



Full wwPDB EM Validation Report ⓘ

Jul 7, 2024 – 06:55 pm BST

PDB ID : 7OTV
EMDB ID : EMD-13067
Title : DNA-PKcs in complex with wortmannin
Authors : Liang, S.; Thomas, S.E.; Blundell, T.L.
Deposited on : 2021-06-10
Resolution : 3.24 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.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

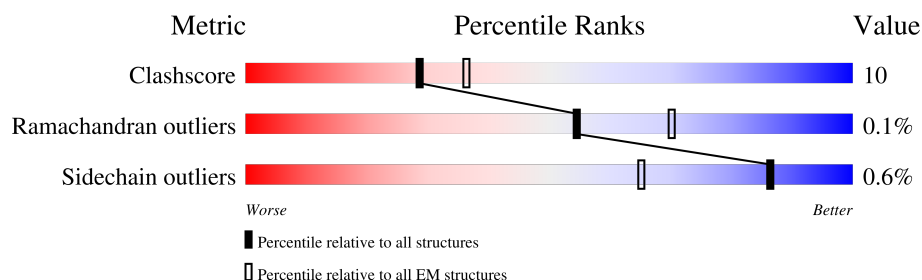
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.24 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	4148	<div> <div>8%</div> <div>69%</div> <div>19%</div> <div>12%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	KWT	A	6101	-	-	X	-

2 Entry composition [i](#)

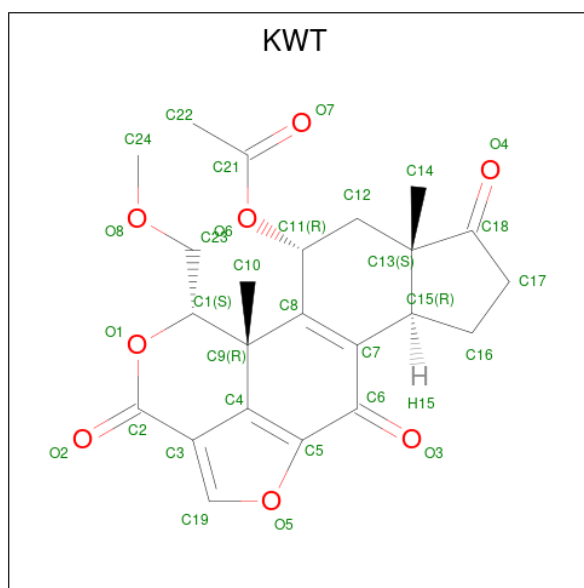
There are 2 unique types of molecules in this entry. The entry contains 29041 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-PKcs.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3656	29010	18609	4903	5307	191	0	0

- Molecule 2 is (1S,6BR,9AS,11R,11BR)-9A,11B-DIMETHYL-1-[(METHYLOXY)METHYL]-3,6,9-TRIOXO-1,6,6B,7,8,9,9A,10,11,11B-DECAHYDRO-3H-FURO[4, 3,2-DE]INDENO[4,5-H][2]BENZOPYRAN-11-YL ACETATE (three-letter code: KWT) (formula: C₂₃H₂₄O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	A	1	31	23	8	0

3 Residue-property plots

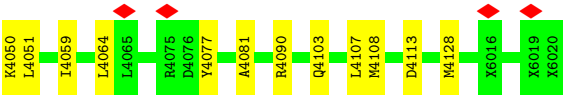
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-PKcs



L2323	F2224	I2137	PRO	GLU	D1821	R1711	S1549	R1445	A1317	I1188	D1005
L2327	F2231	V2138	ARG	ARG	R1822	R1715	V1550	S1446	A1318	I1189	T1006
V2330	L2235	P2139	ALA	LYS	L1824	E1715	F1553	R1447	G1319	V1195	L1009
L2336	T2240	F2145	THR	LYS	L1827	I1718	Y1560	L1448	N1320	P1204	L1010
K2347	L2241	I2151	GLY	TYR	L1836	F1722	S1563	V1452	R1321	L1208	E1011
Q2348	C2244	N2152	ARG	ILE	L1837	Q1725	L1562	L1458	T1322	L1212	D1015
L2349	W2245	E2155	ARG	ILE	E1838	S1726	I1567	I1467	Q1325	L1217	G1016
K2350	L2249	E2158	ARG	LYS	V1845	G1732	E1570	S1470	K1334	V1217	I1017
Q2353	P2252	V2164	ALA	ALA	D1846	T1733	L1572	Q1471	P1324	S1218	V1018
N2354	Y2253	L2165	ASP	ARG	L1932	G1734	K1573	S1472	V1339	F1219	D1019
T2355	R2254	S2166	PRO	ALA	L1934	R1735	L1574	T1473	R1340	L1220	P1020
R2356	L2255	P2167	THR	ASN	D1849	Q1754	L1575	D1474	T1351	I1221	V1021
L2357	L2256	L2168	VAL	GLY	S1853	Q1758	S1585	L1475	T1352	N1222	R1026
D2358	Q2170	L2169	HIS	ASP	R1854	L1759	S1586	H1476	P1353	T1223	G1030
K2359	Q2171	Q2170	ASP	ASP	F1855	E1760	L1597	H1477	L1358	F1224	I1033
F2360	L2171	S2174	VAL	ASP	T1856	L1759	L1597	V1478	L1359	E1225	I1037
S2261	E2175	E2175	LEU	GLY	K1857	E1764	Q1614	V1479	N1365	Q1231	R1062
G2262	N2176	N2176	LEU	PRO	L1858	E1769	K1617	E1482	T1366	S1233	L1037
K2268	N2177	G2178	GLU	TYR	N1859	Q1770	L1618	L1484	G1234	G1234	P1062
D2269	G2178	G2179	GLU	MET	S1861	F1782	I1622	S1485	L1372	L1236	A1081
N2270	G2179	Q1963	LEU	SER	D1864	I1785	K1627	D1495	V1374	T1240	F1082
S2271	E2180	Q1964	THR	LEU	I1867	A1786	W1632	E1496	Q1374	L1241	N1083
V2272	C2092	F1965	LEU	LEU	K1870	R1787	W1633	K1497	T1375	L1242	N1084
L2276	C2093	F1965	ALA	ASP	M1871	R1788	A1634	Q1498	C1377	L1269	I1085
L2277	L2097	S1968	ASP	SER	R1871	R1789	K1635	G1499	E1378	L1280	Y1087
V2280	H2103	E1969	THR	SER	Y1874	S1790	D1636	L1503	S1381	L1261	E1088
N2281	M2104	K1970	LEU	THR	K1875	T1793	E1640	D1504	I1382	E1265	E1097
A2282	H2105	P1971	SER	LEU	R1883	Q1794	T1641	L1505	I1386	C1266	L1104
N2283	L2108	N1974	GLU	GLU	L1884	V1795	K1642	L1514	V1389	Y1267	I1124
D2289	GLY	L1975	MET	MET	P1885	G1796	L1652	F1519	Q1390	T1269	Q1125
A2200	PRO	L1976	SER	SER	D1888	L1798	S1657	C1526	M1392	A1286	Q1126
T2201	PRO	L1981	ASP	PHE	V1889	E1799	S1664	E1526	L1395	L1290	D1129
V2205	GLN	L1984	GLY	ASP	H1890	Y1802	S1664	R1527	L1398	F1296	R1151
P2206	GLY	K1985	THR	PHE	A1891	E1803	D1685	L1528	V1398	S1300	P1158
K2207	ASP	K1985	GLY	SER	K1892	R1806	K1689	L1532	L1402	M1303	P1159
D2208	VAL	ARG	VAL	GLN	S1894	R1811	G1690	L1538	M1403	H1304	L1163
E2209	VAL	TYR	VAL	GLN	K1895	R1812	K1689	L1538	P1410	E1310	L1168
V2210	P2119	TYR	TYR	SER	L1896	S1813	G1690	L1538	T1424	K1311	R1178
L2211	R2120	TYR	TYR	TYR	N1897	F1814	V1693	L1538	T1424	E1310	R1178
K2212	D2121	TYR	TYR	TYR	Q1898	T1815	L1696	L1538	S1427	K1312	E1182
N2213	S2124	SER	SER	SER	R1899	R1816	L1696	L1538	L1431	PHE	C1183
L2214	W2125	GLU	GLU	GLU	F1900	Q1817	L1696	L1538	C1432	GLY	R1184
L2215	L2133	GLU	GLU	ASP	H1901	T1700	L1696	L1538	L1432	T1315	H1185
F2218	L2133	VAL	PRO	ASP	G1902	G1705	L1696	L1538	Q1442	G1316	
L2219		VAL	PRO	ASP	S1903						
M2220		VAL	PRO	ASP	C1904						
K2221		VAL	PRO	ASP	I1905						
V2223		VAL	PRO	ASP	E1907						





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64179	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.589	Depositor
Minimum map value	-1.600	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.22	Depositor
Map size (\AA)	339.04, 339.04, 339.04	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.304, 1.304, 1.304	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: KWT

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	0.33	0/29502	0.46	0/39893

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	29010	0	29193	572	0
2	A	31	0	23	23	0
All	All	29041	0	29216	572	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 10.

