



Full wwPDB EM Validation Report ⓘ

Oct 16, 2025 – 01:51 pm BST

PDB ID : 9SZR / pdb_00009szr
EMDB ID : EMD-55382
Title : shutdown state non-muscle myosin 2A heads region
Authors : Peckham, M.; Carrington, G.
Deposited on : 2025-10-15
Resolution : 6.30 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:

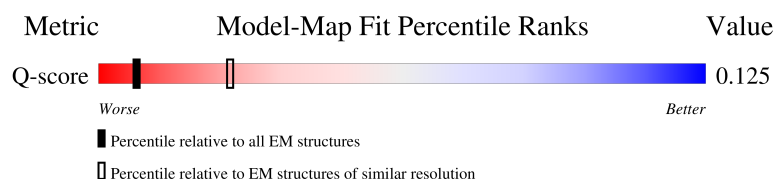
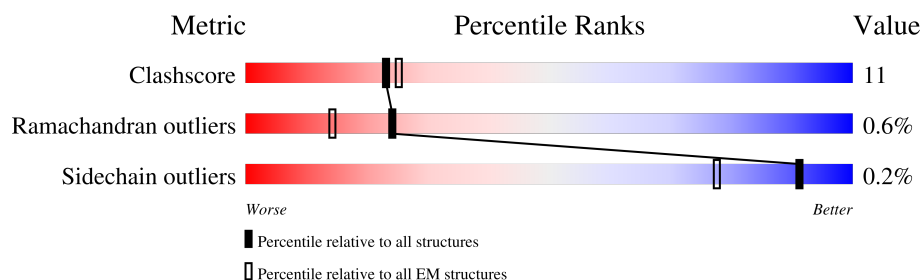
EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up 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) : 2.46

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.30 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	550 (5.80 - 6.80)

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	1960	
1	B	1960	
2	C	151	
2	D	151	

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Mol	Chain	Length	Quality of chain
3	E	172	<div><div></div><div>79%</div><div>9% • 12%</div></div>
3	F	172	<div><div></div><div>78%</div><div>13% 8%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36487 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 Isoform 1 of Myosin-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1947	Total	C	N	O	S	0	0
			15790	9772	2822	3125	71		
1	B	1945	Total	C	N	O	S	0	0
			15770	9761	2816	3122	71		

- Molecule 2 is a protein called Isoform 1 of Myosin light polypeptide 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	150	Total	C	N	O	S	0	0
			1174	729	195	238	12		
2	D	150	Total	C	N	O	S	0	0
			1175	729	195	239	12		

- Molecule 3 is a protein called Myosin regulatory light polypeptide 9.

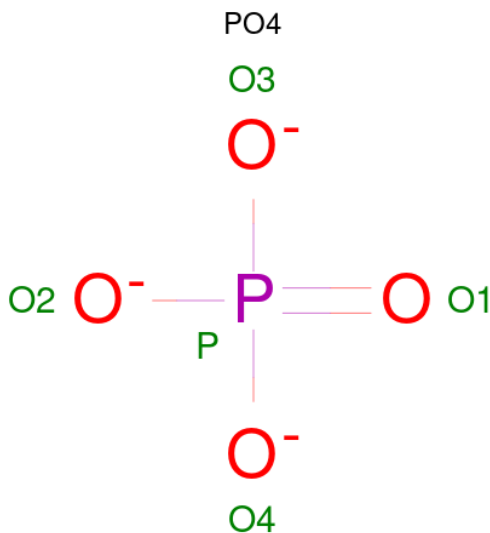
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	152	Total	C	N	O	S	0	0
			1229	771	200	249	9		
3	F	158	Total	C	N	O	S	0	0
			1281	803	212	257	9		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	O	P	0
			5	4	1	

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Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	O	P	0
			5	4	1	

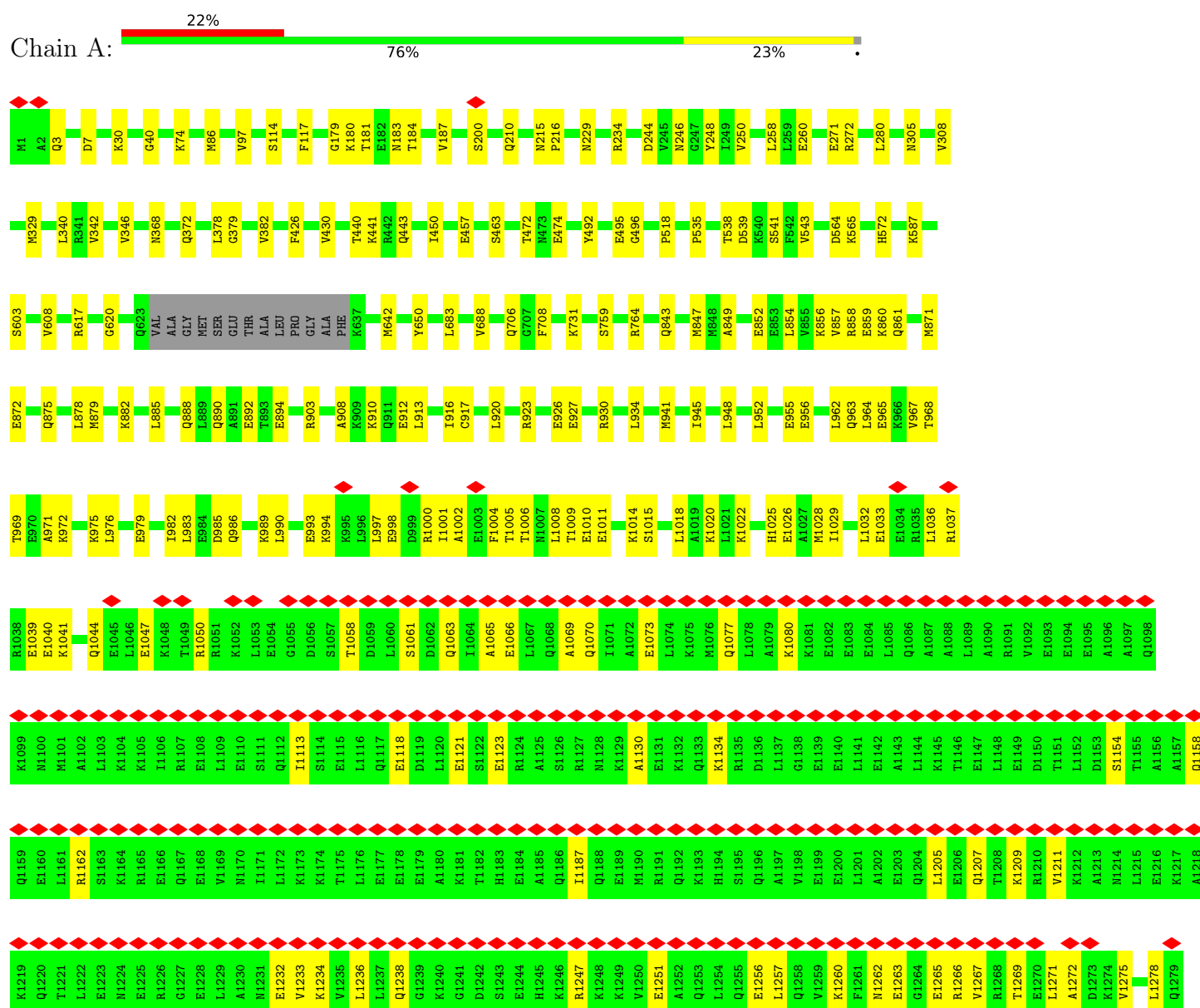
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

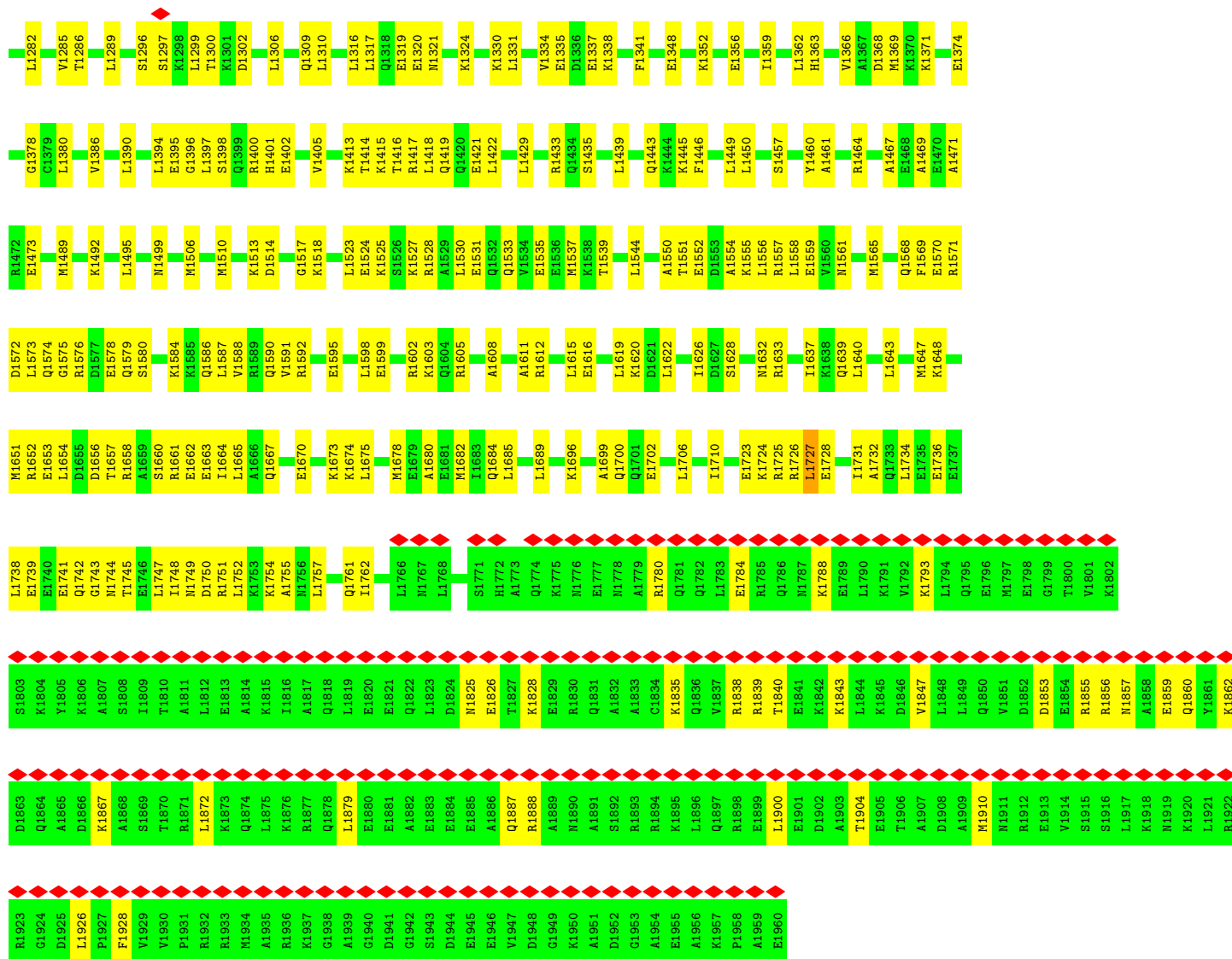
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mg	0
			1	1	
6	B	1	Total	Mg	0
			1	1	
6	E	1	Total	Mg	0
			1	1	
6	F	1	Total	Mg	0
			1	1	

3 Residue-property plots [i](#)

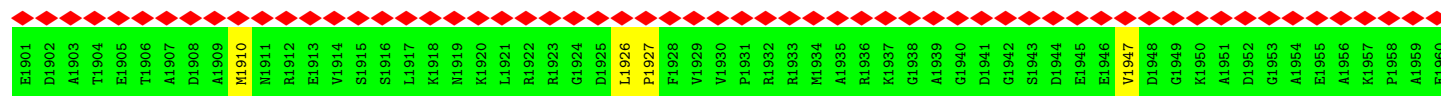
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Isoform 1 of Myosin-9





E1841	Q1761	E1702	L1622	E1545	D1428	V1334	K1260	E1200	E1140	K1080	E1012	R923
K1842	Q1762	R1703	H1625	L1548	L1429	Q1344	F1261	L1201	L1141	K1081	E1013	E926
K1843	L1763	L1706	I1626	T1551	Q1432	Q1434	N1262	A1202	E1142	E1082	K1014	E927
L1844	E1764	L1709	D1627	T1555	Q1434	E1348	G1264	F1203	A1143	E1083	K1016	E928
K1846	R1765	E1709	S1628	K1555	S1435	E1349	E1265	Q1204	L1144	E1084	S1017	Q932
D1847	Q1766	A1711	N1632	L1556	L1439	E1350	E1266	E1206	K1145	L1018	L1018	H933
L1848	N1767	M1712	R1633	L1558	K1442	K1352	V1267	Q1207	T1146	L1085	A1019	A934
L1849	E1768	S1713	K1637	V1560	K1442	H1353	R1268	T1208	E1147	Q1086	K1020	Q935
K1850	L1790	G1715	T1638	M1561	A1451	L1354	E1270	K1209	L1148	A1087	L1021	A936
V1851	K1791	K1716	Q1639	L1562	A1451	L1355	E1271	M1210	E1149	L1088	K1022	E937
D1852	V1792	E1723	L1640	Q1563	T1455	I1359	L1271	A1210	D1150	L1089	M1025	K938
D1853	K1724	K1724	R1641	A1564	I1456	L1362	A1272	V1211	T1151	R1091	K940	K939
L1854	L1727	L1727	K1642	M1565	S1457	H1363	D1273	L1152	L1152	V1092	M1028	K941
R1855	L1794	L1727	L1643	Q1568	A1458	L1366	K1274	A1213	D1153	E1093	T1030	1945
R1856	Q1644	Q1644	Q1644	F1569	K1459	H1363	V1275	M1214	S1154	E1094	D1031	Q946
R1857	M1647	M1647	M1647	R1571	Y1460	V1366	T1276	L1215	T1155	E1095	L1032	E947
E1858	E1653	E1653	E1653	D1572	R1464	M1369	K1277	E1216	A1156	A1096	R1035	E949
E1859	T1657	T1657	T1657	L1573	A1471	L1380	L1278	K1217	A1157	A1097	L1036	E950
Y1861	R1658	R1658	R1658	R1576	R1472	E1384	Q1279	A1218	Q1158	Q1098	R1037	Q951
D1863	A1659	A1659	A1659	E1581	R1472	E1385	V1280	K1219	Q1159	K1099	E1038	E955
K1864	R1661	R1661	R1661	E1582	T1476	V1386	E1281	E1220	L1160	M1100	E1039	E956
A1865	E1662	E1662	E1662	K1583	L1495	R1387	M1285	T1221	L1161	M1101	R1043	R959
D1866	K1663	K1663	K1663	K1584	E1496	R1388	E1286	E1223	R1162	A1102	Q1044	Q960
K1867	E1664	E1664	E1664	K1585	E1496	K1389	G1287	M1224	S1163	L1103	L1046	K961
K1868	L1665	L1665	L1665	Q1586	L1509	L1390	E1287	E1225	K1164	K1104	E1047	L962
S1869	K1669	K1669	K1669	L1587	S1512	Q1391	L1288	E1226	R1165	K1105	L1063	Q963
T1870	E1670	E1670	E1670	R1588	S1512	K1392	L1289	A1226	E1166	I1106	L1063	E970
R1871	M1671	M1671	M1671	R1589	D1514	D1393	S1284	G1227	Q1167	R1107	E1054	L973
L1872	E1672	E1672	E1672	Q1590	D1514	L1394	K1295	E1228	Q1168	E1108	G1065	Q800
K1873	K1673	K1673	K1673	V1591	D1515	G1396	K1297	L1229	V1169	L1109	D1066	K989
L1874	L1675	L1675	L1675	E1592	S1519	L1397	T1298	A1230	N1170	E1110	S1057	E993
K1875	K1676	K1676	K1676	M1594	S1519	R1400	L1299	M1231	I1171	S1111	T1068	K994
K1876	M1682	M1682	M1682	E1595	L1523	E1403	T1300	E1232	K1173	T1113	D1059	K995
R1877	I1683	I1683	I1683	A1596	K1525	K1404	K1301	V1233	K1174	S1114	S1061	L996
Q1878	Q1686	Q1686	Q1686	L1597	S1526	Y1408	D1302	K1234	T1175	E1115	D1062	E997
L1879	E1687	E1687	E1687	D1600	R1528	L1411	E1304	V1235	L1176	L1116	Q1063	D999
E1880	E1688	E1688	E1688	E1601	A1529	E1412	L1306	L1236	E1177	Q1117	I1064	R1000
E1881	L1689	L1689	L1689	Q1604	L1530	K1413	Q1309	L1237	E1178	E1118	A1065	I1001
E1882	A1690	A1690	A1690	R1605	Q1533	T1414	L1310	Q1238	E1179	D1119	E1066	A1002
A1883	A1691	A1691	A1691	E1608	E1536	K1415	Q1311	G1239	A1180	L1120	E1067	E1003
E1884	A1692	A1692	A1692	A1608	M1537	T1416	D1312	K1240	K1181	E1121	Q1068	F1004
E1885	A1695	A1695	A1695	R1612	K1538	R1417	T1313	G1241	T1182	S1122	A1069	T1005
E1886	Q1698	Q1698	Q1698	L1615	Q1540	L1418	Q1314	D1242	H1183	E1123	Q1070	N1007
E1887	A1699	A1699	A1699	L1618	L1541	E1421	E1315	E1244	E1184	R1124	I1071	L1008
R1888	Q1700	Q1700	Q1700	D1618	E1542	L1425	E1319	H1245	A1185	A1125	A1072	E1011
A1889	Q1701	Q1701	Q1701	L1619	E1542	L1425	E1320	K1246	Q1186	S1126	E1073	
E1890	L1776	L1776	L1776	E1777	E1777	E1777	N1321	R1247	I1187	R1127	L1074	
E1891	A1779	A1779	A1779	M1778	M1778	M1778	R1322	K1248	Q1188	M1128	K1075	
E1892	R1780	R1780	R1780	R1780	R1780	R1780	K1330	K1249	E1189	K1129	M1076	
E1893	Q1831	Q1831	Q1831	Q1831	Q1831	Q1831	L1331	V1250	M1190	A1130	Q1077	
E1894	S1892	S1892	S1892	S1892	S1892	S1892	E1251	E1251	R1191	E1131	L1078	
E1895	A1833	A1833	A1833	A1833	A1833	A1833	E1252	A1252	Q1192	K1132	A1079	
E1896	C1834	C1834	C1834	C1834	C1834	C1834	K1193	Q1253	K1193	Q1133		
E1897	K1835	K1835	K1835	K1835	K1835	K1835	H1194	L1254	H1194	K1134		
E1898	Q1836	Q1836	Q1836	Q1836	Q1836	Q1836	S1195	Q1255	S1195	R1135		
E1899	V1837	V1837	V1837	V1837	V1837	V1837	Q1196	E1256	Q1196	L1136		
E1900	R1838	R1838	R1838	R1838	R1838	R1838	A1197	L1257	A1197	L1137		
	R1839	R1839	R1839	R1839	R1839	R1839	V1198	Q1258	V1198	G1138		
	L1900	L1900	L1900	L1900	L1900	L1900	E1199	V1259	E1199	E1139		



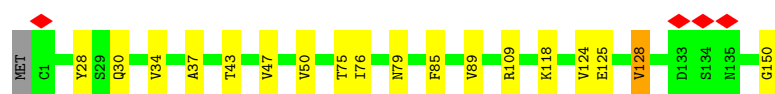
- Molecule 2: Isoform 1 of Myosin light polypeptide 6

Chain C: 87% 12% ..



