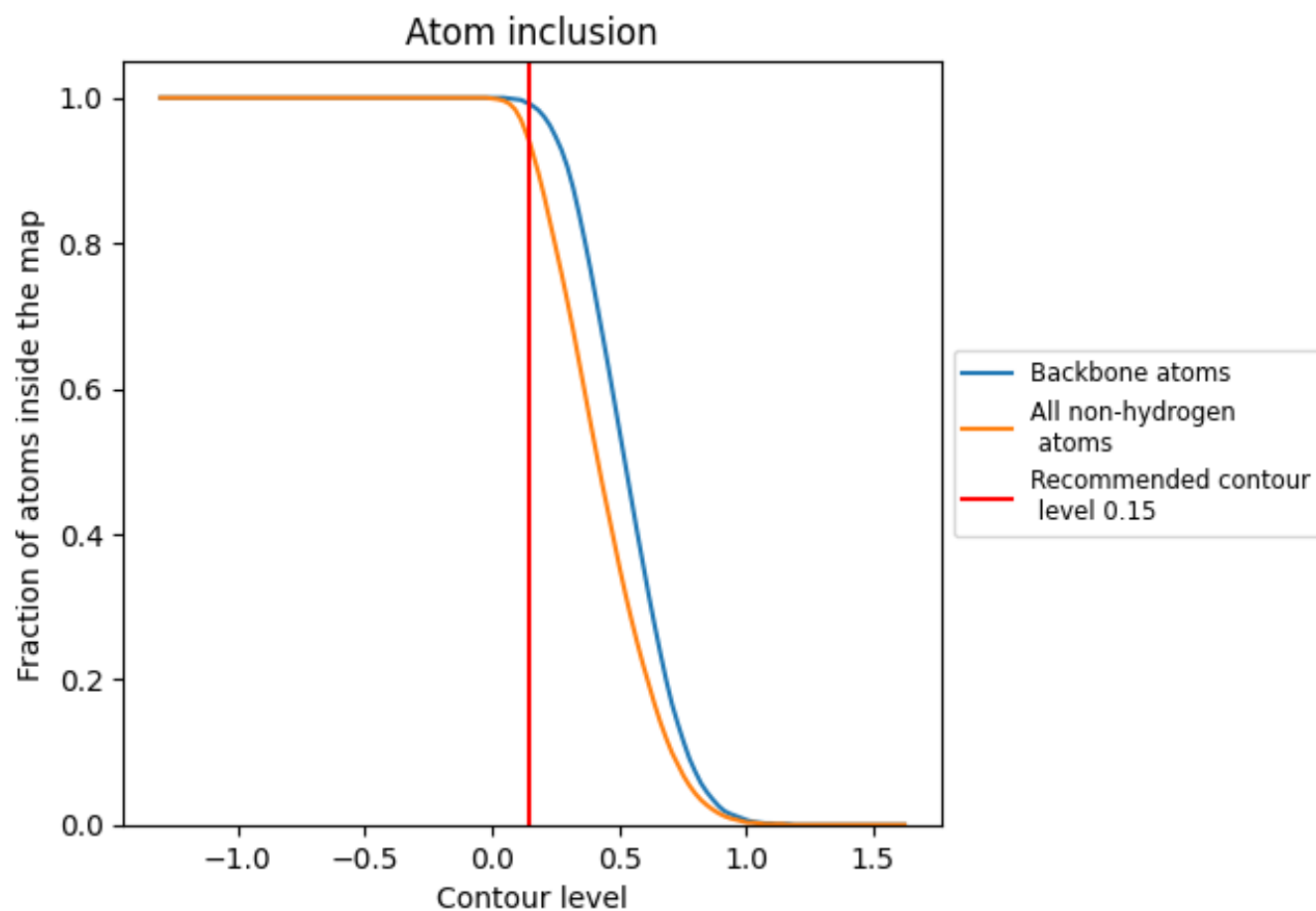
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 94% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9370	0.3720
A	0.9370	0.3720