All (572) 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:3809:THR:CB	1:A:3929:MET:HE1	1.66	1.25
1:A:3809:THR:CB	1:A:3929:MET:CE	2.16	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3751:LEU:HD13	2:A:6101:KWT:H143	1.15	1.09
1:A:3809:THR:HB	1:A:3929:MET:HE3	1.26	1.08
1:A:3809:THR:CG2	1:A:3929:MET:HE1	1.83	1.07
1:A:3809:THR:HB	1:A:3929:MET:CE	1.82	1.03
1:A:3809:THR:OG1	1:A:3929:MET:HE1	1.59	1.02
1:A:3809:THR:OG1	1:A:3929:MET:CE	2.09	1.01
1:A:3811:THR:HG21	2:A:6101:KWT:H223	1.42	1.00
1:A:3751:LEU:CD1	2:A:6101:KWT:H143	1.90	1.00
1:A:3809:THR:HG21	1:A:3929:MET:HE1	1.45	0.98
1:A:3809:THR:CB	1:A:3929:MET:HE3	1.92	0.93
1:A:3444:ALA:HA	1:A:3482:LEU:CD2	1.99	0.93
1:A:3805:TRP:CE3	2:A:6101:KWT:H141	2.04	0.92
1:A:3811:THR:CG2	2:A:6101:KWT:H223	2.00	0.91
1:A:3803:ILE:CD1	2:A:6101:KWT:C6	2.51	0.88
1:A:3751:LEU:HD13	2:A:6101:KWT:C14	2.04	0.85
1:A:3728:VAL:HG22	1:A:3736:LYS:CD	2.07	0.83
1:A:3803:ILE:HD12	2:A:6101:KWT:O3	1.78	0.83
1:A:3728:VAL:HG22	1:A:3736:LYS:HD2	1.60	0.82
1:A:3618:GLY:H	1:A:3633:ILE:HD12	1.46	0.79
1:A:403:GLY:H	1:A:406:ARG:HH12	1.29	0.78
1:A:3444:ALA:O	1:A:3482:LEU:HD21	1.83	0.78
1:A:3751:LEU:HD12	1:A:3805:TRP:CE3	2.18	0.78
1:A:899:ARG:HE	1:A:2568:MET:HB2	1.48	0.78
1:A:3751:LEU:HD21	2:A:6101:KWT:H101	1.67	0.75
1:A:1212:LEU:HD11	1:A:1217:VAL:HA	1.69	0.74
1:A:2796:ALA:O	1:A:2800:ARG:NH1	2.21	0.74
1:A:3298:LEU:HD12	1:A:3333:THR:HG23	1.69	0.73
1:A:3751:LEU:HD12	1:A:3805:TRP:HE3	1.51	0.73
1:A:3288:SER:O	1:A:3289:ARG:NH1	2.20	0.72
1:A:3444:ALA:CA	1:A:3482:LEU:CD2	2.67	0.72
1:A:4050:LYS:HE3	1:A:4059:ILE:HG21	1.71	0.72
1:A:1933:LEU:HD13	1:A:1936:ARG:HB3	1.72	0.71
1:A:3803:ILE:HD12	2:A:6101:KWT:C6	2.19	0.71
1:A:356:ASN:ND2	1:A:404:ASP:O	2.24	0.70
1:A:3444:ALA:HB1	1:A:3482:LEU:HD22	1.73	0.70
1:A:3809:THR:HG21	1:A:3929:MET:CE	2.19	0.70
1:A:3444:ALA:CB	1:A:3482:LEU:HD22	2.21	0.70
1:A:1240:THR:HG22	1:A:1242:LEU:H	1.56	0.70
1:A:1484:LEU:HD11	1:A:1527:ARG:HH12	1.56	0.70
1:A:2151:ILE:HG21	1:A:2188:GLU:HG2	1.73	0.70
1:A:3187:CYS:SG	1:A:3239:LYS:NZ	2.63	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3186:ARG:HD3	1:A:3238:MET:HE3	1.74	0.70
1:A:3520:GLU:OE2	1:A:3524:ASN:ND2	2.25	0.69
1:A:1097:GLU:OE2	1:A:1151:ARG:NH2	2.25	0.69
1:A:3580:ASN:ND2	1:A:3734:ARG:HB2	2.08	0.69
1:A:899:ARG:NH2	1:A:2568:MET:SD	2.65	0.69
1:A:3803:ILE:CD1	2:A:6101:KWT:O3	2.40	0.69
1:A:3281:CYS:HB2	1:A:3329:LEU:HD23	1.75	0.68
1:A:75:SER:H	1:A:78:PHE:HB3	1.59	0.68
1:A:709:LYS:NZ	1:A:713:GLU:OE2	2.27	0.68
1:A:767:GLU:HG2	1:A:851:ILE:HD11	1.75	0.68
1:A:1083:ASN:ND2	1:A:1126:GLN:OE1	2.26	0.68
1:A:3145:ILE:HD11	1:A:3196:LYS:HD2	1.74	0.68
1:A:1185:HIS:NE2	1:A:1265:GLU:OE2	2.26	0.67
1:A:1225:GLU:HB3	1:A:1236:LEU:HB2	1.76	0.67
1:A:3811:THR:HG21	2:A:6101:KWT:C22	2.23	0.67
1:A:16:GLN:NE2	1:A:17:GLU:OE2	2.27	0.67
1:A:38:LEU:O	1:A:41:GLU:HB3	1.95	0.67
1:A:247:GLU:HG2	1:A:285:CYS:HB3	1.76	0.67
1:A:1334:LYS:NZ	1:A:1382:ILE:O	2.28	0.66
1:A:4064:LEU:HD13	1:A:4077:TYR:HB3	1.78	0.66
1:A:3751:LEU:CD2	2:A:6101:KWT:H101	2.26	0.65
1:A:2365:ASN:HD22	1:A:2396:LEU:HD13	1.63	0.64
1:A:3911:ILE:HD12	1:A:3928:PHE:HE1	1.62	0.64
1:A:3495:PHE:HB3	1:A:3502:MET:HE3	1.77	0.64
1:A:90:CYS:O	1:A:93:LEU:HB3	1.98	0.64
1:A:2169:LEU:HD11	1:A:2215:LEU:HD22	1.80	0.64
1:A:1897:ASN:HB3	1:A:1903:SER:HB2	1.81	0.63
1:A:3448:GLU:HB3	1:A:3482:LEU:HD11	1.81	0.63
1:A:3924:HIS:ND1	1:A:3926:ASN:OD1	2.29	0.63
1:A:463:LYS:HD3	1:A:545:LEU:HD22	1.80	0.63
1:A:1151:ARG:NH1	1:A:1163:LEU:O	2.31	0.63
1:A:3009:LYS:O	1:A:3013:TYR:HB3	1.98	0.63
1:A:2563:LEU:HD13	1:A:2812:LEU:HD11	1.80	0.63
1:A:1432:CYS:HB3	1:A:1486:LEU:HD11	1.79	0.62
1:A:3580:ASN:HD21	1:A:3734:ARG:HB2	1.63	0.62
1:A:3992:ARG:NH1	1:A:4103:GLN:OE1	2.33	0.62
1:A:173:LYS:HA	1:A:176:GLU:HG3	1.81	0.62
1:A:3580:ASN:HD21	1:A:3734:ARG:CB	2.11	0.62
1:A:374:LYS:HD2	1:A:423:TYR:HB3	1.82	0.62
1:A:1754:GLN:HA	1:A:1785:ILE:HD11	1.81	0.62
1:A:2439:ILE:O	1:A:2443:MET:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3515:GLN:NE2	1:A:3551:ASN:OD1	2.34	0.61
1:A:3477:GLU:HA	1:A:3477:GLU:OE1	2.01	0.61
1:A:93:LEU:O	1:A:97:GLY:N	2.25	0.61
1:A:2155:GLU:OE2	1:A:2158:ARG:NH2	2.34	0.60
1:A:3666:LEU:O	1:A:3670:MET:HG3	2.01	0.60
1:A:3444:ALA:HA	1:A:3482:LEU:HD21	1.82	0.60
1:A:1358:LEU:HD11	1:A:1410:PRO:HG2	1.84	0.60
1:A:3425:ARG:NH1	1:A:4000:ASN:OD1	2.35	0.60
1:A:3723:ASP:OD1	1:A:3724:GLU:N	2.35	0.60
1:A:3864:ARG:NH1	1:A:3868:VAL:HG21	2.17	0.60
1:A:3284:SER:HB3	1:A:3301:LEU:HD12	1.84	0.59
1:A:3295:GLU:OE2	1:A:3295:GLU:N	2.33	0.59
1:A:3444:ALA:CA	1:A:3482:LEU:HD21	2.32	0.59
1:A:3728:VAL:HG22	1:A:3736:LYS:HD3	1.83	0.59
1:A:108:LYS:HZ2	1:A:156:PHE:HZ	1.51	0.59
1:A:203:GLU:O	1:A:206:THR:OG1	2.20	0.59
1:A:2091:HIS:CE1	1:A:2093:CYS:SG	2.96	0.58
1:A:3154:GLN:OE1	1:A:3226:ASP:N	2.36	0.58
1:A:3444:ALA:HB2	1:A:3478:GLU:HG2	1.85	0.58
1:A:1733:THR:HG22	1:A:1735:ARG:H	1.67	0.58
1:A:1819:PHE:O	1:A:1823:SER:OG	2.22	0.58
1:A:1267:TYR:CD2	1:A:1290:LEU:HD22	2.39	0.58
1:A:2357:GLU:HB3	1:A:2385:LEU:HD21	1.85	0.58
1:A:4081:ALA:O	1:A:4090:ARG:NH1	2.36	0.58
1:A:1871:MET:HG2	1:A:1940:TYR:HA	1.84	0.58
1:A:3646:LYS:H	1:A:3650:LYS:HB3	1.68	0.58
1:A:3684:SER:HB2	1:A:3685:PRO:HD3	1.85	0.58
1:A:1104:LEU:HD23	1:A:1168:LEU:HD21	1.86	0.58
1:A:628:GLU:OE2	1:A:631:ARG:NH2	2.37	0.57
1:A:3929:MET:HG3	1:A:3940:ILE:CD1	2.34	0.57
1:A:4090:ARG:NH2	1:A:4113:ASP:OD2	2.37	0.57
1:A:205:LYS:HG2	1:A:249:PHE:HZ	1.70	0.57
1:A:2361:ILE:HD12	1:A:2389:PHE:HE2	1.67	0.57
1:A:3244:ASP:OD1	1:A:3247:ARG:NH1	2.37	0.57
1:A:2224:PHE:HB2	1:A:2272:VAL:HG11	1.87	0.57
1:A:2347:LYS:O	1:A:2351:GLN:NE2	2.37	0.57
1:A:606:SER:OG	1:A:1026:ARG:NH2	2.37	0.57
1:A:3751:LEU:CD1	2:A:6101:KWT:C14	2.73	0.57
1:A:1541:ALA:HB2	1:A:1550:VAL:HG12	1.87	0.57
1:A:1769:GLU:O	1:A:1822:ARG:NH2	2.24	0.57
1:A:1975:LEU:HD12	1:A:1976:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1125:GLN:NE2	1:A:1129:ASP:OD2	2.37	0.56
1:A:3961:PHE:HE2	1:A:4107:LEU:HD13	1.70	0.56
1:A:1525:CYS:SG	1:A:1574:ASN:ND2	2.78	0.56
1:A:1011:GLU:O	1:A:1015:ASP:N	2.38	0.56
1:A:2406:GLU:OE1	1:A:2441:LYS:NZ	2.34	0.56
1:A:2443:MET:SD	1:A:2476:ILE:HG23	2.46	0.56
1:A:131:LEU:HD22	1:A:173:LYS:HD2	1.85	0.56
1:A:1867:ILE:O	1:A:1871:MET:HG3	2.06	0.56
1:A:3596:LEU:HD12	1:A:3601:VAL:HA	1.88	0.56
1:A:2254:ARG:NH1	1:A:2292:CYS:O	2.39	0.56
1:A:2260:PHE:O	1:A:2270:ASN:ND2	2.38	0.56
1:A:229:SER:HA	1:A:274:LEU:HD13	1.88	0.56
1:A:1754:GLN:HG3	1:A:1785:ILE:HG13	1.88	0.56
1:A:2919:ASP:OD1	1:A:2920:VAL:N	2.38	0.56
1:A:3751:LEU:HD11	2:A:6101:KWT:H101	1.86	0.56
1:A:3803:ILE:HD11	2:A:6101:KWT:C6	2.34	0.56
