



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 07:39 PM UTC

PDB ID : 8JVJ / pdb_00008jvj
EMDB ID : EMD-36676
Title : Structure of human TRPV4 with antagonist A2 and RhoA
Authors : Fan, J.; Lei, X.
Deposited on : 2023-06-28
Resolution : 3.44 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

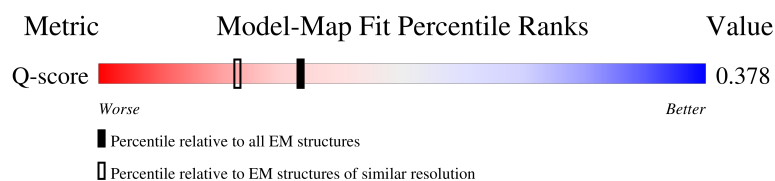
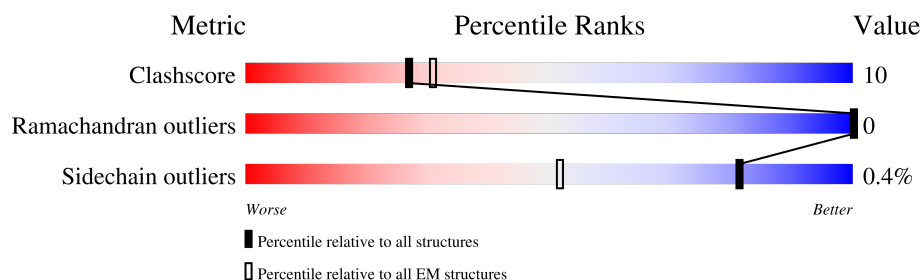
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.44 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13877 (2.94 - 3.94)

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	1144	10% 42% 12% 46%
1	B	1144	10% 44% 11% 46%
1	C	1144	10% 43% 11% 46%
1	D	1144	10% 43% 11% 46%

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Mol	Chain	Length	Quality of chain
2	E	193	
2	F	193	
2	G	193	
2	H	193	

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
3	F9M	B	1201	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25052 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.

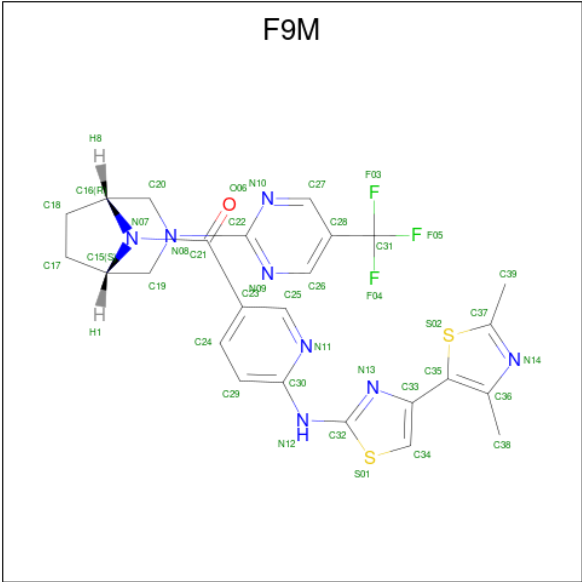
- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 4,3C-GFP.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	620	Total	C	N	O	S	0	0
			4921	3211	817	868	25		
1	B	620	Total	C	N	O	S	0	0
			4921	3211	817	868	25		
1	C	620	Total	C	N	O	S	0	0
			4921	3211	817	868	25		
1	D	620	Total	C	N	O	S	0	0
			4921	3211	817	868	25		

- Molecule 2 is a protein called Transforming protein RhoA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	182	Total	C	N	O	S	0	0
			1303	833	226	236	8		
2	F	182	Total	C	N	O	S	0	0
			1303	833	226	236	8		
2	G	182	Total	C	N	O	S	0	0
			1303	833	226	236	8		
2	H	182	Total	C	N	O	S	0	0
			1303	833	226	236	8		

- Molecule 3 is [6-[[4-(2,4-dimethyl-1,3-thiazol-5-yl)-1,3-thiazol-2-yl]amino]pyridin-3-yl]-[(1 {S},5 {R})-3-[5-(trifluoromethyl)pyrimidin-2-yl]-3,8-diazabicyclo[3.2.1]octan-8-yl]methanone (CCD ID: F9M) (formula: C₂₅H₂₃F₃N₈OS₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	F	N	O	S	0
			39	25	3	8	1	2	
3	B	1	Total	C	F	N	O	S	0
			39	25	3	8	1	2	
3	C	1	Total	C	F	N	O	S	0
			39	25	3	8	1	2	
3	D	1	Total	C	F	N	O	S	0
			39	25	3	8	1	2	



[illegible]

GLY
SER
GLY
GLY
SER
ALA
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

- Molecule 1: Transient receptor potential cation channel subfamily V member 4,3C-GFP



MET	ALA	ASP	SER	GLY	PRO	ARG	ALA	ALA	GLY	PRO	GLY	GLU	VAL	ALA	ALA	GLU	LEU	PRO	GLY	ASP	SER	GLY	THR	PRO	GLY	GLY	GLU	ALA	PHE	PRO	LEU	SER	SER	LEU	ALA	ASN	LEU	PHE	GLY	GLU	GLY	ASP	GLY	SER	SER	LEU	SER	PRO	PRO	ALA	ASP	ALA	GLY	PRO	ARG	ALA	GLY	PRO
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GLY	ASP	GLY	GLY	ARG	PRO	ARG	ASN	LEU	ARG	MET	LYS	PHE	GLN	GLY	PHE	ARG	LYS	GLY	VAL	PRO	ASN	PRO	PRO	ILE	ASP	LEU	LEU	GLU	THR	LEU	TYR	GLU	VAL	VAL	PRO	GLY	PRO	LYS	LYS	ALA	PRO	PRO	MET	ASP	SER	SER	LEU	PHE	ASP	TYR	GLY	THR	THR	ARG	HIS	HIS	SER	SER	SER	ASP	ASN
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[illegible]

E218
R219
R223
R224
R225
F226
I227
D233
Y234
Y335
Y336
R237
E255
E258
Y259
Q260
J261
A262
E278
L289
Y303
D313
M314
R320
T323
H326
V329
D333
M338
F341
M345
L362
V365
L371
M376
K379
I383

I385	D408	P413	L418	Y419	D420	L421	L424	D425	T426	E430	V433	I436	S441	K442	I443	E444	K445	R446	M449	V452	E453	P454	I455	V463	F466	G467	A468	V469	I473	V476	M482	L494	E495	G496	P498	P499	Y502	R503	L504	T505	V506
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D607	Y508	L509	R510	L511	A512	G513	E514	V515	L518	F519	L523	F524	F525	F526	I529	K530	D531	L532	F533	M534	K535	K536	C537	P538	G539	V540	M541	S542	L543	F544	L545	D546	G547	S548	F549	Q550	L551	L552	F561	V562	S563	A564	A565	L566	Y567	L568	A569	G570	L571	F572	A573	Y574	L575	V576
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[illegible]

GLN	THR	ASN	CYS	THR	VAL	PRO	THR	TYR	PRO	PRO	SER	SER	ARG	D662	T685	T686	T687	T688	T689	F674	K675	G679	M680	L683	E684	K690	G691	P692	T696	T697	L698	L699	Y702	I703	T704	L705	T706	F707	L710	L711	M712	M713	L714	T715	A716	L717	M718	G719	E720	T721	T722	G723	V724	V725	V726	V727	V728	V729	V730	V731	V732	V733	V734	V735	V736	V737	V738	V739	V740	V741	V742	V743	V744	V745	V746	V747	V748	V749	V750	V751	V752	V753	V754	V755	V756	V757	V758	V759	V760	V761	V762	V763	V764	V765	V766	V767	V768	V769	V770	V771	V772	V773	V774	V775	V776	V777	V778	V779	V780	V781	V782	V783	V784	V785	V786	V787	V788	V789	V790	V791	V792	V793	V794	V795	V796	V797	V798	V799	V800	V801	V802	V803	V804	V805	V806	V807	V808	V809	V810	V811	V812	V813	V814	V815	V816	V817	V818	V819	V820	V821	V822	V823	V824	V825	V826	V827	V828	V829	V830	V831	V832	V833	V834	V835	V836	V837	V838	V839	V840	V841	V842	V843	V844	V845	V846	V847	V848	V849	V850	V851	V852	V853	V854	V855	V856	V857	V858	V859	V860	V861	V862	V863	V864	V865	V866	V867	V868	V869	V870	V871	V872	V873	V874	V875	V876	V877	V878	V879	V880	V881	V882	V883	V884	V885	V886	V887	V888	V889	V890	V891	V892	V893	V894	V895	V896	V897	V898	V899	V900	V901	V902	V903	V904	V905	V906	V907	V908	V909	V910	V911	V912	V913	V914	V915	V916	V917	V918	V919	V920	V921	V922	V923	V924	V925	V926	V927	V928	V929	V930	V931	V932	V933	V934	V935	V936	V937	V938	V939	V940	V941	V942	V943	V944	V945	V946	V947	V948	V949	V950	V951	V952	V953	V954	V955	V956	V957	V958	V959	V960	V961	V962	V963	V964	V965	V966	V967	V968	V969	V970	V971	V972	V973	V974	V975	V976	V977	V978	V979	V980	V981	V982	V983	V984	V985	V986	V987	V988	V989	V990	V991	V992	V993	V994	V995	V996	V997	V998	V999	V1000	V1001	V1002	V1003	V1004	V1005	V1006	V1007	V1008	V1009	V1010	V1011	V1012	V1013	V1014	V1015	V1016	V1017	V1018	V1019	V1020	V1021	V1022	V1023	V1024	V1025	V1026	V1027	V1028	V1029	V1030	V1031	V1032	V1033	V1034	V1035	V1036	V1037	V1038	V1039	V1040	V1041	V1042	V1043	V1044	V1045	V1046	V1047	V1048	V1049	V1050	V1051	V1052	V1053	V1054	V1055	V1056	V1057	V1058	V1059	V1060	V1061	V1062	V1063	V1064	V1065	V1066	V1067	V1068	V1069	V1070	V1071	V1072	V1073	V1074	V1075	V1076	V1077	V1078	V1079	V1080	V1081	V1082	V1083	V1084	V1085	V1086	V1087	V1088	V1089	V1090	V1091	V1092	V1093	V1094	V1095	V1096	V1097	V1098	V1099	V1100	V1101	V1102	V1103	V1104	V1105	V1106	V1107	V1108	V1109	V1110	V1111	V1112	V1113	V1114	V1115	V1116	V1117	V1118	V1119	V1120	V1121	V1122	V1123	V1124	V1125	V1126	V1127	V1128	V1129	V1130	V1131	V1132	V1133	V1134	V1135	V1136	V1137	V1138	V1139	V1140	V1141	V1142	V1143	V1144	V1145	V1146	V1147	V1148	V1149	V1150	V1151	V1152	V1153	V1154	V1155	V1156	V1157	V1158	V1159	V1160	V1161	V1162	V1163	V1164	V1165	V1166	V1167	V1168	V1169	V1170	V1171	V1172	V1173	V1174	V1175	V1176	V1177	V1178	V1179	V1180	V1181	V1182	V1183	V1184	V1185	V1186	V1187	V1188	V1189	V1190	V1191	V1192	V1193	V1194	V1195	V1196	V1197	V1198	V1199	V1200	V1201	V1202	V1203	V1204	V1205	V1206	V1207	V1208	V1209	V1210	V1211	V1212	V1213	V1214	V1215	V1216	V1217	V1218	V1219	V1220	V1221	V1222	V1223	V1224	V1225	V1226	V1227	V1228	V1229	V1230	V1231	V1232	V1233	V1234	V1235	V1236	V1237	V1238	V1239	V1240	V1241	V1242	V1243	V1244	V1245	V1246	V1247	V1248	V1249	V1250	V1251	V1252	V1253	V1254	V1255	V1256	V1257	V1258	V1259	V1260	V1261	V1262	V1263	V1264	V1265	V1266	V1267	V1268	V1269	V1270	V1271	V1272	V1273	V1274	V1275	V1276	V1277	V1278	V1279	V1280	V1281	V1282	V1283	V1284	V1285	V1286	V1287	V1288	V1289	V1290	V1291	V1292	V1293	V1294	V1295	V1296	V1297	V1298	V1299	V1300	V1301	V1302	V1303	V1304	V1305	V1306	V1307	V1308	V1309	V1310	V1311	V1312	V1313	V1314	V1315	V1316	V1317	V1318	V1319	V1320	V1321	V1322	V1323	V1324	V1325	V1326	V1327	V1328	V1329	V1330	V1331	V1332	V1333	V1334	V1335	V1336	V1337	V1338	V1339	V1340	V1341	V1342	V1343	V1344	V1345	V1346	V1347	V1348	V1349	V1350	V1351	V1352	V1353	V1354	V1355	V1356	V1357	V1358	V1359	V1360	V1361	V1362	V1363	V1364	V1365	V1366	V1367	V1368	V1369	V1370	V1371	V1372	V1373	V1374	V1375	V1376	V1377	V1378	V1379	V1380	V1381	V1382	V1383	V1384	V1385	V1386	V1387	V1388	V1389	V1390	V1391	V1392	V1393	V1394	V1395	V1396	V1397	V1398	V1399	V1400	V1401	V1402	V1403	V1404	V1405	V1406	V1407	V1408	V1409	V1410	V1411	V1412	V1413	V1414	V1415	V1416	V1417	V1418	V1419	V1420	V1421	V1422	V1423	V1424	V1425	V1426	V1427	V1428	V1429	V1430	V1431	V1432	V1433	V1434	V1435	V1436	V1437	V1438	V1439	V1440	V1441	V1442	V1443	V1444	V1445	V1446	V1447	V1448	V1449	V1450	V1451	V1452	V1453	V1454	V1455	V1456	V1457	V1458	V1459	V1460	V1461	V1462	V1463	V1464	V1465	V1466	V1467	V1468	V1469	V1470	V1471	V1472	V1473	V1474	V1475	V1476	V1477	V1478	V1479	V1480	V1481	V1482	V1483	V1484	V1485	V1486	V1487	V1488	V1489	V1490	V1491	V1492	V1493	V1494	V1495	V1496	V1497	V1498	V1499	V1500	V1501	V1502	V1503	V1504	V1505	V1506	V1507	V1508	V1509	V1510	V1511	V1512	V1513	V1514	V1515	V1516	V1517	V1518	V1519	V1520	V1521	V1522	V1523	V1524	V1525	V1526	V1527	V1528	V1529	V1530	V1531	V1532	V1533	V1534	V1535	V1536	V1537	V1538	V1539	V1540	V1541	V1542	V1543	V1544	V1545	V1546	V1547	V1548	V1549	V1550	V1551	V1552	V1553	V1554	V1555	V1556	V1557	V1558	V1559	V1560	V15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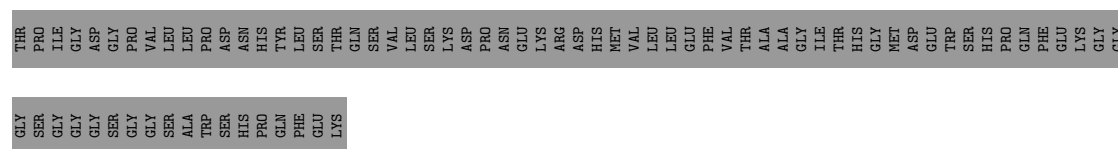
Q724	V725	S726	F727	E728	S729	W730	W731	W732	W733	E745	F748	F756	R775	F778	R779	W788	ASN	GLN	ASN	ASN	GLY	ILE	ILE	ILE	ASN	ASN	GLU	ASP	PRO	GLY	LYS	ASN	ASN	GLU	THR	THR	GLN	TYR	TYR	GLY	PHE	SER	SER	HIS	THR	VAL	GLY	ARG	LEU	LEU	ARG	ARG	ASP	ARG	TRP	SER	SER	SER	VAL	VAL
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