- Molecule 2: Isoform 1 of Myosin light polypeptide 6

Chain D: 87% 11% ..



- Molecule 3: Myosin regulatory light polypeptide 9

Chain E: 79% 9% 12%



- Molecule 3: Myosin regulatory light polypeptide 9

Chain F: 78% 13% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15167	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	36.94	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.051	Depositor
Minimum map value	-0.432	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	839.68, 839.68, 839.68	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.64, 1.64, 1.64	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, ADP

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	0.06	0/15951	0.14	0/21339
1	B	0.06	0/15930	0.14	0/21311
2	C	0.09	0/1189	0.19	0/1594
2	D	0.10	0/1190	0.21	0/1594
3	E	0.07	0/1252	0.18	0/1685
3	F	0.07	0/1305	0.18	0/1755
All	All	0.06	0/36817	0.15	0/49278

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

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	15790	0	15952	532	0
1	B	15770	0	15927	539	0
2	C	1174	0	1138	11	0
2	D	1175	0	1138	10	0
3	E	1229	0	1154	13	0
3	F	1281	0	1215	12	0
4	A	27	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	27	0	12	1	0
5	A	5	0	0	1	0
5	B	5	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
All	All	36487	0	36548	794	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 11.

All (794) 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:1570:GLU:HA	1:A:1574:GLN:HB2	1.44	0.96
1:A:971:ALA:HB2	1:B:1687:GLU:HG3	1.49	0.94
1:A:1595:GLU:HG2	1:B:1594:MET:HG3	1.53	0.90
1:A:847:MET:HE1	1:B:843:GLN:HB3	1.52	0.90
1:A:1317:LEU:HD13	1:B:1316:LEU:HD23	1.52	0.89
1:A:1573:LEU:HD11	1:B:1569:PHE:HA	1.53	0.89
1:A:1415:LYS:HE2	1:B:1411:LEU:HD22	1.54	0.89
1:A:1446:PHE:HA	1:A:1450:LEU:HD13	1.58	0.85
1:B:131:SER:O	1:B:135:VAL:HG23	1.76	0.85
1:A:1665:LEU:HD22	1:B:1664:ILE:HB	1.59	0.84
1:A:1334:VAL:HG12	1:B:1334:VAL:HG12	1.59	0.83
1:B:131:SER:HA	1:B:134:ILE:HG12	1.60	0.83
1:A:1665:LEU:HD21	1:B:1661:ARG:HA	1.59	0.83
1:A:1080:LYS:HE2	1:B:1800:THR:HB	1.61	0.82
1:A:1523:LEU:HD13	1:B:1524:GLU:HG3	1.62	0.80
1:A:916:ILE:HG22	1:B:917:CYS:HB2	1.64	0.79
1:A:857:VAL:HG12	1:B:857:VAL:HG12	1.64	0.79
1:A:1706:LEU:HD12	1:B:1706:LEU:HB2	1.63	0.78
1:A:1647:MET:HE1	1:B:1643:LEU:HD22	1.66	0.77
1:A:1066:GLU:HB3	1:B:1788:LYS:HD3	1.67	0.77
1:B:1829:GLU:HA	1:B:1832:ALA:HB3	1.66	0.77
1:A:1338:LYS:HD3	1:B:1334:VAL:HG13	1.68	0.74
1:A:1591:VAL:HA	1:B:1591:VAL:HG21	1.69	0.74
1:A:1727:LEU:HD12	1:B:1724:LYS:HG2	1.70	0.73
1:B:1439:LEU:HD23	1:B:1442:LYS:HE2	1.71	0.73
1:A:913:LEU:HD13	1:B:914:GLU:HB2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1008:LEU:HA	1:B:1008:LEU:HD13	1.71	0.73
1:A:1661:ARG:HA	1:A:1664:ILE:HG12	1.70	0.72
1:B:1349:GLU:OE1	1:B:1352:LYS:NZ	2.23	0.72
1:A:180:LYS:N	4:A:2001:ADP:O3B	2.23	0.72
1:A:1665:LEU:HD13	1:B:1664:ILE:HD12	1.71	0.72
1:A:1006:THR:HG22	1:B:1301:LYS:HG2	1.72	0.72
1:B:1671:ASN:HA	1:B:1674:LYS:HE2	1.72	0.72
2:C:19:ASP:OD2	3:E:132:ARG:NH1	2.23	0.72
1:A:1706:LEU:HG	1:B:1703:ARG:HA	1.70	0.72
1:B:948:LEU:HD21	1:B:1669:LYS:HD3	1.70	0.72
1:A:229:ASN:ND2	4:A:2001:ADP:O2A	2.23	0.71
1:A:1073:GLU:HG3	1:B:1792:VAL:HG13	1.71	0.71
1:B:1592:ARG:NH1	1:B:1595:GLU:OE1	2.22	0.71
1:A:114:SER:OG	1:A:117:PHE:O	2.08	0.71
1:B:1588:VAL:HA	1:B:1591:VAL:HG12	1.72	0.71
1:A:989:LYS:HD2	1:A:1710:ILE:HG23	1.73	0.70
1:A:843:GLN:HB3	1:A:847:MET:HG3	1.74	0.70
1:B:229:ASN:ND2	4:B:2001:ADP:O2A	2.24	0.70
1:A:941:MET:HE1	1:B:938:LYS:HD3	1.74	0.69
1:B:517:LYS:NZ	1:B:519:ALA:O	2.26	0.69
1:A:910:LYS:HA	1:B:910:LYS:HG3	1.73	0.69
1:A:1026:GLU:HA	1:A:1029:ILE:HG22	1.73	0.69
1:B:819:TYR:OH	3:F:94:ASN:O	2.09	0.69
2:C:4:SER:O	2:C:8:THR:OG1	2.09	0.69
1:B:840:VAL:HG23	3:F:39:MET:HE1	1.74	0.69
1:B:959:ARG:NH1	1:B:963:GLN:OE1	2.26	0.68
1:A:1317:LEU:HD11	1:B:1313:THR:HA	1.75	0.68
1:A:917:CYS:HB2	1:B:916:ILE:HG22	1.75	0.68
1:B:821:LYS:NZ	3:F:137:GLU:OE1	2.27	0.68
1:A:923:ARG:HA	1:A:926:GLU:HG2	1.76	0.67
1:A:1015:SER:HB2	1:B:1018:LEU:HD12	1.74	0.67
1:B:1018:LEU:HA	1:B:1021:LEU:HD12	1.76	0.67
1:B:642:MET:SD	1:B:642:MET:N	2.67	0.67
3:E:119:GLU:OE1	3:E:123:ARG:NH2	2.27	0.67
1:A:1702:GLU:HB3	1:B:1703:ARG:HD3	1.77	0.67
1:B:1000:ARG:HH22	1:B:1315:GLU:HB2	1.58	0.67
1:A:1578:GLU:OE2	1:A:1579:GLN:NE2	2.27	0.67
1:A:1723:GLU:OE2	1:A:1726:ARG:NH1	2.27	0.67
1:A:1751:ARG:HG3	1:B:1028:MET:HE1	1.77	0.67
1:B:74:LYS:NZ	1:B:91:CYS:SG	2.68	0.66
1:A:1464:ARG:HG2	1:B:1460:TYR:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1586:GLN:O	1:B:1590:GLN:NE2	2.28	0.66
1:B:250:VAL:O	1:B:440:THR:OG1	2.13	0.65
1:A:1256:GLU:OE1	1:A:1260:LYS:NZ	2.30	0.65
1:B:272:ARG:NE	1:B:308:VAL:O	2.30	0.65
1:B:1594:MET:O	1:B:1598:LEU:HB2	1.97	0.65
1:A:1247:ARG:NH1	1:A:1251:GLU:OE2	2.28	0.65
1:A:1398:SER:OG	1:A:1402:GLU:OE2	2.10	0.65
1:A:1366:VAL:HG13	1:B:1369:MET:HE1	1.79	0.64
1:A:472:THR:OG1	1:A:650:TYR:OH	2.08	0.64
1:A:1415:LYS:NZ	1:A:1419:GLN:OE1	2.27	0.64
1:A:1867:LYS:HZ1	1:B:1143:ALA:HA	1.61	0.64
2:C:19:ASP:O	2:C:21:THR:N	2.30	0.64
1:A:997:LEU:HB3	1:B:997:LEU:HB3	1.79	0.64
1:A:975:LYS:HE2	1:B:1695:ALA:HB2	1.78	0.64
1:A:1555:LYS:HD2	1:B:1551:THR:HB	1.79	0.63
1:B:803:GLN:O	1:B:807:THR:OG1	2.11	0.63
1:B:1557:ARG:O	1:B:1561:ASN:ND2	2.26	0.63
1:A:916:ILE:HG22	1:A:920:LEU:HD12	1.81	0.63
1:A:1620:LYS:NZ	1:B:901:GLU:OE2	2.31	0.63
1:A:1011:GLU:HB2	1:B:1011:GLU:HG3	1.81	0.63
1:A:1738:LEU:HD22	1:B:1734:LEU:HD23	1.79	0.63
1:A:847:MET:HE2	1:B:847:MET:HB2	1.81	0.63
1:A:1065:ALA:HB2	1:B:1785:ARG:HG2	1.81	0.63
1:A:1282:LEU:HD12	1:B:1285:VAL:HG11	1.81	0.63
1:A:181:THR:OG1	4:A:2001:ADP:O1B	2.07	0.63
1:A:1123:GLU:OE2	1:B:1127:ARG:NE	2.32	0.63
1:A:1555:LYS:HB3	1:B:1555:LYS:HE2	1.81	0.63
1:B:904:ALA:O	1:B:907:THR:OG1	2.16	0.62
1:A:1286:THR:HA	1:A:1289:LEU:HD21	1.82	0.62
1:A:250:VAL:O	1:A:440:THR:OG1	2.17	0.62
1:B:1894:ARG:NH2	1:B:1897:GLN:OE1	2.32	0.62
1:B:131:SER:CA	1:B:134:ILE:HG12	2.28	0.62
1:B:1660:SER:HB2	1:B:1664:ILE:HD12	1.81	0.62
1:A:1306:LEU:HB3	1:B:1306:LEU:HB3	1.81	0.62
1:A:875:GLN:HG2	1:B:878:LEU:HD12	1.80	0.62
1:A:1262:ASN:OD1	1:A:1266:ARG:NE	2.28	0.62
1:A:1362:LEU:HB3	1:B:1362:LEU:HB3	1.80	0.62
1:A:1510:MET:HE1	1:A:1525:LYS:HB2	1.81	0.62
1:A:1853:ASP:OD1	1:A:1856:ARG:NH2	2.27	0.62
1:B:1759:ILE:O	1:B:1763:ASN:ND2	2.30	0.62
1:A:1591:VAL:HG12	1:B:1591:VAL:HG11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1754:LYS:HZ3	1:B:1032:LEU:HD21	1.65	0.61
1:A:975:LYS:HD3	1:B:1691:ALA:HB1	1.82	0.61
1:A:913:LEU:HD22	1:B:914:GLU:HG3	1.83	0.61
1:A:1633:ARG:HB2	1:B:1633:ARG:HB2	1.82	0.61
1:B:567:ASP:OD2	1:B:580:LYS:NZ	2.34	0.61
1:A:964:LEU:HD11	1:B:1686:GLN:HG3	1.82	0.61
1:A:1640:LEU:HD11	1:B:1643:LEU:HD12	1.82	0.61
1:B:1384:GLU:HA	1:B:1387:LYS:HG2	1.83	0.61
1:A:1605:ARG:HG3	1:B:1601:GLU:HB3	1.82	0.60
1:A:1044:GLN:NE2	1:A:1761:GLN:OE1	2.34	0.60
1:A:1602:ARG:HG3	1:B:1598:LEU:HD22	1.82	0.60
1:B:838:LEU:CB	1:B:841:SER:HB3	2.31	0.60
1:A:1011:GLU:HG3	1:B:1012:GLU:HA	1.83	0.60
1:B:1589:ARG:NH1	1:B:1593:GLU:OE2	2.30	0.60
1:A:234:ARG:NE	1:A:260:GLU:OE1	2.35	0.60
1:B:1571:ARG:NH2	3:E:111:GLU:O	2.32	0.60
1:B:1601:GLU:O	1:B:1605:ARG:N	2.28	0.60
2:C:101:GLY:O	2:C:139:ASN:ND2	2.33	0.60
1:A:1706:LEU:HD21	1:B:1703:ARG:HD2	1.84	0.60
1:B:1412:GLU:O	1:B:1416:THR:HG23	2.01	0.60
1:A:1661:ARG:HG2	1:B:1661:ARG:HD3	1.84	0.59
1:B:1316:LEU:O	1:B:1320:GLU:HG2	2.02	0.59
1:A:969:THR:HG21	1:B:970:GLU:HG2	1.83	0.59
1:A:1272:ALA:HB2	1:B:1271:LEU:HD13	1.85	0.59
1:A:1670:GLU:HA	1:A:1673:LYS:HE3	1.84	0.59
1:A:1738:LEU:HA	1:B:1738:LEU:HD21	1.85	0.59
1:A:964:LEU:HD13	1:B:1683:ILE:HA	1.83	0.59
1:A:1551:THR:HG21	1:B:1548:LEU:CD1	2.33	0.59
1:A:1569:PHE:CD1	1:A:1573:LEU:HD12	2.38	0.59
1:B:1538:LYS:NZ	1:B:1542:GLU:OE2	2.26	0.59
1:A:1316:LEU:HD23	1:A:1319:GLU:OE2	2.03	0.59
1:A:1401:HIS:O	1:A:1405:VAL:HG23	2.02	0.59
1:A:1535:GLU:O	1:A:1539:THR:HG23	2.03	0.59
1:A:1633:ARG:HH11	1:A:1637:ILE:HD12	1.67	0.59
1:A:271:GLU:O	1:A:305:ASN:ND2	2.36	0.58
1:A:910:LYS:HD2	1:B:913:LEU:HD12	1.85	0.58
1:A:1445:LYS:O	1:A:1449:LEU:N	2.36	0.58
1:A:1446:PHE:O	1:A:1450:LEU:HB2	2.03	0.58
1:A:1825:ASN:HA	1:A:1828:LYS:HE2	1.85	0.58
1:B:994:LYS:CE	1:B:1713:SER:HB3	2.34	0.58
1:A:1320:GLU:OE1	1:A:1324:LYS:NZ	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1536:GLU:O	1:B:1539:THR:OG1	2.16	0.58
1:A:1233:VAL:HA	1:A:1236:LEU:CD2	2.34	0.58
1:A:1565:MET:SD	1:A:1568:GLN:NE2	2.77	0.58
1:A:1745:THR:O	1:A:1749:ASN:ND2	2.26	0.58
1:B:1564:ALA:HB1	3:E:104:ASN:HD22	1.68	0.58
1:B:234:ARG:NH2	5:B:2002:PO4:O3	2.37	0.58
1:A:997:LEU:HB2	1:B:997:LEU:HD13	1.85	0.58
1:A:1568:GLN:HB3	1:A:1572:ASP:OD2	2.04	0.57
1:B:993:GLU:HG2	1:B:1316:LEU:HD22	1.86	0.57
1:A:1495:LEU:HB3	1:B:1495:LEU:HB3	1.85	0.57
1:A:1558:LEU:HD22	1:B:1559:GLU:HG2	1.86	0.57
1:A:1397:LEU:HA	1:A:1400:ARG:HH11	1.70	0.57
1:A:847:MET:CE	1:B:847:MET:HB2	2.34	0.57
1:B:459:PHE:O	1:B:462:ASN:ND2	2.37	0.57
1:A:872:GLU:HG2	1:B:871:MET:HE3	1.85	0.57
1:A:1555:LYS:NZ	1:A:1559:GLU:OE2	2.29	0.57
1:A:1728:GLU:HA	1:A:1731:ILE:HG22	1.85	0.57
1:A:379:GLY:O	1:A:603:SER:OG	2.18	0.57
1:A:1565:MET:HB3	1:B:1565:MET:HE1	1.84	0.57
1:A:1619:LEU:HD22	1:B:1615:LEU:HD22	1.87	0.57
1:B:995:LYS:HE3	1:B:1712:ASN:ND2	2.19	0.57
1:A:1571:ARG:O	1:A:1575:GLY:HA3	2.05	0.57
1:A:1887:GLN:OE1	1:A:1888:ARG:NH1	2.37	0.57
1:B:94:GLU:N	1:B:94:GLU:OE1	2.37	0.57
1:B:898:GLU:HA	1:B:901:GLU:HG2	1.86	0.57
1:A:1471:ALA:HA	1:B:1471:ALA:HB2	1.87	0.57
1:A:910:LYS:HG3	1:B:910:LYS:HA	1.86	0.56
1:B:463:SER:OG	1:B:584:TRP:NE1	2.37	0.56
1:A:857:VAL:HG21	1:B:854:LEU:HD11	1.87	0.56
1:A:879:MET:O	1:A:882:LYS:HG3	2.05	0.56
1:A:1573:LEU:HD22	1:B:1572:ASP:HB2	1.87	0.56
1:A:1793:LYS:HE3	1:B:1794:LEU:HD21	1.87	0.56
1:A:871:MET:HE1	1:B:868:LEU:HD21	1.86	0.56
1:A:1926:LEU:HB2	1:A:1928:PHE:CE2	2.40	0.56
1:A:948:LEU:HD11	1:B:945:ILE:HG23	1.86	0.56
1:A:964:LEU:HB2	1:B:1683:ILE:HG12	1.86	0.56
1:A:1205:LEU:HD11	1:A:1209:LYS:HE3	1.88	0.56
1:A:1005:THR:HG22	1:B:1004:PHE:CD2	2.41	0.56
1:A:1544:LEU:CD1	1:B:1541:LEU:HG	2.36	0.56
1:B:838:LEU:HB2	1:B:841:SER:HB3	1.88	0.56
1:A:1033:GLU:OE2	1:A:1754:LYS:NZ	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1278:LEU:HD13	1:B:1278:LEU:HB2	1.88	0.56
1:A:1738:LEU:CD2	1:B:1734:LEU:HD23	2.35	0.56
1:A:1628:SER:O	1:A:1632:ASN:ND2	2.36	0.56
1:A:1368:ASP:O	1:A:1371:LYS:HG3	2.06	0.56
1:A:1584:LYS:HA	1:A:1587:LEU:HD12	1.87	0.56
1:B:1263:GLU:OE1	1:B:1266:ARG:NH2	2.34	0.56
1:A:683:LEU:HD11	1:A:688:VAL:HG21	1.87	0.55
1:A:1544:LEU:HD11	1:B:1541:LEU:HG	1.87	0.55
1:A:1552:GLU:O	1:A:1556:LEU:HG	2.07	0.55
1:A:1570:GLU:O	1:A:1575:GLY:N	2.39	0.55
1:A:1599:GLU:OE2	1:A:1602:ARG:NH2	2.39	0.55
1:B:1412:GLU:O	1:B:1415:LYS:HG2	2.06	0.55
1:A:972:LYS:O	1:A:976:LEU:N	2.32	0.55
1:A:1366:VAL:HG23	1:B:1366:VAL:HG23	1.86	0.55
1:A:1855:ARG:NH2	1:B:1132:LYS:HD3	2.21	0.55
1:A:1571:ARG:O	1:A:1571:ARG:NH1	2.33	0.55
1:B:1319:GLU:OE2	1:B:1322:ARG:NH1	2.36	0.55
1:A:955:GLU:OE1	1:B:959:ARG:NE	2.32	0.55
1:B:1604:GLN:O	1:B:1608:ALA:N	2.38	0.55
1:A:234:ARG:NH2	1:A:457:GLU:OE2	2.39	0.55
1:B:105:TYR:O	1:B:109:LEU:N	2.37	0.55
1:A:1533:GLN:O	1:A:1537:MET:HG2	2.07	0.55
1:A:1696:LYS:HD2	1:B:1692:ALA:HA	1.88	0.55
1:B:951:GLN:O	1:B:955:GLU:HG2	2.06	0.55
1:B:1031:ASP:OD2	1:B:1035:ARG:NH1	2.28	0.55
1:B:1533:GLN:O	1:B:1537:MET:HG2	2.07	0.55
1:A:1010:GLU:OE2	1:A:1014:LYS:HE3	2.07	0.55
1:A:1467:ALA:CB	1:B:1464:ARG:HG2	2.37	0.55
1:A:1724:LYS:HB3	1:A:1725:ARG:NH1	2.22	0.55
1:B:1145:LYS:O	1:B:1149:GLU:HG3	2.07	0.55
1:A:1495:LEU:HD11	1:B:1496:GLU:HG3	1.88	0.55
1:A:945:ILE:HG13	1:B:945:ILE:HG13	1.89	0.54
1:A:1286:THR:HA	1:A:1289:LEU:CD2	2.36	0.54
1:A:1696:LYS:O	1:A:1700:GLN:HG2	2.07	0.54
1:A:875:GLN:HE21	1:B:878:LEU:HD11	1.72	0.54
1:A:1415:LYS:CE	1:B:1411:LEU:HD22	2.33	0.54
1:B:1594:MET:HB3	1:B:1598:LEU:HD12	1.88	0.54
1:A:1233:VAL:HA	1:A:1236:LEU:HD21	1.89	0.54
1:A:1296:SER:O	1:A:1300:THR:HG23	2.07	0.54
1:B:348:GLN:OE1	1:B:351:ASN:ND2	2.41	0.54
1:A:538:THR:H	1:A:541:SER:HG	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:847:MET:CE	1:B:843:GLN:HB3	2.34	0.54
1:A:1398:SER:HA	1:A:1401:HIS:CD2	2.42	0.54
1:A:1460:TYR:HB3	1:B:1460:TYR:HB2	1.88	0.54
1:A:1661:ARG:HA	1:A:1664:ILE:CG1	2.38	0.54
1:A:1879:LEU:HD13	1:B:1879:LEU:HD22	1.88	0.54
1:B:206:GLU:OE1	1:B:206:GLU:N	2.40	0.54
1:B:1281:GLU:O	1:B:1285:VAL:HG23	2.07	0.54
1:A:706:GLN:O	1:A:764:ARG:NH1	2.40	0.54
1:A:1015:SER:HB2	1:B:1018:LEU:CD1	2.37	0.54
1:A:1727:LEU:HG	1:B:1724:LYS:HE2	1.90	0.54
1:A:463:SER:OG	1:A:587:LYS:NZ	2.39	0.54
1:A:1018:LEU:HD13	1:B:1019:ALA:HA	1.90	0.54
1:A:1706:LEU:CD2	1:B:1703:ARG:HD2	2.38	0.54