1:A:1224:PHE:HD2	1:A:1267:TYR:HE1	1.54	0.55
1:A:3406:ALA:O	1:A:3409:VAL:HG12	2.06	0.55
1:A:205:LYS:HG2	1:A:249:PHE:CZ	2.41	0.55
1:A:771:ASN:OD1	1:A:854:ARG:NH2	2.40	0.55
1:A:56:SER:HA	1:A:59:PHE:CD2	2.42	0.55
1:A:1874:TYR:HE2	1:A:1940:TYR:HE1	1.54	0.55
1:A:3710:LYS:HB2	1:A:3711:PRO:HD2	1.88	0.55
1:A:3639:GLU:O	1:A:3643:HIS:N	2.28	0.55
1:A:3680:LEU:HD23	1:A:3682:GLU:H	1.71	0.55
1:A:3751:LEU:HD22	1:A:3803:ILE:HD11	1.88	0.55
1:A:3097:ASP:OD1	1:A:3098:ARG:N	2.37	0.55
1:A:2168:LEU:HD22	1:A:2189:ILE:HD11	1.89	0.55
1:A:13:LEU:HD23	1:A:14:ARG:HE	1.70	0.55
1:A:1812:LEU:O	1:A:1815:THR:N	2.36	0.55
1:A:1442:GLN:HG3	1:A:1445:ARG:HH12	1.71	0.54
1:A:1920:TYR:HE1	1:A:1963:GLN:CB	2.20	0.54
1:A:1961:PHE:O	1:A:1961:PHE:CD1	2.59	0.54
1:A:3735:PRO:HG3	2:A:6101:KWT:H102	1.89	0.54
1:A:4027:TRP:HE3	1:A:4030:GLU:HB3	1.72	0.54
1:A:1267:TYR:HD2	1:A:1290:LEU:HD22	1.72	0.54
1:A:1815:THR:O	1:A:1818:SER:OG	2.25	0.54
1:A:3137:GLU:OE1	1:A:3186:ARG:NH2	2.35	0.54
1:A:3661:ASP:HA	1:A:3664:ASN:HD21	1.72	0.54
1:A:129:ASP:OD1	1:A:129:ASP:N	2.40	0.54
1:A:849:GLU:OE1	1:A:3108:GLN:NE2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3605:ASN:OD1	1:A:3606:ILE:N	2.40	0.54
1:A:3608:LYS:O	1:A:3611:GLU:HG3	2.07	0.54
1:A:1351:THR:HG22	1:A:1353:PRO:HD2	1.90	0.54
1:A:901:MET:SD	1:A:2535:THR:OG1	2.64	0.54
1:A:1920:TYR:CE1	1:A:1963:GLN:CB	2.91	0.54
1:A:1759:LEU:HD12	1:A:1785:ILE:HD13	1.88	0.54
1:A:3495:PHE:HB3	1:A:3502:MET:CE	2.38	0.54
1:A:56:SER:HA	1:A:59:PHE:HD2	1.73	0.53
1:A:59:PHE:HA	1:A:62:ASP:HB2	1.91	0.53
1:A:2999:LEU:HD21	1:A:3015:SER:O	2.09	0.53
1:A:2474:TYR:HD2	1:A:2517:LEU:HD12	1.74	0.53
1:A:2918:PRO:HB2	1:A:2922:ARG:HH22	1.73	0.53
1:A:1634:ALA:O	1:A:1642:LYS:NZ	2.29	0.53
1:A:79:ARG:HA	1:A:82:ARG:HB2	1.90	0.53
1:A:2411:LEU:HD11	1:A:2415:LEU:HD23	1.90	0.53
1:A:2091:HIS:HE1	1:A:2093:CYS:SG	2.32	0.53
1:A:355:ASN:HB3	1:A:358:GLU:HG2	1.90	0.53
1:A:1528:LEU:HD21	1:A:1567:ILE:HG23	1.90	0.53
1:A:131:LEU:O	1:A:135:LEU:HG	2.08	0.53
1:A:301:CYS:O	1:A:309:LYS:NZ	2.38	0.53
1:A:3661:ASP:HA	1:A:3664:ASN:ND2	2.24	0.53
1:A:796:LEU:HD23	1:A:855:VAL:HG13	1.90	0.52
1:A:3033:GLU:HG3	1:A:3034:PRO:HD3	1.91	0.52
1:A:170:VAL:O	1:A:171:LEU:HD22	2.10	0.52
1:A:267:VAL:HG23	1:A:268:PRO:HD3	1.90	0.52
1:A:1484:LEU:HD11	1:A:1527:ARG:NH1	2.22	0.52
1:A:1685:ASP:OD1	1:A:1685:ASP:N	2.42	0.52
1:A:1378:GLU:HG2	1:A:1378:GLU:O	2.10	0.52
1:A:3627:ALA:HB3	1:A:3683:CYS:HB2	1.91	0.52
1:A:3348:LEU:O	1:A:3352:GLU:HG2	2.09	0.52
1:A:3496:ILE:HD11	1:A:3521:ILE:HD11	1.92	0.52
1:A:3791:TYR:CE1	1:A:3940:ILE:HG22	2.45	0.52
1:A:13:LEU:O	1:A:14:ARG:NE	2.43	0.52
1:A:2933:ILE:HD11	1:A:3121:LEU:HD22	1.91	0.52
1:A:3751:LEU:HD11	2:A:6101:KWT:C10	2.39	0.51
1:A:1086:TYR:O	1:A:1087:ARG:HB2	2.11	0.51
1:A:2457:PRO:O	1:A:2460:GLU:HG2	2.10	0.51
1:A:3646:LYS:N	1:A:3650:LYS:HB3	2.25	0.51
1:A:1374:GLN:HE22	1:A:1381:SER:HB3	1.76	0.51
1:A:1575:LEU:H	1:A:1575:LEU:HD23	1.76	0.51
1:A:2205:VAL:HB	1:A:2208:ASP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2555:LEU:HD11	1:A:2854:PHE:HA	1.91	0.51
1:A:3507:ASP:HB3	1:A:3540:TYR:CD1	2.45	0.51
1:A:1519:PHE:CG	1:A:1570:GLU:HG3	2.45	0.51
1:A:2522:ARG:HG2	1:A:2561:PHE:HE1	1.76	0.51
1:A:967:PRO:HD3	1:A:1010:LEU:HD12	1.93	0.51
1:A:3622:ALA:HB3	1:A:3625:LEU:HB2	1.92	0.51
1:A:2806:LYS:HG3	1:A:2857:CYS:HB2	1.93	0.51
1:A:36:ARG:HH21	1:A:39:GLY:HA3	1.76	0.51
1:A:708:VAL:HG22	1:A:740:ILE:HG23	1.92	0.51
1:A:3053:LEU:HD11	1:A:3088:LEU:HD13	1.92	0.51
1:A:1037:LEU:HD23	1:A:1085:ILE:HB	1.93	0.50
1:A:3243:ILE:HD13	1:A:3259:LEU:HD13	1.92	0.50
1:A:3944:HIS:NE2	1:A:4020:MET:SD	2.84	0.50
1:A:1224:PHE:HD2	1:A:1267:TYR:CE1	2.28	0.50
1:A:2256:ILE:HG22	1:A:2260:PHE:HE2	1.76	0.50
1:A:242:PRO:O	1:A:245:SER:OG	2.24	0.50
1:A:2091:HIS:CE1	1:A:2093:CYS:HG	2.30	0.50
1:A:2828:GLU:O	1:A:2832:ILE:HG12	2.11	0.50
1:A:3629:ARG:O	1:A:3633:ILE:HG12	2.11	0.50
1:A:1818:SER:HA	1:A:1821:ASP:HB3	1.94	0.50
1:A:3596:LEU:HB2	1:A:3601:VAL:HG22	1.94	0.50
1:A:403:GLY:O	1:A:406:ARG:NH1	2.45	0.49
1:A:1782:PHE:HA	1:A:1785:ILE:HG22	1.94	0.49
1:A:23:ASP:HA	1:A:30:ALA:HB1	1.93	0.49
1:A:1234:GLY:HA2	1:A:1259:LEU:HD22	1.93	0.49
1:A:2376:ASP:OD1	1:A:2404:ARG:NE	2.41	0.49
1:A:3751:LEU:CD1	2:A:6101:KWT:H101	2.42	0.49
1:A:3227:ILE:HD12	1:A:3227:ILE:H	1.78	0.49
1:A:3791:TYR:CZ	1:A:3940:ILE:HG22	2.47	0.49
1:A:2097:LEU:HD12	1:A:2145:PHE:HZ	1.77	0.49
1:A:1726:SER:O	1:A:1726:SER:OG	2.27	0.49
1:A:2365:ASN:ND2	1:A:2396:LEU:HD13	2.27	0.49
1:A:3809:THR:CG2	1:A:3929:MET:CE	2.62	0.49
1:A:3911:ILE:CD1	1:A:3928:PHE:HE1	2.25	0.49
1:A:975:ASP:OD1	1:A:976:VAL:N	2.45	0.49
1:A:3929:MET:SD	2:A:6101:KWT:O4	2.70	0.49
1:A:1006:THR:HG22	1:A:1009:LEU:HB2	1.94	0.49
1:A:1339:VAL:HG23	1:A:1398:VAL:HG21	1.95	0.49
1:A:3805:TRP:CE3	2:A:6101:KWT:C14	2.88	0.49
1:A:1864:ASP:HA	1:A:1867:ILE:HG12	1.95	0.49
1:A:3062:LEU:HD13	1:A:3093:GLN:NE2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1208:LEU:HD21	1:A:1220:LEU:HD11	1.94	0.49
1:A:1532:LEU:HD11	1:A:1560:TYR:HB2	1.94	0.49
1:A:1817:GLN:OE1	1:A:1936:ARG:NH2	2.41	0.49
1:A:2269:ASP:OD1	1:A:2269:ASP:N	2.46	0.49
1:A:2313:LYS:HA	1:A:2316:TYR:CE2	2.48	0.49
1:A:2368:THR:HG23	1:A:2372:PRO:HA	1.93	0.49
1:A:2415:LEU:HD12	1:A:2420:PHE:CD1	2.48	0.49
1:A:3151:LEU:HD21	1:A:3197:LEU:HA	1.95	0.49
1:A:59:PHE:HB3	1:A:63:PHE:CE1	2.47	0.48
1:A:3444:ALA:HA	1:A:3482:LEU:HD23	1.92	0.48
1:A:346:TYR:HB3	1:A:350:ARG:HH12	1.78	0.48
1:A:1586:SER:O	1:A:1632:TRP:NE1	2.43	0.48
1:A:1470:SER:HB3	1:A:1476:HIS:CD2	2.48	0.48
1:A:2940:ARG:HG2	1:A:2957:LEU:HD22	1.95	0.48
1:A:3104:GLN:OE1	1:A:3139:GLN:NE2	2.46	0.48
1:A:3444:ALA:C	1:A:3482:LEU:HD21	2.33	0.48
1:A:1933:LEU:HD12	1:A:1937:ARG:HG3	1.95	0.48
1:A:3616:ALA:O	1:A:3629:ARG:NH2	2.47	0.48
1:A:1871:MET:HE1	1:A:1936:ARG:HH21	1.79	0.48
1:A:2259:LYS:HB3	1:A:2272:VAL:HG23	1.94	0.48
1:A:253:LEU:HD11	1:A:271:GLY:HA3	1.95	0.48
1:A:1082:PHE:HA	1:A:1085:ILE:HG12	1.94	0.48
1:A:2304:VAL:HG12	1:A:2323:LEU:HD11	1.96	0.48
1:A:2786:LYS:O	1:A:2788:SER:N	2.47	0.48
1:A:3587:ASP:OD2	1:A:3733:ARG:NH1	2.45	0.48
1:A:2261:SER:OG	1:A:2262:GLY:N	2.46	0.48
1:A:2301:GLN:OE1	1:A:2305:ASN:ND2	2.46	0.48
1:A:2877:SER:OG	1:A:2925:GLU:HB3	2.13	0.48
1:A:3446:VAL:O	1:A:3450:MET:HG2	2.13	0.48
1:A:3728:VAL:HG12	1:A:3734:ARG:HD3	1.96	0.48
1:A:1009:LEU:HD21	1:A:1062:ARG:NH1	2.29	0.47
1:A:1471:GLN:N	1:A:1471:GLN:OE1	2.48	0.47
1:A:2542:LEU:HD21	1:A:2558:ALA:HA	1.95	0.47
1:A:1934:LEU:O	1:A:1938:ARG:N	2.43	0.47
1:A:2206:PRO:O	1:A:2210:VAL:HG23	2.14	0.47
1:A:2432:GLN:OE1	1:A:2464:HIS:NE2	2.45	0.47
1:A:2551:GLU:OE2	1:A:2849:SER:OG	2.28	0.47