PRO	ARG	VAL	VAL	GLU	LEU	ASN	LYS	ASN	ASN	SER	ASN	PRO	ASP	GLU	VAL	VAL	VAL	VAL	PRO	LEU	ASP	SER	MET	GLY	ASN	ASN	PRO	ARG	CYS	ASP	GLY	HIS	GLN	GLN	GLY	TYR	PRO	ARG	LYS	TRP	ARG	ARG	THR	ASP	ASP	ALA	PRO	LEU	ALA	ALA	ALA	LEU	GLU	VAL	VAL	LEU	PHE	GLN	PRO	GLY	SER	LYS	GLY	GLU
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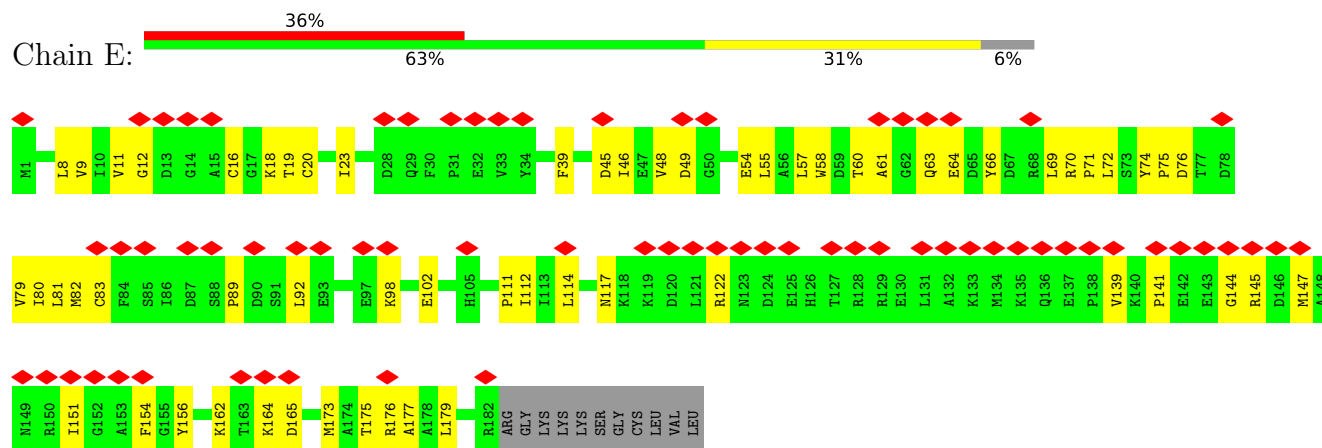
GLU LEU PHE THR GLY VAL VAL PRO ILE LEU VAL GLU LEU ASP GLY ASP ASN HIS PHE LYS SER VAL ARG GLY GLU GLY GLU GLY ASP ALA THR GLY LYS LEU LEU LEU PHE CYS THR THR GLY LEU LEU PRO VAL PRO TRP PRO THR LEU VAL THR THR LEU

TYR	GLY	VAL	GLN	CYS	PHE	SER	ARG	THR	TYR	PRO	PRO	ASP	ASP	HIS	ASP	MET	LYS	ARG	HIS	PHE	PHE	LYS	ALA	SER	ALA	SER	MET	PRO	GLU	GLY	TYR	VAL	GLN	GLU	ARG	THR	THR	ILE	SER	SER	PHE	LYS	ASP	ASP	GLY	GLY	THR	TYR	LYS	THR	ARG	ALA	GLU	GLU	VAL	VAL	LYS	PHE	GLU	GLY	ASP	THR	LEU	VAL	ASN	ARG	ILE	ILE	GLU	LEU
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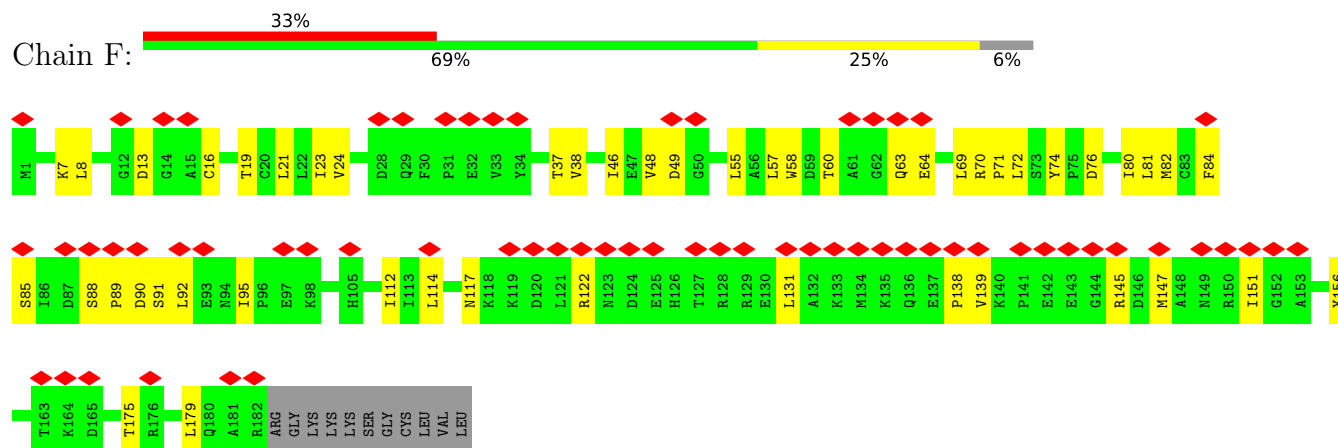
LYS
ILE
GLY
ASP
PHE
LYS
GLU
ASP
GLY
ASN
LEU
ILE
GLY
HIS
LYS
LEU
GLU
TYR
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PHE
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ASP
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ASN



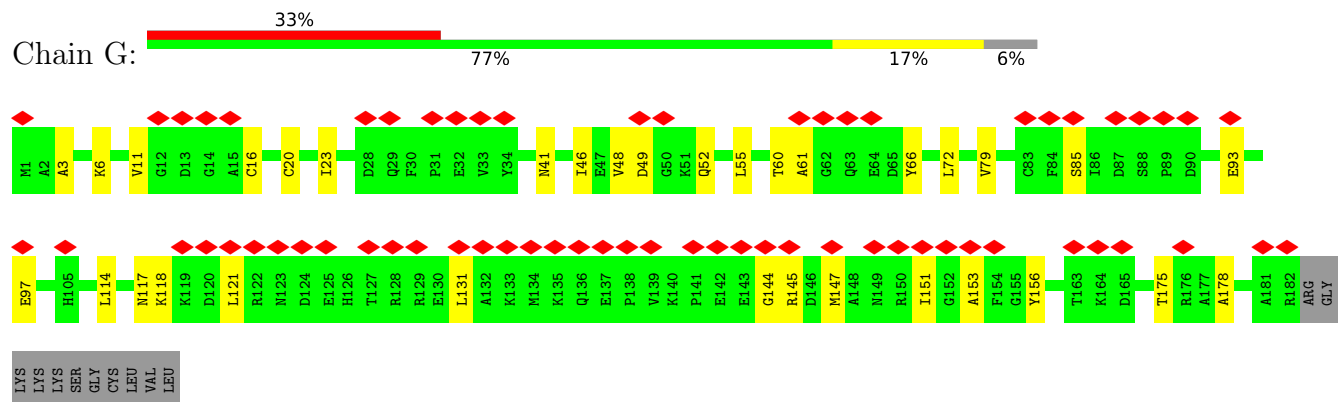
- Molecule 2: Transforming protein RhoA



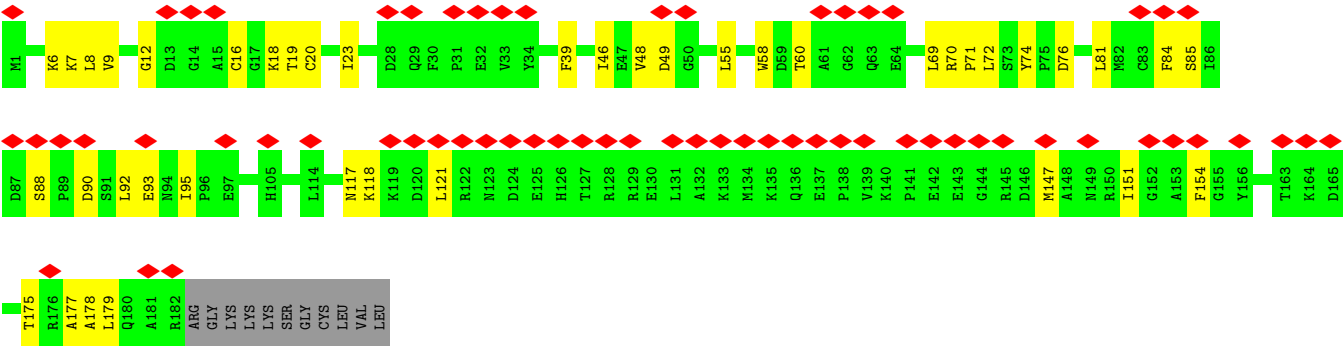
- Molecule 2: Transforming protein RhoA



- Molecule 2: Transforming protein RhoA



- Molecule 2: Transforming protein RhoA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47803	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.511	Depositor
Minimum map value	-1.572	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.28	Depositor
Map size ($\text{\AA}$)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	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: F9M

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	0.17	0/5038	0.35	0/6838
1	B	0.12	0/5038	0.32	0/6838
1	C	0.16	0/5038	0.37	0/6838
1	D	0.16	0/5038	0.37	0/6838
2	E	0.12	0/1330	0.38	0/1818
2	F	0.13	0/1330	0.36	0/1818
2	G	0.12	0/1330	0.34	0/1818
2	H	0.11	0/1330	0.35	0/1818
All	All	0.15	0/25472	0.35	0/34624