1:B:928:GLU:O	1:B:932:GLN:HG2	2.06	0.54
1:B:956:GLU:OE2	1:B:960:GLN:NE2	2.41	0.54
1:B:1155:THR:HG22	1:B:1158:GLN:HG2	1.88	0.54
1:A:1513:LYS:HA	1:B:1513:LYS:HE2	1.88	0.54
1:A:1685:LEU:HD12	1:B:1682:MET:HG2	1.90	0.54
1:A:1706:LEU:HD12	1:B:1706:LEU:CB	2.34	0.54
1:B:76:ASN:N	1:B:77:PRO:HA	2.22	0.54
1:B:199:LYS:O	1:B:201:LYS:N	2.40	0.54
1:A:975:LYS:HG3	1:B:1698:GLN:HE22	1.72	0.54
1:A:1011:GLU:HB3	1:B:1015:SER:HB3	1.90	0.54
1:A:1699:ALA:HB1	1:B:1699:ALA:CB	2.38	0.54
1:B:1712:ASN:O	1:B:1716:LYS:HB2	2.08	0.54
1:A:1530:LEU:CD1	1:B:1527:LYS:HD3	2.39	0.53
1:B:1349:GLU:O	1:B:1352:LYS:HG2	2.08	0.53
1:B:1641:ARG:O	1:B:1644:GLN:HG3	2.09	0.53
3:F:57:LEU:HD13	3:F:64:PRO:HB3	1.89	0.53
1:A:1394:LEU:HG	1:B:1394:LEU:HG	1.90	0.53
1:A:1643:LEU:HG	1:B:1640:LEU:HD11	1.88	0.53
1:A:1734:LEU:CD1	1:B:1731:ILE:HG23	2.37	0.53
1:A:474:GLU:OE1	1:A:572:HIS:ND1	2.41	0.53
1:A:857:VAL:HG11	1:B:858:ARG:HG3	1.89	0.53
1:A:1047:GLU:HG2	1:B:1046:LEU:HD13	1.89	0.53
1:A:1576:ARG:O	1:A:1580:SER:N	2.20	0.53
1:A:885:LEU:CD1	1:B:882:LYS:HG3	2.38	0.53
1:A:1022:LYS:HE2	1:B:1025:HIS:NE2	2.23	0.53
1:A:1233:VAL:HG21	1:B:1229:LEU:HD11	1.90	0.53
1:A:1744:ASN:HB3	1:A:1748:ILE:HD12	1.89	0.53
1:A:983:LEU:HD12	1:B:980:GLN:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1867:LYS:NZ	1:B:1143:ALA:HA	2.23	0.53
1:B:1618:ASP:O	1:B:1622:LEU:HG	2.08	0.53
1:B:1731:ILE:HA	1:B:1734:LEU:HD12	1.91	0.53
1:B:1846:ASP:HA	1:B:1849:LEU:CD2	2.39	0.53
1:A:250:VAL:HG21	1:A:443:GLN:O	2.09	0.53
1:B:46:LEU:HA	1:B:56:VAL:HG12	1.90	0.53
1:A:1495:LEU:O	1:A:1499:ASN:ND2	2.37	0.53
1:A:1857:ASN:HA	1:A:1860:GLN:HG2	1.91	0.53
1:B:932:GLN:O	1:B:935:GLN:HG3	2.08	0.53
1:A:74:LYS:NZ	1:A:1421:GLU:OE1	2.31	0.53
1:A:1366:VAL:HG13	1:B:1369:MET:CE	2.38	0.53
1:A:1742:GLN:NE2	1:B:1741:GLU:OE2	2.41	0.53
1:B:956:GLU:HG2	1:B:959:ARG:HH21	1.74	0.53
1:A:1422:LEU:HD22	1:B:1418:LEU:CD1	2.39	0.52
1:B:1585:LYS:O	1:B:1589:ARG:HB2	2.09	0.52
1:A:1414:THR:HA	1:A:1417:ARG:HG2	1.89	0.52
1:A:1602:ARG:HG3	1:B:1598:LEU:CD2	2.39	0.52
1:B:605:ASP:OD2	1:B:608:VAL:HG23	2.09	0.52
1:B:1523:LEU:O	1:B:1527:LYS:HG2	2.09	0.52
1:B:1846:ASP:O	1:B:1849:LEU:HG	2.09	0.52
1:A:1257:LEU:HD12	1:B:1254:LEU:HD11	1.90	0.52
1:A:1510:MET:SD	1:A:1525:LYS:HD3	2.49	0.52
1:A:903:ARG:HG3	1:B:903:ARG:HA	1.90	0.52
1:A:1573:LEU:CD1	1:B:1569:PHE:HA	2.34	0.52
1:A:888:GLN:O	1:A:892:GLU:HG2	2.09	0.52
1:A:976:LEU:HG	1:B:973:LEU:HG	1.92	0.52
1:B:1234:LYS:HA	1:B:1237:LEU:HD21	1.90	0.52
1:A:200:SER:OG	2:C:122:GLU:OE2	2.22	0.52
1:A:1608:ALA:CB	1:B:1605:ARG:HG3	2.39	0.52
1:B:934:LEU:HD23	1:B:937:GLU:OE2	2.09	0.52
1:A:1374:GLU:O	1:A:1378:GLY:N	2.37	0.52
1:A:1665:LEU:HD22	1:B:1664:ILE:CB	2.35	0.52
1:B:1830:ARG:O	1:B:1831:GLN:N	2.43	0.52
3:F:81:ASN:ND2	3:F:84:MET:SD	2.82	0.52
1:A:1278:LEU:HD13	1:B:1278:LEU:CB	2.40	0.52
1:A:1352:LYS:HE2	1:A:1356:GLU:OE2	2.10	0.52
1:A:1626:ILE:HG12	1:B:1626:ILE:HG13	1.92	0.52
1:A:1647:MET:HE3	1:A:1648:LYS:HE3	1.92	0.52
1:A:1741:GLU:O	1:A:1745:THR:HG23	2.10	0.52
1:B:1581:GLU:O	1:B:1584:LYS:HG2	2.10	0.52
1:A:920:LEU:HD12	1:B:917:CYS:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1829:GLU:HA	1:B:1832:ALA:CB	2.39	0.52
1:A:1282:LEU:CD1	1:B:1285:VAL:HG11	2.40	0.52
1:A:1657:THR:O	1:A:1661:ARG:N	2.37	0.52
1:A:1840:THR:HG23	1:B:1844:LEU:HD22	1.92	0.52
1:B:1564:ALA:HB2	3:E:101:VAL:HG23	1.91	0.52
1:A:1348:GLU:OE1	1:B:1352:LYS:HD3	2.11	0.51
1:A:1359:ILE:HG23	1:B:1362:LEU:CD1	2.40	0.51
1:A:1445:LYS:HB3	1:A:1449:LEU:CD1	2.40	0.51
1:B:1557:ARG:O	1:B:1560:VAL:HG12	2.10	0.51
1:A:1275:VAL:HG13	1:B:1278:LEU:HD11	1.92	0.51
1:A:1872:LEU:HG	1:B:1875:LEU:CD1	2.40	0.51
1:B:1846:ASP:HA	1:B:1849:LEU:HD21	1.91	0.51
1:A:1551:THR:HG21	1:B:1548:LEU:HD13	1.93	0.51
1:A:1633:ARG:HA	1:B:1633:ARG:HG3	1.92	0.51
1:B:162:MET:O	1:B:165:ARG:NH1	2.42	0.51
1:A:1598:LEU:HD11	1:B:1595:GLU:CG	2.41	0.51
1:A:882:LYS:HE2	1:B:878:LEU:HD22	1.93	0.51
1:A:1073:GLU:CG	1:B:1792:VAL:HG13	2.41	0.51
1:A:1464:ARG:HB3	1:B:1460:TYR:O	2.10	0.51
1:A:1587:LEU:O	1:A:1591:VAL:HG13	2.11	0.51
1:B:1583:LYS:HA	1:B:1583:LYS:HE2	1.92	0.51
1:A:1443:GLN:HA	1:A:1446:PHE:CD2	2.45	0.51
1:A:1732:ALA:HB1	1:B:1016:LYS:HD3	1.91	0.51
1:A:378:LEU:O	1:A:608:VAL:HG21	2.09	0.51
1:B:417:LEU:HD21	1:B:596:ILE:HG21	1.93	0.51
1:A:1028:MET:CE	1:B:1029:ILE:HD13	2.40	0.51
1:A:1233:VAL:HG22	1:B:1233:VAL:HG22	1.91	0.51
1:A:1394:LEU:CD2	1:B:1394:LEU:HG	2.41	0.51
1:A:1467:ALA:HB2	1:B:1464:ARG:HG2	1.92	0.51
1:A:1862:LYS:HE2	1:B:1861:TYR:CZ	2.46	0.51
1:A:1523:LEU:HD13	1:B:1524:GLU:CG	2.39	0.51
1:A:1910:MET:SD	1:B:1910:MET:HE2	2.51	0.51
1:B:998:GLU:OE1	1:B:1712:ASN:HB3	2.11	0.51
1:A:1263:GLU:O	1:A:1267:VAL:HG23	2.11	0.50
1:A:1640:LEU:HA	1:B:1640:LEU:HD13	1.92	0.50
1:B:1581:GLU:HA	1:B:1584:LYS:HG2	1.93	0.50
1:B:1660:SER:HB2	1:B:1664:ILE:CD1	2.41	0.50
1:A:1154:SER:O	1:A:1158:GLN:HG3	2.12	0.50
1:A:1640:LEU:CD1	1:B:1643:LEU:HD12	2.41	0.50
1:A:1648:LYS:HE2	1:A:1648:LYS:HA	1.93	0.50
1:A:1744:ASN:HB3	1:A:1748:ILE:CD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1622:LEU:HD12	1:B:1619:LEU:HG	1.92	0.50
1:A:1591:VAL:HG12	1:B:1591:VAL:CG1	2.40	0.50
1:A:1741:GLU:HB3	1:B:1741:GLU:HB3	1.94	0.50
1:A:1856:ARG:HH11	1:B:1135:ARG:HD3	1.77	0.50
1:A:1080:LYS:HE2	1:B:1800:THR:CB	2.38	0.50
1:A:1362:LEU:HD11	1:B:1359:ILE:HG23	1.93	0.50
1:A:1648:LYS:HB3	1:A:1652:ARG:CZ	2.42	0.50
1:A:1660:SER:O	1:A:1664:ILE:HG12	2.12	0.50
1:A:1755:ALA:HB1	1:B:1759:ILE:HD11	1.92	0.50
1:B:1270:GLU:OE1	1:B:1274:LYS:NZ	2.44	0.50
1:B:1559:GLU:O	1:B:1562:LEU:HG	2.12	0.50
1:A:967:VAL:CG1	1:B:1687:GLU:HB2	2.41	0.50
1:A:1622:LEU:HD12	1:B:1619:LEU:CD1	2.41	0.50
1:B:478:GLN:NE2	1:B:507:ASP:OD1	2.45	0.50
1:B:947:GLU:O	1:B:950:GLU:HG2	2.11	0.50
1:B:1000:ARG:HH12	1:B:1315:GLU:HB3	1.76	0.50
1:B:1797:MET:HA	1:B:1800:THR:HG22	1.94	0.50
1:A:849:ALA:O	1:A:852:GLU:HG3	2.12	0.50
1:A:1598:LEU:HD11	1:B:1595:GLU:HG2	1.94	0.50
1:B:1234:LYS:HA	1:B:1237:LEU:CD2	2.42	0.50
1:B:1926:LEU:HB3	1:B:1927:PRO:HD2	1.94	0.50
1:A:861:GLN:NE2	1:B:860:LYS:HB3	2.27	0.50
1:A:871:MET:SD	1:B:868:LEU:HG	2.52	0.50
1:A:878:LEU:HD13	1:B:879:MET:HB2	1.93	0.50
1:A:1020:LYS:HD3	1:B:1289:LEU:HG	1.94	0.50
1:A:1573:LEU:HD13	1:B:1572:ASP:HB2	1.93	0.50
1:A:1598:LEU:CD2	1:B:1599:GLU:HG2	2.42	0.50
1:B:1389:LYS:HA	1:B:1389:LYS:HE2	1.94	0.49
1:A:1706:LEU:HB3	1:B:1706:LEU:HD12	1.94	0.49
1:B:1386:VAL:O	1:B:1390:LEU:HG	2.12	0.49
1:A:1069:ALA:O	1:B:1792:VAL:HG11	2.13	0.49
1:A:1380:LEU:HA	1:B:1380:LEU:HD13	1.93	0.49
1:A:1530:LEU:HD12	1:B:1527:LYS:HD3	1.93	0.49
1:A:1633:ARG:CB	1:B:1633:ARG:HB2	2.42	0.49
1:B:956:GLU:HG2	1:B:959:ARG:NH2	2.28	0.49
1:A:983:LEU:HD21	1:B:1701:GLN:OE1	2.12	0.49
1:A:1061:SER:OG	1:B:1781:GLN:NE2	2.45	0.49
1:A:1573:LEU:HD22	1:B:1572:ASP:CB	2.42	0.49
1:A:1734:LEU:HD13	1:B:1731:ILE:HG23	1.95	0.49
1:B:1830:ARG:C	1:B:1833:ALA:HB3	2.38	0.49
1:A:1316:LEU:HA	1:A:1319:GLU:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1738:LEU:HA	1:B:1738:LEU:CD2	2.42	0.49
1:A:1847:VAL:HG12	1:B:1847:VAL:HG12	1.95	0.49
1:A:368:ASN:ND2	1:B:715:GLN:OE1	2.46	0.48
1:A:1506:MET:CE	1:B:1509:LEU:HD11	2.43	0.48
1:A:1736:GLU:HG2	1:B:1016:LYS:O	2.13	0.48
1:A:1748:ILE:HG22	1:B:1748:ILE:HG22	1.94	0.48
1:A:1643:LEU:CD1	1:B:1647:MET:HE2	2.42	0.48
1:B:1657:THR:HA	1:B:1660:SER:OG	2.12	0.48
1:A:882:LYS:HE2	1:B:878:LEU:CD2	2.44	0.48
1:A:1429:LEU:HD11	1:A:1433:ARG:HD3	1.95	0.48
1:A:1653:GLU:HA	1:A:1656:ASP:OD2	2.13	0.48
1:B:837:LEU:O	1:B:842:ARG:HG3	2.13	0.48
1:A:184:THR:HG23	1:A:450:ILE:HG21	1.95	0.48
1:A:1015:SER:HB3	1:B:1015:SER:HA	1.95	0.48
1:A:1559:GLU:HG3	1:B:1558:LEU:HD13	1.94	0.48
2:D:43:THR:O	2:D:47:VAL:HG23	2.13	0.48
1:B:417:LEU:HD21	1:B:596:ILE:CG2	2.42	0.48
1:B:1569:PHE:CZ	1:B:1573:LEU:HD11	2.48	0.48
1:A:964:LEU:CD1	1:B:1683:ILE:HA	2.43	0.48
1:A:1330:LYS:O	1:A:1334:VAL:HG23	2.13	0.48
1:A:1359:ILE:HD11	1:B:1355:LEU:O	2.14	0.48
2:D:85:PHE:O	2:D:89:VAL:HG23	2.14	0.48
1:A:1286:THR:O	1:A:1289:LEU:HG	2.14	0.48
1:A:1843:LYS:O	1:A:1847:VAL:HG23	2.14	0.48
1:B:463:SER:O	1:B:465:GLU:N	2.47	0.48
1:A:1879:LEU:HB2	1:B:1879:LEU:HD21	1.95	0.48
1:B:1551:THR:O	1:B:1555:LYS:HB2	2.14	0.48
1:B:1758:GLN:HB3	1:B:1762:ILE:CD1	2.44	0.48
2:D:50:VAL:HG11	2:D:76:ILE:HG13	1.96	0.48
1:A:1647:MET:CE	1:B:1643:LEU:HD22	2.39	0.48
1:B:1164:LYS:HE2	1:B:1164:LYS:HA	1.96	0.48
1:A:963:GLN:HB2	1:B:962:LEU:HD13	1.96	0.48
1:A:1306:LEU:CD2	1:B:1310:LEU:HD22	2.44	0.48
1:B:1043:ARG:O	1:B:1047:GLU:HG3	2.13	0.48
1:B:1229:LEU:O	1:B:1233:VAL:HG23	2.14	0.48
1:A:941:MET:HB3	1:B:941:MET:HB3	1.95	0.47
1:A:1020:LYS:HB3	1:B:1289:LEU:CD2	2.44	0.47
1:B:1294:SER:O	1:B:1298:LYS:HB2	2.14	0.47
1:B:229:ASN:OD1	1:B:230:ASP:N	2.47	0.47
1:B:1400:ARG:NH2	1:B:1403:GLU:OE1	2.41	0.47
1:A:878:LEU:HD12	1:B:875:GLN:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:GLY:O	1:B:183:ASN:ND2	2.48	0.47
1:A:1025:HIS:CD2	1:B:1022:LYS:HE2	2.50	0.47
1:A:1130:ALA:O	1:A:1134:LYS:HG3	2.14	0.47
1:A:1362:LEU:CD1	1:B:1359:ILE:HG23	2.45	0.47
1:A:1657:THR:HG22	1:A:1661:ARG:HE	1.79	0.47
1:A:857:VAL:HG21	1:B:854:LEU:CD1	2.43	0.47
1:A:1445:LYS:HB3	1:A:1449:LEU:HD12	1.97	0.47
1:B:840:VAL:HG11	3:F:35:GLU:OE1	2.14	0.47
1:A:183:ASN:O	1:A:187:VAL:HG23	2.14	0.47
1:A:272:ARG:NH1	1:A:308:VAL:O	2.44	0.47
1:A:1233:VAL:HA	1:A:1236:LEU:HG	1.97	0.47
1:B:1758:GLN:HB3	1:B:1762:ILE:HD12	1.96	0.47
1:A:964:LEU:CB	1:B:1683:ILE:HG12	2.45	0.47
1:A:1026:GLU:CA	1:A:1029:ILE:HG22	2.43	0.47
1:A:1309:GLN:HB2	1:B:1310:LEU:HD21	1.97	0.47
1:A:1654:LEU:HD12	1:B:1653:GLU:HB3	1.96	0.47
1:A:859:GLU:OE2	1:A:860:LYS:HG2	2.15	0.47
1:A:1233:VAL:O	1:A:1236:LEU:HG	2.14	0.47
1:A:1369:MET:HB3	1:B:1369:MET:HB3	1.97	0.47
1:A:1398:SER:HA	1:A:1401:HIS:NE2	2.30	0.47
1:A:1418:LEU:HB3	1:B:1418:LEU:HD21	1.97	0.47
3:F:48:ILE:N	3:F:80:ILE:O	2.47	0.47
1:A:1039:GLU:HG3	1:B:1036:LEU:HD11	1.97	0.47
1:A:1275:VAL:HG23	1:B:1275:VAL:HG23	1.97	0.47
1:A:1573:LEU:HD13	1:B:1572:ASP:CB	2.44	0.47
1:A:1524:GLU:OE2	1:B:1512:SER:HB2	2.15	0.46
1:A:1754:LYS:NZ	1:B:1032:LEU:HD21	2.29	0.46
1:A:1780:ARG:NH1	1:A:1784:GLU:OE2	2.48	0.46
1:A:1835:LYS:O	1:A:1838:ARG:HG2	2.15	0.46
1:B:913:LEU:HA	1:B:916:ILE:HD12	1.95	0.46
1:A:872:GLU:HG2	1:B:871:MET:CE	2.45	0.46
1:B:1584:LYS:HB2	1:B:1588:VAL:CG2	2.46	0.46
1:A:856:LYS:O	1:A:859:GLU:HG3	2.15	0.46
1:A:986:GLN:OE1	1:B:1702:GLU:HB2	2.15	0.46
1:A:1063:GLN:O	1:A:1066:GLU:HG2	2.15	0.46
1:A:1588:VAL:O	1:A:1592:ARG:HG2	2.15	0.46
1:B:838:LEU:O	1:B:842:ARG:HG3	2.16	0.46
1:B:1388:ARG:O	1:B:1392:LYS:HG2	2.15	0.46
1:B:1421:GLU:O	1:B:1425:LEU:HD23	2.16	0.46
1:B:1711:ALA:O	1:B:1715:GLY:HA3	2.16	0.46
1:A:244:ASP:OD1	1:A:248:TYR:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1461:ALA:O	1:A:1464:ARG:HG3	2.15	0.46
1:A:1573:LEU:HD13	1:B:1572:ASP:OD2	2.15	0.46
1:B:796:ARG:NH1	2:D:150:GLY:OXT	2.47	0.46
1:B:1639:GLN:O	1:B:1643:LEU:HG	2.15	0.46
2:C:23:ASP:O	2:C:25:LYS:N	2.48	0.46
3:F:42:GLN:NE2	3:F:55:ASP:OD2	2.48	0.46
1:A:1506:MET:HE3	1:B:1509:LEU:HD11	1.97	0.46
1:B:221:PHE:O	1:B:422:TYR:OH	2.33	0.46
1:B:1305:ALA:O	1:B:1309:GLN:HG3	2.16	0.46
1:B:1778:ASN:O	1:B:1782:GLN:HG3	2.16	0.46
1:A:923:ARG:CA	1:A:926:GLU:HG2	2.45	0.46
1:A:923:ARG:O	1:A:926:GLU:HG2	2.16	0.46
1:A:1446:PHE:HA	1:A:1450:LEU:CD1	2.38	0.46
1:A:1615:LEU:HD23	1:B:1612:ARG:HD2	1.96	0.46
1:A:1689:LEU:HD13	1:B:1689:LEU:N	2.30	0.46
1:A:1302:ASP:HB3	1:B:1303:PHE:CE1	2.51	0.46
1:A:1022:LYS:NZ	1:A:1026:GLU:OE2	2.43	0.46
1:A:1435:SER:O	1:A:1439:LEU:HG	2.16	0.46
1:A:1682:MET:HA	1:B:1682:MET:HG2	1.98	0.46
1:A:1751:ARG:HG2	1:B:1035:ARG:NH2	2.31	0.46
1:B:578:ASP:OD1	1:B:578:ASP:N	2.49	0.46
1:B:1127:ARG:NH1	1:B:1131:GLU:OE2	2.49	0.46
1:B:1699:ALA:O	1:B:1703:ARG:N	2.40	0.46
1:A:1033:GLU:HB3	1:A:1037:ARG:NH1	2.31	0.46
1:A:1359:ILE:HG23	1:B:1362:LEU:HD11	1.97	0.46
1:B:1296:SER:O	1:B:1300:THR:HG23	2.15	0.46
1:B:1647:MET:HE3	1:B:1647:MET:HB3	1.88	0.46
3:E:120:ASP:OD1	3:E:121:TYR:N	2.48	0.46
3:F:160:ARG:O	3:F:164:HIS:N	2.49	0.46
1:A:1066:GLU:O	1:A:1070:GLN:HG3	2.16	0.46
1:A:1661:ARG:HD3	1:B:1657:THR:HB	1.97	0.46
1:B:1527:LYS:HE2	1:B:1530:LEU:HD12	1.97	0.46
3:F:120:ASP:OD1	3:F:121:TYR:N	2.49	0.46
1:A:885:LEU:HD11	1:B:882:LYS:HG3	1.98	0.45
1:A:923:ARG:HA	1:A:926:GLU:CG	2.46	0.45
1:A:1205:LEU:HD13	1:B:1205:LEU:HD12	1.98	0.45
1:B:76:ASN:OD1	1:B:76:ASN:C	2.58	0.45
1:B:1396:GLY:O	1:B:1400:ARG:HG2	2.16	0.45
1:A:908:ALA:O	1:A:912:GLU:HG2	2.16	0.45
1:A:1118:GLU:OE1	1:B:1192:GLN:NE2	2.49	0.45
1:A:1309:GLN:CB	1:B:1310:LEU:HD21	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1587:LEU:O	1:A:1591:VAL:HG22	2.16	0.45
1:A:1670:GLU:O	1:A:1674:LYS:HG3	2.16	0.45
1:A:1674:LYS:O	1:A:1678:MET:HG2	2.16	0.45
1:B:338:GLY:O	1:B:342:VAL:HG23	2.16	0.45