1:A:3753:LYS:HD2	1:A:3753:LYS:HA	1.56	0.47
1:A:397:LEU:HD21	1:A:438:LEU:HD22	1.95	0.47
1:A:195:ASN:O	1:A:198:ARG:HG3	2.15	0.47
1:A:540:MET:SD	1:A:540:MET:N	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1572:LEU:HD21	1:A:1618:LEU:HD22	1.96	0.47
1:A:1912:THR:O	1:A:1916:ILE:HG12	2.14	0.47
1:A:3444:ALA:HB2	1:A:3478:GLU:CG	2.44	0.47
1:A:439:VAL:O	1:A:442:GLN:HB3	2.15	0.47
1:A:3729:MET:SD	1:A:3729:MET:N	2.87	0.47
1:A:3733:ARG:HH21	1:A:3755:GLY:C	2.18	0.47
1:A:1323:SER:O	1:A:1325:GLN:N	2.48	0.47
1:A:3809:THR:OG1	1:A:3929:MET:SD	2.73	0.47
1:A:12:LEU:O	1:A:16:GLN:HG2	2.14	0.47
1:A:726:LEU:HD21	1:A:754:MET:SD	2.55	0.47
1:A:1689:LYS:O	1:A:1693:VAL:HG13	2.15	0.47
1:A:2121:ASP:OD1	1:A:2121:ASP:N	2.43	0.47
1:A:3344:GLU:OE2	1:A:3348:LEU:HD23	2.15	0.47
1:A:3803:ILE:CD1	2:A:6101:KWT:C5	2.92	0.47
1:A:63:PHE:O	1:A:66:LEU:HB2	2.15	0.46
1:A:3186:ARG:HD3	1:A:3238:MET:CE	2.44	0.46
1:A:180:LEU:HA	1:A:230:LEU:HD21	1.98	0.46
1:A:3137:GLU:CD	1:A:3186:ARG:HE	2.19	0.46
1:A:3789:ARG:NH2	1:A:3806:LEU:HD11	2.31	0.46
1:A:14:ARG:O	1:A:18:THR:HG23	2.15	0.46
1:A:1793:THR:O	1:A:1797:LEU:HG	2.15	0.46
1:A:2539:LEU:HD13	1:A:2562:LEU:HD11	1.97	0.46
1:A:3066:ASP:OD1	1:A:3067:LYS:N	2.48	0.46
1:A:1300:SER:O	1:A:1300:SER:OG	2.32	0.46
1:A:2785:ILE:O	1:A:2789:SER:HB2	2.16	0.46
1:A:2884:LEU:HD12	1:A:3116:SER:HB2	1.96	0.46
1:A:942:LEU:HD11	1:A:991:LEU:HD21	1.97	0.46
1:A:1711:ARG:NH2	1:A:1760:GLU:OE1	2.48	0.46
1:A:3410:ILE:HD11	1:A:3456:LEU:HB3	1.98	0.46
1:A:3959:MET:HE3	1:A:3959:MET:H	1.81	0.46
1:A:1372:LEU:HD13	1:A:1402:LEU:HD23	1.98	0.46
1:A:1586:SER:O	1:A:1586:SER:OG	2.34	0.46
1:A:2213:ASN:OD1	1:A:2214:ARG:N	2.48	0.46
1:A:586:GLN:HB2	1:A:613:HIS:CD2	2.51	0.46
1:A:1715:GLU:HA	1:A:1718:ILE:HG12	1.98	0.46
1:A:3313:SER:HA	1:A:3316:LEU:HB2	1.96	0.46
1:A:242:PRO:C	1:A:246:ARG:HE	2.20	0.45
1:A:1478:SER:O	1:A:1482:GLU:HG3	2.17	0.45
1:A:1572:LEU:HB3	1:A:1614:GLN:HE21	1.81	0.45
1:A:2183:HIS:CE1	1:A:2186:VAL:HG23	2.52	0.45
1:A:3447:VAL:HG22	1:A:3468:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3369:ASP:OD1	1:A:3369:ASP:N	2.49	0.45
1:A:3484:THR:HG23	1:A:3513:ALA:HA	1.97	0.45
1:A:1496:GLU:OE1	1:A:1496:GLU:N	2.42	0.45
1:A:225:LYS:HZ3	1:A:253:LEU:HD13	1.81	0.45
1:A:2471:GLU:HA	1:A:2517:LEU:HD11	1.98	0.45
1:A:3636:PHE:CE2	1:A:3670:MET:HG2	2.52	0.45
1:A:189:MET:SD	1:A:189:MET:N	2.90	0.45
1:A:1484:LEU:HD21	1:A:1527:ARG:HH22	1.80	0.45
1:A:2576:MET:HB3	1:A:2787:HIS:CD2	2.52	0.45
1:A:861:SER:O	1:A:3167:ARG:NH1	2.46	0.45
1:A:1188:ILE:HD13	1:A:1269:THR:HG21	1.98	0.45
1:A:1538:LEU:HD12	1:A:1553:PHE:CE1	2.52	0.45
1:A:1935:GLU:OE2	1:A:1938:ARG:NE	2.34	0.45
1:A:154:SER:HA	1:A:157:TYR:HD2	1.82	0.45
1:A:1221:ILE:HD12	1:A:1221:ILE:H	1.82	0.45
1:A:2327:LEU:HA	1:A:2330:VAL:HG12	1.99	0.45
1:A:2930:TYR:HA	1:A:2933:ILE:HG22	1.98	0.45
1:A:100:ILE:HB	1:A:102:PRO:HD3	1.98	0.45
1:A:1158:PRO:N	1:A:1159:PRO:HD2	2.31	0.45
1:A:2361:ILE:HD12	1:A:2389:PHE:CE2	2.51	0.45
1:A:2863:CYS:SG	1:A:2895:GLU:HG3	2.57	0.45
1:A:487:LEU:HD12	1:A:490:ILE:HD11	1.99	0.45
1:A:2372:PRO:O	1:A:2374:LEU:N	2.50	0.45
1:A:3751:LEU:HD21	2:A:6101:KWT:C10	2.42	0.45
1:A:3603:LYS:HB3	1:A:3606:ILE:HG22	1.98	0.44
1:A:849:GLU:OE2	1:A:852:ARG:NH1	2.50	0.44
1:A:3467:ARG:O	1:A:3471:ILE:HG12	2.17	0.44
1:A:3779:SER:OG	1:A:3780:ALA:N	2.50	0.44
1:A:3878:VAL:HG21	1:A:4128:MET:HB3	1.98	0.44
1:A:346:TYR:HD1	1:A:366:TYR:HH	1.63	0.44
1:A:1786:ALA:HB2	1:A:1827:LEU:HD23	1.99	0.44
1:A:221:ALA:O	1:A:225:LYS:HE3	2.18	0.44
1:A:404:ASP:HB2	1:A:1732:GLY:O	2.17	0.44
1:A:1696:LEU:HA	1:A:1696:LEU:HD23	1.81	0.44
1:A:1864:ASP:N	1:A:1864:ASP:OD1	2.50	0.44
1:A:2522:ARG:HG2	1:A:2561:PHE:CE1	2.52	0.44
1:A:2559:THR:O	1:A:2563:LEU:HB2	2.16	0.44
1:A:3088:LEU:HD23	1:A:3088:LEU:HA	1.74	0.44
1:A:3383:GLN:O	1:A:3387:GLU:HG3	2.17	0.44
1:A:3604:LYS:HA	1:A:3607:GLU:HG2	2.00	0.44
1:A:114:VAL:HG12	1:A:130:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:GLU:HB3	1:A:153:PHE:CE1	2.53	0.44
1:A:493:LYS:O	1:A:625:ASN:ND2	2.51	0.44
1:A:2463:SER:O	1:A:2463:SER:OG	2.31	0.44
1:A:2575:PRO:HA	1:A:2786:LYS:H	1.83	0.44
1:A:3588:TRP:CD1	1:A:3613:MET:HB2	2.52	0.44
1:A:1231:GLN:O	1:A:1233:SER:N	2.47	0.44
1:A:1427:SER:O	1:A:1431:LEU:HD23	2.18	0.44
1:A:1770:GLN:N	1:A:1770:GLN:OE1	2.51	0.44
1:A:1458:LEU:HD13	1:A:1467:ILE:HD11	2.00	0.44
1:A:3229:SER:OG	1:A:3232:ARG:NH1	2.43	0.44
1:A:225:LYS:HZ3	1:A:253:LEU:HD22	1.82	0.43
1:A:275:PHE:CZ	1:A:293:LEU:HD21	2.52	0.43
1:A:1019:ASP:HA	1:A:1026:ARG:HH11	1.82	0.43
1:A:1124:ILE:HG23	1:A:1182:GLU:HG2	2.00	0.43
1:A:1690:GLY:HA2	1:A:1693:VAL:HG22	2.00	0.43
1:A:2506:LEU:HD23	1:A:2506:LEU:HA	1.83	0.43
1:A:3285:HIS:HD2	1:A:3298:LEU:HD11	1.83	0.43
1:A:3793:VAL:HG13	1:A:3803:ILE:HG22	1.99	0.43
1:A:3881:ASP:OD1	1:A:3881:ASP:N	2.50	0.43
1:A:3981:TYR:HD1	1:A:4108:MET:HE2	1.83	0.43
1:A:671:SER:O	1:A:675:ARG:HG3	2.18	0.43
1:A:1365:ASN:OD1	1:A:1366:THR:N	2.51	0.43
1:A:1448:LEU:HD21	1:A:1514:LEU:HD11	1.99	0.43
1:A:1585:SER:O	1:A:1585:SER:OG	2.27	0.43
1:A:2945:SER:HB2	1:A:2946:GLU:OE1	2.17	0.43
1:A:59:PHE:O	1:A:63:PHE:N	2.52	0.43
1:A:864:GLY:O	1:A:868:LYS:NZ	2.43	0.43
1:A:1376:LEU:HD13	1:A:1403:MET:HE1	2.00	0.43
1:A:2415:LEU:HD12	1:A:2420:PHE:CG	2.53	0.43
1:A:2877:SER:HG	1:A:2925:GLU:HB3	1.84	0.43
1:A:3095:ASP:N	1:A:3095:ASP:OD1	2.52	0.43
1:A:3587:ASP:CG	1:A:3733:ARG:HH12	2.21	0.43
1:A:923:ASP:C	1:A:925:GLN:H	2.21	0.43
1:A:1802:TYR:O	1:A:1806:ARG:HG2	2.19	0.43
1:A:3714:GLU:N	1:A:3714:GLU:OE1	2.51	0.43
1:A:3789:ARG:HG2	1:A:3938:ILE:HG12	2.01	0.43
1:A:1622:ILE:HG21	1:A:1652:ILE:HD11	2.00	0.43
1:A:1636:ASP:N	1:A:1636:ASP:OD1	2.50	0.43
1:A:3626:GLY:HA3	1:A:3684:SER:O	2.19	0.43
1:A:355:ASN:OD1	1:A:356:ASN:N	2.52	0.43
1:A:770:LEU:HD12	1:A:770:LEU:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1242:LEU:HA	1:A:1310:GLU:HB2	2.01	0.43
1:A:3449:LYS:HA	1:A:3449:LYS:HD3	1.72	0.43
1:A:12:LEU:HA	1:A:15:LEU:HB3	2.00	0.43
1:A:1086:TYR:C	1:A:1088:GLU:H	2.22	0.43
1:A:1640:GLU:OE1	1:A:1640:GLU:N	2.50	0.43
1:A:2921:LEU:O	1:A:2925:GLU:HG2	2.19	0.43
1:A:3077:ILE:HG13	1:A:3078:LEU:N	2.34	0.43
1:A:3727:THR:HG22	1:A:3729:MET:SD	2.59	0.43
1:A:579:LEU:HD23	1:A:579:LEU:HA	1.88	0.43
1:A:991:LEU:HD23	1:A:991:LEU:HA	1.85	0.43
1:A:1225:GLU:OE2	1:A:1267:TYR:OH	2.27	0.43
1:A:3444:ALA:CA	1:A:3482:LEU:HD22	2.42	0.43
1:A:79:ARG:O	1:A:82:ARG:HB2	2.19	0.42
1:A:131:LEU:HD12	1:A:132:ILE:N	2.33	0.42
1:A:253:LEU:HD12	1:A:254:LYS:N	2.34	0.42
1:A:737:PRO:HD2	1:A:740:ILE:HD12	2.01	0.42
1:A:1195:VAL:HG11	1:A:1204:PRO:HA	2.00	0.42
1:A:1476:HIS:HB3	1:A:1479:VAL:HG22	2.01	0.42
1:A:2887:PRO:HB2	1:A:3895:GLU:HG3	2.00	0.42