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	4921	0	4932	114	0
1	B	4921	0	4932	89	0
1	C	4921	0	4932	99	0
1	D	4921	0	4932	101	0
2	E	1303	0	1210	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1303	0	1210	33	0
2	G	1303	0	1210	22	0
2	H	1303	0	1210	25	0
3	A	39	0	0	3	0
3	B	39	0	0	0	0
3	C	39	0	0	0	0
3	D	39	0	0	0	0
All	All	25052	0	24568	492	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 (492) 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:C:466:PHE:CD2	1:C:748:PHE:HE2	1.88	0.92
1:C:466:PHE:CE2	1:C:748:PHE:HE2	1.90	0.89
2:H:16:CYS:O	2:H:117:ASN:ND2	2.08	0.86
1:D:466:PHE:CD2	1:D:748:PHE:HE2	1.97	0.83
1:A:466:PHE:CD2	1:A:748:PHE:HE2	1.96	0.82
1:D:466:PHE:HD2	1:D:748:PHE:HE2	1.24	0.81
2:G:16:CYS:O	2:G:117:ASN:ND2	2.15	0.80
1:C:466:PHE:CE2	1:C:748:PHE:CE2	2.71	0.79
2:F:82:MET:O	2:F:114:LEU:HA	1.83	0.79
1:B:635:LEU:HD22	1:B:695:PHE:HE1	1.48	0.79
1:A:579:VAL:HG11	1:D:635:LEU:HD11	1.66	0.78
1:C:475:VAL:HG22	1:C:592:PHE:CD2	2.18	0.78
1:C:631:ALA:HB1	1:D:579:VAL:HG13	1.67	0.75
1:D:466:PHE:CD2	1:D:748:PHE:CE2	2.76	0.73
1:D:466:PHE:HD2	1:D:748:PHE:CE2	2.05	0.72
1:A:531:ASP:OD2	1:A:550:GLN:NE2	2.22	0.70
1:C:635:LEU:HD22	1:C:695:PHE:HZ	1.57	0.70
1:B:691:TYR:OH	1:C:572:GLU:O	2.09	0.69
1:D:617:PHE:CD2	1:D:713:MET:HE3	2.28	0.69
1:A:506:VAL:HG12	1:A:510:ARG:HE	1.57	0.69
2:E:79:VAL:HG23	2:E:111:PRO:HB2	1.75	0.69
1:D:590:LEU:HB3	1:D:603:SER:HB2	1.73	0.69
1:A:466:PHE:CE2	1:A:748:PHE:HE2	2.11	0.68
2:G:85:SER:HA	2:G:117:ASN:OD1	1.93	0.68
1:C:408:ASP:OD2	1:C:779:ARG:NH2	2.25	0.68
1:A:463:TRP:CH2	1:A:468:ALA:HA	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:ARG:HB3	1:B:736:GLN:HE21	1.59	0.67
1:B:214:LEU:HD13	1:B:260:GLN:HE22	1.59	0.67
1:A:597:LYS:HB3	1:A:733:TRP:CZ3	2.30	0.67
1:B:408:ASP:HB2	1:B:418:LEU:HD22	1.76	0.67
1:D:289:LEU:HD21	1:D:314:MET:HG3	1.77	0.67
2:H:8:LEU:HB2	2:H:55:LEU:HD11	1.77	0.66
1:A:491:TYR:O	1:A:510:ARG:NH1	2.27	0.66
1:C:594:ARG:HD3	1:C:736:GLN:HG2	1.76	0.66
1:A:437:LEU:HD11	1:A:449:MET:HB3	1.79	0.65
1:B:631:ALA:HB1	1:C:579:VAL:HG13	1.77	0.65
2:F:16:CYS:O	2:F:117:ASN:ND2	2.30	0.65
1:A:482:MET:HE1	1:A:585:GLY:HA3	1.78	0.65
1:B:333:ASP:HB2	1:B:338:ASN:HD22	1.61	0.65
1:C:466:PHE:CD2	1:C:748:PHE:CE2	2.79	0.65
2:F:122:ARG:NH2	2:F:139:VAL:O	2.29	0.65
2:F:82:MET:HE2	2:F:95:ILE:HG23	1.78	0.65
1:A:463:TRP:CE2	1:A:468:ALA:HB2	2.32	0.64
1:D:278:GLU:OE1	1:D:320:ARG:NH2	2.30	0.64
1:C:463:TRP:CZ2	1:C:468:ALA:HA	2.33	0.64
2:E:122:ARG:NH2	2:E:139:VAL:O	2.31	0.64
1:A:278:GLU:OE1	1:A:320:ARG:NH2	2.31	0.63
1:A:475:VAL:HG22	1:A:592:PHE:HB3	1.81	0.63
1:C:218:GLU:OE2	1:C:219:ARG:NH1	2.31	0.63
1:C:463:TRP:CE2	1:C:468:ALA:HA	2.34	0.62
2:G:46:ILE:HG21	2:G:175:THR:HG21	1.80	0.62
1:B:452:VAL:HG12	1:B:454:PRO:HD2	1.79	0.62
1:B:278:GLU:OE1	1:B:320:ARG:NH2	2.33	0.62
2:E:46:ILE:HD11	2:E:175:THR:HG21	1.82	0.62
1:A:631:ALA:HB1	1:B:579:VAL:HG13	1.82	0.62
1:C:466:PHE:HE2	1:C:748:PHE:CE2	2.17	0.62
1:D:466:PHE:CZ	1:D:745:GLU:HG3	2.35	0.62
2:F:131:LEU:HD12	2:F:138:PRO:HD3	1.80	0.62
1:B:258:VAL:HA	1:B:262:ALA:HB3	1.82	0.62
1:B:289:LEU:HD21	1:B:314:MET:HG3	1.82	0.61
1:B:631:ALA:HB2	1:C:582:LEU:HD22	1.81	0.61
1:C:149:PHE:HA	1:C:153:ILE:HD11	1.81	0.61
1:C:289:LEU:HD21	1:C:314:MET:HG3	1.81	0.61
1:D:166:LEU:HD13	1:D:216:ILE:HD11	1.83	0.61
1:C:408:ASP:HB2	1:C:418:LEU:HD22	1.82	0.61
1:A:408:ASP:HB2	1:A:418:LEU:HD22	1.82	0.61
1:B:633:VAL:HA	1:B:636:LEU:HD13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:553:TYR:HE1	1:C:588:ASN:HB3	1.65	0.61
1:C:278:GLU:OE2	1:C:320:ARG:NH2	2.34	0.60
2:E:12:GLY:O	2:E:18:LYS:NZ	2.35	0.60
1:A:463:TRP:CZ2	1:A:468:ALA:HA	2.37	0.60
2:F:19:THR:O	2:F:23:ILE:HG12	2.00	0.60
1:D:408:ASP:OD2	1:D:779:ARG:NH2	2.25	0.60
1:B:155:PHE:HA	1:B:158:VAL:HG12	1.83	0.60
1:B:616:ARG:HH22	1:C:598:LEU:HD12	1.67	0.59
1:B:475:VAL:HG22	1:B:592:PHE:HB3	1.85	0.59
1:D:150:ASN:H	1:D:153:ILE:HD11	1.67	0.59
1:C:391:ARG:HG2	1:C:419:TYR:HE2	1.68	0.59
1:C:249:ARG:HG2	1:C:297:GLN:HE21	1.67	0.59
1:A:466:PHE:CE2	1:A:748:PHE:CE2	2.90	0.59
1:A:572:GLU:O	1:D:691:TYR:OH	2.20	0.59
1:D:628:TYR:HD2	1:D:702:TYR:HD1	1.51	0.59
2:H:12:GLY:O	2:H:18:LYS:NZ	2.35	0.59
1:C:452:VAL:HG12	1:C:454:PRO:HD2	1.84	0.58
1:C:685:MET:HA	1:C:688:SER:HB3	1.85	0.58
2:F:88:SER:OG	2:F:90:ASP:OD1	2.20	0.58
1:A:218:GLU:OE2	1:A:219:ARG:NE	2.35	0.58
1:D:237:ARG:NH1	2:H:76:ASP:OD2	2.36	0.58
2:F:80:ILE:HD11	2:F:112:ILE:HG13	1.85	0.58
1:C:628:TYR:CE1	1:D:583:VAL:HG13	2.37	0.58
1:D:408:ASP:HB2	1:D:418:LEU:HD22	1.85	0.58
1:C:545:ILE:HG22	1:C:546:ASP:H	1.68	0.58
1:B:232:ARG:HB3	2:F:72:LEU:HD23	1.86	0.58
1:B:505:THR:HA	1:B:508:TYR:HD1	1.68	0.57
1:A:442:LYS:NZ	1:A:445:ASN:HB2	2.19	0.57
1:A:466:PHE:CD2	1:A:748:PHE:CE2	2.86	0.57
1:B:408:ASP:OD2	1:B:779:ARG:NH1	2.37	0.57
1:B:712:ASN:HA	1:B:715:ILE:HB	1.86	0.57
1:D:441:SER:O	1:D:446:ARG:NH2	2.36	0.57
1:C:232:ARG:HB3	2:G:72:LEU:HD23	1.86	0.57
2:F:8:LEU:HD11	2:F:81:LEU:HG	1.86	0.57
1:D:424:LEU:HD22	1:D:455:ILE:HD11	1.85	0.57
1:A:289:LEU:HD21	1:A:314:MET:HG3	1.86	0.57
1:B:323:THR:HG1	1:B:326:HIS:HD1	1.51	0.57
1:C:635:LEU:HD22	1:C:695:PHE:CZ	2.37	0.57
1:D:371:LEU:HD11	1:D:379:LYS:HD3	1.86	0.57
1:D:534:MET:HE2	1:D:534:MET:HA	1.87	0.57
1:A:418:LEU:HA	1:A:779:ARG:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ASP:O	1:A:219:ARG:HG2	2.05	0.56
1:B:237:ARG:NH1	2:F:76:ASP:OD2	2.31	0.56
1:D:421:LEU:HD23	1:D:778:PHE:HB2	1.86	0.56
2:E:80:ILE:HD11	2:E:112:ILE:HG13	1.86	0.56
3:A:1201:F9M:S01	3:A:1201:F9M:C29	2.93	0.56
1:C:549:PHE:CD2	1:C:591:TYR:HB2	2.41	0.56
1:D:333:ASP:HB2	1:D:338:ASN:HD22	1.70	0.56
1:B:329:VAL:HG22	1:B:385:ILE:HD13	1.87	0.56
1:D:323:THR:HG21	1:D:365:VAL:HG11	1.87	0.56
1:B:375:MET:HG2	1:B:433:VAL:HG22	1.88	0.56
1:C:719:GLY:HA3	1:D:722:VAL:HG11	1.88	0.56
1:D:552:LEU:HD11	1:D:611:PHE:HE2	1.69	0.56
1:A:590:LEU:HB3	1:A:603:SER:HB2	1.88	0.55
1:C:475:VAL:HA	1:C:592:PHE:CE2	2.41	0.55
2:E:61:ALA:HB3	2:E:66:TYR:HD2	1.72	0.55
2:H:46:ILE:HG21	2:H:175:THR:HG21	1.87	0.55
1:D:469:VAL:HG23	1:D:469:VAL:O	2.07	0.55
1:D:463:TRP:CE2	1:D:468:ALA:HA	2.41	0.55
1:D:567:TYR:HB2	1:D:574:TYR:CE1	2.40	0.55
1:B:442:LYS:NZ	1:B:445:ASN:HB2	2.22	0.55
1:B:191:GLY:HA3	1:B:232:ARG:HG3	1.89	0.55
1:B:715:ILE:HG12	1:C:718:MET:HE3	1.87	0.55
1:A:566:LEU:O	1:A:570:GLY:N	2.39	0.55
1:A:691:TYR:HB3	1:A:694:VAL:HG22	1.88	0.55
2:E:154:PHE:CE2	2:E:173:MET:HE3	2.42	0.55
1:A:475:VAL:CG2	1:A:592:PHE:HB3	2.37	0.55
3:A:1201:F9M:C25	3:A:1201:F9M:C15	2.85	0.55
1:A:559:LEU:HA	1:A:562:VAL:HG12	1.87	0.54
1:A:323:THR:HG21	1:A:365:VAL:HG11	1.89	0.54
2:F:46:ILE:HG21	2:F:175:THR:HG21	1.89	0.54
1:A:635:LEU:HD22	1:B:579:VAL:HG21	1.90	0.54
1:D:547:GLY:HA2	1:D:550:GLN:NE2	2.22	0.54
1:D:729:SER:HA	1:D:732:ILE:HG22	1.90	0.54
2:E:9:VAL:HG12	2:E:58:TRP:HB2	1.88	0.54
2:H:85:SER:HA	2:H:117:ASN:OD1	2.07	0.54
1:D:502:TYR:HH	1:D:567:TYR:HH	1.56	0.54
1:A:622:LEU:HA	1:A:625:MET:HE3	1.90	0.54
2:H:19:THR:HG23	2:H:39:PHE:HB2	1.88	0.54
1:A:698:LEU:HD11	1:B:583:VAL:HG21	1.90	0.54
1:D:463:TRP:O	1:D:468:ALA:N	2.30	0.54
2:E:16:CYS:O	2:E:117:ASN:ND2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:ASP:O	1:C:219:ARG:HG2	2.07	0.54
2:E:114:LEU:O	2:E:156:TYR:HA	2.08	0.54
1:D:424:LEU:HD23	1:D:433:VAL:HB	1.89	0.54
1:C:482:MET:HE1	1:C:585:GLY:HA3	1.90	0.53
2:F:69:LEU:HA	2:F:72:LEU:HD13	1.90	0.53
1:B:635:LEU:HD22	1:B:695:PHE:CE1	2.36	0.53
1:D:233:ASP:OD1	1:D:236:TYR:N	2.41	0.53
2:H:9:VAL:HG12	2:H:58:TRP:HB2	1.90	0.53
2:H:69:LEU:HA	2:H:72:LEU:HD13	1.90	0.53
1:D:218:GLU:HB3	1:D:223:MET:HE2	1.90	0.53
1:A:190:THR:HA	1:A:233:ASP:HB2	1.91	0.53
2:H:48:VAL:HG23	2:H:49:ASP:H	1.74	0.53
1:D:452:VAL:HG12	1:D:454:PRO:HD2	1.90	0.53
1:C:469:VAL:HG23	1:C:469:VAL:O	2.09	0.52
1:D:614:LEU:HG	1:D:618:LEU:HD23	1.90	0.52
2:F:8:LEU:HB2	2:F:55:LEU:HD11	1.91	0.52
1:B:328:LEU:HD21	1:B:345:MET:HB3	1.91	0.52
1:B:371:LEU:HD11	1:B:379:LYS:HD3	1.89	0.52
1:D:234:ILE:HD12	1:D:237:ARG:HE	1.74	0.52
1:B:590:LEU:HD22	1:B:603:SER:HB3	1.91	0.52
2:E:74:TYR:N	2:E:75:PRO:HD2	2.25	0.52
2:G:61:ALA:HB3	2:G:66:TYR:HD2	1.75	0.52
1:A:694:VAL:HG11	1:B:576:ALA:HB1	1.92	0.52
1:C:202:LEU:HD23	1:C:207:ASN:HB2	1.91	0.52
2:F:147:MET:O	2:F:151:ILE:HG12	2.10	0.52
1:B:218:GLU:HA	1:B:223:MET:HB2	1.91	0.51
1:B:587:MET:HE2	1:B:610:LEU:HD13	1.93	0.51
2:H:8:LEU:HD13	2:H:55:LEU:HD21	1.92	0.51
1:A:215:ASP:O	1:A:218:GLU:HG3	2.10	0.51
1:C:590:LEU:HB3	1:C:603:SER:HB2	1.92	0.51
1:A:237:ARG:NH1	2:E:76:ASP:OD1	2.39	0.51
2:E:8:LEU:HD21	2:E:81:LEU:HD12	1.91	0.51
1:A:471:PHE:CE2	1:A:595:GLY:CA	2.94	0.51
1:C:633:VAL:HG11	1:C:666:PHE:HD1	1.76	0.51
1:C:559:LEU:HB3	1:C:581:ALA:HB2	1.92	0.51
2:H:60:THR:HB	2:H:70:ARG:HG2	1.91	0.51
1:B:711:LEU:O	1:B:715:ILE:HG13	2.11	0.51
2:F:8:LEU:HD21	2:F:81:LEU:HD12	1.93	0.51
2:G:144:GLY:HA3	2:G:156:TYR:CE2	2.45	0.51
1:A:393:GLU:HA	1:A:403:SER:HB2	1.92	0.50
1:A:507:ASP:HA	1:A:510:ARG:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:LEU:HD11	1:B:564:ALA:HB2	1.92	0.50
1:C:195:LEU:HB2	1:C:226:PHE:CZ	2.45	0.50
2:H:8:LEU:HD21	2:H:81:LEU:HD12	1.93	0.50
1:D:215:ASP:O	1:D:218:GLU:HG3	2.11	0.50
1:A:375:MET:HG2	1:A:433:VAL:HG22	1.93	0.50
1:D:215:ASP:O	1:D:219:ARG:HG2	2.11	0.50
1:A:401:HIS:O	1:A:775:ARG:NH2	2.44	0.50
2:F:84:PHE:HB3	2:F:95:ILE:HD11	1.93	0.50
2:H:88:SER:OG	2:H:90:ASP:OD2	2.30	0.50
1:D:195:LEU:HB2	1:D:226:PHE:CZ	2.46	0.50
2:G:48:VAL:HG23	2:G:49:ASP:H	1.76	0.50
1:A:463:TRP:CE2	1:A:468:ALA:CB	2.95	0.50
1:B:601:THR:O	1:B:605:MET:HG3	2.12	0.50
2:G:114:LEU:O	2:G:156:TYR:HA	2.10	0.50
1:B:339:THR:HG21	1:B:384:GLY:HA3	1.92	0.50
2:F:48:VAL:HG23	2:F:49:ASP:H	1.76	0.50
1:C:748:PHE:HB3	1:C:752:LEU:HD23	1.94	0.50
1:A:747:SER:OG	3:A:1201:F9M:C38	2.60	0.49
1:C:552:LEU:HD11	1:C:611:PHE:HE2	1.77	0.49
1:A:166:LEU:HD13	1:A:216:ILE:HD11	1.94	0.49
1:B:443:ILE:HD13	1:B:446:ARG:HH22	1.76	0.49
1:C:763:THR:HB	1:C:774:ARG:HD2	1.94	0.49
1:C:375:MET:HG2	1:C:433:VAL:HG22	1.95	0.49
1:D:192:LYS:HG3	1:D:196:PRO:HB2	1.95	0.49
1:A:466:PHE:HD2	1:A:748:PHE:HE2	1.56	0.49
1:C:616:ARG:HH22	1:D:598:LEU:HD12	1.77	0.49
1:A:408:ASP:OD1	1:A:779:ARG:NH2	2.37	0.49
1:A:452:VAL:HG12	1:A:454:PRO:HD2	1.95	0.49
1:A:767:SER:N	1:A:771:THR:O	2.44	0.48
1:B:525:PHE:HB2	1:B:557:SER:HB2	1.95	0.48
1:D:420:ASP:OD2	1:D:775:ARG:HD3	2.13	0.48
1:D:375:MET:HG2	1:D:433:VAL:HG22	1.95	0.48
1:A:525:PHE:HB2	1:A:557:SER:HB2	1.94	0.48
1:B:531:ASP:OD2	1:B:550:GLN:NE2	2.34	0.48
1:D:625:MET:HE2	1:D:702:TYR:OH	2.13	0.48
2:E:71:PRO:HA	2:E:74:TYR:CD2	2.48	0.48
2:F:63:GLN:HG3	2:F:64:GLU:OE1	2.13	0.48
1:A:622:LEU:HA	1:A:625:MET:HG2	1.95	0.48
1:C:445:ASN:HB3	1:C:449:MET:HE2	1.96	0.48
1:C:559:LEU:HD21	1:C:580:PHE:HD1	1.78	0.48
1:A:704:ILE:O	1:A:708:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:VAL:O	1:B:473:ILE:HG12	2.13	0.48
1:B:628:TYR:CE1	1:C:583:VAL:HG13	2.49	0.48
1:C:471:PHE:CZ	1:C:595:GLY:HA3	2.49	0.48
1:D:149:PHE:HB2	1:D:172:PHE:CD2	2.48	0.48
1:D:597:LYS:HG3	1:D:733:TRP:CZ3	2.48	0.48
1:D:442:LYS:HE2	1:D:442:LYS:HA	1.95	0.48
1:A:475:VAL:HA	1:A:592:PHE:HD1	1.77	0.48
1:C:463:TRP:CD1	1:C:468:ALA:HB2	2.48	0.48
1:C:463:TRP:CH2	1:C:468:ALA:HA	2.49	0.48
1:D:473:ILE:O	1:D:476:VAL:HG22	2.13	0.47
2:E:8:LEU:HD23	2:E:57:LEU:HD23	1.94	0.47
1:A:525:PHE:CE1	1:A:529:ILE:HD11	2.49	0.47
1:B:297:GLN:OE1	1:B:300:ILE:HD12	2.13	0.47
1:D:466:PHE:HB3	1:D:756:PHE:CD2	2.50	0.47
1:A:463:TRP:CZ3	1:A:468:ALA:HA	2.49	0.47
1:B:715:ILE:O	1:B:718:MET:HG3	2.14	0.47
2:E:8:LEU:HB2	2:E:55:LEU:HD11	1.96	0.47
2:E:147:MET:O	2:E:151:ILE:HG12	2.13	0.47
1:A:329:VAL:HG22	1:A:385:ILE:HD13	1.97	0.47
1:A:680:MET:N	1:A:680:MET:HE2	2.29	0.47
1:B:234:ILE:HD12	1:B:237:ARG:HE	1.80	0.47
1:D:566:LEU:O	1:D:570:GLY:N	2.47	0.47
1:A:328:LEU:HG	1:A:342:VAL:HG13	1.95	0.47
1:A:386:PHE:HE2	1:A:452:VAL:HG21	1.79	0.47
1:B:207:ASN:O	1:B:253:TYR:OH	2.31	0.47
1:C:715:ILE:HD11	1:D:717:LEU:HB3	1.96	0.47
2:E:69:LEU:HA	2:E:72:LEU:HD13	1.97	0.47
2:E:154:PHE:CE2	2:E:177:ALA:HB2	2.50	0.47
2:F:16:CYS:HB2	2:F:117:ASN:HD21	1.79	0.47
2:H:6:LYS:NZ	2:H:178:ALA:O	2.48	0.47
1:A:195:LEU:HB2	1:A:226:PHE:CZ	2.50	0.47
1:D:426:THR:HG21	1:D:430:GLU:H	1.80	0.47
1:B:767:SER:N	1:B:771:THR:O	2.47	0.46
1:C:218:GLU:HB3	1:C:223:MET:HG3	1.97	0.46
2:F:37:THR:HG23	2:F:38:VAL:HG22	1.97	0.46
1:C:421:LEU:HD23	1:C:778:PHE:HB2	1.97	0.46
1:D:214:LEU:HB3	1:D:223:MET:HE1	1.98	0.46
2:H:147:MET:O	2:H:151:ILE:HG12	2.15	0.46
1:B:635:LEU:HD12	1:C:579:VAL:HG21	1.97	0.46
2:H:7:LYS:HE3	2:H:58:TRP:CE2	2.50	0.46
1:A:463:TRP:NE1	1:A:468:ALA:HB2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:TYR:CD2	1:B:702:TYR:HD1	2.33	0.46
2:F:13:ASP:OD2	2:F:13:ASP:N	2.46	0.46
1:B:219:ARG:HA	1:B:219:ARG:NE	2.30	0.46
1:C:225:GLU:OE2	2:G:41:ASN:ND2	2.27	0.46
1:D:498:PRO:HD2	1:D:571:ILE:HA	1.96	0.46
1:A:255:GLU:HG2	1:A:303:TYR:CZ	2.50	0.46
1:B:761:MET:O	1:B:761:MET:HG3	2.16	0.46
1:C:192:LYS:HG3	1:C:196:PRO:HB2	1.97	0.46
1:D:202:LEU:HD23	1:D:207:ASN:HB2	1.98	0.46
2:G:93:GLU:O	2:G:97:GLU:HG3	2.16	0.46
1:A:405:LYS:HD2	1:A:419:TYR:CZ	2.50	0.46
1:D:633:VAL:HG11	1:D:666:PHE:HD1	1.81	0.46
2:G:3:ALA:HA	2:G:52:GLN:O	2.16	0.46
1:A:338:ASN:HA	1:A:341:PHE:CE1	2.51	0.45
1:A:598:LEU:HB3	1:D:616:ARG:NH1	2.31	0.45
1:A:386:PHE:CE2	1:A:452:VAL:HG21	2.51	0.45
1:A:679:GLY:C	1:A:680:MET:HE2	2.42	0.45
1:D:258:VAL:HA	1:D:262:ALA:HB3	1.98	0.45
1:D:323:THR:OG1	1:D:326:HIS:ND1	2.42	0.45
1:A:475:VAL:HA	1:A:592:PHE:CD1	2.51	0.45
2:E:176:ARG:HA	2:E:179:LEU:HG	1.99	0.45
1:D:383:ILE:HD13	1:D:449:MET:HG3	1.98	0.45
2:F:71:PRO:HA	2:F:74:TYR:CD2	2.51	0.45
1:A:192:LYS:HG3	1:A:196:PRO:HB2	1.99	0.45
1:B:598:LEU:O	1:B:602:TYR:HD1	2.00	0.45
1:C:486:THR:HG22	1:C:582:LEU:HD11	1.96	0.45
1:C:518:LEU:HD11	1:C:564:ALA:HB2	1.99	0.45
1:C:421:LEU:HD13	1:C:425:ASP:HB3	1.98	0.45
1:D:710:LEU:O	1:D:714:LEU:HG	2.17	0.45
1:D:562:VAL:O	1:D:566:LEU:HG	2.16	0.45
2:E:66:TYR:O	2:E:70:ARG:HG3	2.17	0.45
2:F:7:LYS:HE2	2:F:58:TRP:CE2	2.51	0.45
1:C:664:GLU:O	1:C:668:THR:HG23	2.16	0.45
1:B:478:TYR:HE2	1:B:589:ALA:HA	1.81	0.45
1:D:413:PRO:HG3	1:D:788:TRP:HH2	1.80	0.45
1:A:207:ASN:O	1:A:253:TYR:OH	2.28	0.45
2:E:45:ASP:OD1	2:E:54:GLU:HG2	2.17	0.45
1:C:313:ASP:OD1	1:C:313:ASP:N	2.50	0.44
1:A:218:GLU:HB3	1:A:223:MET:HG3	1.99	0.44
1:B:372:SER:OG	1:B:375:MET:HG3	2.17	0.44
1:C:628:TYR:HD2	1:C:702:TYR:CD1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:12:GLY:HA3	2:E:83:CYS:SG	2.57	0.44
1:A:614:LEU:HG	1:A:618:LEU:HD23	1.99	0.44
1:B:682:ASP:OD1	1:B:682:ASP:N	2.49	0.44
2:H:175:THR:O	2:H:179:LEU:HG	2.17	0.44
1:A:202:LEU:HD23	1:A:207:ASN:HB2	1.99	0.44
1:A:552:LEU:HD21	1:A:607:GLN:HE22	1.82	0.44
1:A:763:THR:HB	1:A:774:ARG:HD2	2.00	0.44
1:B:328:LEU:HD12	1:B:331:ILE:HD11	2.00	0.44
1:C:329:VAL:HG22	1:C:385:ILE:HD13	1.99	0.44
2:E:60:THR:OG1	2:E:70:ARG:HG2	2.18	0.44
2:E:63:GLN:HG3	2:E:64:GLU:OE1	2.17	0.44
1:C:249:ARG:HG2	1:C:297:GLN:NE2	2.32	0.44
1:C:584:LEU:HG	1:C:588:ASN:HD21	1.82	0.44
1:A:163:THR:HG22	1:A:209:THR:HG22	2.00	0.44
1:A:691:TYR:HB2	1:A:695:PHE:HE1	1.82	0.44
1:D:255:GLU:HG2	1:D:303:TYR:CZ	2.53	0.44
2:F:60:THR:HB	2:F:70:ARG:HG2	1.99	0.44
1:C:247:GLU:OE2	1:C:248:ARG:NH2	2.51	0.44
1:C:635:LEU:HB2	1:D:579:VAL:HG21	1.99	0.44
1:A:748:PHE:HB3	1:A:752:LEU:HD23	2.00	0.44
1:C:153:ILE:HG13	1:C:154:LEU:N	2.32	0.44
2:G:11:VAL:HG12	2:G:60:THR:HG21	1.99	0.44
1:A:471:PHE:HE2	1:A:595:GLY:HA3	1.82	0.43
1:A:573:ALA:O	1:A:577:VAL:HG22	2.17	0.43
1:C:258:VAL:HA	1:C:262:ALA:HB3	2.00	0.43
2:E:82:MET:HE3	2:E:82:MET:HB2	1.85	0.43
2:G:145:ARG:NH2	2:G:156:TYR:O	2.50	0.43
1:A:582:LEU:HD23	1:A:586:TRP:HD1	1.83	0.43
1:B:418:LEU:HD23	1:B:418:LEU:H	1.82	0.43
1:B:482:MET:HE1	1:B:585:GLY:HA3	2.00	0.43
1:B:713:MET:SD	1:B:714:LEU:N	2.91	0.43
2:E:98:LYS:O	2:E:102:GLU:HG3	2.18	0.43
1:C:767:SER:N	1:C:771:THR:O	2.43	0.43
1:D:313:ASP:N	1:D:313:ASP:OD1	2.49	0.43
1:A:466:PHE:HD2	1:A:748:PHE:CE2	2.34	0.43
1:B:323:THR:HG1	1:B:326:HIS:CE1	2.37	0.43
2:E:165:ASP:OD1	2:E:165:ASP:N	2.51	0.43
1:D:218:GLU:OE2	1:D:219:ARG:NE	2.48	0.43
1:A:607:GLN:OE1	1:A:607:GLN:HA	2.19	0.43
1:B:313:ASP:N	1:B:313:ASP:OD1	2.49	0.43
1:B:671:LEU:HA	1:B:674:PHE:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:VAL:HG22	1:D:385:ILE:HD13	2.00	0.43
1:D:442:LYS:HG3	1:D:444:GLU:OE1	2.19	0.43
2:E:20:CYS:HA	2:E:23:ILE:HG22	2.01	0.43
2:F:89:PRO:O	2:F:92:LEU:HG	2.18	0.43
1:D:518:LEU:HD11	1:D:564:ALA:HB2	1.99	0.43
2:E:48:VAL:HG23	2:E:49:ASP:H	1.83	0.43
2:G:6:LYS:NZ	2:G:178:ALA:O	2.49	0.43
1:A:362:LEU:O	1:A:365:VAL:HG12	2.19	0.43
1:A:424:LEU:HD23	1:A:433:VAL:HB	2.01	0.43
1:B:323:THR:HG21	1:B:365:VAL:HG11	2.00	0.43
1:B:345:MET:HE2	1:B:345:MET:HB2	1.93	0.43
1:B:608:LYS:HE2	1:B:608:LYS:HB3	1.83	0.43
1:B:698:LEU:HD23	1:B:698:LEU:HA	1.87	0.43
1:B:711:LEU:HD12	1:C:714:LEU:HD13	2.01	0.43
1:C:418:LEU:HD23	1:C:418:LEU:H	1.83	0.43
1:D:155:PHE:HA	1:D:158:VAL:HG12	2.01	0.43
1:D:195:LEU:HB3	1:D:196:PRO:HD3	2.01	0.43
2:E:19:THR:HG23	2:E:39:PHE:HB2	2.01	0.43
1:A:418:LEU:HD23	1:A:418:LEU:H	1.84	0.43
1:A:421:LEU:HD13	1:A:425:ASP:HB3	2.01	0.43
1:C:155:PHE:HA	1:C:158:VAL:HG12	2.00	0.43
1:A:317:GLN:HG2	1:A:323:THR:HG22	1.99	0.42
1:B:697:ILE:O	1:B:701:THR:HG23	2.19	0.42
1:C:255:GLU:HG2	1:C:303:TYR:CZ	2.54	0.42
1:A:633:VAL:HG12	1:B:490:TYR:HE1	1.84	0.42
1:C:635:LEU:HG	1:D:575:LEU:HB3	2.02	0.42
1:A:313:ASP:OD1	1:A:313:ASP:N	2.50	0.42
1:B:307:ASN:ND2	1:B:310:LYS:O	2.50	0.42
1:B:514:GLU:O	1:B:518:LEU:HD23	2.19	0.42
1:C:223:MET:O	1:C:227:ILE:HG12	2.19	0.42
2:F:21:LEU:HA	2:F:24:VAL:HG12	2.01	0.42
1:A:505:THR:HA	1:A:508:TYR:HD2	1.83	0.42
2:G:131:LEU:HD23	2:G:131:LEU:HA	1.86	0.42
1:C:510:ARG:HA	1:C:510:ARG:HD3	1.89	0.42
2:F:92:LEU:HD23	2:F:139:VAL:HG22	2.02	0.42
1:A:576:ALA:O	1:A:579:VAL:HG12	2.20	0.42
1:B:502:TYR:HA	1:B:507:ASP:HB3	2.02	0.42
1:A:155:PHE:HA	1:A:158:VAL:HG12	2.02	0.42
1:A:383:ILE:HD13	1:A:449:MET:SD	2.60	0.42
1:A:437:LEU:HD21	1:A:449:MET:HB2	2.02	0.42
1:B:636:LEU:HD12	1:B:695:PHE:HZ	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:562:VAL:HG22	1:C:566:LEU:HD23	2.01	0.42
1:C:697:ILE:O	1:C:701:THR:HG23	2.20	0.42
1:C:721:THR:OG1	1:C:725:VAL:HG23	2.19	0.42
1:D:466:PHE:HZ	1:D:745:GLU:HG3	1.83	0.42
2:E:8:LEU:HD12	2:E:79:VAL:HG13	2.02	0.42
2:E:11:VAL:HG12	2:E:60:THR:HG21	2.01	0.42
2:F:8:LEU:HD23	2:F:57:LEU:HD23	2.01	0.42
1:A:691:TYR:HB2	1:A:695:PHE:CE1	2.55	0.42
1:B:442:LYS:HZ2	1:B:445:ASN:N	2.17	0.42
1:C:345:MET:HB2	1:C:345:MET:HE3	1.79	0.42
1:A:179:ARG:HB3	1:A:222:ASN:ND2	2.34	0.42
1:A:218:GLU:HA	1:A:223:MET:HB2	2.01	0.42
1:B:218:GLU:HB3	1:B:223:MET:SD	2.60	0.42
1:B:219:ARG:HA	1:B:219:ARG:CZ	2.50	0.42
2:H:84:PHE:HB3	2:H:95:ILE:HD11	2.01	0.42
1:A:333:ASP:HB2	1:A:338:ASN:HD22	1.85	0.42
1:A:590:LEU:HB3	1:A:603:SER:CB	2.50	0.42
1:A:608:LYS:HB3	1:A:608:LYS:HE2	1.79	0.42
1:B:223:MET:O	1:B:227:ILE:HG13	2.19	0.42
2:E:89:PRO:O	2:E:92:LEU:HG	2.20	0.42
2:E:144:GLY:HA3	2:E:156:TYR:CE2	2.55	0.42
1:C:232:ARG:HH11	2:G:72:LEU:HD22	1.85	0.41
1:C:333:ASP:HB2	1:C:338:ASN:HD22	1.85	0.41
1:D:498:PRO:HA	1:D:499:PRO:C	2.45	0.41
2:H:71:PRO:HA	2:H:74:TYR:CD2	2.55	0.41
1:D:224:ARG:HH22	2:H:39:PHE:HE1	1.69	0.41
1:D:721:THR:O	1:D:725:VAL:HG23	2.20	0.41
2:F:88:SER:O	2:F:91:SER:OG	2.36	0.41
2:G:79:VAL:HB	2:G:178:ALA:HB2	2.00	0.41
2:H:154:PHE:HD2	2:H:177:ALA:HB2	1.86	0.41
1:A:248:ARG:HD2	1:A:248:ARG:HA	1.80	0.41
1:A:342:VAL:HG12	1:A:385:ILE:HD12	2.02	0.41
1:B:289:LEU:HD11	1:B:301:VAL:HG13	2.02	0.41
1:C:584:LEU:HA	1:C:587:MET:HG2	2.01	0.41
1:D:601:THR:HB	1:D:605:MET:HE1	2.02	0.41
2:E:145:ARG:NH2	2:E:156:TYR:HD2	2.17	0.41
2:F:145:ARG:NH2	2:F:156:TYR:HD2	2.18	0.41
2:H:20:CYS:HA	2:H:23:ILE:HG22	2.03	0.41
1:D:338:ASN:HA	1:D:341:PHE:CE1	2.56	0.41
1:D:482:MET:HE1	1:D:585:GLY:CA	2.50	0.41
2:F:175:THR:O	2:F:179:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:147:MET:O	2:G:151:ILE:HG12	2.20	0.41
1:A:442:LYS:NZ	1:A:444:GLU:HB2	2.35	0.41
1:D:183:GLU:HA	1:D:186:ARG:HD2	2.02	0.41
1:D:223:MET:HE3	1:D:260:GLN:HG2	2.02	0.41
1:D:418:LEU:H	1:D:418:LEU:HD23	1.86	0.41
1:D:609:ILE:HG12	1:D:717:LEU:HD21	2.02	0.41
2:G:118:LYS:HB3	2:G:121:LEU:HG	2.02	0.41
1:A:463:TRP:CE3	1:A:467:GLY:C	2.98	0.41
1:C:169:LEU:HD22	1:C:216:ILE:HD13	2.02	0.41
1:C:438:VAL:O	1:C:446:ARG:NE	2.52	0.41
2:H:92:LEU:HD12	2:H:93:GLU:N	2.36	0.41
1:B:170:LEU:HB3	1:B:171:PRO:HD3	2.03	0.41
1:B:184:GLU:HB2	1:B:185:PHE:HD2	1.86	0.41
1:C:195:LEU:HB3	1:C:196:PRO:HD3	2.02	0.41
1:C:289:LEU:HD11	1:C:301:VAL:HG13	2.01	0.41
1:D:345:MET:HE2	1:D:345:MET:HB2	1.93	0.41
1:C:434:LEU:HD12	1:C:434:LEU:HA	1.96	0.41
1:C:442:LYS:NZ	1:C:445:ASN:HB2	2.36	0.41
1:D:223:MET:O	1:D:227:ILE:HG13	2.20	0.41
1:D:379:LYS:HB3	1:D:436:ILE:CG2	2.50	0.41
2:E:162:LYS:O	2:E:164:LYS:NZ	2.54	0.41
2:G:151:ILE:HD11	2:G:153:ALA:HB2	2.03	0.41
2:H:118:LYS:HB3	2:H:121:LEU:HG	2.03	0.41
1:A:284:PHE:CD2	1:A:291:LEU:HD13	2.56	0.41
1:A:590:LEU:O	1:A:593:THR:OG1	2.29	0.41
1:A:597:LYS:O	1:A:601:THR:OG1	2.17	0.41
1:B:393:GLU:HA	1:B:403:SER:HB2	2.02	0.41
1:B:635:LEU:HD21	1:B:691:TYR:HD2	1.86	0.41
1:C:179:ARG:HB3	1:C:222:ASN:ND2	2.36	0.41
1:D:149:PHE:HA	1:D:153:ILE:HD11	2.03	0.41
1:D:552:LEU:HD11	1:D:611:PHE:CE2	2.53	0.41
2:F:85:SER:HA	2:F:117:ASN:OD1	2.21	0.41
2:G:55:LEU:HD13	2:G:175:THR:HG22	2.02	0.41
1:A:332:ALA:HB2	1:A:342:VAL:HG11	2.02	0.41
1:A:425:ASP:HB2	1:A:458:LEU:HD21	2.03	0.41
1:A:583:VAL:HG13	1:D:628:TYR:HE1	1.86	0.41
1:A:512:ALA:HA	1:A:515:VAL:HG22	2.04	0.40
1:B:362:LEU:O	1:B:365:VAL:HG12	2.21	0.40
1:C:737:TRP:NE1	1:C:741:ILE:HD11	2.36	0.40
1:D:463:TRP:CZ2	1:D:468:ALA:HA	2.56	0.40
1:D:628:TYR:CD2	1:D:702:TYR:HD1	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:PHE:CE2	1:A:595:GLY:HA3	2.56	0.40
1:C:323:THR:OG1	1:C:326:HIS:ND1	2.44	0.40
1:C:546:ASP:HB2	1:C:736:GLN:HE22	1.85	0.40
1:D:362:LEU:O	1:D:365:VAL:HG12	2.21	0.40
1:B:413:PRO:HG3	1:B:785:TRP:CZ3	2.57	0.40
1:B:549:PHE:CE2	1:B:607:GLN:HG2	2.55	0.40
1:C:485:PHE:CE1	1:C:582:LEU:HD12	2.56	0.40
1:C:543:LEU:O	1:C:548:SER:HB3	2.21	0.40
1:D:725:VAL:O	1:D:729:SER:HB2	2.21	0.40
2:E:57:LEU:O	2:E:58:TRP:HD1	2.05	0.40
2:G:20:CYS:HA	2:G:23:ILE:HG22	2.02	0.40
1:A:426:THR:HG21	1:A:430:GLU:H	1.86	0.40
1:D:597:LYS:HA	1:D:733:TRP:CH2	2.57	0.40
1:D:599:THR:HA	1:D:602:TYR:HB2	2.03	0.40
2:E:122:ARG:HH22	2:E:141:PRO:HD3	1.86	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	616/1144 (54%)	589 (96%)	27 (4%)	0	100	100
1	B	616/1144 (54%)	596 (97%)	20 (3%)	0	100	100
1	C	616/1144 (54%)	589 (96%)	27 (4%)	0	100	100
1	D	616/1144 (54%)	594 (96%)	22 (4%)	0	100	100
2	E	180/193 (93%)	174 (97%)	6 (3%)	0	100	100
2	F	180/193 (93%)	173 (96%)	7 (4%)	0	100	100
2	G	180/193 (93%)	173 (96%)	7 (4%)	0	100	100
2	H	180/193 (93%)	174 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3184/5348 (60%)	3062 (96%)	122 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	525/991 (53%)	521 (99%)	4 (1%)	73	77
1	B	525/991 (53%)	525 (100%)	0	100	100
1	C	525/991 (53%)	521 (99%)	4 (1%)	73	77
1	D	525/991 (53%)	523 (100%)	2 (0%)	84	82
2	E	120/167 (72%)	120 (100%)	0	100	100
2	F	120/167 (72%)	120 (100%)	0	100	100
2	G	120/167 (72%)	120 (100%)	0	100	100
2	H	120/167 (72%)	120 (100%)	0	100	100
All	All	2580/4632 (56%)	2570 (100%)	10 (0%)	81	82