1:B:426:PHE:O	1:B:430:VAL:HG23	2.16	0.45
1:A:1271:LEU:HD12	1:B:1268:ARG:HG3	1.97	0.45
1:A:1359:ILE:HG13	1:B:1359:ILE:CG1	2.45	0.45
1:A:1559:GLU:CG	1:B:1558:LEU:HD13	2.46	0.45
1:A:1675:LEU:HD22	1:B:1674:LYS:CB	2.46	0.45
1:A:1748:ILE:CG2	1:B:1748:ILE:HG22	2.46	0.45
1:B:1393:ASP:O	1:B:1397:LEU:HG	2.17	0.45
1:A:993:GLU:CB	1:B:994:LYS:HD2	2.47	0.45
1:A:1390:LEU:O	1:A:1394:LEU:N	2.44	0.45
1:A:1469:ALA:O	1:A:1473:GLU:HG2	2.16	0.45
1:B:840:VAL:H	3:F:39:MET:HE2	1.82	0.45
1:B:1020:LYS:O	1:B:1024:LYS:HG3	2.16	0.45
1:B:1633:ARG:HH11	1:B:1637:ILE:HD12	1.81	0.45
1:B:1723:GLU:O	1:B:1727:LEU:HG	2.17	0.45
2:D:124:VAL:HG12	2:D:128:VAL:HG23	1.98	0.45
1:A:210:GLN:NE2	1:A:329:MET:O	2.47	0.45
1:A:979:GLU:HA	1:B:1698:GLN:HG2	1.99	0.45
1:A:1611:ALA:O	1:A:1615:LEU:HD23	2.16	0.45
1:B:1572:ASP:O	1:B:1576:ARG:HG2	2.16	0.45
1:B:1659:ALA:O	1:B:1663:GLU:HG2	2.16	0.45
1:A:1317:LEU:CD1	1:B:1316:LEU:HD23	2.35	0.45
3:F:26:ASP:OD1	3:F:27:GLN:N	2.48	0.45
1:B:892:GLU:HA	1:B:895:LEU:HD12	1.98	0.45
1:B:1588:VAL:CA	1:B:1591:VAL:HG12	2.45	0.45
2:C:18:PHE:O	2:C:20:ARG:N	2.46	0.45
1:A:1158:GLN:OE1	1:A:1162:ARG:NH2	2.47	0.45
1:A:1331:LEU:HD11	1:B:1330:LYS:HB3	1.99	0.45
1:A:1571:ARG:NH1	1:A:1579:GLN:HE22	2.14	0.45
1:A:1050:ARG:HG3	1:B:1053:LEU:HD12	1.97	0.45
1:A:1058:THR:HA	1:B:1781:GLN:NE2	2.31	0.45
1:A:1586:GLN:O	1:A:1590:GLN:N	2.44	0.45
1:A:1826:GLU:OE1	1:B:1830:ARG:HD2	2.16	0.45
1:B:1515:ASP:OD2	1:B:1519:SER:OG	2.35	0.45
1:A:1310:LEU:HB2	1:B:1310:LEU:CD1	2.47	0.45
1:A:1401:HIS:CE1	1:A:1402:GLU:HG3	2.52	0.45
1:B:67:VAL:HG12	1:B:71:ASP:HB2	1.99	0.45
1:B:940:LYS:HE3	1:B:1662:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1451:ALA:O	1:B:1455:THR:HG23	2.17	0.45
1:A:1040:GLU:HG2	1:B:1039:GLU:HG3	1.99	0.44
1:A:1457:SER:HA	1:B:1457:SER:HB2	1.99	0.44
1:A:1835:LYS:O	1:A:1839:ARG:HG3	2.16	0.44
1:A:1036:LEU:HA	1:B:1036:LEU:CD1	2.47	0.44
1:B:1780:ARG:NH1	1:B:1784:GLU:OE2	2.50	0.44
3:E:119:GLU:OE2	3:E:123:ARG:NH1	2.49	0.44
1:A:372:GLN:HG2	1:A:382:VAL:HG11	1.98	0.44
1:A:843:GLN:HB3	1:A:847:MET:CG	2.46	0.44
1:A:854:LEU:HD12	1:A:858:ARG:HG3	1.98	0.44
1:A:1289:LEU:N	1:B:1289:LEU:HD13	2.32	0.44
1:A:1362:LEU:HD22	1:B:1363:HIS:HA	1.99	0.44
1:A:1363:HIS:HA	1:B:1362:LEU:HD22	1.99	0.44
1:A:1065:ALA:CB	1:B:1785:ARG:HG2	2.44	0.44
1:A:1285:VAL:HG12	1:B:1285:VAL:HG12	2.00	0.44
1:B:917:CYS:O	1:B:921:GLU:HG2	2.17	0.44
1:A:1008:LEU:CA	1:B:1008:LEU:HD13	2.46	0.44
1:A:1289:LEU:HB3	1:B:1289:LEU:HA	2.00	0.44
1:A:1445:LYS:HB3	1:A:1449:LEU:HG	1.98	0.44
1:B:1310:LEU:HA	1:B:1313:THR:OG1	2.17	0.44
1:B:1428:ASP:O	1:B:1432:GLN:HG2	2.17	0.44
1:A:913:LEU:HD22	1:B:914:GLU:CG	2.48	0.44
1:A:1386:VAL:CG1	1:B:1387:LYS:HE3	2.47	0.44
1:B:843:GLN:O	1:B:847:MET:N	2.39	0.44
1:B:1148:LEU:O	1:B:1152:LEU:HG	2.17	0.44
1:B:1459:LYS:O	1:B:1463:GLU:HG2	2.17	0.44
1:A:495:GLU:OE2	1:A:759:SER:OG	2.25	0.44
1:A:617:ARG:NH1	1:A:642:MET:SD	2.91	0.44
1:B:1294:SER:HA	1:B:1297:SER:OG	2.17	0.44
1:B:1344:GLN:O	1:B:1348:GLU:HG2	2.18	0.44
2:D:28:TYR:OH	2:D:47:VAL:O	2.36	0.44
1:A:843:GLN:O	1:A:847:MET:HB2	2.17	0.44
1:A:1296:SER:HA	1:A:1299:LEU:HD12	1.99	0.44
1:B:901:GLU:O	1:B:905:ARG:HG3	2.18	0.44
1:B:1545:GLU:OE1	1:B:1548:LEU:HD23	2.18	0.44
1:B:1588:VAL:HA	1:B:1591:VAL:CG1	2.45	0.44
1:A:1234:LYS:O	1:A:1238:GLN:HB2	2.18	0.44
1:A:1386:VAL:O	1:A:1390:LEU:HG	2.18	0.44
1:A:1569:PHE:CE1	1:A:1573:LEU:HD12	2.53	0.44
1:B:61:ASN:ND2	1:B:61:ASN:O	2.50	0.44
1:B:1414:THR:O	1:B:1417:ARG:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:ASP:OD1	1:A:989:LYS:HE2	2.18	0.43
1:A:1066:GLU:CB	1:B:1788:LYS:HD3	2.43	0.43
1:A:1317:LEU:HD23	1:B:1320:GLU:HG3	1.98	0.43
1:A:1550:ALA:O	1:A:1554:ALA:N	2.43	0.43
1:A:1595:GLU:O	1:A:1599:GLU:HB2	2.17	0.43
1:A:1663:GLU:O	1:A:1667:GLN:HG3	2.18	0.43
1:B:796:ARG:NE	2:D:37:ALA:O	2.48	0.43
1:B:1476:THR:HG21	2:C:68:GLN:NE2	2.32	0.43
1:A:1321:ASN:OD1	1:B:989:LYS:HG2	2.18	0.43
1:A:1337:GLU:O	1:A:1341:PHE:HB2	2.18	0.43
1:A:1599:GLU:OE1	1:A:1603:LYS:NZ	2.27	0.43
1:B:932:GLN:HA	1:B:935:GLN:CG	2.48	0.43
2:D:109:ARG:NH2	2:D:125:GLU:OE1	2.47	0.43
1:A:426:PHE:O	1:A:430:VAL:HG23	2.19	0.43
1:A:1011:GLU:CB	1:B:1011:GLU:HG3	2.48	0.43
1:A:1557:ARG:O	1:A:1561:ASN:ND2	2.31	0.43
1:A:1657:THR:HB	1:A:1661:ARG:HD2	2.00	0.43
3:E:81:ASN:O	3:E:85:PHE:N	2.40	0.43
1:A:3:GLN:NE2	1:A:7:ASP:OD2	2.49	0.43
1:A:1612:ARG:O	1:A:1616:GLU:HG3	2.18	0.43
1:A:1657:THR:CG2	1:A:1661:ARG:HE	2.31	0.43
1:B:1432:GLN:HA	1:B:1435:SER:HG	1.83	0.43
1:A:1558:LEU:HD12	1:B:1555:LYS:HD3	2.00	0.43
1:B:1568:GLN:OE1	3:E:104:ASN:ND2	2.52	0.43
1:B:1752:LEU:HG	1:B:1756:ASN:ND2	2.33	0.43
1:A:968:THR:HG22	1:B:1686:GLN:HB3	2.01	0.43
1:A:1297:SER:O	1:A:1300:THR:OG1	2.34	0.43
1:A:1514:ASP:O	1:A:1518:LYS:HB2	2.18	0.43
1:A:1528:ARG:NH2	1:B:1509:LEU:HD21	2.34	0.43
1:A:1745:THR:O	1:A:1749:ASN:HB2	2.18	0.43
1:A:998:GLU:HG3	1:B:997:LEU:HD11	2.01	0.43
1:A:1002:ALA:O	1:A:1006:THR:HG23	2.19	0.43
1:A:1331:LEU:O	1:A:1335:GLU:HG3	2.19	0.43
1:A:1527:LYS:O	1:A:1531:GLU:HG2	2.18	0.43
1:A:1660:SER:O	1:A:1664:ILE:HG23	2.19	0.43
1:B:1525:LYS:O	1:B:1528:ARG:HG2	2.19	0.43
1:B:1759:ILE:O	1:B:1763:ASN:HB2	2.19	0.43
1:B:1875:LEU:O	1:B:1879:LEU:HD23	2.18	0.43
1:A:923:ARG:O	1:A:927:GLU:HG2	2.18	0.43
1:A:962:LEU:HD22	1:B:963:GLN:HG2	2.01	0.43
1:A:1413:LYS:HA	1:A:1416:THR:HG1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1675:LEU:HD22	1:B:1674:LYS:HB3	2.01	0.43
1:A:1900:LEU:O	1:A:1904:THR:HG23	2.19	0.43
1:B:1013:GLU:OE2	1:B:1730:ARG:NH1	2.52	0.43
1:B:1142:GLU:O	1:B:1146:THR:HG23	2.18	0.43
1:A:443:GLN:CD	1:B:1592:ARG:HE	2.27	0.43
1:A:564:ASP:OD1	1:A:565:LYS:N	2.52	0.43
1:B:6:ALA:O	1:B:11:TYR:N	2.52	0.43
1:B:131:SER:HB2	1:B:134:ILE:HD11	2.00	0.43
1:B:934:LEU:O	1:B:937:GLU:HG2	2.19	0.43
1:B:1527:LYS:HE2	1:B:1527:LYS:HA	2.01	0.43
1:A:1026:GLU:HA	1:A:1029:ILE:CG2	2.45	0.43
1:A:1619:LEU:HD22	1:B:1615:LEU:CD2	2.49	0.43
1:A:1825:ASN:HA	1:A:1828:LYS:CE	2.47	0.43
1:B:1472:ARG:O	1:B:1476:THR:HG23	2.18	0.43
1:A:280:LEU:HD13	1:A:340:LEU:HD22	2.01	0.42
1:A:890:GLN:O	1:A:894:GLU:HG2	2.18	0.42
1:A:903:ARG:HG3	1:B:906:LEU:HD12	2.01	0.42
1:A:930:ARG:HH21	1:A:934:LEU:HD11	1.84	0.42
1:A:1762:ILE:HG23	1:B:1766:LEU:HD22	2.01	0.42
1:B:342:VAL:O	1:B:346:VAL:HG23	2.18	0.42
1:A:492:TYR:OH	1:A:708:PHE:N	2.49	0.42
1:A:1187:ILE:HD13	1:B:1186:GLN:OE1	2.19	0.42
1:A:1739:GLU:HB2	1:B:1020:LYS:HG2	2.01	0.42
1:B:737:LYS:O	1:B:741:VAL:HG23	2.18	0.42
1:B:1404:LYS:O	1:B:1408:TYR:N	2.41	0.42
1:B:1597:GLU:HG2	1:B:1598:LEU:N	2.33	0.42
1:A:1330:LYS:CB	1:B:1331:LEU:HD11	2.50	0.42
1:A:1788:LYS:HE2	1:A:1788:LYS:HA	2.01	0.42
1:A:539:ASP:O	1:A:543:VAL:HG23	2.19	0.42
1:A:1008:LEU:HD13	1:B:1008:LEU:HA	2.01	0.42
1:A:1275:VAL:HG23	1:B:1275:VAL:CG2	2.49	0.42
1:A:1552:GLU:O	1:A:1555:LYS:HG2	2.19	0.42
1:A:1665:LEU:HD13	1:B:1664:ILE:CD1	2.47	0.42
1:B:995:LYS:HG2	1:B:1712:ASN:CG	2.44	0.42
1:B:1002:ALA:HA	1:B:1005:THR:OG1	2.19	0.42
1:B:1233:VAL:O	1:B:1237:LEU:HD23	2.20	0.42
1:B:1828:LYS:O	1:B:1831:GLN:N	2.52	0.42
1:A:440:THR:OG1	1:A:441:LYS:N	2.49	0.42
1:A:1296:SER:HB3	1:B:1296:SER:HB3	2.00	0.42
1:A:1710:ILE:CG2	1:B:1706:LEU:HD13	2.50	0.42
1:B:838:LEU:HB3	1:B:841:SER:HB3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1588:VAL:O	1:B:1592:ARG:HB2	2.20	0.42
2:D:75:THR:O	2:D:79:ASN:ND2	2.52	0.42
1:A:1006:THR:HA	1:B:1301:LYS:HG3	2.01	0.42
1:A:1037:ARG:O	1:A:1041:LYS:HG2	2.19	0.42
1:A:1113:ILE:CD1	1:B:1109:LEU:HG	2.49	0.42
1:A:1739:GLU:OE1	1:B:1024:LYS:NZ	2.42	0.42
1:B:868:LEU:O	1:B:872:GLU:HG3	2.18	0.42
1:B:1557:ARG:HA	1:B:1560:VAL:HG12	2.00	0.42
2:C:133:ASP:OD1	2:C:137:CYS:N	2.53	0.42
3:E:34:LYS:O	3:E:38:ASN:ND2	2.53	0.42
1:A:1233:VAL:HA	1:A:1236:LEU:CG	2.50	0.42
1:A:1302:ASP:O	1:A:1306:LEU:HG	2.20	0.42
1:A:1661:ARG:CA	1:A:1664:ILE:HG12	2.45	0.42
1:A:234:ARG:NH1	1:A:457:GLU:OE1	2.52	0.42
1:A:1285:VAL:CG1	1:B:1285:VAL:HG12	2.49	0.42
1:A:1626:ILE:HD12	1:B:1622:LEU:HD22	2.02	0.42
1:B:184:THR:HG23	1:B:450:ILE:HG21	2.00	0.42
2:D:30:GLN:O	2:D:34:VAL:HG23	2.20	0.42
3:E:63:ASN:N	3:E:64:PRO:CD	2.82	0.42
1:B:477:GLN:NE2	1:B:695:ASN:O	2.53	0.42
1:B:1429:LEU:HD13	1:B:1433:ARG:NH2	2.34	0.42
1:B:1706:LEU:O	1:B:1710:ILE:N	2.49	0.42
1:A:86:MET:SD	1:A:97:VAL:HG13	2.60	0.42
1:A:1032:LEU:HD13	1:B:1032:LEU:HB2	2.02	0.42
1:A:1232:GLU:O	1:A:1236:LEU:HD23	2.19	0.42
1:A:1320:GLU:HB3	1:A:1324:LYS:NZ	2.35	0.42
1:A:1622:LEU:CD1	1:B:1619:LEU:HG	2.50	0.42
1:A:1680:ALA:O	1:A:1684:GLN:HG2	2.20	0.42
1:B:1595:GLU:HA	1:B:1599:GLU:HG2	2.02	0.42
1:A:965:GLU:HA	1:A:968:THR:OG1	2.20	0.41
1:A:990:LEU:CD2	1:B:1709:GLU:HG3	2.49	0.41
1:B:190:TYR:O	1:B:194:VAL:HG23	2.20	0.41
1:A:215:ASN:HB2	1:A:216:PRO:HD3	2.01	0.41
1:A:234:ARG:NH1	5:A:2002:PO4:O3	2.53	0.41
1:A:854:LEU:CD1	1:A:858:ARG:HG3	2.50	0.41
1:A:1857:ASN:O	1:A:1860:GLN:HG2	2.20	0.41
1:B:1673:LYS:HA	1:B:1676:LYS:HE3	2.02	0.41
1:A:1394:LEU:CD1	1:B:1390:LEU:HD22	2.50	0.41
1:A:1859:GLU:HB3	1:B:1139:GLU:OE1	2.20	0.41
1:B:1641:ARG:HA	1:B:1644:GLN:HG2	2.02	0.41
1:A:903:ARG:CG	1:B:906:LEU:HD12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1272:ALA:HB2	1:B:1271:LEU:CD1	2.50	0.41
1:A:246:ASN:ND2	2:C:132:GLU:OE2	2.54	0.41
1:A:903:ARG:HD2	1:B:902:LEU:CB	2.50	0.41
1:A:982:ILE:HG23	1:B:1702:GLU:OE1	2.20	0.41
1:A:1207:GLN:O	1:A:1211:VAL:HG23	2.21	0.41
1:A:1626:ILE:CD1	1:B:1622:LEU:HD22	2.51	0.41
1:A:1658:ARG:O	1:A:1662:GLU:HB2	2.19	0.41
1:B:1571:ARG:HH12	3:E:113:ALA:CB	2.34	0.41
1:A:975:LYS:O	1:B:1698:GLN:NE2	2.53	0.41
1:A:1489:MET:HG2	1:A:1492:LYS:HE3	2.03	0.41
1:A:1664:ILE:HG13	1:A:1665:LEU:N	2.35	0.41
1:A:1752:LEU:HD21	1:B:1752:LEU:HA	2.03	0.41
1:A:1757:LEU:O	1:A:1761:GLN:NE2	2.53	0.41
1:B:1537:MET:N	1:B:1537:MET:HE2	2.36	0.41
1:B:1660:SER:O	1:B:1664:ILE:N	2.37	0.41
1:B:1661:ARG:O	1:B:1665:LEU:HB2	2.20	0.41
1:A:179:GLY:O	1:A:183:ASN:ND2	2.52	0.41
1:A:1121:GLU:OE1	1:B:1191:ARG:NH1	2.50	0.41
1:A:1622:LEU:O	1:A:1626:ILE:HG13	2.21	0.41
1:B:1218:ALA:O	1:B:1222:LEU:HD23	2.21	0.41
1:B:1773:ALA:O	1:B:1777:GLU:HG2	2.21	0.41
1:A:1008:LEU:HD13	1:B:1007:ASN:C	2.46	0.41
1:A:1415:LYS:HG2	1:A:1419:GLN:OE1	2.21	0.41
1:B:898:GLU:O	1:B:901:GLU:HG2	2.20	0.41
1:B:1350:GLU:HA	1:B:1353:HIS:CD2	2.55	0.41
1:B:1584:LYS:HB2	1:B:1588:VAL:HG21	2.01	0.41
1:A:952:LEU:O	1:A:956:GLU:HB2	2.21	0.41
1:A:1001:ILE:HD13	1:B:1001:ILE:CG1	2.51	0.41
1:A:1366:VAL:HG23	1:B:1366:VAL:CG2	2.49	0.41
1:A:1368:ASP:OD1	1:A:1371:LYS:HE3	2.21	0.41
1:A:1390:LEU:HD22	1:B:1394:LEU:HD12	2.03	0.41
1:A:1445:LYS:HD3	1:A:1449:LEU:HD11	2.02	0.41
1:A:1699:ALA:HB1	1:B:1699:ALA:HB2	2.03	0.41
1:B:131:SER:CB	1:B:134:ILE:HD11	2.50	0.41
1:B:923:ARG:HH21	1:B:926:GLU:HG3	1.86	0.41
1:B:1385:GLU:O	1:B:1389:LYS:HG2	2.20	0.41
1:B:1589:ARG:O	1:B:1593:GLU:HG2	2.21	0.41
1:B:1625:HIS:HA	1:B:1628:SER:OG	2.21	0.41
1:B:1793:LYS:O	1:B:1797:MET:HG2	2.21	0.41
1:A:857:VAL:HG12	1:B:857:VAL:CG1	2.43	0.41
1:A:861:GLN:HA	1:B:861:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:994:LYS:HE2	1:A:998:GLU:OE2	2.21	0.41
1:A:998:GLU:O	1:A:1001:ILE:HG22	2.21	0.41
1:A:1000:ARG:HB3	1:A:1004:PHE:CE2	2.56	0.41
1:A:1647:MET:HG2	1:A:1651:MET:SD	2.60	0.41
1:A:1661:ARG:HH12	1:B:1658:ARG:HA	1.85	0.41
1:B:837:LEU:HD23	1:B:838:LEU:N	2.35	0.41
1:A:1009:THR:OG1	1:B:1301:LYS:HG3	2.20	0.40
1:A:1265:GLU:O	1:A:1269:THR:HG23	2.22	0.40
1:A:1457:SER:HB3	1:B:1457:SER:HB3	2.03	0.40
1:A:1576:ARG:NE	1:A:1579:GLN:OE1	2.39	0.40
1:A:1743:GLY:O	1:A:1747:LEU:HG	2.21	0.40
1:A:1750:ASP:HB3	1:B:1028:MET:HE2	2.03	0.40
1:B:1232:GLU:O	1:B:1236:LEU:HD13	2.21	0.40
1:A:1077:GLN:HA	1:A:1080:LYS:HD2	2.03	0.40
1:B:509:GLN:N	1:B:510:PRO:CD	2.84	0.40
1:B:1571:ARG:HH12	3:E:113:ALA:HB2	1.86	0.40
1:B:1628:SER:O	1:B:1632:ASN:ND2	2.51	0.40
1:B:1757:LEU:O	1:B:1761:GLN:N	2.50	0.40
1:A:342:VAL:O	1:A:346:VAL:HG23	2.20	0.40
1:A:1395:GLU:HG3	1:A:1396:GLY:N	2.35	0.40
1:A:1527:LYS:HG3	1:B:1527:LYS:NZ	2.37	0.40
1:B:226:THR:N	1:B:229:ASN:O	2.49	0.40
1:B:945:ILE:O	1:B:949:GLU:HG2	2.21	0.40
1:B:1330:LYS:O	1:B:1334:VAL:HG23	2.21	0.40
1:B:1362:LEU:O	1:B:1366:VAL:HG23	2.22	0.40
1:A:1029:ILE:HD11	1:B:1028:MET:HB3	2.03	0.40
1:A:1586:GLN:HB3	1:A:1590:GLN:OE1	2.22	0.40
1:A:1639:GLN:O	1:A:1643:LEU:HD23	2.21	0.40
1:B:997:LEU:HD23	1:B:1312:ASP:OD2	2.21	0.40
1:B:1476:THR:HG21	2:C:68:GLN:HE22	1.87	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	1943/1960 (99%)	1865 (96%)	69 (4%)	9 (0%)	25	64
1	B	1939/1960 (99%)	1850 (95%)	81 (4%)	8 (0%)	30	68
2	C	148/151 (98%)	134 (90%)	11 (7%)	3 (2%)	6	31
2	D	148/151 (98%)	134 (90%)	12 (8%)	2 (1%)	9	40
3	E	150/172 (87%)	130 (87%)	19 (13%)	1 (1%)	19	57
3	F	156/172 (91%)	133 (85%)	18 (12%)	5 (3%)	3	21
All	All	4484/4566 (98%)	4246 (95%)	210 (5%)	28 (1%)	24	60