1:A:3700:GLU:HA	1:A:3718:ARG:HA	2.00	0.42
1:A:3875:GLU:O	1:A:3878:VAL:HG12	2.19	0.42
1:A:192:ASN:N	1:A:192:ASN:OD1	2.52	0.42
1:A:1627:LYS:HD2	1:A:1627:LYS:HA	1.84	0.42
1:A:236:LYS:HD3	1:A:246:ARG:HH12	1.84	0.42
1:A:466:LEU:HB3	1:A:560:LEU:HD22	2.01	0.42
1:A:1391:VAL:HG13	1:A:1392:MET:SD	2.59	0.42
1:A:3681:LYS:O	1:A:3685:PRO:HD2	2.19	0.42
1:A:3816:LEU:HD21	1:A:3883:LEU:HD13	2.01	0.42
1:A:251:PHE:HA	1:A:254:LYS:HZ2	1.84	0.42
1:A:287:LEU:HG	1:A:326:MET:SD	2.59	0.42
1:A:563:LEU:O	1:A:567:GLU:HG2	2.19	0.42
1:A:1820:VAL:HG12	1:A:1824:LEU:HD23	2.00	0.42
1:A:3065:ILE:HD13	1:A:3065:ILE:HA	1.91	0.42
1:A:3260:LYS:HA	1:A:3260:LYS:HD2	1.83	0.42
1:A:3483:MET:O	1:A:3483:MET:HG3	2.16	0.42
1:A:3582:GLU:HG2	1:A:3583:LEU:N	2.34	0.42
1:A:1358:LEU:HD21	1:A:1410:PRO:HB2	2.01	0.42
1:A:2486:ASP:HB3	1:A:2489:SER:HB2	2.01	0.42
1:A:3012:GLU:HB2	1:A:3047:SER:HB2	2.02	0.42
1:A:3913:ILE:HG21	1:A:3987:ALA:HB3	2.02	0.42
1:A:174:VAL:O	1:A:177:LEU:HG	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ASN:OD1	1:A:196:LEU:N	2.52	0.42
1:A:1395:LEU:O	1:A:1398:VAL:HG22	2.20	0.42
1:A:3227:ILE:O	1:A:3228:SER:HB3	2.19	0.42
1:A:3819:THR:HG21	1:A:3886:ALA:HB2	2.00	0.42
1:A:3879:PRO:HB2	1:A:3882:LEU:HG	2.01	0.42
1:A:60:SER:OG	1:A:61:ARG:N	2.53	0.42
1:A:1424:THR:HG23	1:A:1427:SER:H	1.85	0.42
1:A:2220:MET:HB3	1:A:2255:LEU:HD22	2.01	0.42
1:A:2576:MET:HB3	1:A:2787:HIS:NE2	2.34	0.42
1:A:3318:LYS:O	1:A:3322:ALA:HB3	2.19	0.42
1:A:3917:ILE:HD13	1:A:4051:LEU:HD21	2.01	0.42
1:A:3922:ASP:O	1:A:3923:ARG:NE	2.49	0.42
1:A:29:LEU:HD13	1:A:32:HIS:HB3	2.02	0.42
1:A:202:GLY:HA2	1:A:205:LYS:HE2	2.02	0.42
1:A:275:PHE:HZ	1:A:293:LEU:HD21	1.84	0.42
1:A:469:ALA:HB2	1:A:479:ILE:HD11	2.02	0.42
1:A:1218:SER:O	1:A:1222:ASN:ND2	2.52	0.42
1:A:1718:ILE:O	1:A:1722:PHE:HB2	2.20	0.42
1:A:42:CYS:HA	1:A:88:PHE:CE1	2.55	0.42
1:A:3542:PHE:HZ	1:A:3555:VAL:HG11	1.84	0.42
1:A:3751:LEU:HD12	1:A:3805:TRP:CZ3	2.52	0.42
1:A:523:THR:HG23	1:A:525:LYS:H	1.85	0.42
1:A:1030:GLY:O	1:A:1033:ILE:HG22	2.20	0.42
1:A:1448:LEU:O	1:A:1452:VAL:HG13	2.20	0.42
1:A:2917:PRO:HB2	1:A:2919:ASP:OD1	2.20	0.42
1:A:3138:ILE:O	1:A:3142:ILE:HG12	2.20	0.42
1:A:3537:SER:HA	1:A:3540:TYR:CE2	2.55	0.42
1:A:4107:LEU:HD23	1:A:4107:LEU:HA	1.79	0.42
1:A:251:PHE:HA	1:A:254:LYS:NZ	2.35	0.41
1:A:2349:LEU:HA	1:A:2352:HIS:CE1	2.56	0.41
1:A:3100:LYS:O	1:A:3103:ILE:HG22	2.20	0.41
1:A:3506:LEU:HD23	1:A:3506:LEU:HA	1.81	0.41
1:A:3929:MET:HE2	1:A:3929:MET:HB3	1.95	0.41
1:A:31:GLY:HA2	1:A:34:LEU:HB2	2.03	0.41
1:A:35:ILE:HG21	1:A:80:GLU:HB3	2.02	0.41
1:A:438:LEU:O	1:A:442:GLN:N	2.49	0.41
1:A:765:LEU:HA	1:A:765:LEU:HD23	1.72	0.41
1:A:853:ILE:HA	1:A:3111:MET:HE1	2.00	0.41
1:A:995:PHE:HB3	1:A:1005:ASP:OD1	2.19	0.41
1:A:1178:ARG:O	1:A:1184:ARG:NH2	2.51	0.41
1:A:2411:LEU:HA	1:A:2411:LEU:HD12	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2455:LEU:HD22	1:A:2498:ILE:HG23	2.01	0.41
1:A:109:ASN:OD1	1:A:110:THR:N	2.53	0.41
1:A:296:VAL:HG23	1:A:297:LEU:HD12	2.03	0.41
1:A:2166:SER:OG	1:A:2167:PRO:HD3	2.20	0.41
1:A:2397:CYS:O	1:A:2400:VAL:HG12	2.20	0.41
1:A:36:ARG:NE	1:A:36:ARG:HA	2.36	0.41
1:A:68:PHE:O	1:A:71:LYS:HB2	2.20	0.41
1:A:623:PHE:CE2	1:A:665:GLY:HA3	2.54	0.41
1:A:733:LEU:HD12	1:A:733:LEU:HA	1.85	0.41
1:A:2802:PRO:HG2	1:A:2803:ILE:HD12	2.02	0.41
1:A:3911:ILE:CD1	1:A:3928:PHE:CE1	3.03	0.41
1:A:803:SER:HB3	1:A:852:ARG:HE	1.86	0.41
1:A:2097:LEU:HD23	1:A:2097:LEU:HA	1.81	0.41
1:A:3006:ALA:HB3	1:A:3257:LYS:HE2	2.01	0.41
1:A:2252:PRO:C	1:A:2254:ARG:H	2.23	0.41
1:A:3271:ASP:HB2	1:A:3315:TYR:CE2	2.55	0.41
1:A:220:LEU:O	1:A:224:LEU:HG	2.21	0.41
1:A:240:GLU:HB3	1:A:242:PRO:HD2	2.01	0.41
1:A:1758:LEU:HD23	1:A:1758:LEU:HA	1.84	0.41
1:A:3687:MET:HB3	1:A:3722:PHE:CD1	2.56	0.41
1:A:128:LEU:HD13	1:A:131:LEU:HD21	2.02	0.41
1:A:3953:LEU:HD22	1:A:4026:SER:HB3	2.02	0.41
1:A:363:ILE:HD13	1:A:363:ILE:HA	1.97	0.41
1:A:442:GLN:HG3	1:A:461:ILE:HD11	2.02	0.41
1:A:1081:ALA:O	1:A:1085:ILE:HG23	2.21	0.41
1:A:1220:LEU:O	1:A:1223:THR:OG1	2.27	0.41
1:A:1240:THR:HG23	1:A:1296:PHE:CG	2.56	0.41
1:A:1261:LEU:CD1	1:A:1340:ARG:HG3	2.51	0.41
1:A:1431:LEU:HD11	1:A:1447:ARG:NH2	2.35	0.41
1:A:1795:VAL:HG21	1:A:1838:GLU:HG3	2.03	0.41
1:A:1836:LEU:HD21	1:A:1883:ARG:HH21	1.85	0.41
1:A:2276:LEU:HD23	1:A:2276:LEU:HA	1.92	0.41
1:A:2277:LEU:O	1:A:2280:VAL:HG12	2.21	0.41
1:A:2411:LEU:C	1:A:2413:PHE:H	2.24	0.41
1:A:2425:ARG:HG2	1:A:2460:GLU:OE2	2.21	0.41
1:A:2891:ARG:HD2	1:A:2891:ARG:HA	1.85	0.41
1:A:3011:LEU:O	1:A:3016:THR:OG1	2.21	0.41
1:A:3523:ASP:OD1	1:A:3561:LYS:NZ	2.31	0.41
1:A:3526:PRO:C	1:A:3528:ALA:H	2.23	0.41
1:A:4015:ASN:O	1:A:4018:GLN:HG3	2.20	0.41
1:A:1754:GLN:HE22	1:A:1788:ARG:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1871:MET:O	1:A:1875:LYS:HG3	2.20	0.41
1:A:2133:LEU:HD23	1:A:2164:TRP:CZ3	2.56	0.41
1:A:2392:VAL:O	1:A:2396:LEU:HD23	2.21	0.41
1:A:3728:VAL:CG1	1:A:3734:ARG:HD3	2.51	0.41
1:A:865:GLN:H	1:A:865:GLN:HG2	1.73	0.40
1:A:1374:GLN:HE22	1:A:1381:SER:CB	2.33	0.40
1:A:1980:ASN:OD1	1:A:1981:LEU:N	2.49	0.40
1:A:2165:LEU:HD12	1:A:2165:LEU:HA	1.81	0.40
1:A:2211:LEU:HA	1:A:2214:ARG:HG2	2.02	0.40
1:A:2300:PHE:O	1:A:2304:VAL:HG13	2.21	0.40
1:A:3192:LYS:HE2	1:A:3192:LYS:HB2	1.90	0.40
1:A:313:LEU:HA	1:A:313:LEU:HD23	1.86	0.40
1:A:888:ARG:HB3	1:A:3889:ARG:HH21	1.85	0.40
1:A:1867:ILE:HA	1:A:1870:LYS:HE3	2.03	0.40
1:A:1945:TYR:O	1:A:1949:ILE:HG12	2.21	0.40
1:A:2164:TRP:C	1:A:2167:PRO:HD2	2.42	0.40
1:A:2392:VAL:HG12	1:A:2396:LEU:HD23	2.03	0.40
1:A:3227:ILE:HG22	1:A:3228:SER:N	2.36	0.40
1:A:3521:ILE:HD12	1:A:3521:ILE:HA	1.91	0.40
1:A:3558:ILE:HD13	1:A:3558:ILE:HA	1.96	0.40
1:A:249:PHE:O	1:A:252:VAL:HG12	2.21	0.40
1:A:346:TYR:HB3	1:A:350:ARG:NH1	2.36	0.40
1:A:3153:SER:OG	1:A:3154:GLN:N	2.55	0.40
1:A:165:LYS:HB2	1:A:167:PRO:HD2	2.03	0.40
1:A:1086:TYR:CE2	1:A:1087:ARG:HG3	2.56	0.40
1:A:1575:LEU:HD11	1:A:1617:LYS:HG3	2.03	0.40
1:A:1790:SER:O	1:A:1794:GLN:HG3	2.21	0.40
1:A:2231:PHE:O	1:A:2235:LEU:HD23	2.21	0.40
1:A:2430:GLU:O	1:A:2434:VAL:HG22	2.21	0.40
1:A:2785:ILE:HD12	1:A:2785:ILE:HA	1.96	0.40
1:A:3259:LEU:HD12	1:A:3259:LEU:HA	1.92	0.40
1:A:3756:GLU:HA	1:A:4022:LYS:NZ	2.37	0.40
1:A:3816:LEU:HA	1:A:3816:LEU:HD23	1.86	0.40
1:A:397:LEU:HD22	1:A:437:HIS:HB3	2.03	0.40
1:A:961:LEU:HD23	1:A:961:LEU:HA	1.94	0.40
1:A:1562:LEU:HD23	1:A:1562:LEU:HA	1.85	0.40
1:A:1597:LEU:HD23	1:A:1597:LEU:HA	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	3602/4148 (87%)	3293 (91%)	305 (8%)	4 (0%)	51	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3481	SER
1	A	2787	HIS
1	A	3406	ALA
1	A	1968	SER