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	473	ILE
1	A	474	ASN
1	A	475	VAL
1	A	736	GLN
1	C	469	VAL
1	C	470	SER
1	C	473	ILE
1	C	475	VAL
1	D	469	VAL
1	D	473	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	A	309	HIS
1	A	368	ASN
1	A	474	ASN
1	B	260	GLN
1	B	338	ASN
1	B	474	ASN
1	B	736	GLN
1	C	307	ASN
1	D	309	HIS
1	D	368	ASN
1	D	474	ASN
1	D	712	ASN
2	E	63	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are 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
3	F9M	B	1201	-	44,44,44	6.14	32 (72%)	59,66,66	6.34	26 (44%)
3	F9M	A	1201	-	44,44,44	5.98	32 (72%)	59,66,66	6.37	26 (44%)
3	F9M	D	1201	-	44,44,44	6.16	32 (72%)	59,66,66	6.27	23 (38%)
3	F9M	C	1201	-	44,44,44	6.15	32 (72%)	59,66,66	6.31	22 (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
3	F9M	B	1201	-	-	13/26/47/47	0/6/6/6
3	F9M	A	1201	-	-	4/26/47/47	0/7/6/6
3	F9M	D	1201	-	-	6/26/47/47	0/6/6/6
3	F9M	C	1201	-	-	4/26/47/47	0/6/6/6