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	276	ILE
2	C	20	ARG
1	B	838	LEU
3	E	154	ASN
3	F	16	ARG
1	A	535	PRO
1	B	464	PHE
2	D	118	LYS
3	F	146	PRO
1	A	258	LEU
1	A	731	LYS
1	B	315	ASP
2	C	118	LYS
1	A	30	LYS
1	A	40	GLY
1	B	283	GLY
1	B	378	LEU
1	B	1947	VAL
3	F	24	MET
2	C	24	GLY
3	F	79	PRO
1	A	518	PRO
3	F	14	PRO
1	A	496	GLY
1	A	620	GLY
1	A	1517	GLY
1	B	312	GLY

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Mol	Chain	Res	Type
2	D	128	VAL

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	1708/1716 (100%)	1707 (100%)	1 (0%)	92	95
1	B	1706/1716 (99%)	1702 (100%)	4 (0%)	92	94
2	C	129/130 (99%)	127 (98%)	2 (2%)	58	73
2	D	129/130 (99%)	129 (100%)	0	100	100
3	E	132/151 (87%)	131 (99%)	1 (1%)	79	85
3	F	138/151 (91%)	138 (100%)	0	100	100
All	All	3942/3994 (99%)	3934 (100%)	8 (0%)	91	94

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1727	LEU
1	B	76	ASN
1	B	300	TYR
1	B	619	ILE
1	B	683	LEU
2	C	13	GLU
2	C	70	LEU
3	E	85	PHE

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

Mol	Chain	Res	Type
1	A	99	HIS
1	A	100	ASN
1	A	246	ASN
1	A	493	GLN

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Mol	Chain	Res	Type
1	A	665	ASN
1	A	667	ASN
1	A	676	HIS
1	A	710	ASN
1	A	875	GLN
1	A	886	GLN
1	A	918	HIS
1	A	942	GLN
1	A	951	GLN
1	A	1432	GLN
1	A	1491	GLN
1	A	1501	GLN
1	A	1700	GLN
1	B	19	ASN
1	B	100	ASN
1	B	126	ASN
1	B	665	ASN
1	B	875	GLN
1	B	886	GLN
1	B	918	HIS
1	B	942	GLN
1	B	943	GLN
1	B	980	GLN
1	B	1042	GLN
1	B	1311	GLN
1	B	1353	HIS
1	B	1365	GLN
1	B	1431	HIS
1	B	1501	GLN
1	B	1521	HIS
1	B	1563	GLN
1	B	1686	GLN
1	B	1698	GLN
1	B	1758	GLN
1	B	1781	GLN
1	B	1795	GLN
1	B	1864	GLN
2	C	7	GLN
2	C	68	GLN
2	D	131	HIS
3	E	38	ASN
3	E	104	ASN

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Mol	Chain	Res	Type
3	F	31	GLN
3	F	38	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are 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	ADP	B	2001	-	24,29,29	0.96	1 (4%)	29,45,45	1.53	5 (17%)
5	PO4	A	2002	6	4,4,4	1.52	1 (25%)	6,6,6	0.45	0
5	PO4	B	2002	6	4,4,4	1.50	1 (25%)	6,6,6	0.46	0
4	ADP	A	2001	6	24,29,29	0.96	1 (4%)	29,45,45	1.52	4 (13%)

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	ADP	B	2001	-	-	2/12/32/32	0/3/3/3
4	ADP	A	2001	6	-	2/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2002	PO4	P-O1	2.61	1.57	1.50
5	B	2002	PO4	P-O1	2.59	1.56	1.50
4	B	2001	ADP	C5-C4	2.41	1.47	1.40
4	A	2001	ADP	C5-C4	2.40	1.47	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001	ADP	PA-O3A-PB	-3.76	119.91	132.83
4	A	2001	ADP	PA-O3A-PB	-3.69	120.15	132.83
4	B	2001	ADP	N3-C2-N1	-3.66	122.96	128.68
4	A	2001	ADP	N3-C2-N1	-3.65	122.97	128.68
4	B	2001	ADP	C3'-C2'-C1'	3.30	105.95	100.98
4	A	2001	ADP	C3'-C2'-C1'	3.27	105.91	100.98
4	A	2001	ADP	C4-C5-N7	-2.82	106.47	109.40
4	B	2001	ADP	C4-C5-N7	-2.79	106.49	109.40
4	B	2001	ADP	C2-N1-C6	2.03	122.22	118.75

There are no chirality outliers.