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	3196/3671 (87%)	3178 (99%)	18 (1%)	86	93

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	ARG
1	A	924	ARG
1	A	1321	ARG
1	A	1811	ARG
1	A	2105	HIS
1	A	3355	LYS
1	A	3477	GLU

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Mol	Chain	Res	Type
1	A	3478	GLU
1	A	3483	MET
1	A	3696	ARG
1	A	3729	MET
1	A	3733	ARG
1	A	3752	VAL
1	A	3753	LYS
1	A	3806	LEU
1	A	3864	ARG
1	A	3929	MET
1	A	3940	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1083	ASN
1	A	1374	GLN
1	A	1574	ASN
1	A	2091	HIS
1	A	2305	ASN
1	A	2351	GLN
1	A	2365	ASN
1	A	3139	GLN
1	A	3515	GLN
1	A	3580	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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	$\# Z > 2$
2	KWT	A	6101	-	30,35,35	3.76	14 (46%)	35,57,57	8.34	13 (37%)

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
2	KWT	A	6101	-	-	0/7/75/75	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6101	KWT	C9-C4	12.13	1.64	1.53
2	A	6101	KWT	C9-C8	10.58	1.63	1.53
2	A	6101	KWT	O1-C2	5.41	1.43	1.35
2	A	6101	KWT	C15-C7	4.96	1.59	1.52
2	A	6101	KWT	C5-C6	4.19	1.54	1.49
2	A	6101	KWT	C3-C2	3.81	1.58	1.49
2	A	6101	KWT	C10-C9	3.35	1.58	1.53
2	A	6101	KWT	C3-C4	3.27	1.42	1.38
2	A	6101	KWT	C7-C6	3.27	1.54	1.47
2	A	6101	KWT	C8-C7	2.88	1.41	1.35
2	A	6101	KWT	O6-C21	2.71	1.41	1.35
2	A	6101	KWT	C23-C1	2.52	1.56	1.50
2	A	6101	KWT	C12-C11	2.40	1.57	1.52
2	A	6101	KWT	C12-C13	2.16	1.57	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6101	KWT	C5-C4-C3	46.16	124.83	107.42
2	A	6101	KWT	C19-C3-C4	13.01	132.11	110.89
2	A	6101	KWT	C12-C13-C15	-5.07	102.98	109.34
2	A	6101	KWT	C11-O6-C21	3.98	123.10	117.06
2	A	6101	KWT	C16-C17-C18	-3.45	102.23	105.70
2	A	6101	KWT	C5-C6-C7	3.02	119.90	118.14
2	A	6101	KWT	C4-C9-C8	3.01	116.45	110.28
2	A	6101	KWT	C14-C13-C15	2.80	117.25	112.08
2	A	6101	KWT	C14-C13-C18	2.54	109.86	105.18
2	A	6101	KWT	C1-O1-C2	2.40	125.86	119.35
2	A	6101	KWT	C17-C18-C13	2.35	110.91	108.59
2	A	6101	KWT	O1-C2-O2	2.30	120.16	117.60
2	A	6101	KWT	O3-C6-C5	-2.22	117.54	121.37

There are no chirality outliers.

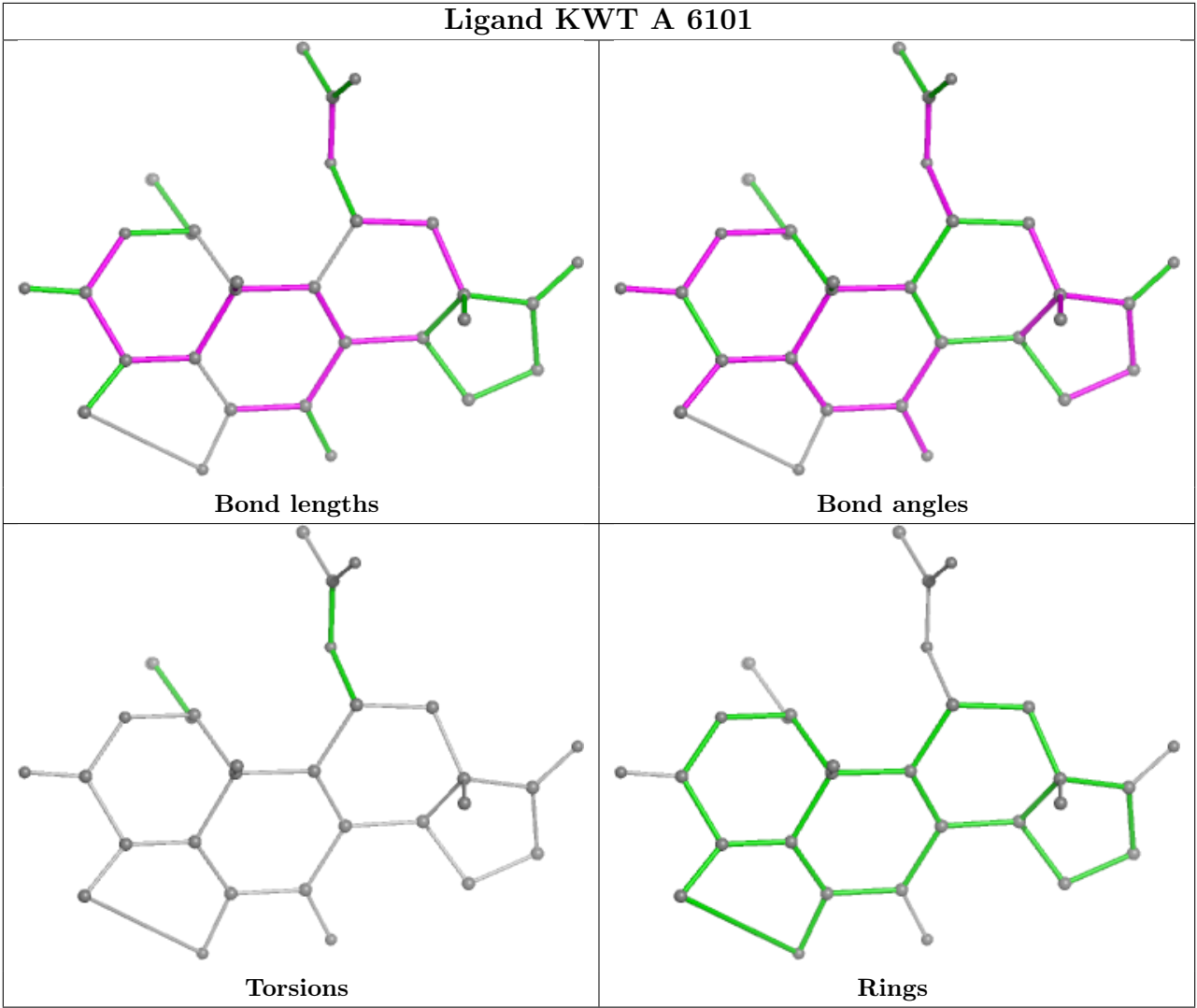
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	6101	KWT	23	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4128:MET	C	6001:UNK	N	84.17

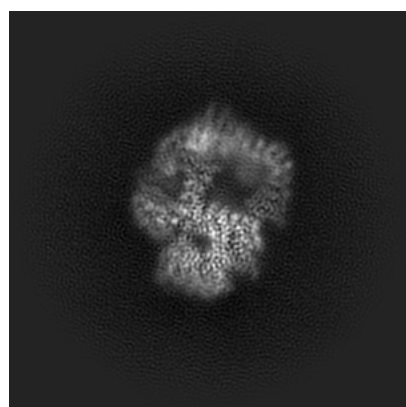
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13067. These allow visual inspection of the internal detail of the map and identification of artifacts.

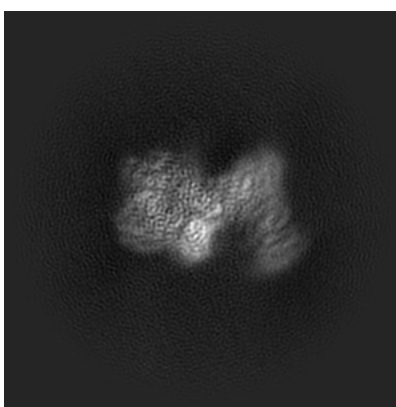
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

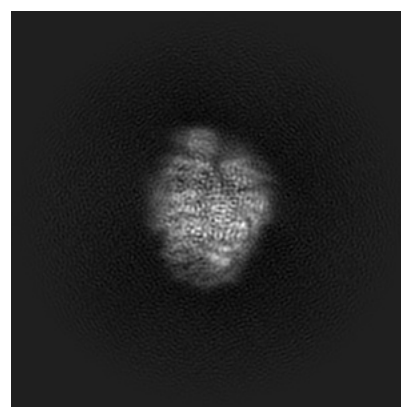
6.1.1 Primary map



X



Y

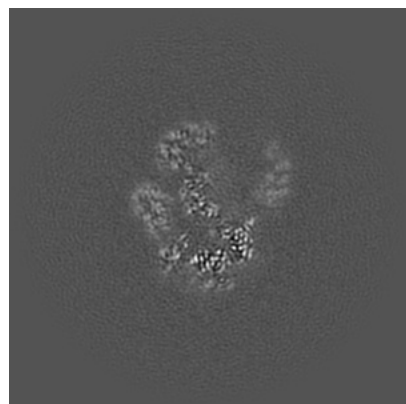


Z

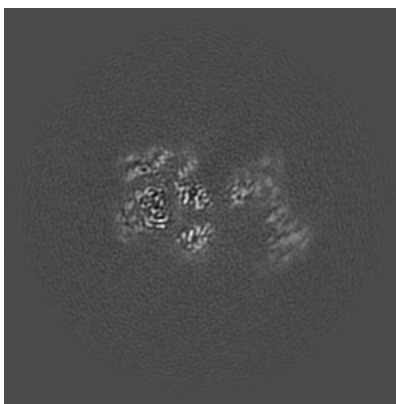
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

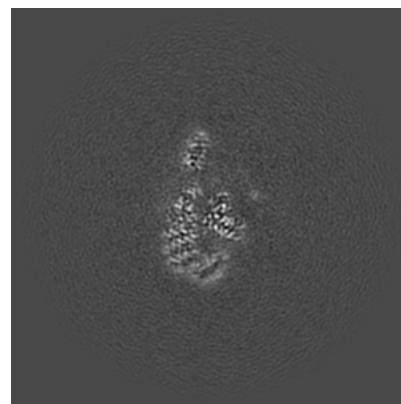
6.2.1 Primary map



X Index: 130



Y Index: 130

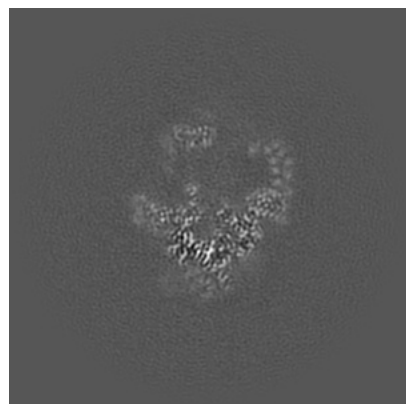


Z Index: 130

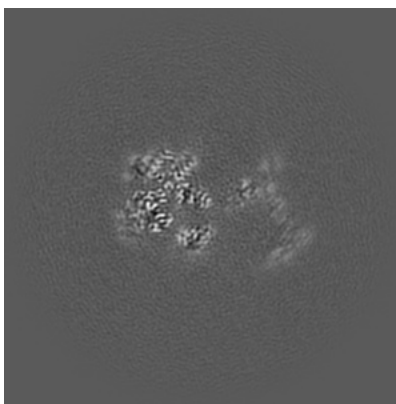
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