All (128) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1201	F9M	C32-S01	-14.92	1.54	1.74
3	D	1201	F9M	C32-S01	-14.68	1.54	1.74
3	C	1201	F9M	C32-S01	-14.64	1.54	1.74
3	B	1201	F9M	C32-S01	-14.62	1.54	1.74
3	A	1201	F9M	C35-S02	-11.64	1.50	1.74
3	D	1201	F9M	C35-S02	-11.14	1.51	1.74
3	B	1201	F9M	C35-S02	-11.02	1.51	1.74
3	C	1201	F9M	C35-S02	-11.00	1.51	1.74
3	D	1201	F9M	C36-N14	9.58	1.57	1.38
3	C	1201	F9M	C36-N14	9.56	1.57	1.38
3	B	1201	F9M	C36-N14	9.53	1.57	1.38
3	A	1201	F9M	C36-N14	9.27	1.56	1.38
3	C	1201	F9M	C22-N09	9.03	1.49	1.34
3	D	1201	F9M	C22-N10	9.02	1.49	1.34
3	C	1201	F9M	C26-C28	8.81	1.49	1.38
3	B	1201	F9M	C26-C28	8.79	1.49	1.38
3	D	1201	F9M	C27-C28	8.78	1.49	1.38
3	B	1201	F9M	C25-C23	8.77	1.53	1.39
3	C	1201	F9M	C22-N10	8.72	1.49	1.34
3	D	1201	F9M	C25-C23	8.72	1.53	1.39
3	B	1201	F9M	C33-N13	8.69	1.57	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1201	F9M	C27-C28	8.66	1.49	1.38
3	B	1201	F9M	C22-N09	8.61	1.48	1.34
3	D	1201	F9M	C33-N13	8.59	1.57	1.38
3	D	1201	F9M	C22-N09	8.59	1.48	1.34
3	B	1201	F9M	C22-N10	8.56	1.48	1.34
3	D	1201	F9M	C26-C28	8.56	1.49	1.38
3	C	1201	F9M	C33-N13	8.56	1.56	1.38
3	A	1201	F9M	C34-S01	-8.54	1.50	1.71
3	C	1201	F9M	C27-C28	8.51	1.49	1.38
3	C	1201	F9M	C25-C23	8.46	1.52	1.39
3	A	1201	F9M	C26-C28	8.45	1.49	1.38
3	A	1201	F9M	C25-C23	8.45	1.52	1.39
3	D	1201	F9M	C34-S01	-8.32	1.51	1.71
3	C	1201	F9M	C34-S01	-8.30	1.51	1.71
3	B	1201	F9M	C34-S01	-8.27	1.51	1.71
3	A	1201	F9M	C27-C28	8.22	1.48	1.38
3	A	1201	F9M	C22-N10	8.22	1.48	1.34
3	B	1201	F9M	C30-N11	8.21	1.49	1.34
3	A	1201	F9M	C37-S02	-8.17	1.52	1.73
3	D	1201	F9M	C30-N11	8.15	1.49	1.34
3	A	1201	F9M	C33-N13	8.14	1.56	1.38
3	A	1201	F9M	C22-N09	8.12	1.48	1.34
3	C	1201	F9M	C30-N11	8.03	1.48	1.34
3	A	1201	F9M	C30-N11	7.81	1.48	1.34
3	D	1201	F9M	C37-S02	-7.76	1.53	1.73
3	C	1201	F9M	C37-S02	-7.71	1.54	1.73
3	B	1201	F9M	C37-S02	-7.65	1.54	1.73
3	B	1201	F9M	C32-N13	7.30	1.42	1.31
3	D	1201	F9M	C32-N13	7.17	1.42	1.31
3	C	1201	F9M	C32-N13	7.16	1.42	1.31
3	B	1201	F9M	C25-N11	7.05	1.48	1.34
3	D	1201	F9M	C25-N11	7.00	1.48	1.34
3	C	1201	F9M	C25-N11	6.85	1.48	1.34
3	C	1201	F9M	C29-C24	6.85	1.49	1.38
3	A	1201	F9M	C25-N11	6.82	1.48	1.34
3	A	1201	F9M	C16-N07	-6.74	1.39	1.47
3	A	1201	F9M	C15-N07	-6.73	1.39	1.47
3	D	1201	F9M	C29-C24	6.68	1.49	1.38
3	D	1201	F9M	C24-C23	6.68	1.49	1.39
3	B	1201	F9M	C29-C24	6.66	1.49	1.38
3	C	1201	F9M	C24-C23	6.66	1.49	1.39
3	B	1201	F9M	C24-C23	6.59	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1201	F9M	C32-N13	6.55	1.41	1.31
3	A	1201	F9M	C24-C23	6.14	1.48	1.39
3	C	1201	F9M	C29-C30	6.13	1.53	1.39
3	B	1201	F9M	C32-N12	6.09	1.45	1.36
3	A	1201	F9M	C29-C24	6.08	1.48	1.38
3	D	1201	F9M	C29-C30	6.05	1.53	1.39
3	C	1201	F9M	C16-N07	-6.05	1.40	1.47
3	B	1201	F9M	C29-C30	6.03	1.53	1.39
3	D	1201	F9M	C16-N07	-6.02	1.40	1.47
3	C	1201	F9M	C32-N12	5.96	1.45	1.36
3	D	1201	F9M	C32-N12	5.90	1.45	1.36
3	D	1201	F9M	C15-N07	-5.87	1.40	1.47
3	C	1201	F9M	C15-N07	-5.84	1.40	1.47
3	B	1201	F9M	C16-N07	-5.83	1.40	1.47
3	B	1201	F9M	C15-N07	-5.82	1.40	1.47
3	A	1201	F9M	C29-C30	5.67	1.52	1.39
3	D	1201	F9M	C27-N10	5.56	1.45	1.34
3	C	1201	F9M	C26-N09	5.55	1.45	1.34
3	A	1201	F9M	C32-N12	5.47	1.45	1.36
3	B	1201	F9M	C26-N09	5.46	1.45	1.34
3	B	1201	F9M	C27-N10	5.35	1.45	1.34
3	D	1201	F9M	C26-N09	5.35	1.45	1.34
3	C	1201	F9M	C21-N07	5.34	1.45	1.35
3	B	1201	F9M	C21-N07	5.33	1.45	1.35
3	C	1201	F9M	C27-N10	5.30	1.45	1.34
3	D	1201	F9M	C21-N07	5.18	1.45	1.35
3	C	1201	F9M	C20-N08	5.18	1.56	1.46
3	A	1201	F9M	C27-N10	5.11	1.44	1.34
3	A	1201	F9M	C26-N09	5.10	1.44	1.34
3	D	1201	F9M	C20-N08	4.86	1.55	1.46
3	B	1201	F9M	C20-N08	4.84	1.55	1.46
3	D	1201	F9M	C19-N08	4.81	1.55	1.46
3	B	1201	F9M	C19-N08	4.76	1.55	1.46
3	A	1201	F9M	C20-N08	4.67	1.55	1.46
3	C	1201	F9M	C19-N08	4.66	1.55	1.46
3	B	1201	F9M	C22-N08	4.66	1.45	1.35
3	D	1201	F9M	C22-N08	4.64	1.45	1.35
3	C	1201	F9M	C22-N08	4.56	1.45	1.35
3	C	1201	F9M	C34-C33	4.51	1.44	1.36
3	D	1201	F9M	C34-C33	4.41	1.44	1.36
3	A	1201	F9M	C21-N07	4.36	1.43	1.35
3	B	1201	F9M	C34-C33	4.34	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1201	F9M	C33-C35	4.25	1.53	1.44
3	B	1201	F9M	C33-C35	4.20	1.53	1.44
3	C	1201	F9M	C35-C36	4.08	1.44	1.37
3	D	1201	F9M	C33-C35	4.07	1.52	1.44
3	A	1201	F9M	C34-C33	4.07	1.43	1.36
3	A	1201	F9M	C22-N08	4.05	1.44	1.35
3	B	1201	F9M	C35-C36	4.02	1.44	1.37
3	D	1201	F9M	C35-C36	3.99	1.44	1.37
3	A	1201	F9M	C19-N08	3.97	1.53	1.46
3	A	1201	F9M	C18-C17	-3.60	1.44	1.54
3	D	1201	F9M	C37-N14	3.56	1.42	1.31
3	B	1201	F9M	C37-N14	3.52	1.42	1.31
3	C	1201	F9M	C37-N14	3.50	1.42	1.31
3	C	1201	F9M	C18-C17	-3.46	1.44	1.54
3	D	1201	F9M	C18-C17	-3.41	1.44	1.54
3	B	1201	F9M	C18-C17	-3.41	1.44	1.54
3	A	1201	F9M	C37-N14	3.40	1.41	1.31
3	A	1201	F9M	C33-C35	3.13	1.51	1.44
3	A	1201	F9M	C35-C36	3.02	1.42	1.37
3	B	1201	F9M	C30-N12	2.36	1.45	1.40
3	C	1201	F9M	C30-N12	2.29	1.45	1.40
3	D	1201	F9M	C30-N12	2.19	1.45	1.40
3	A	1201	F9M	O06-C21	-2.07	1.18	1.22