All (4) torsion outliers are listed below:

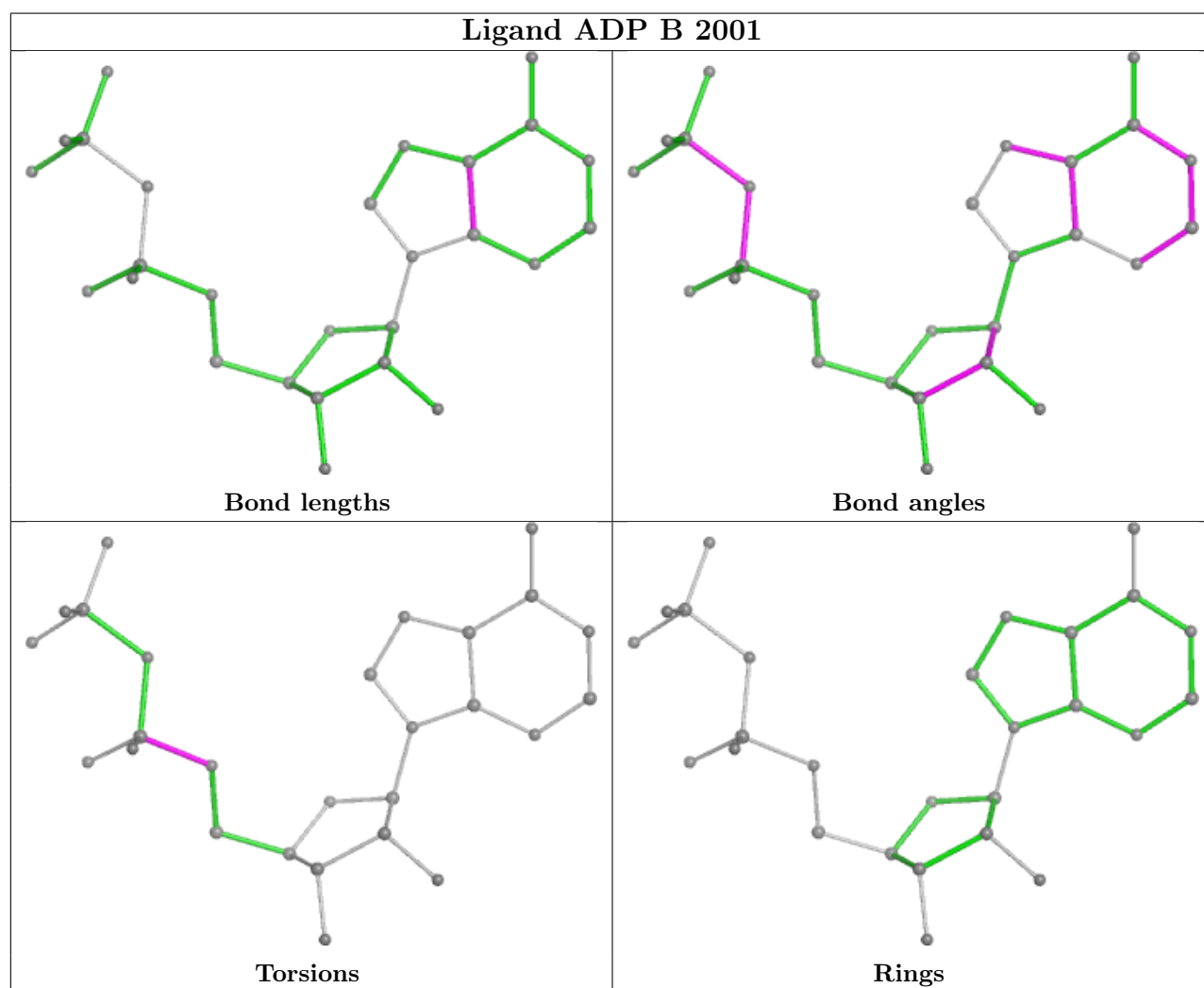
Mol	Chain	Res	Type	Atoms
4	A	2001	ADP	C5'-O5'-PA-O1A
4	A	2001	ADP	C5'-O5'-PA-O3A
4	B	2001	ADP	C5'-O5'-PA-O3A
4	B	2001	ADP	C5'-O5'-PA-O1A

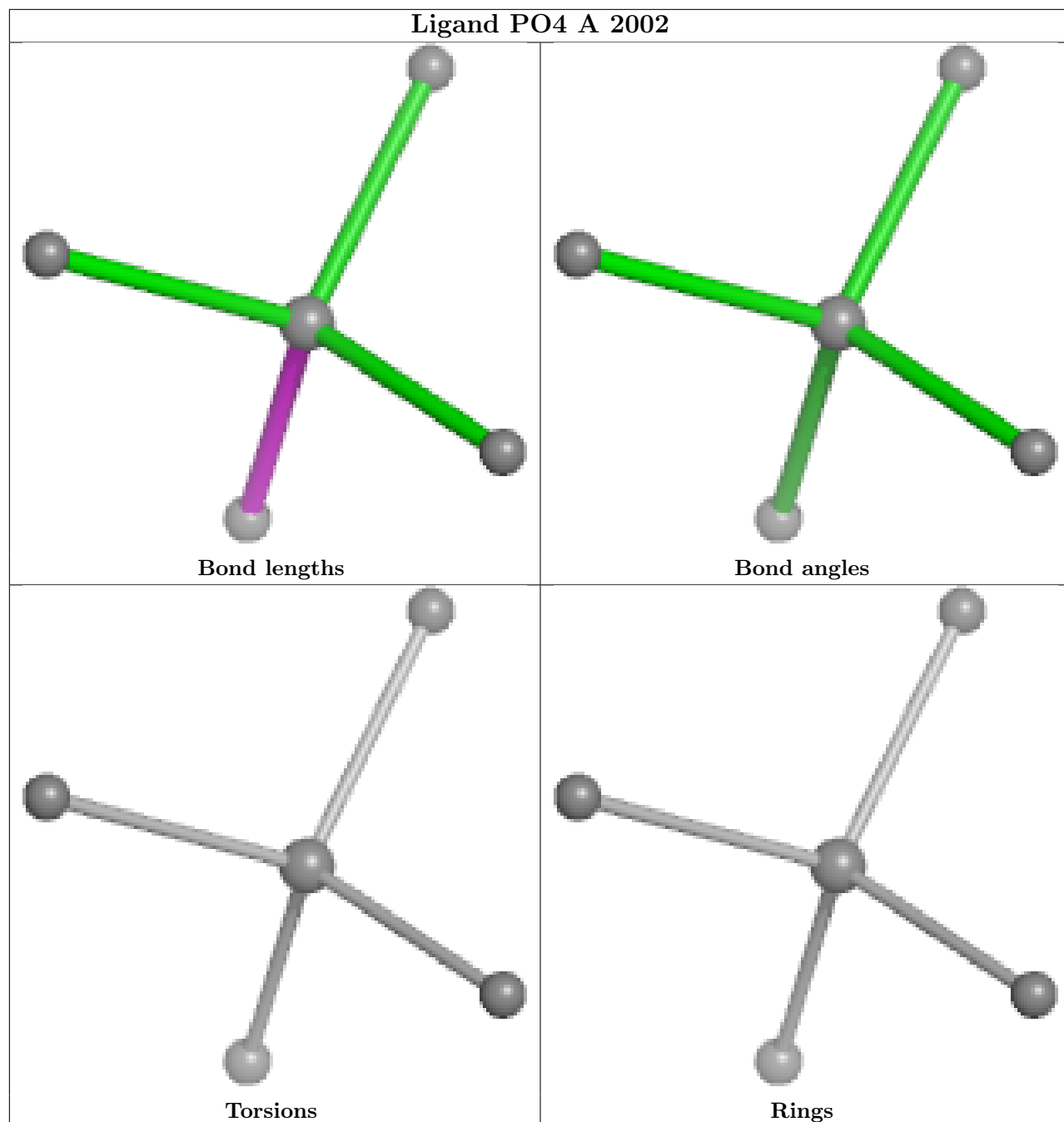
There are no ring outliers.

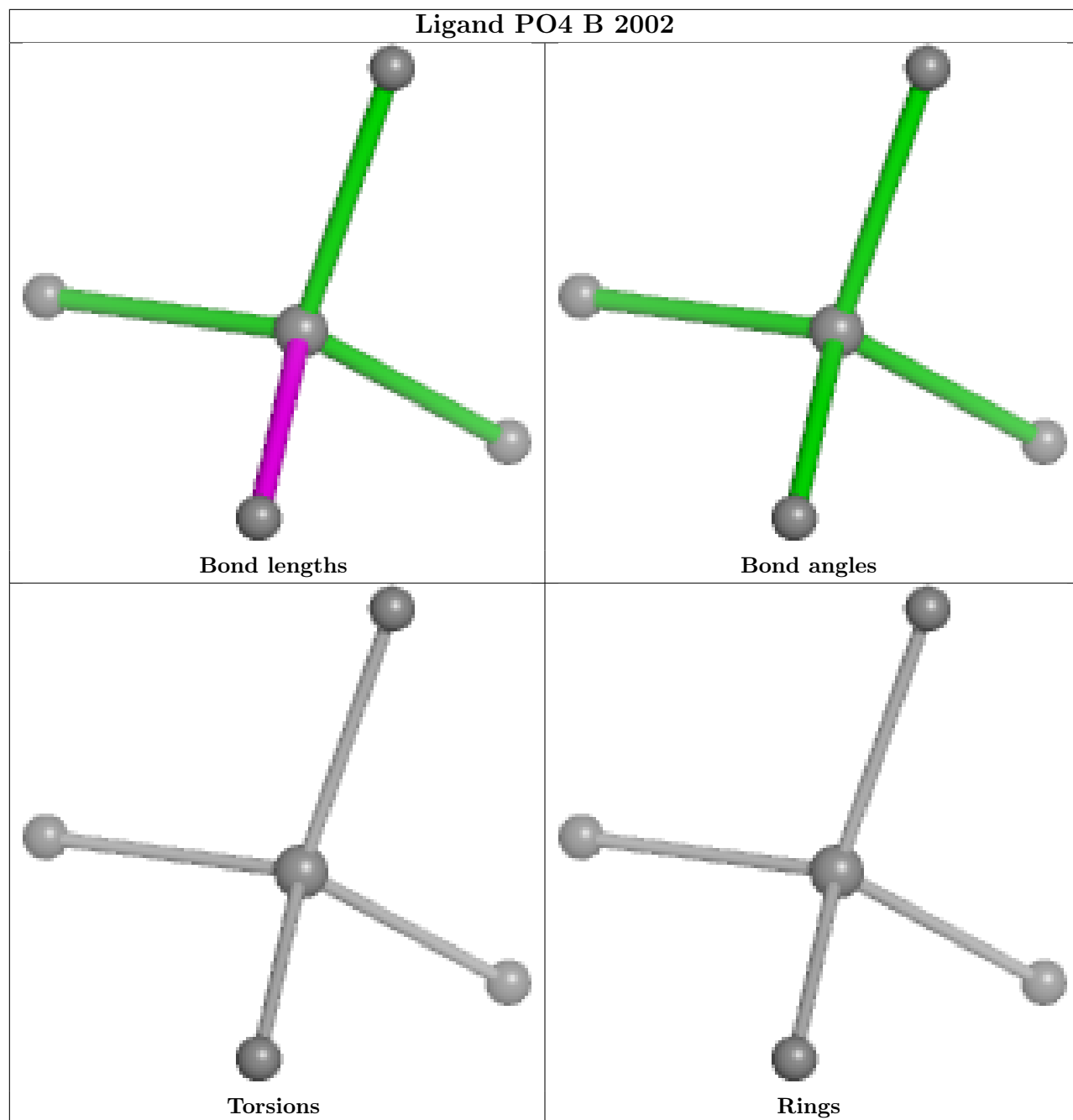
4 monomers are involved in 6 short contacts:

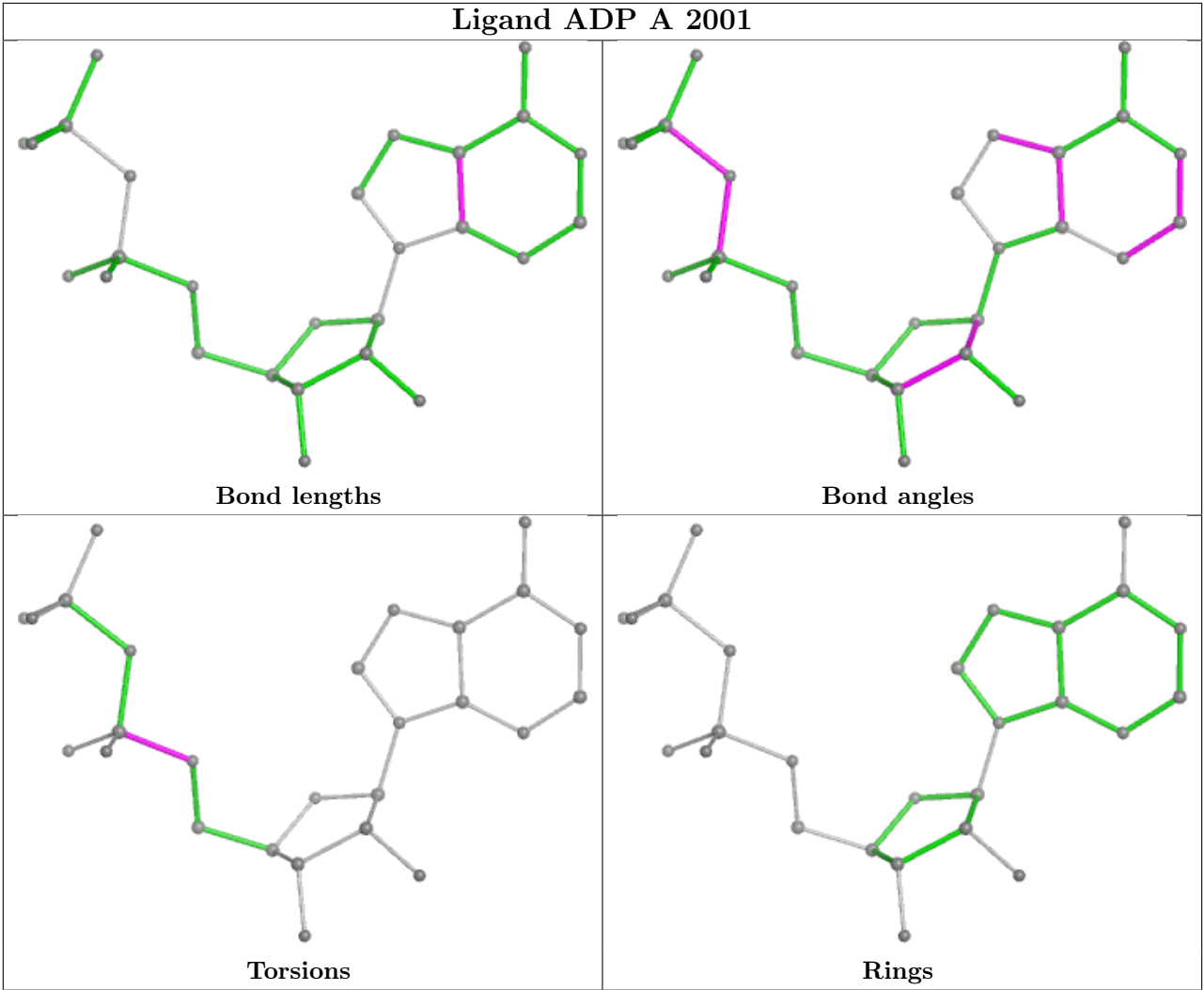
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2001	ADP	1	0
5	A	2002	PO4	1	0
5	B	2002	PO4	1	0
4	A	2001	ADP	3	0

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	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1830:ARG	C	1831:GLN	N	3.54

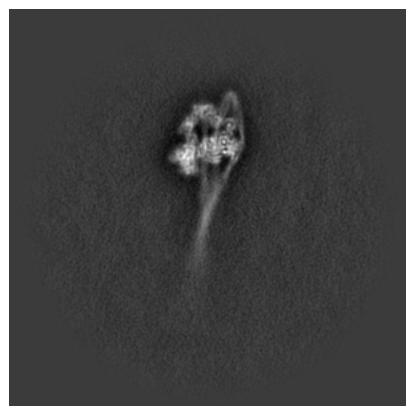
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55382. These allow visual inspection of the internal detail of the map and identification of artifacts.