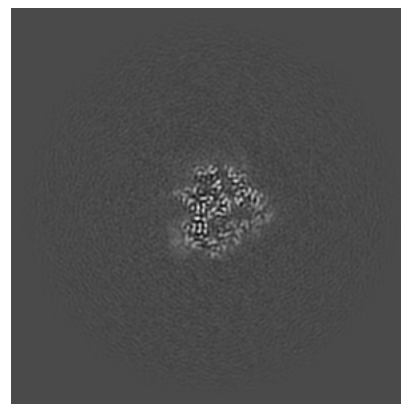
6.3.1 Primary map



X Index: 121



Y Index: 132

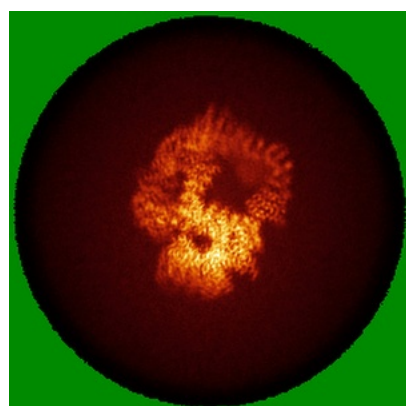


Z Index: 101

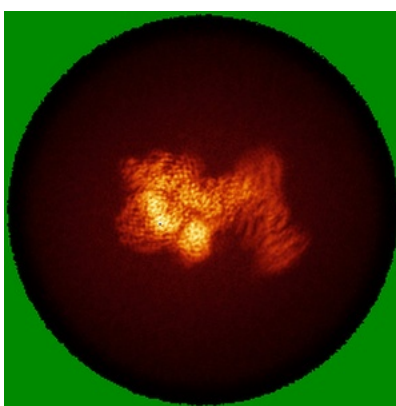
The images above show the largest variance slices of the map in three orthogonal directions.

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

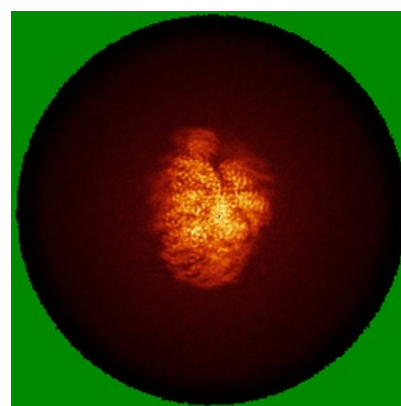
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.22. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

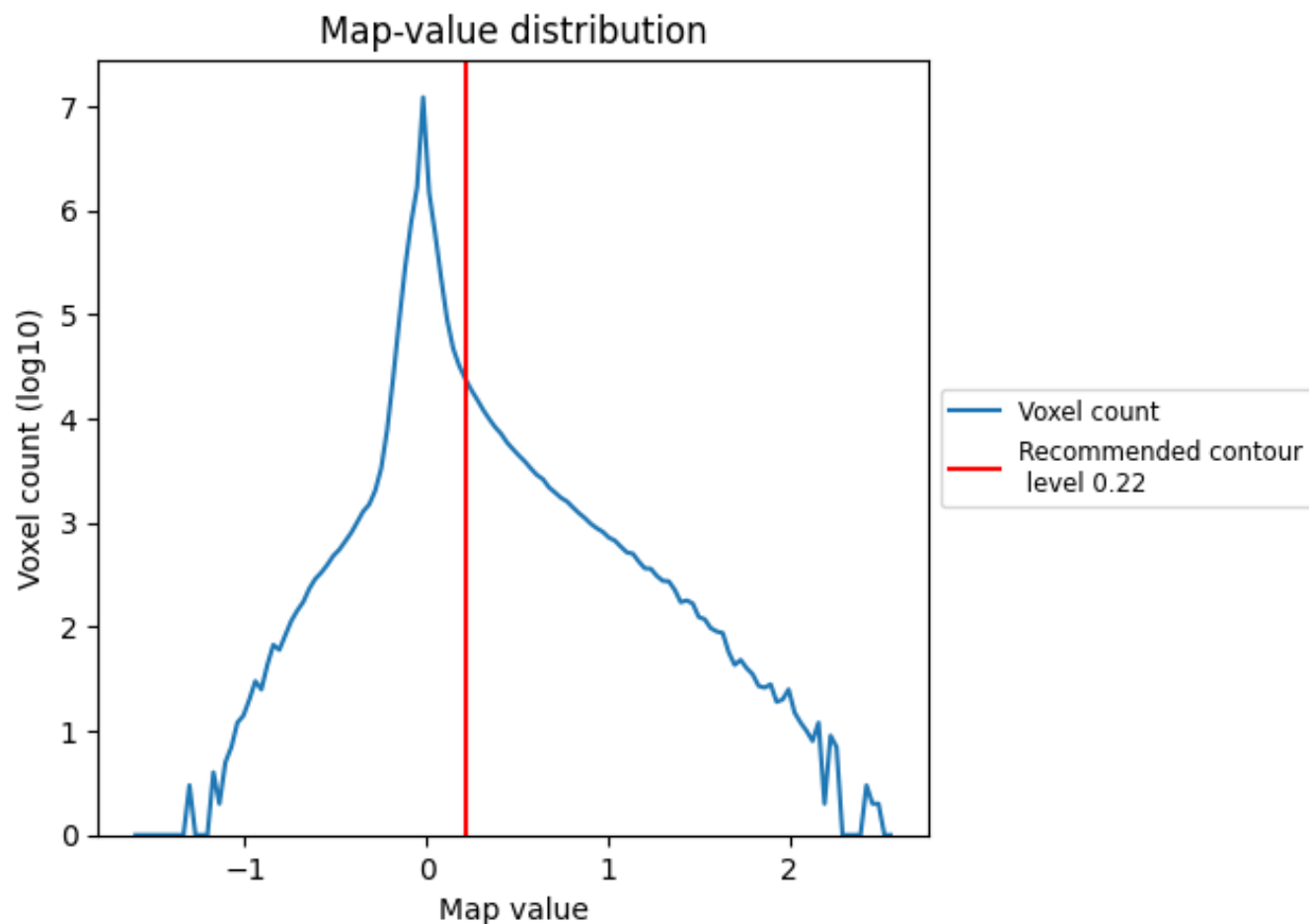
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

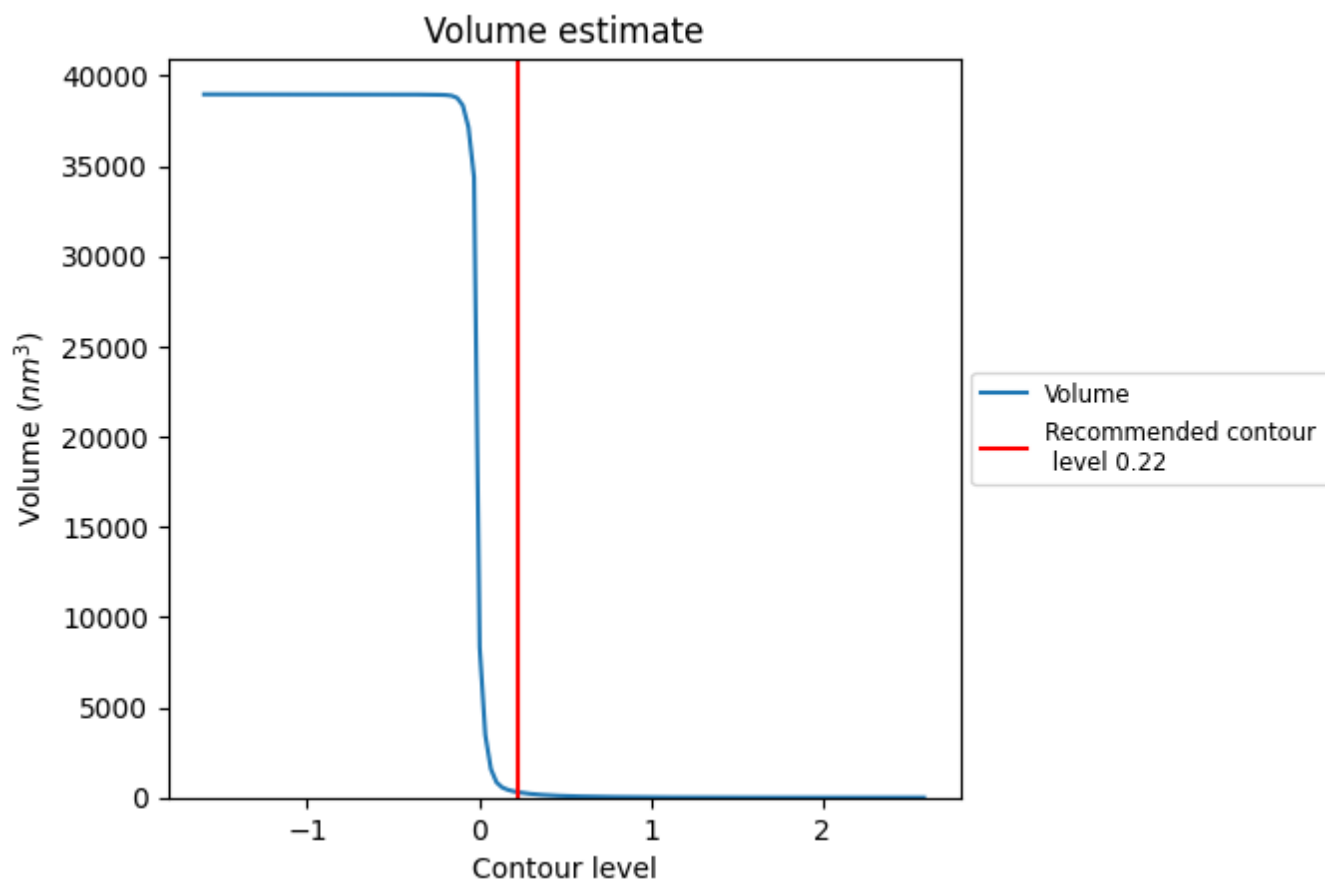
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