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1201	F9M	C37-S02-C35	34.47	107.81	89.55
3	B	1201	F9M	C37-S02-C35	34.30	107.72	89.55
3	D	1201	F9M	C37-S02-C35	34.16	107.65	89.55
3	A	1201	F9M	C37-S02-C35	33.53	107.32	89.55
3	A	1201	F9M	C34-S01-C32	25.48	108.22	88.40
3	B	1201	F9M	C34-S01-C32	25.05	107.89	88.40
3	C	1201	F9M	C34-S01-C32	24.75	107.65	88.40
3	D	1201	F9M	C34-S01-C32	24.68	107.60	88.40
3	A	1201	F9M	C35-C36-N14	-10.51	107.60	114.97
3	D	1201	F9M	C35-C36-N14	-10.04	107.93	114.97
3	C	1201	F9M	C35-C36-N14	-9.92	108.01	114.97
3	C	1201	F9M	S02-C37-N14	-9.68	107.97	114.64
3	B	1201	F9M	C35-C36-N14	-9.66	108.20	114.97
3	B	1201	F9M	S02-C37-N14	-9.55	108.06	114.64
3	A	1201	F9M	S02-C37-N14	-9.52	108.08	114.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1201	F9M	S02-C37-N14	-9.47	108.12	114.64
3	B	1201	F9M	S01-C32-N13	-8.03	107.26	115.69
3	C	1201	F9M	S01-C32-N13	-7.70	107.61	115.69
3	D	1201	F9M	S01-C32-N13	-7.43	107.88	115.69
3	A	1201	F9M	S01-C32-N13	-7.42	107.90	115.69
3	A	1201	F9M	C18-C16-C20	-6.04	106.02	111.70
3	A	1201	F9M	C27-C28-C26	6.02	120.35	114.63
3	C	1201	F9M	C27-N10-C22	5.65	120.68	115.68
3	B	1201	F9M	C34-C33-N13	-5.64	107.67	115.43
3	C	1201	F9M	C34-C33-N13	-5.59	107.74	115.43
3	D	1201	F9M	C26-N09-C22	5.59	120.63	115.68
3	D	1201	F9M	C27-C28-C26	5.57	119.92	114.63
3	B	1201	F9M	C27-C28-C26	5.50	119.86	114.63
3	C	1201	F9M	C27-C28-C26	5.48	119.83	114.63
3	A	1201	F9M	C17-C15-C19	-5.46	106.56	111.70
3	D	1201	F9M	C34-C33-N13	-5.32	108.11	115.43
3	B	1201	F9M	C26-N09-C22	5.12	120.21	115.68
3	B	1201	F9M	C27-N10-C22	5.05	120.15	115.68
3	A	1201	F9M	C30-N12-C32	-4.72	120.80	126.67
3	B	1201	F9M	C18-C16-C20	-4.69	107.29	111.70
3	B	1201	F9M	N10-C22-N09	-4.56	119.99	127.06
3	A	1201	F9M	C27-N10-C22	4.54	119.70	115.68
3	A	1201	F9M	C26-N09-C22	4.49	119.66	115.68
3	C	1201	F9M	C28-C27-N10	-4.43	119.22	123.38
3	D	1201	F9M	C28-C26-N09	-4.33	119.32	123.38
3	A	1201	F9M	C34-C33-N13	-4.32	109.49	115.43
3	D	1201	F9M	N10-C22-N08	4.31	121.38	116.90
3	D	1201	F9M	C18-C16-C20	-4.25	107.70	111.70
3	C	1201	F9M	C18-C16-C20	-4.24	107.71	111.70
3	D	1201	F9M	C17-C15-C19	-4.21	107.74	111.70
3	B	1201	F9M	C17-C15-C19	-4.18	107.77	111.70
3	D	1201	F9M	N10-C22-N09	-4.17	120.60	127.06
3	C	1201	F9M	N10-C22-N09	-4.05	120.78	127.06
3	A	1201	F9M	N10-C22-N09	-3.95	120.93	127.06
3	A	1201	F9M	C28-C27-N10	-3.95	119.67	123.38
3	A	1201	F9M	C28-C26-N09	-3.93	119.69	123.38
3	C	1201	F9M	N09-C22-N08	3.89	120.94	116.90
3	A	1201	F9M	C38-C36-N14	3.84	127.02	119.32
3	B	1201	F9M	C28-C26-N09	-3.83	119.79	123.38
3	C	1201	F9M	C17-C15-C19	-3.70	108.22	111.70
3	B	1201	F9M	C28-C27-N10	-3.60	120.00	123.38
3	B	1201	F9M	C36-C35-S02	-3.43	107.80	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1201	F9M	C36-C35-S02	-3.41	107.81	109.94
3	C	1201	F9M	C16-C20-N08	3.35	113.79	109.47
3	B	1201	F9M	N09-C22-N08	3.33	120.36	116.90
3	D	1201	F9M	C27-N10-C22	3.23	118.54	115.68
3	D	1201	F9M	C38-C36-N14	3.15	125.64	119.32
3	B	1201	F9M	C25-N11-C30	3.14	120.78	117.83
3	A	1201	F9M	C33-C34-S01	-3.11	106.64	110.24
3	C	1201	F9M	C17-C15-N07	3.09	105.04	101.68
3	A	1201	F9M	C24-C23-C25	3.08	121.04	117.61
3	A	1201	F9M	C33-C35-C36	-2.98	125.69	129.60
3	B	1201	F9M	C38-C36-N14	2.97	125.28	119.32
3	D	1201	F9M	C36-C35-S02	-2.95	108.09	109.94
3	A	1201	F9M	C15-C19-N08	-2.76	105.92	109.47
3	A	1201	F9M	C17-C15-N07	2.74	104.66	101.68
3	A	1201	F9M	C16-C20-N08	2.74	112.99	109.47
3	C	1201	F9M	S01-C32-N12	2.72	129.31	121.37
3	C	1201	F9M	C26-N09-C22	2.72	118.09	115.68
3	D	1201	F9M	C25-N11-C30	2.68	120.35	117.83
3	C	1201	F9M	C38-C36-N14	2.65	124.64	119.32
3	B	1201	F9M	N10-C22-N08	2.65	119.65	116.90
3	A	1201	F9M	C23-C25-N11	-2.62	119.73	123.59
3	A	1201	F9M	N09-C22-N08	2.59	119.59	116.90
3	B	1201	F9M	C23-C25-N11	-2.56	119.83	123.59
3	D	1201	F9M	C28-C27-N10	-2.54	121.00	123.38
3	B	1201	F9M	S01-C32-N12	2.51	128.69	121.37
3	D	1201	F9M	C23-C25-N11	-2.49	119.93	123.59
3	A	1201	F9M	N10-C22-N08	2.49	119.48	116.90
3	A	1201	F9M	S01-C32-N12	2.36	128.25	121.37
3	D	1201	F9M	C24-C23-C25	2.30	120.17	117.61
3	C	1201	F9M	C25-N11-C30	2.25	119.94	117.83
3	D	1201	F9M	S01-C32-N12	2.24	127.91	121.37
3	B	1201	F9M	C33-C35-C36	-2.21	126.70	129.60
3	B	1201	F9M	C17-C15-N07	2.17	104.04	101.68
3	D	1201	F9M	C17-C15-N07	2.15	104.02	101.68
3	C	1201	F9M	C19-N08-C22	-2.12	116.24	120.29
3	B	1201	F9M	C29-C30-N11	-2.12	119.39	122.61
3	C	1201	F9M	C28-C26-N09	-2.11	121.40	123.38
3	B	1201	F9M	C16-C20-N08	2.06	112.12	109.47
3	D	1201	F9M	C18-C16-N07	2.02	103.87	101.68
3	B	1201	F9M	C24-C23-C25	2.01	119.85	117.61

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1201	F9M	N09-C22-N08-C20
3	B	1201	F9M	N09-C22-N08-C19
3	B	1201	F9M	N10-C22-N08-C20
3	B	1201	F9M	N10-C22-N08-C19
3	C	1201	F9M	N10-C22-N08-C19
3	D	1201	F9M	N11-C30-N12-C32
3	C	1201	F9M	N09-C22-N08-C19
3	A	1201	F9M	N09-C22-N08-C19
3	D	1201	F9M	C29-C30-N12-C32
3	D	1201	F9M	N09-C22-N08-C19
3	B	1201	F9M	N13-C32-N12-C30
3	D	1201	F9M	N13-C32-N12-C30
3	A	1201	F9M	N10-C22-N08-C19
3	B	1201	F9M	S01-C32-N12-C30
3	D	1201	F9M	S01-C32-N12-C30
3	D	1201	F9M	N10-C22-N08-C19
3	A	1201	F9M	C29-C30-N12-C32
3	A	1201	F9M	N11-C30-N12-C32
3	B	1201	F9M	N11-C30-N12-C32
3	B	1201	F9M	C29-C30-N12-C32
3	B	1201	F9M	C27-C28-C31-F04
3	C	1201	F9M	S01-C32-N12-C30
3	B	1201	F9M	N13-C33-C35-S02
3	C	1201	F9M	N13-C32-N12-C30
3	B	1201	F9M	N13-C33-C35-C36
3	B	1201	F9M	C27-C28-C31-F03
3	B	1201	F9M	C27-C28-C31-F05

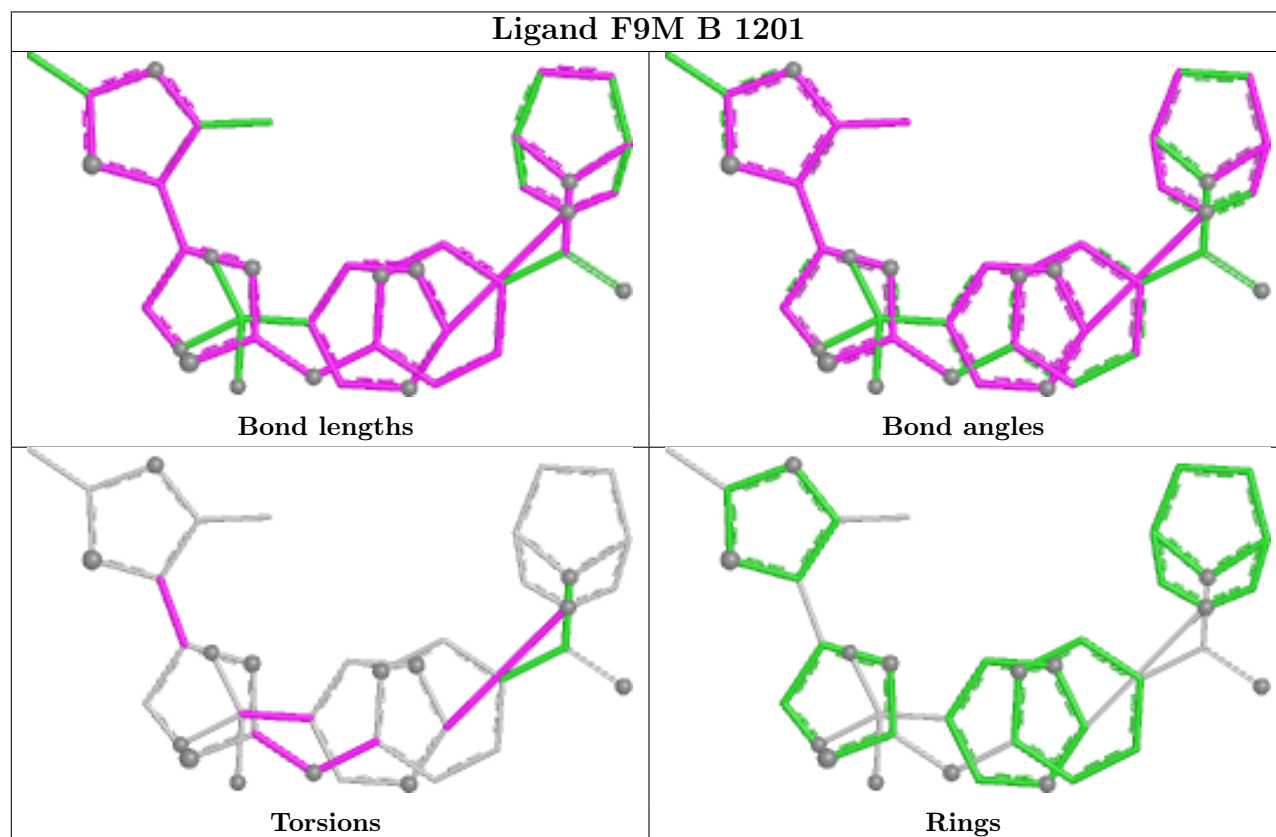
There are no ring outliers.

1 monomer is involved in 3 short contacts:

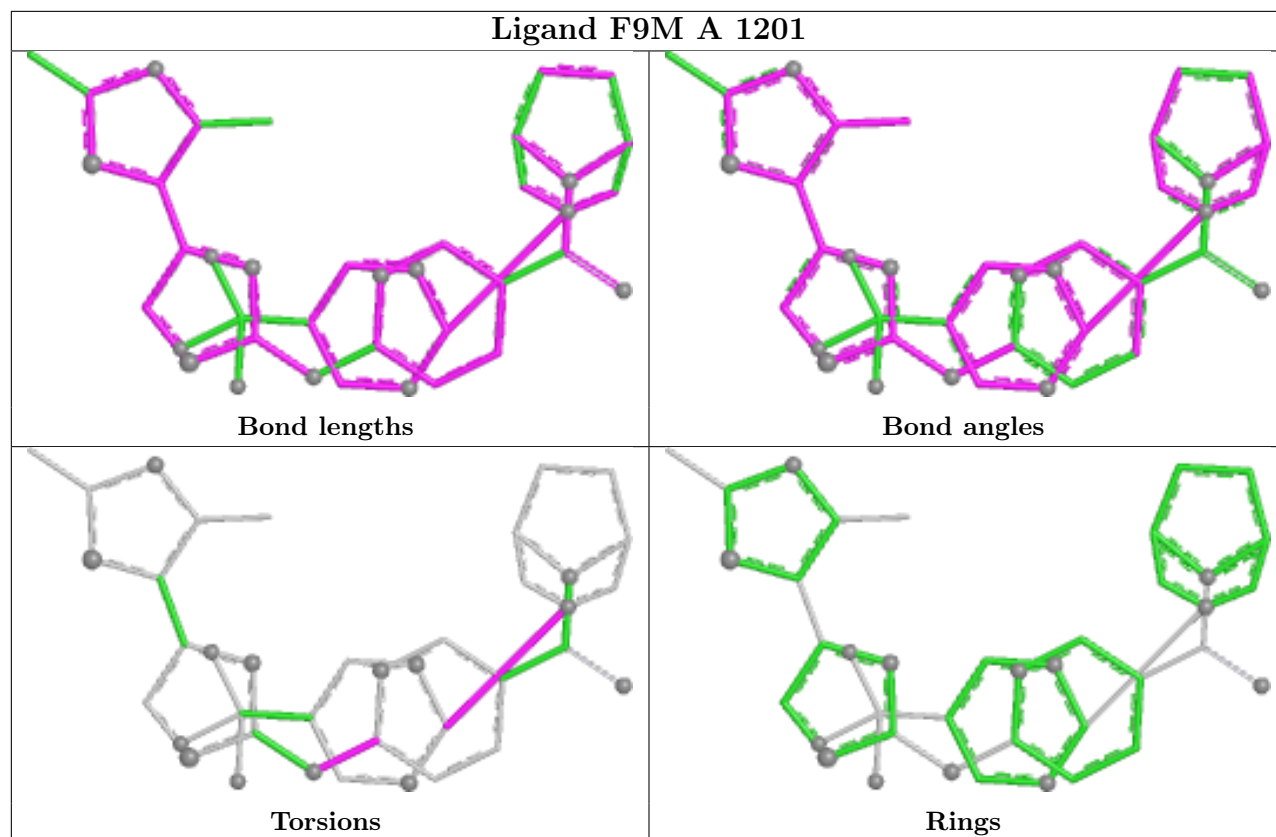
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1201	F9M	3	0

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

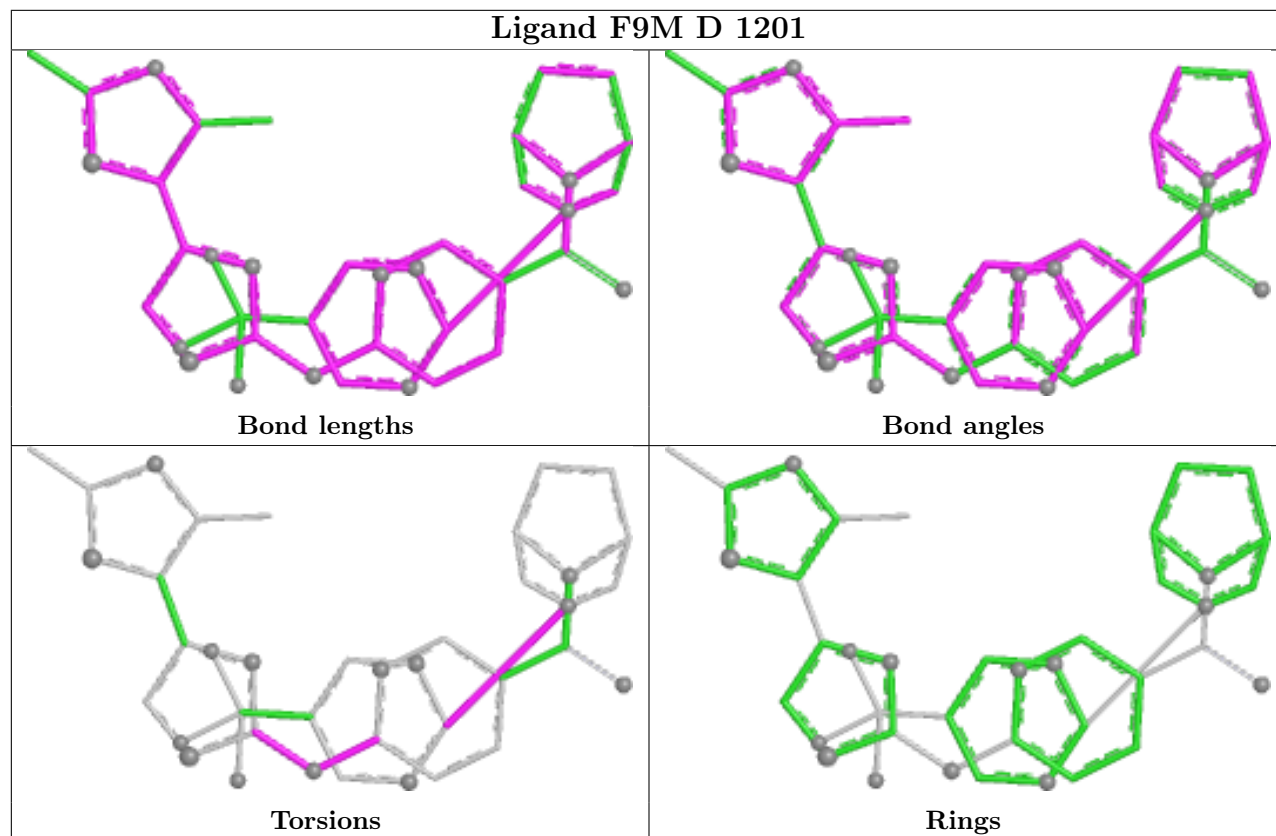
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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