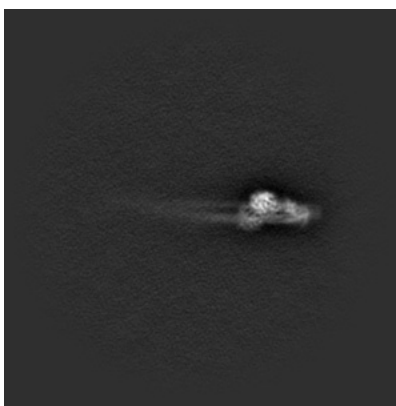
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

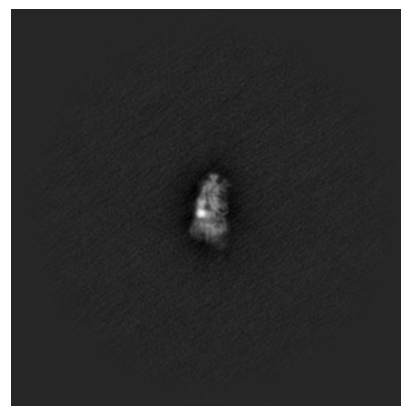
6.1.1 Primary map



X

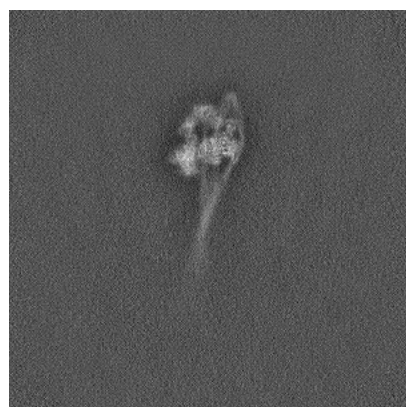


Y

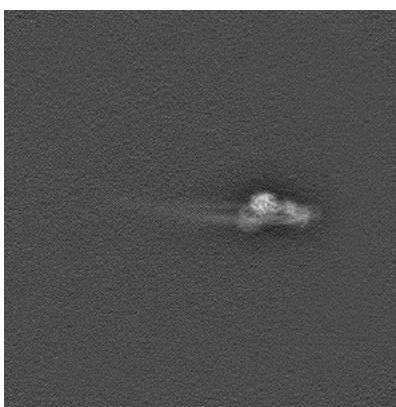


Z

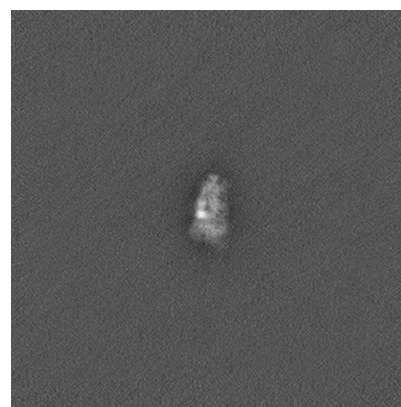
6.1.2 Raw map



X



Y

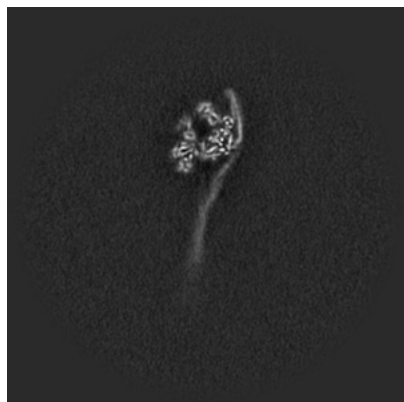


Z

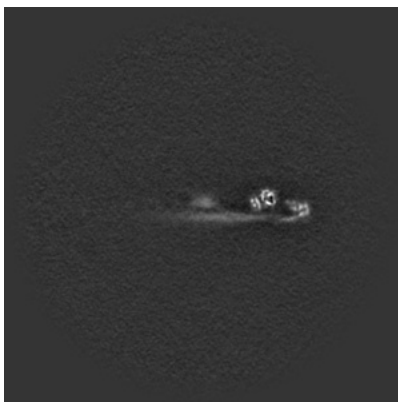
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

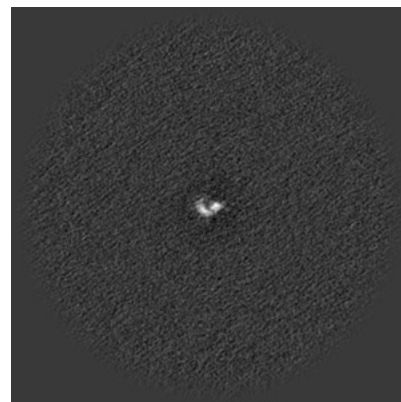
6.2.1 Primary map



X Index: 256



Y Index: 256

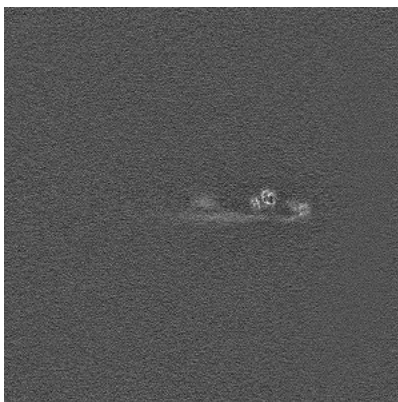


Z Index: 256

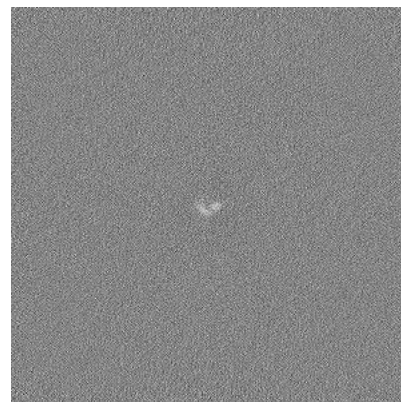
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

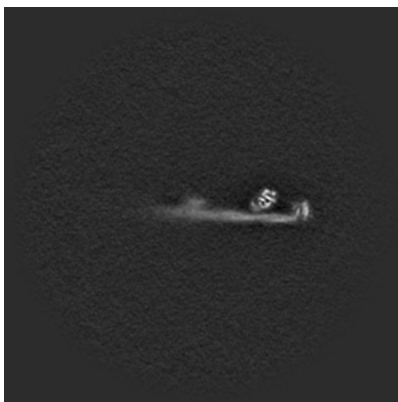
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

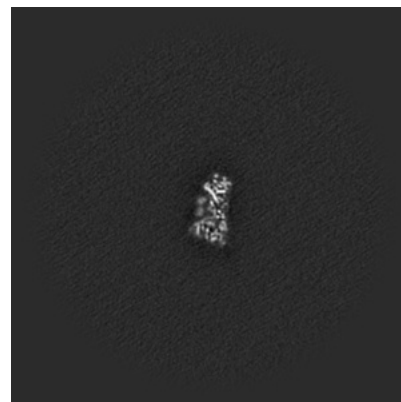
6.3.1 Primary map



X Index: 260

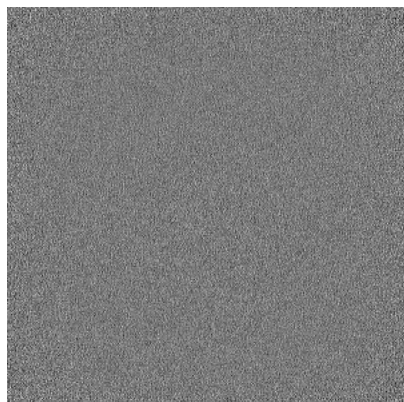


Y Index: 251

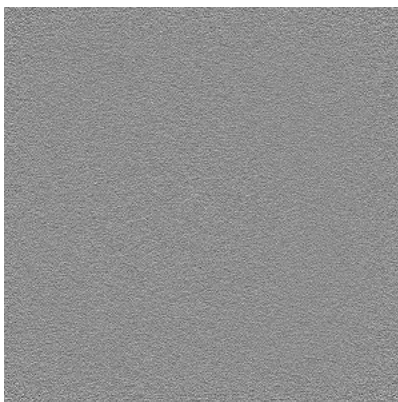


Z Index: 328

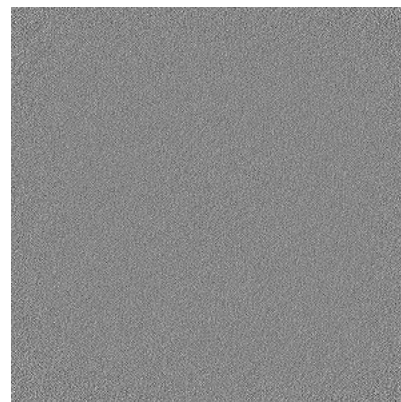
6.3.2 Raw map



X Index: 0



Y Index: 0

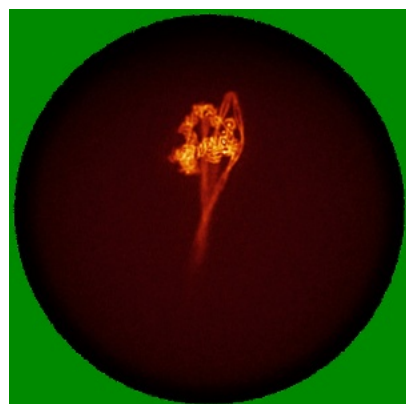


Z Index: 511

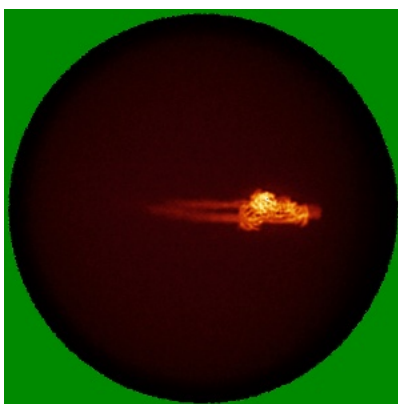
The images above show the largest variance slices of the map in three orthogonal directions.

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

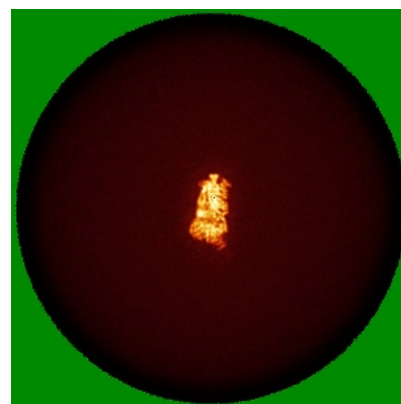
6.4.1 Primary map



X

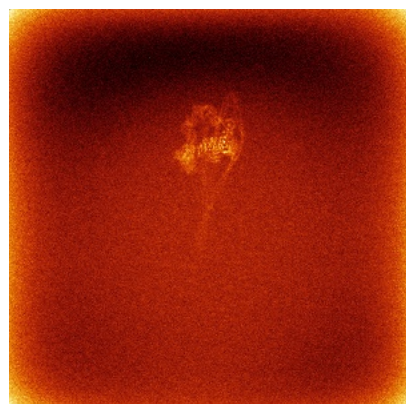


Y

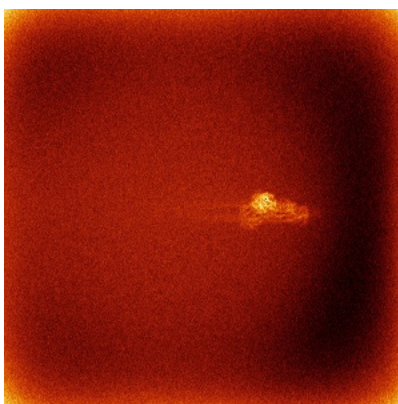


Z

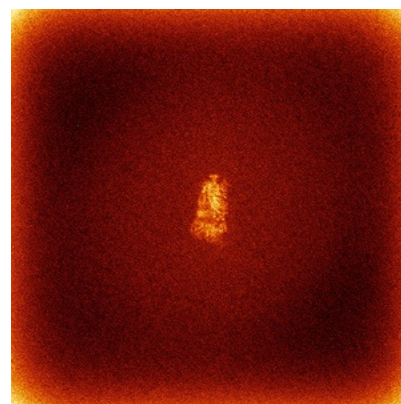
6.4.2 Raw map



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.

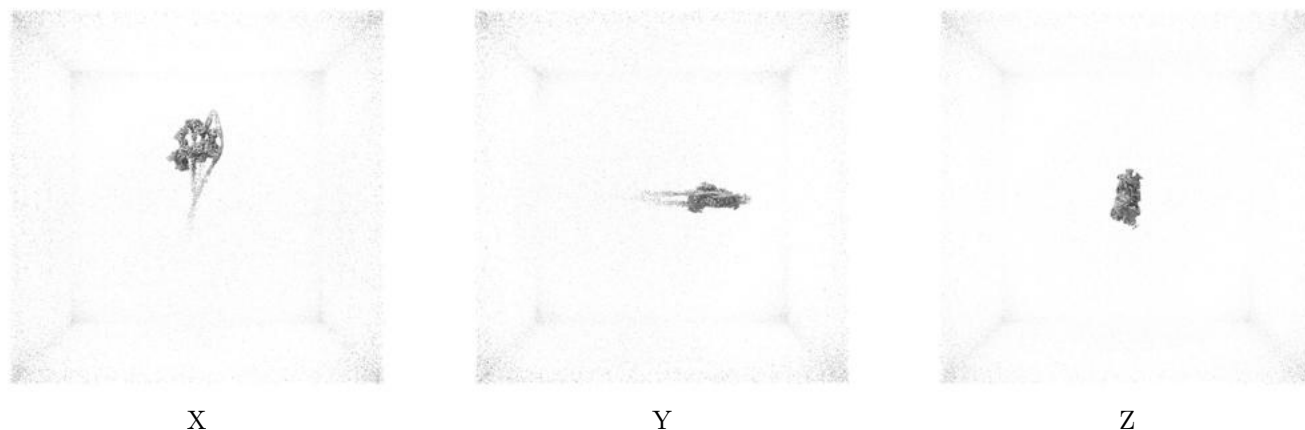
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

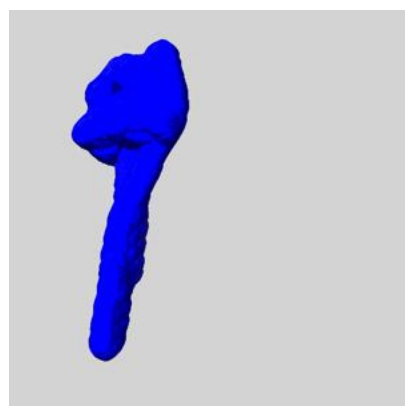
6.6 Mask visualisation [i](#)

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

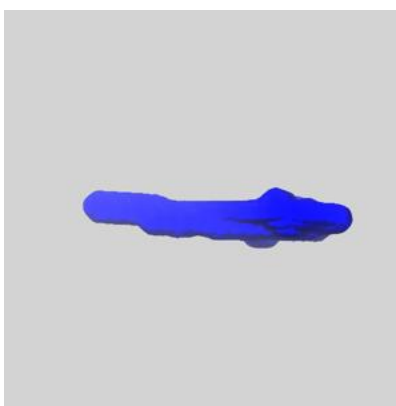
A mask typically either:

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

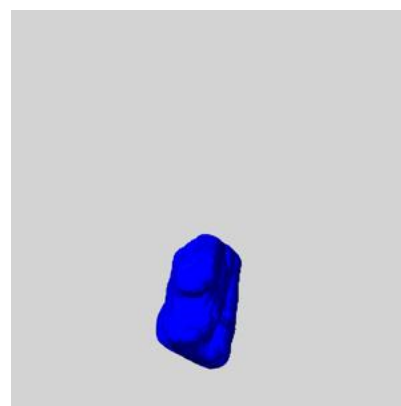
6.6.1 emd_55382_msk_1.map [i](#)