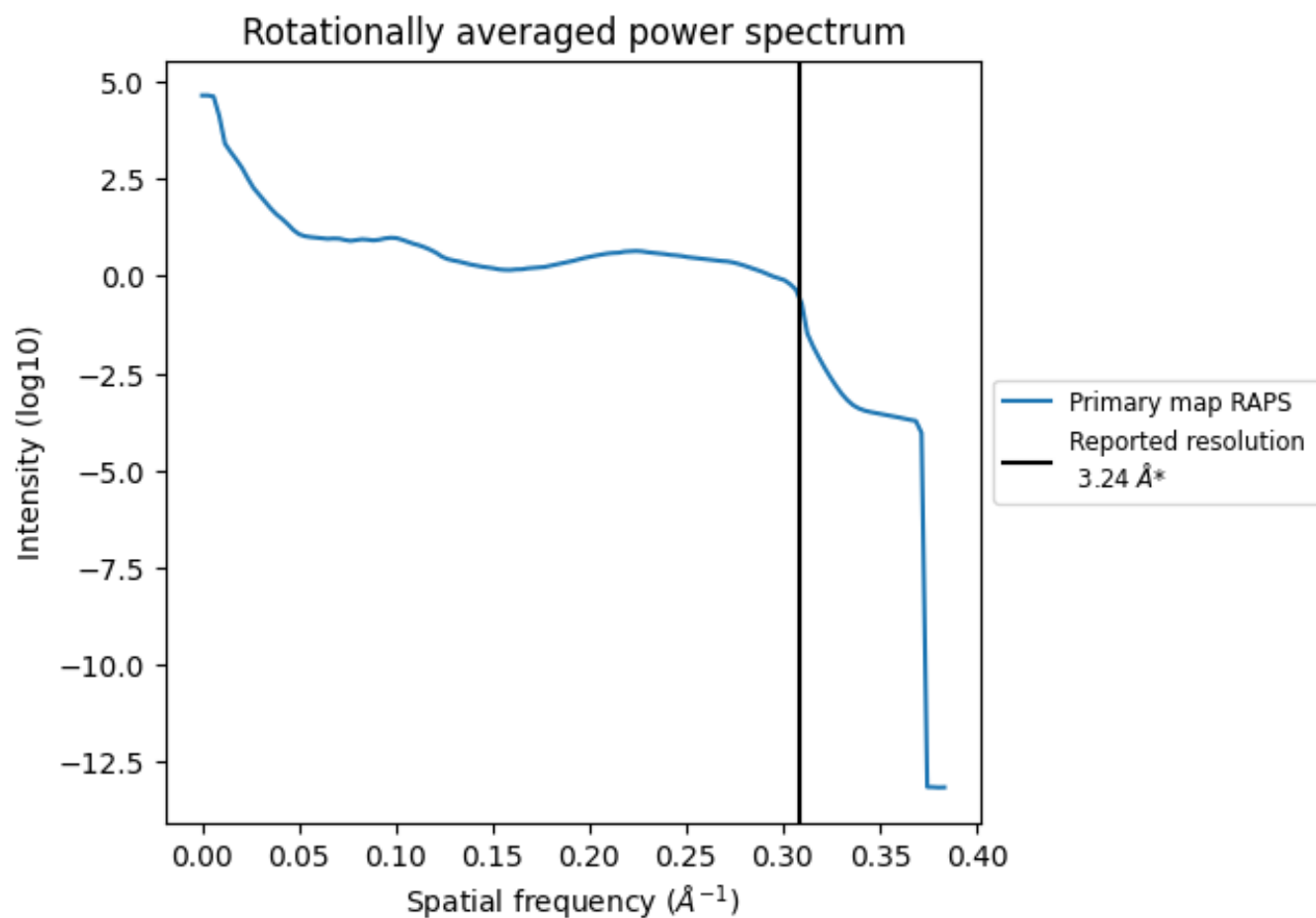
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 311 nm³; this corresponds to an approximate mass of 281 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 0.309 Å⁻¹

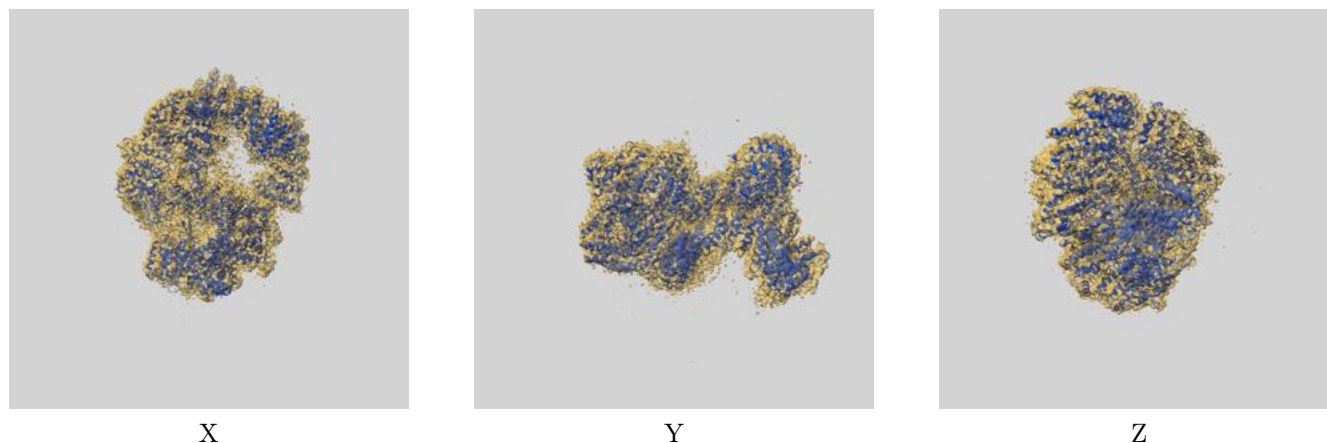
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

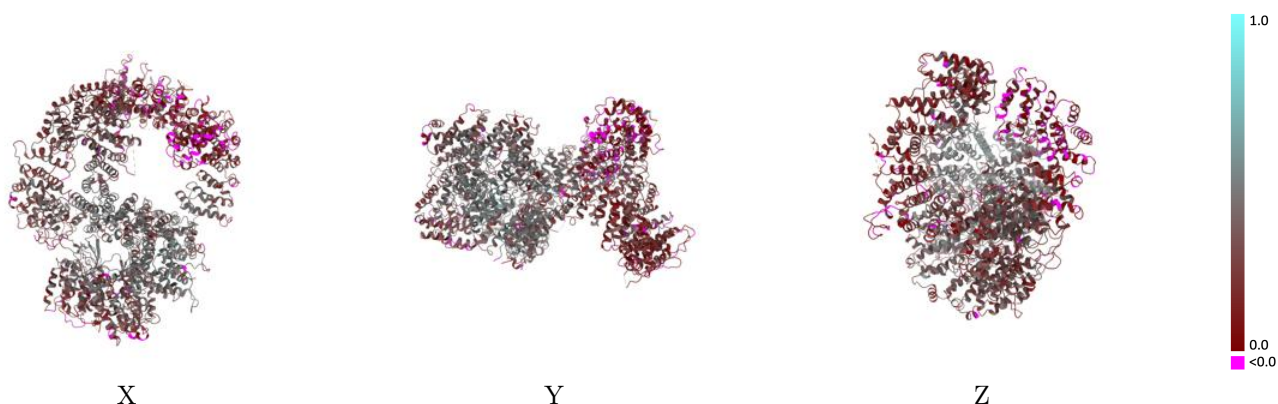
This section contains information regarding the fit between EMDB map EMD-13067 and PDB model 7OTV. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



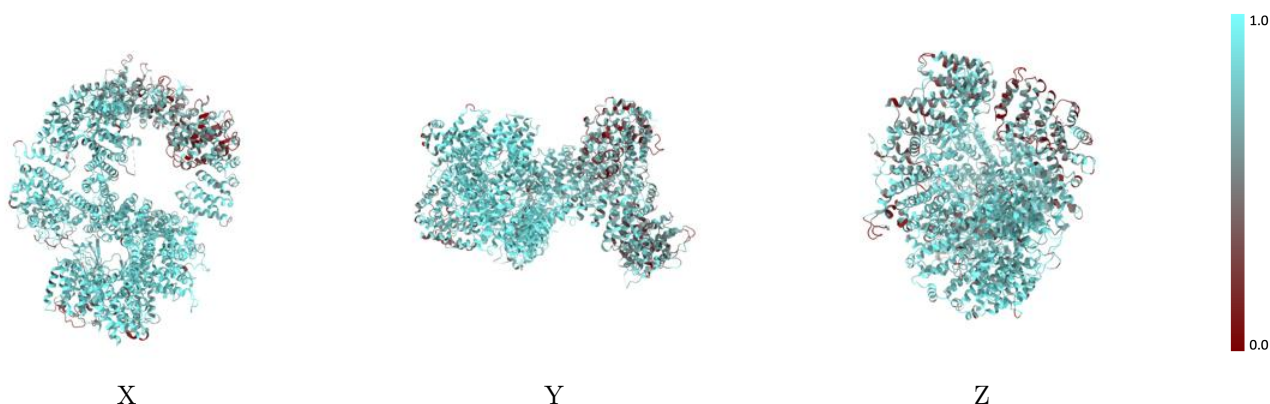
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



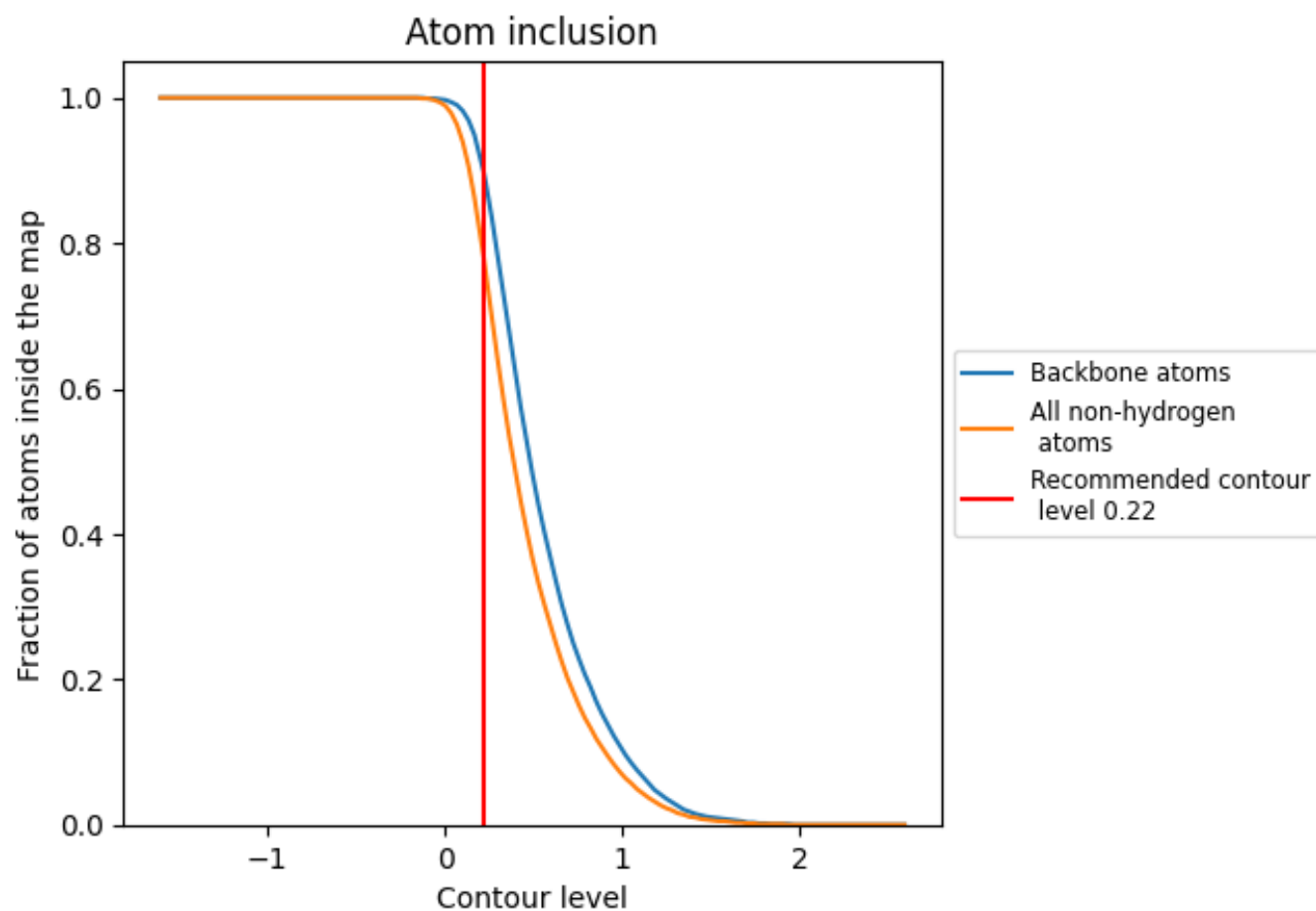
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.22).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 78% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7790	<div></div> 0.3080
A	<div></div> 0.7790	<div></div> 0.3080