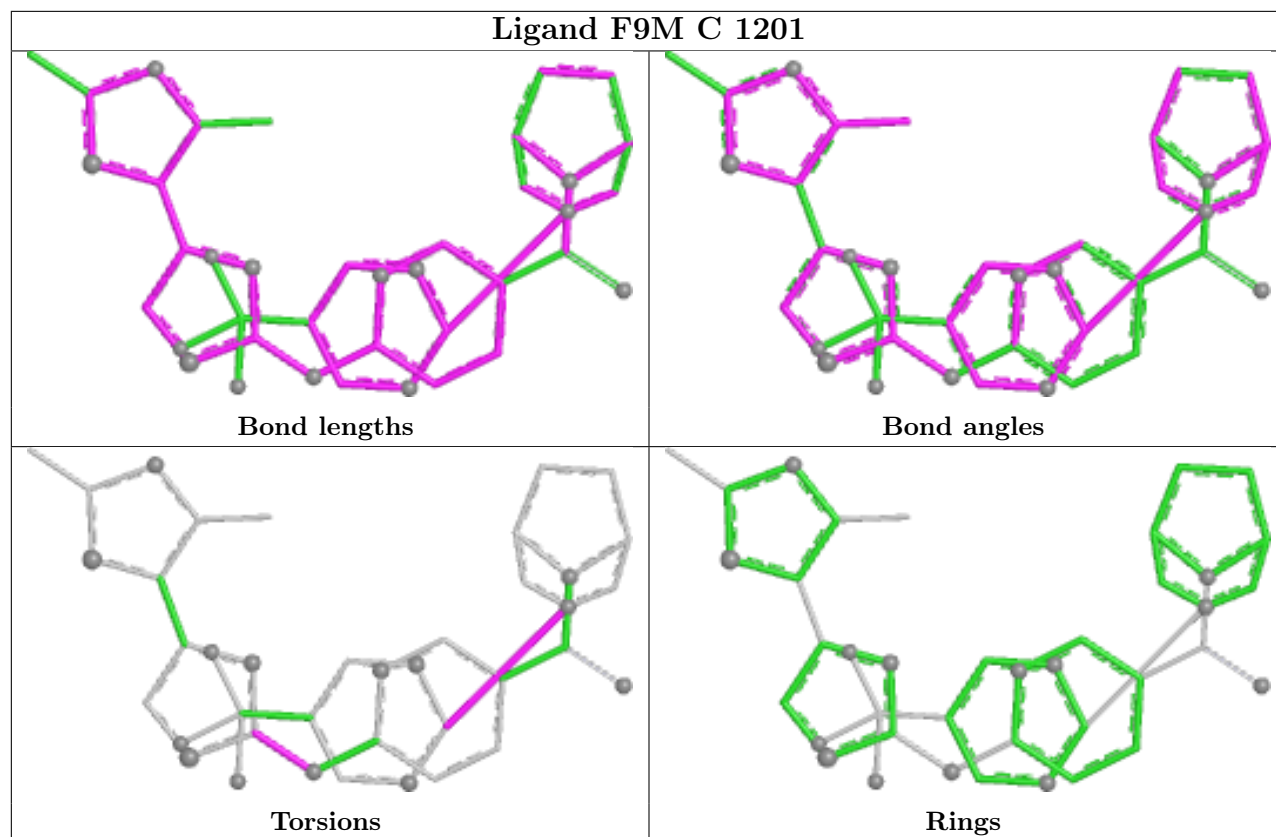


Ligand F9M A 1201



Ligand F9M D 1201





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

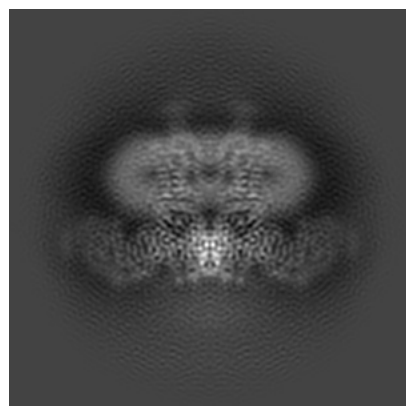
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36676. These allow visual inspection of the internal detail of the map and identification of artifacts.

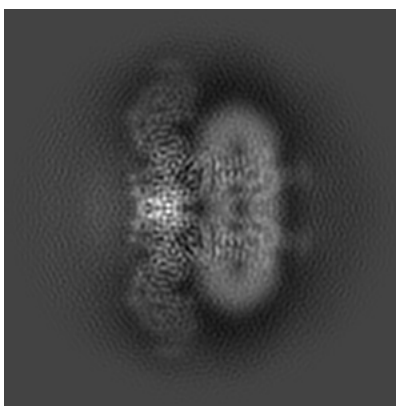
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

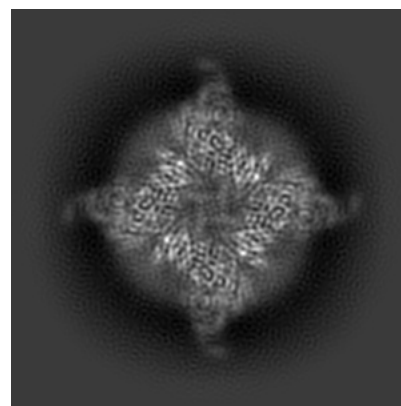
6.1.1 Primary map



X

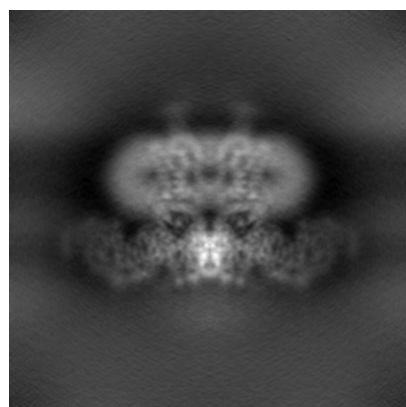


Y

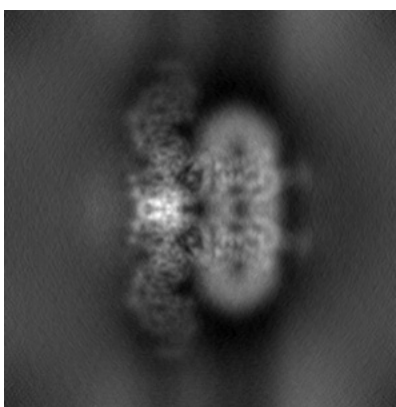


Z

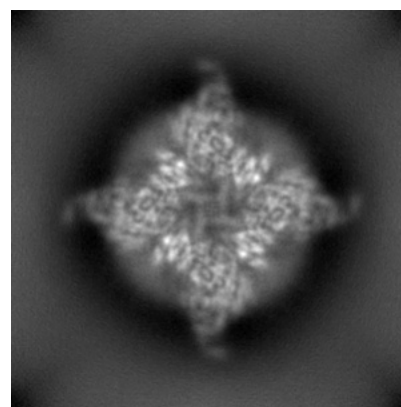
6.1.2 Raw map



X



Y

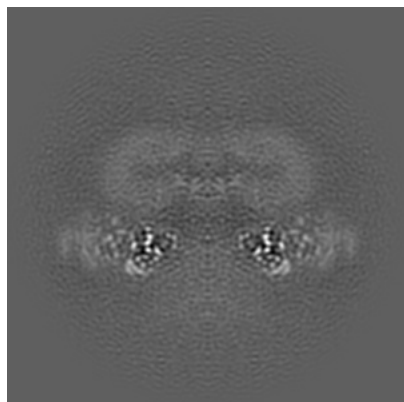


Z

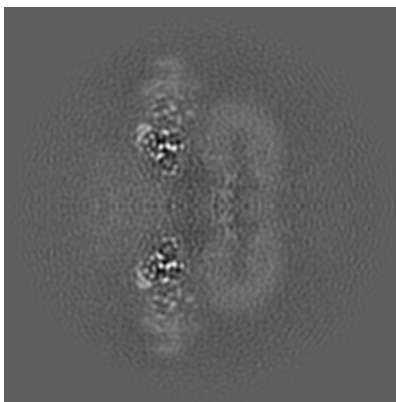
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

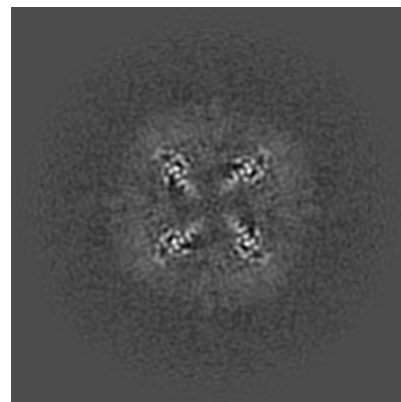
6.2.1 Primary map



X Index: 128

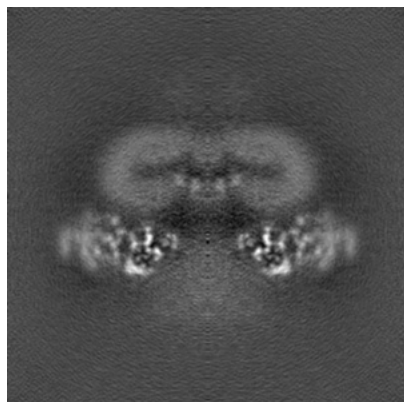


Y Index: 128

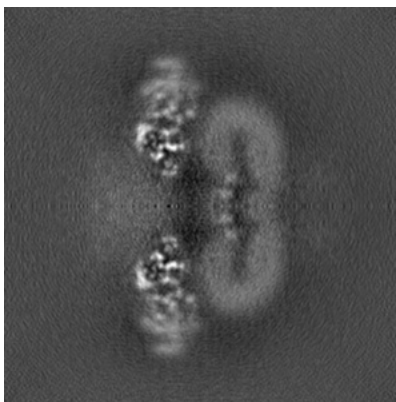


Z Index: 128

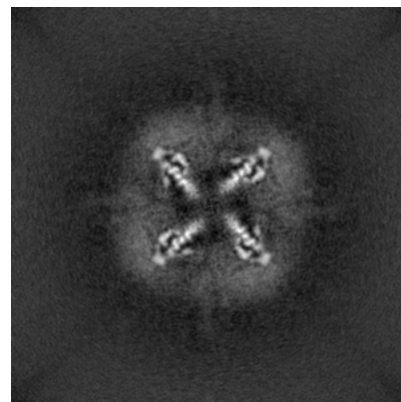
6.2.2 Raw map



X Index: 128



Y Index: 128

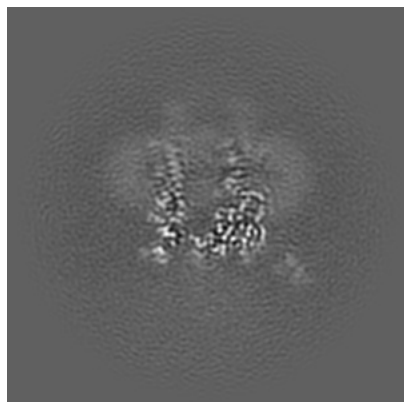


Z Index: 128

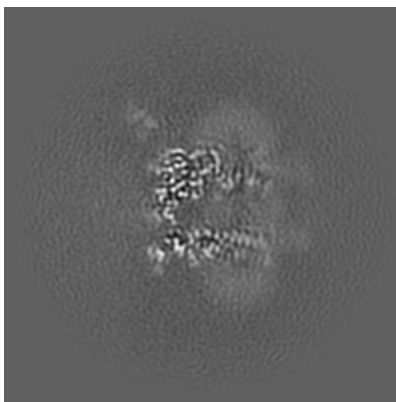
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

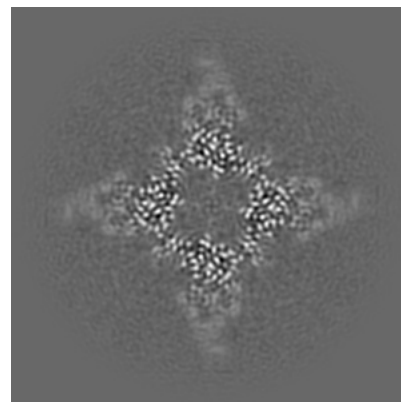
6.3.1 Primary map



X Index: 102

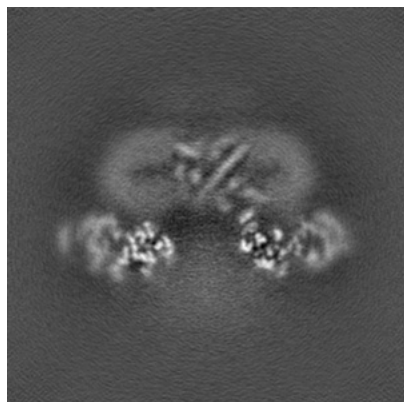


Y Index: 154

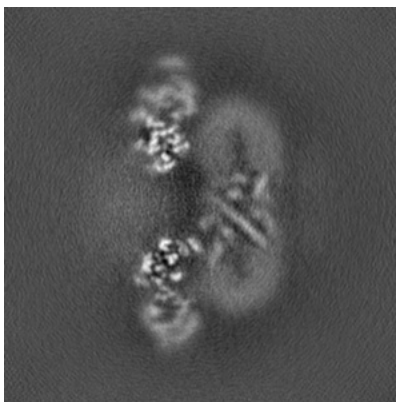


Z Index: 105

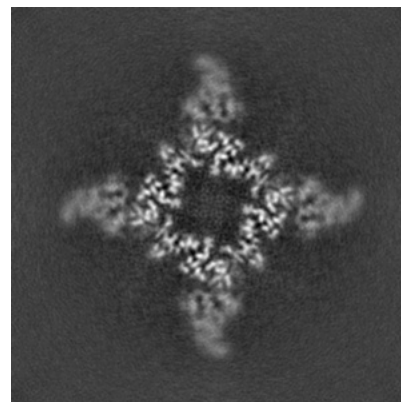
6.3.2 Raw map



X Index: 134



Y Index: 134

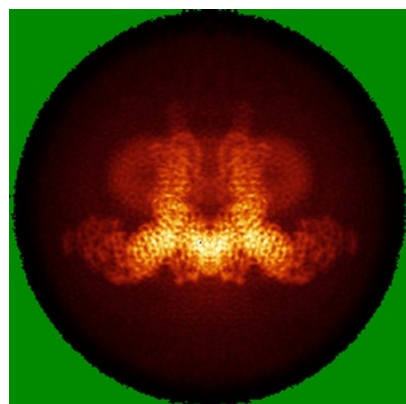


Z Index: 109

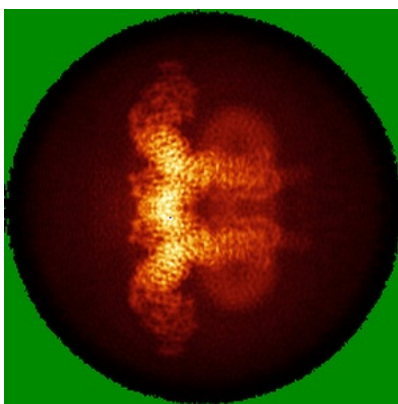
The images above show the largest variance slices of the map in three orthogonal directions.