X



Y

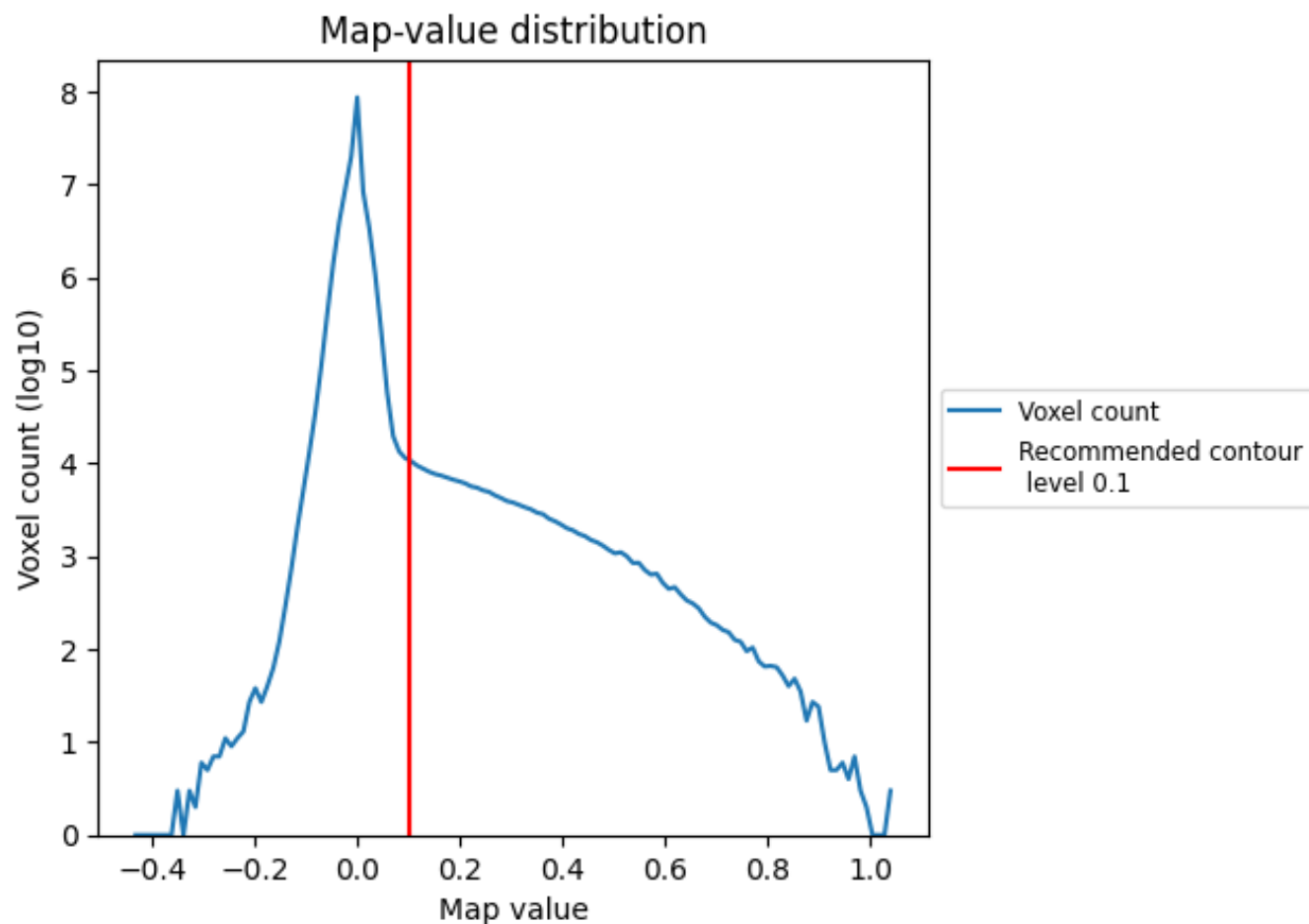


Z

7 Map analysis [i](#)

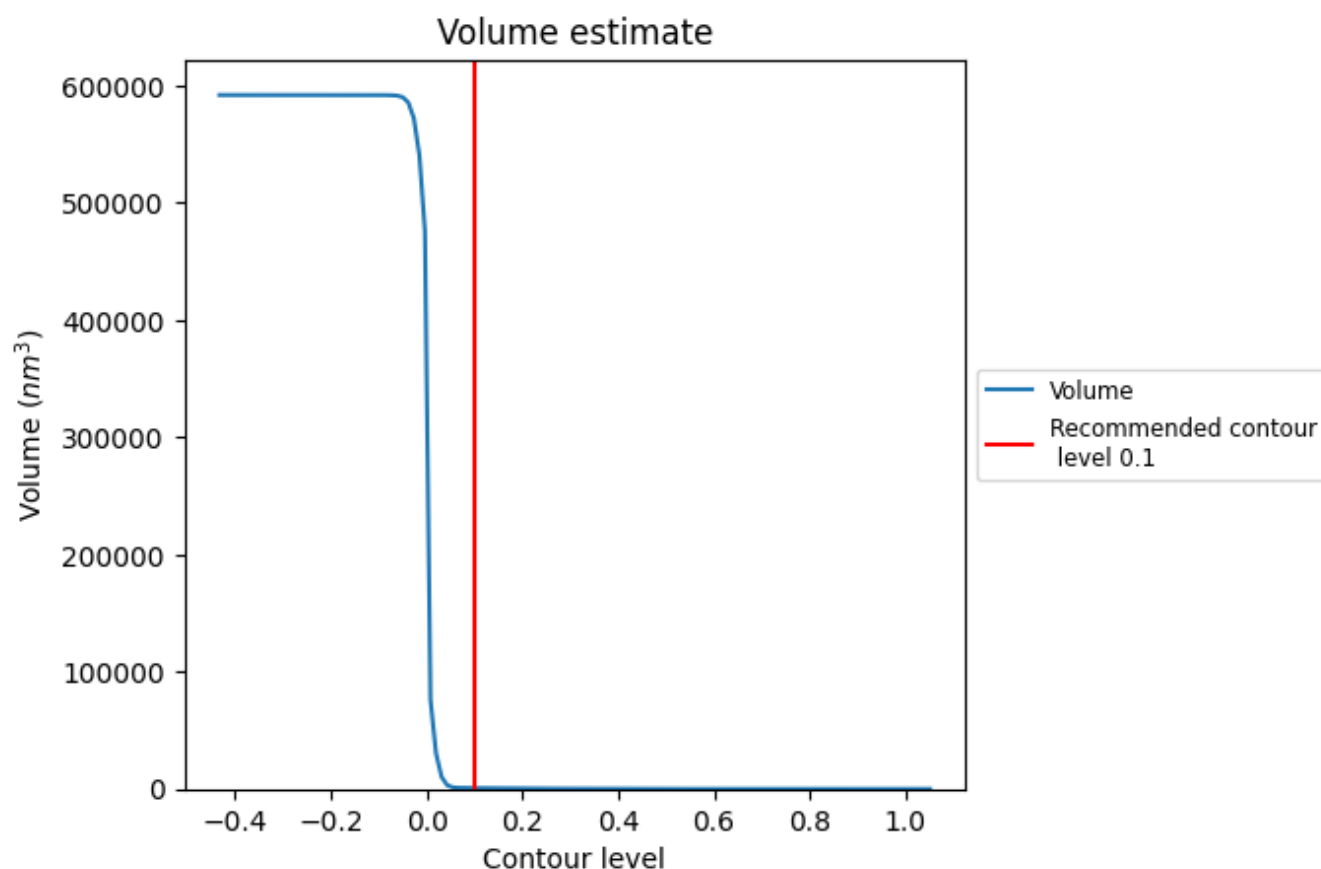
This section contains the results of statistical analysis of the map.

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.

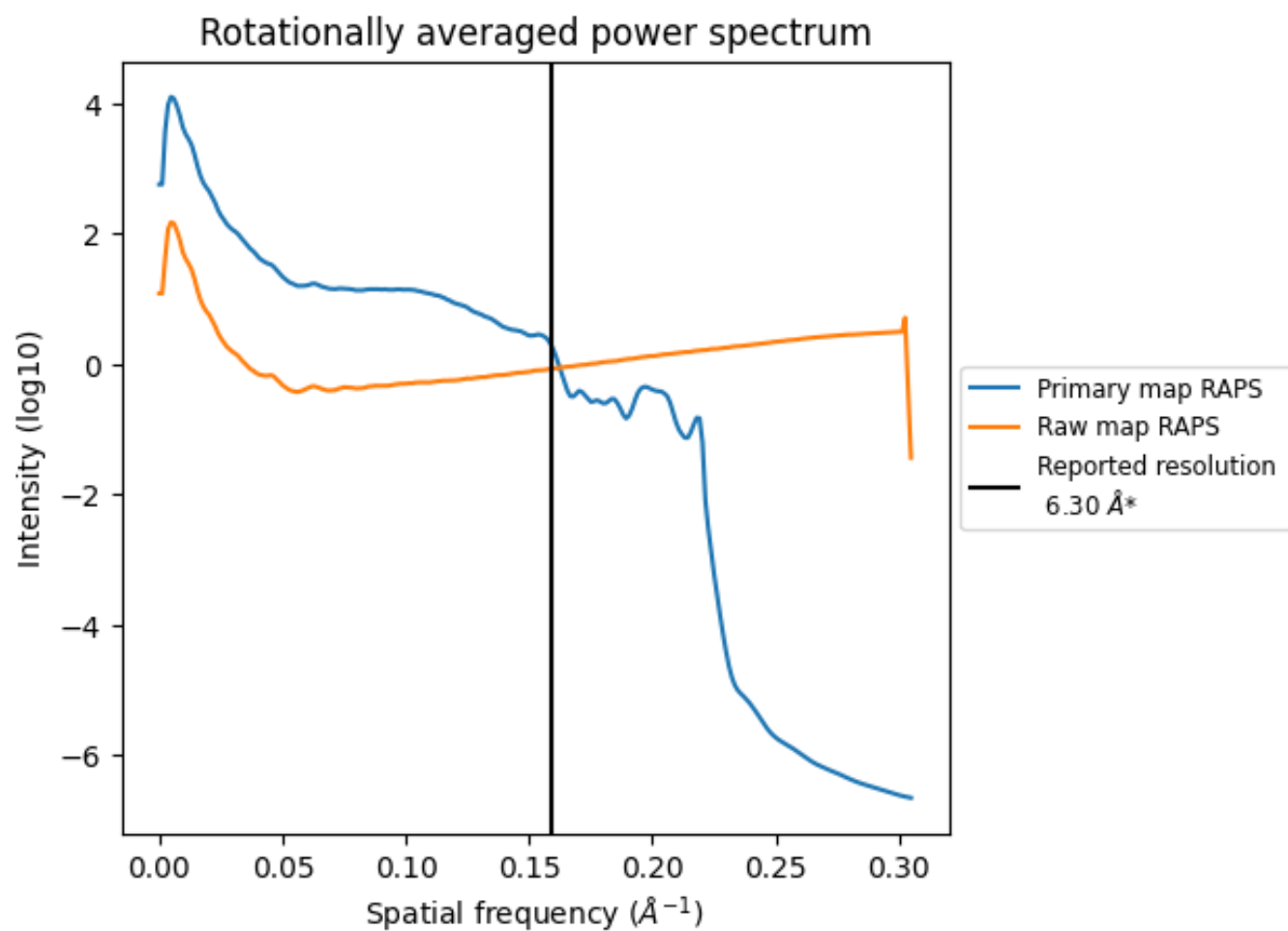
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 737 nm³; this corresponds to an approximate mass of 666 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 ⓘ

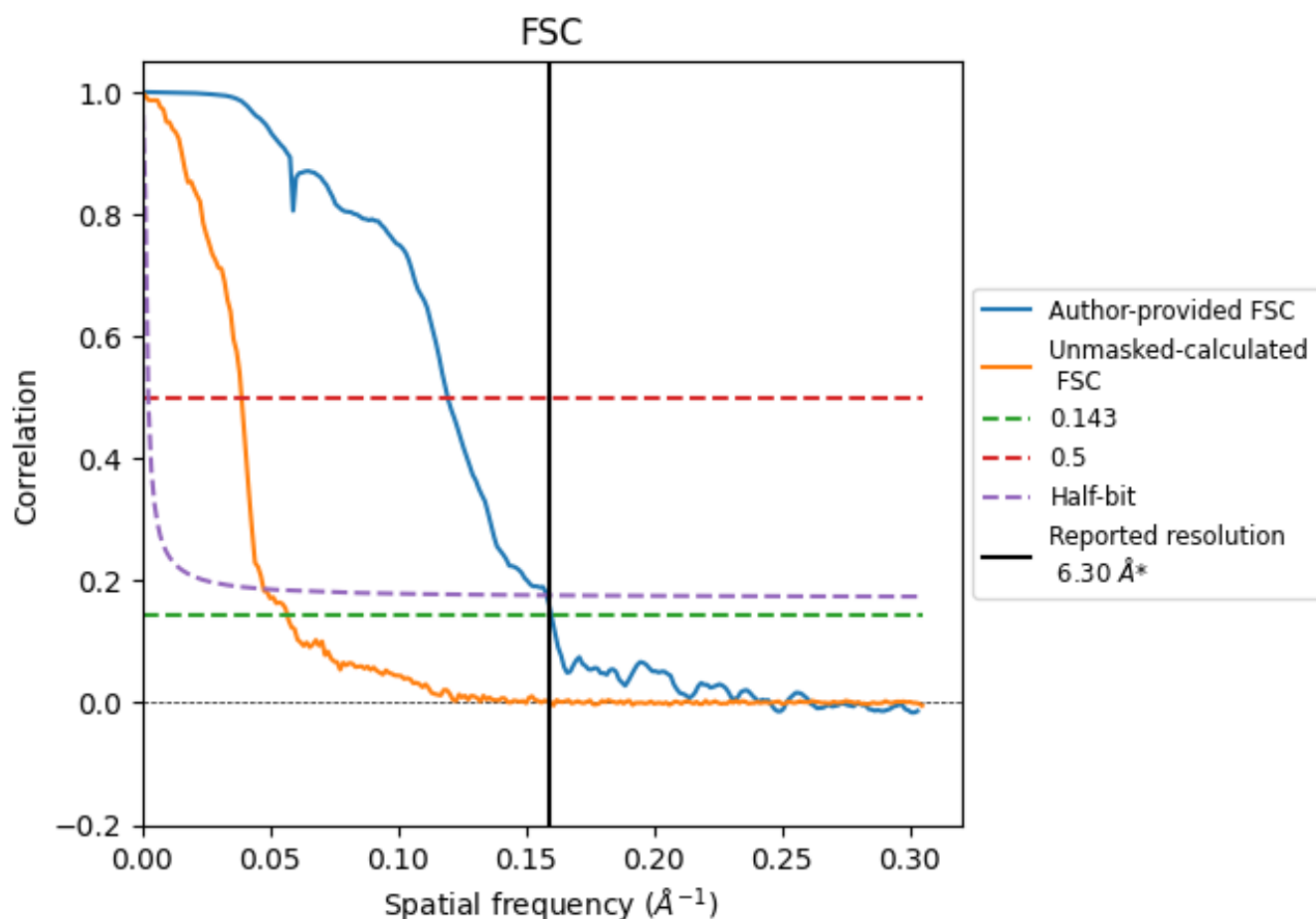


*Reported resolution corresponds to spatial frequency of 0.159 \AA^{-1}

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 0.159 \AA^{-1}

8.2 Resolution estimates [i](#)

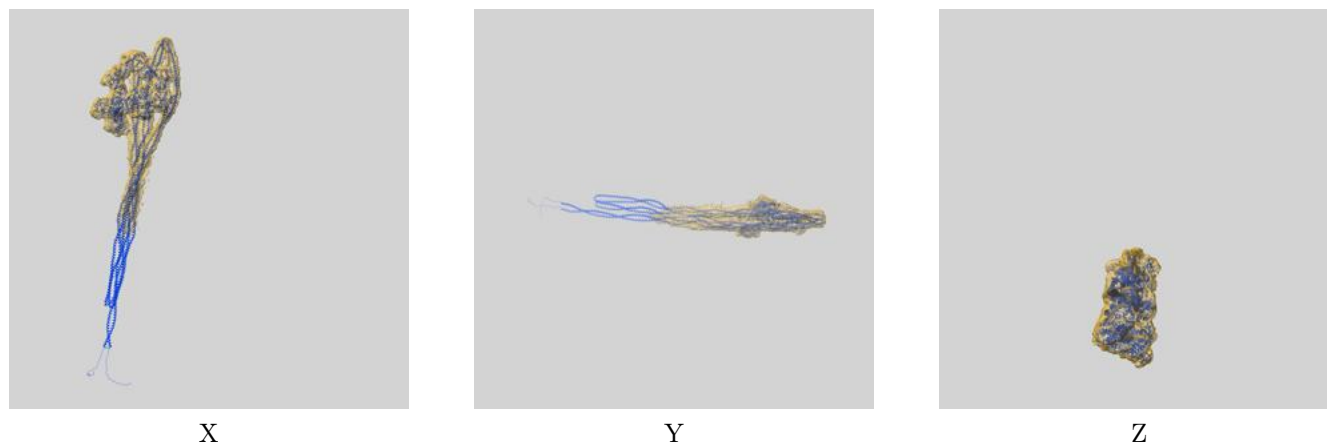
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.30	-	-
Author-provided FSC curve	6.25	8.38	6.33
Unmasked-calculated*	17.64	25.77	21.05

*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 17.64 differs from the reported value 6.3 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55382 and PDB model 9SZR. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



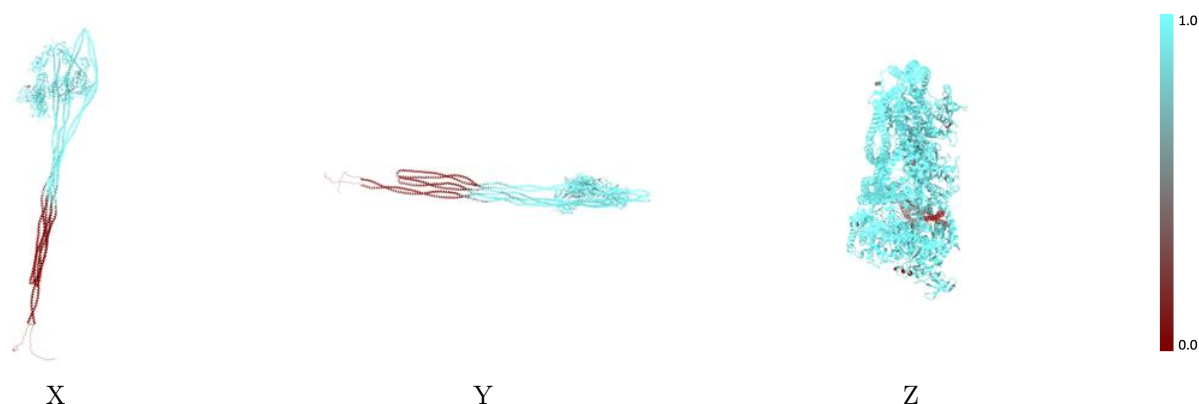
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



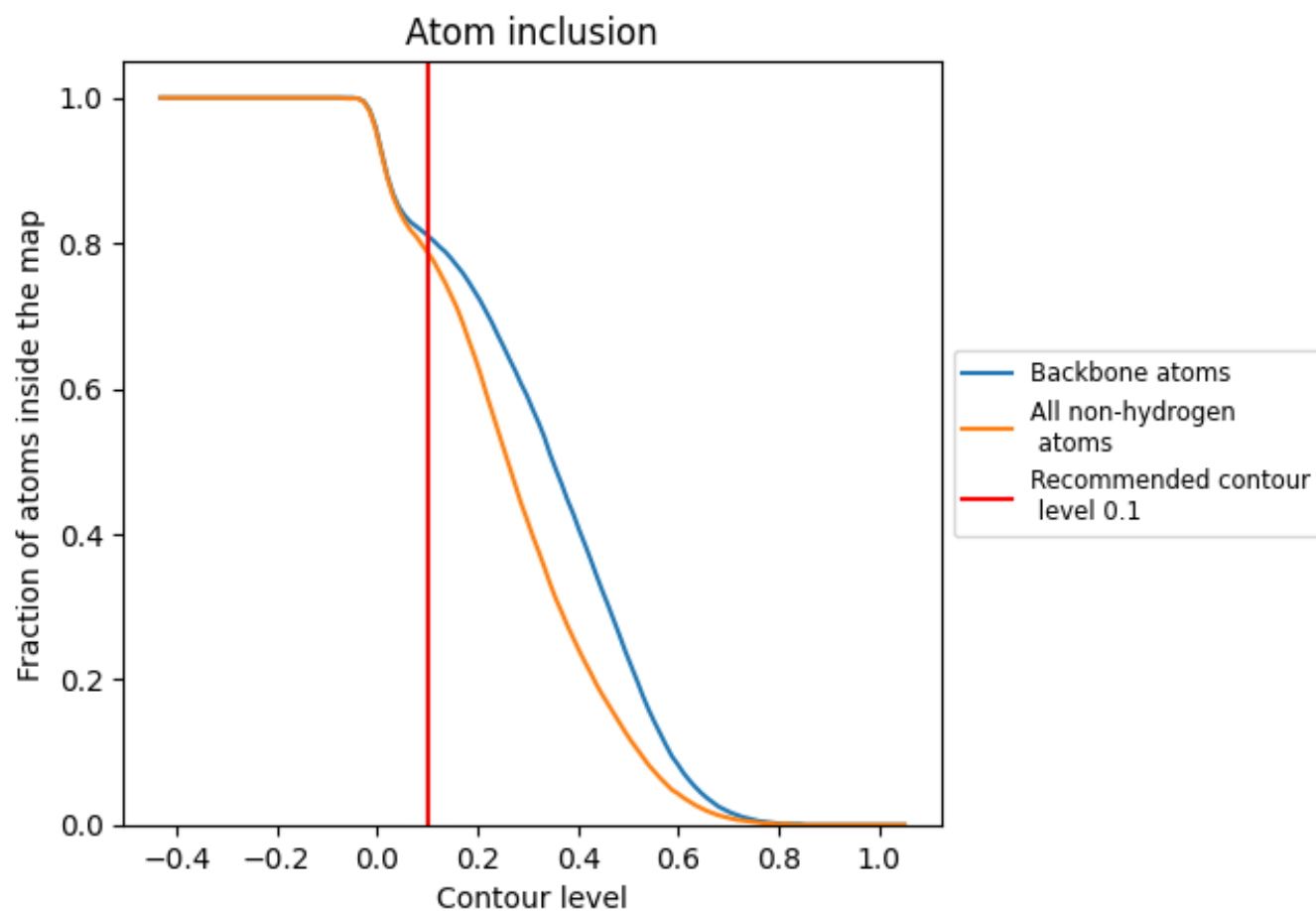
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 79% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7870	<div></div> 0.1250
A	<div></div> 0.7570	<div></div> 0.1240
B	<div></div> 0.7610	<div></div> 0.1180
C	<div></div> 0.9710	<div></div> 0.1800
D	<div></div> 0.9530	<div></div> 0.1540
E	<div></div> 0.9720	<div></div> 0.1440
F	<div></div> 0.9890	<div></div> 0.1340

1.0

0.0

<0.0