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

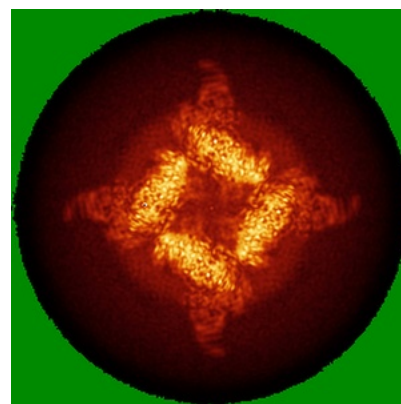
6.4.1 Primary map



X

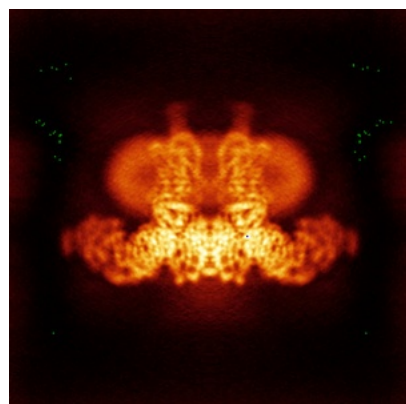


Y

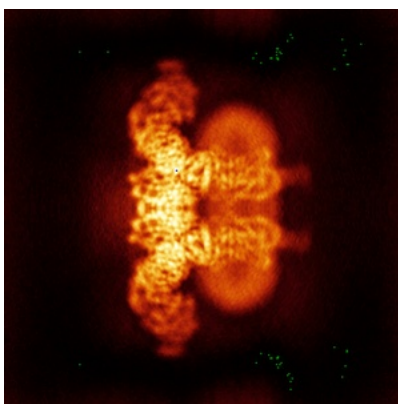


Z

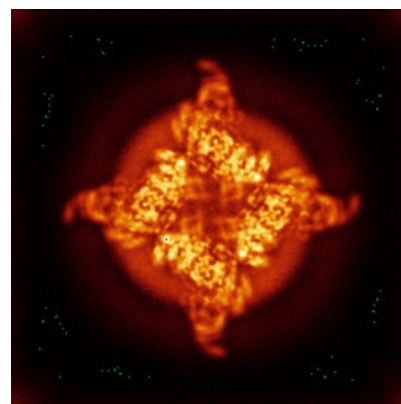
6.4.2 Raw map



X



Y

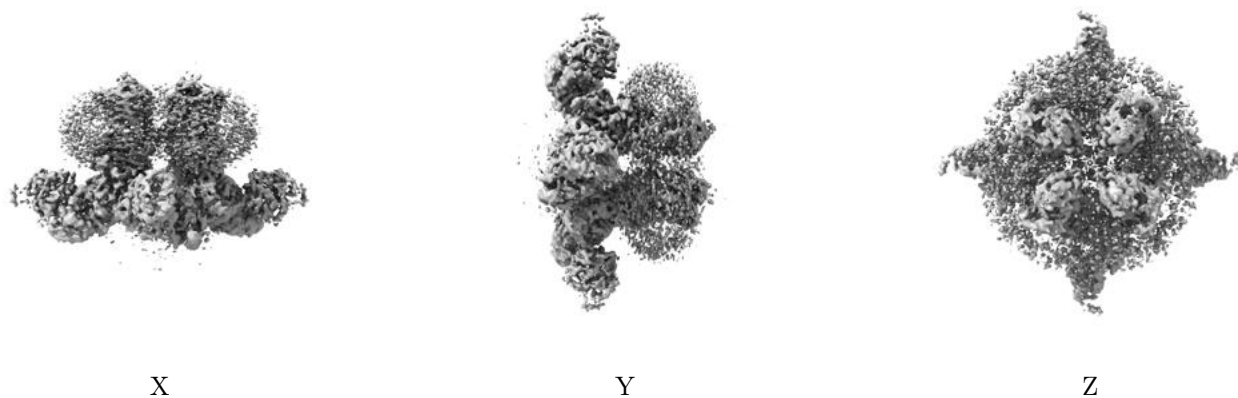


Z

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.

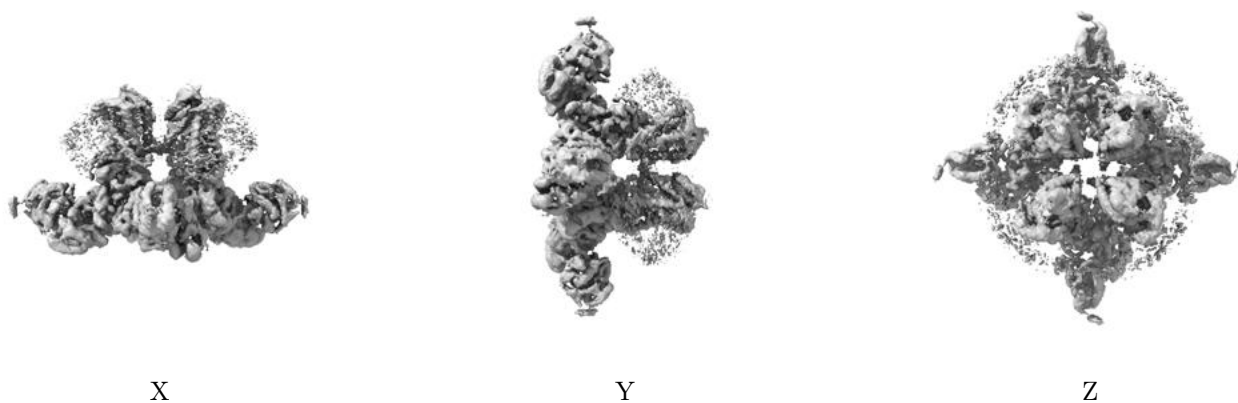
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

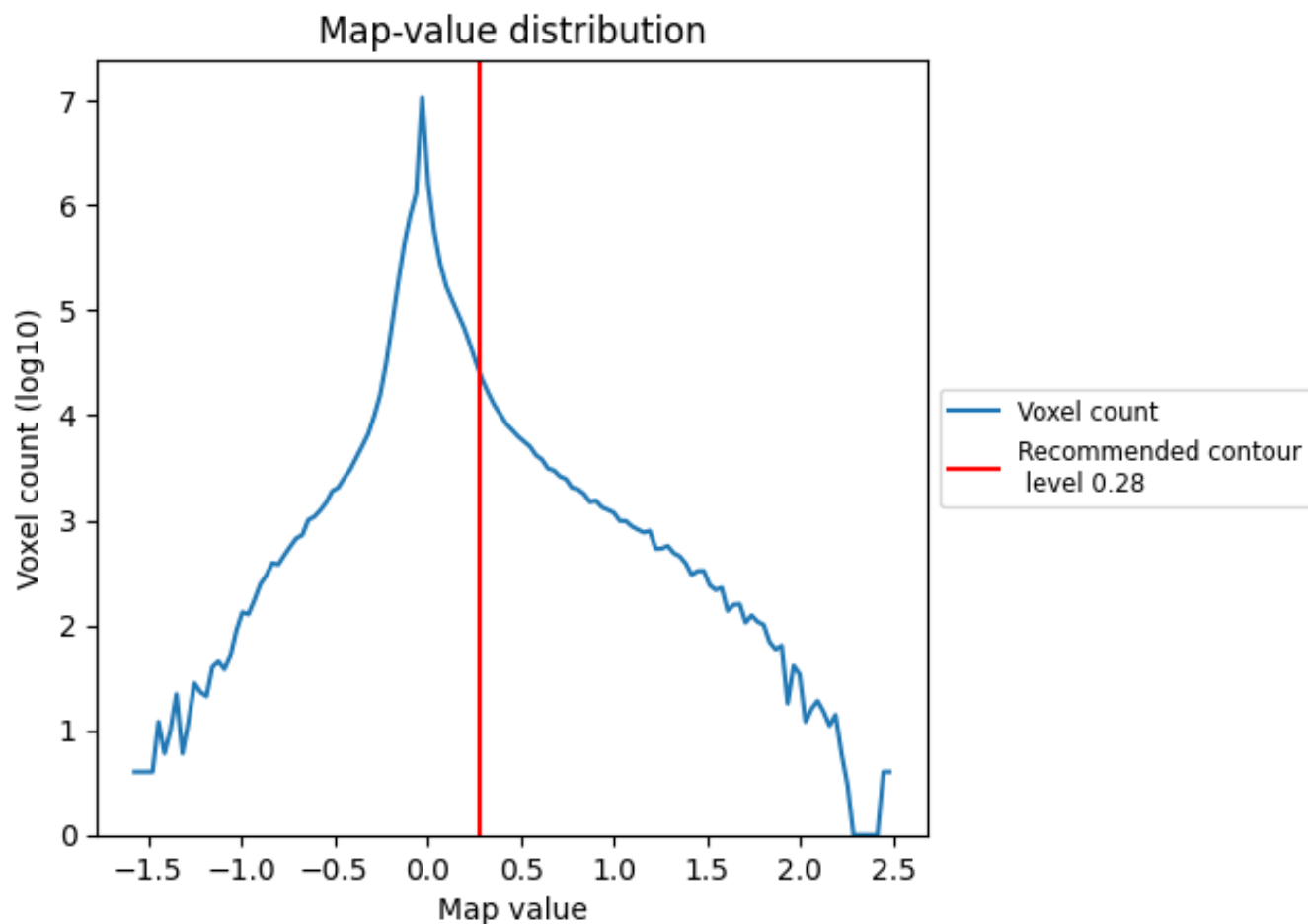
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

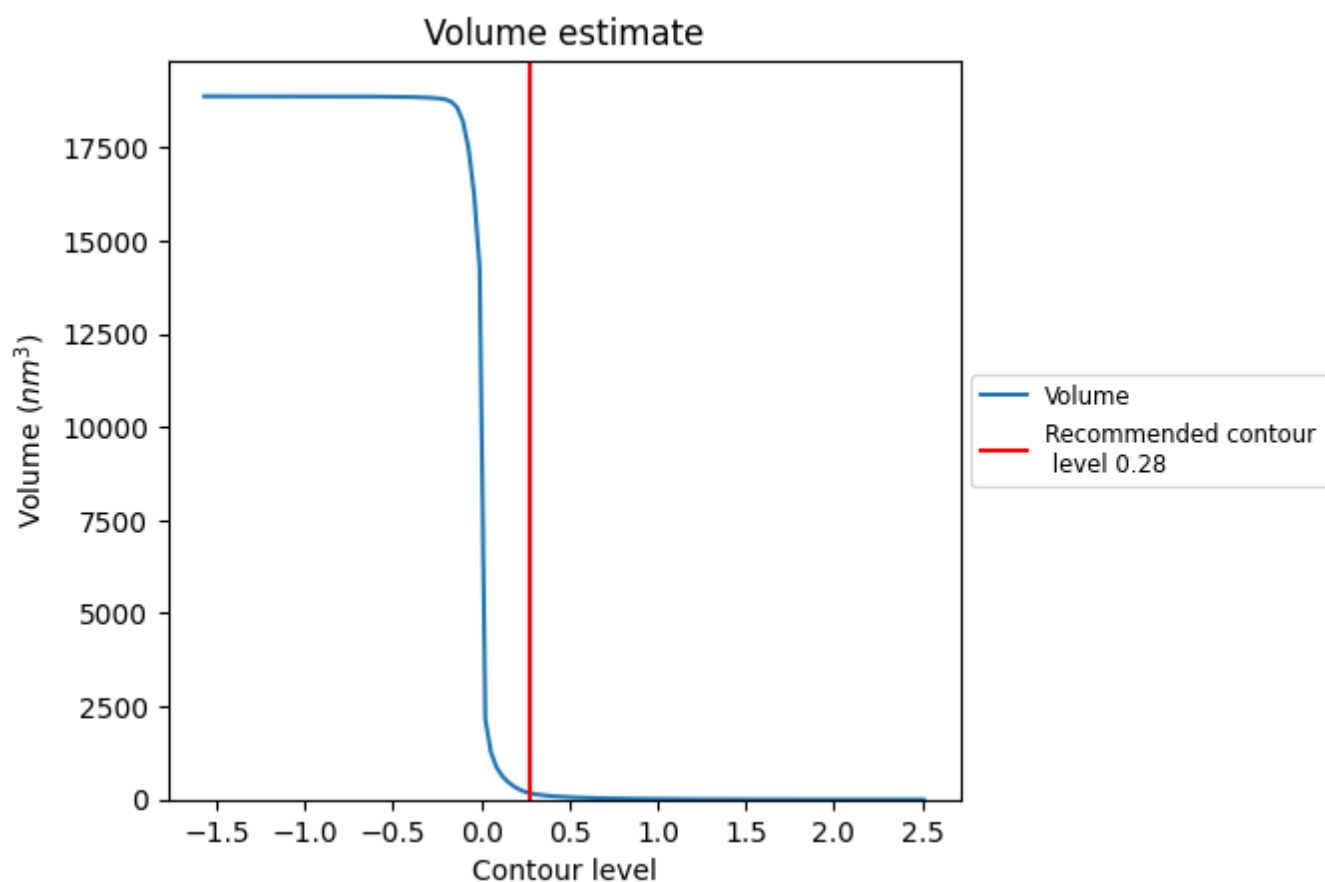
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

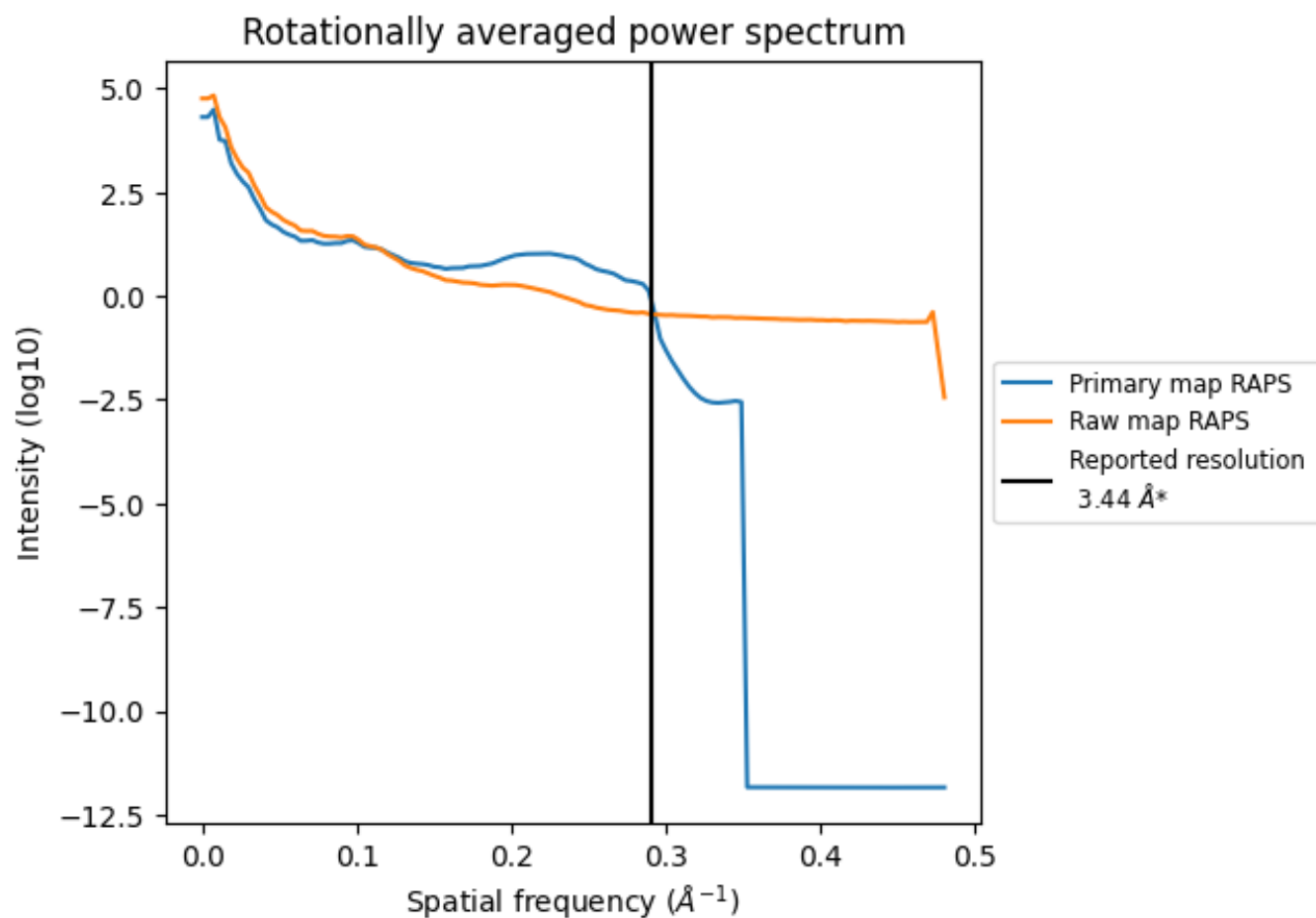
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 167 nm³; this corresponds to an approximate mass of 151 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 ⓘ

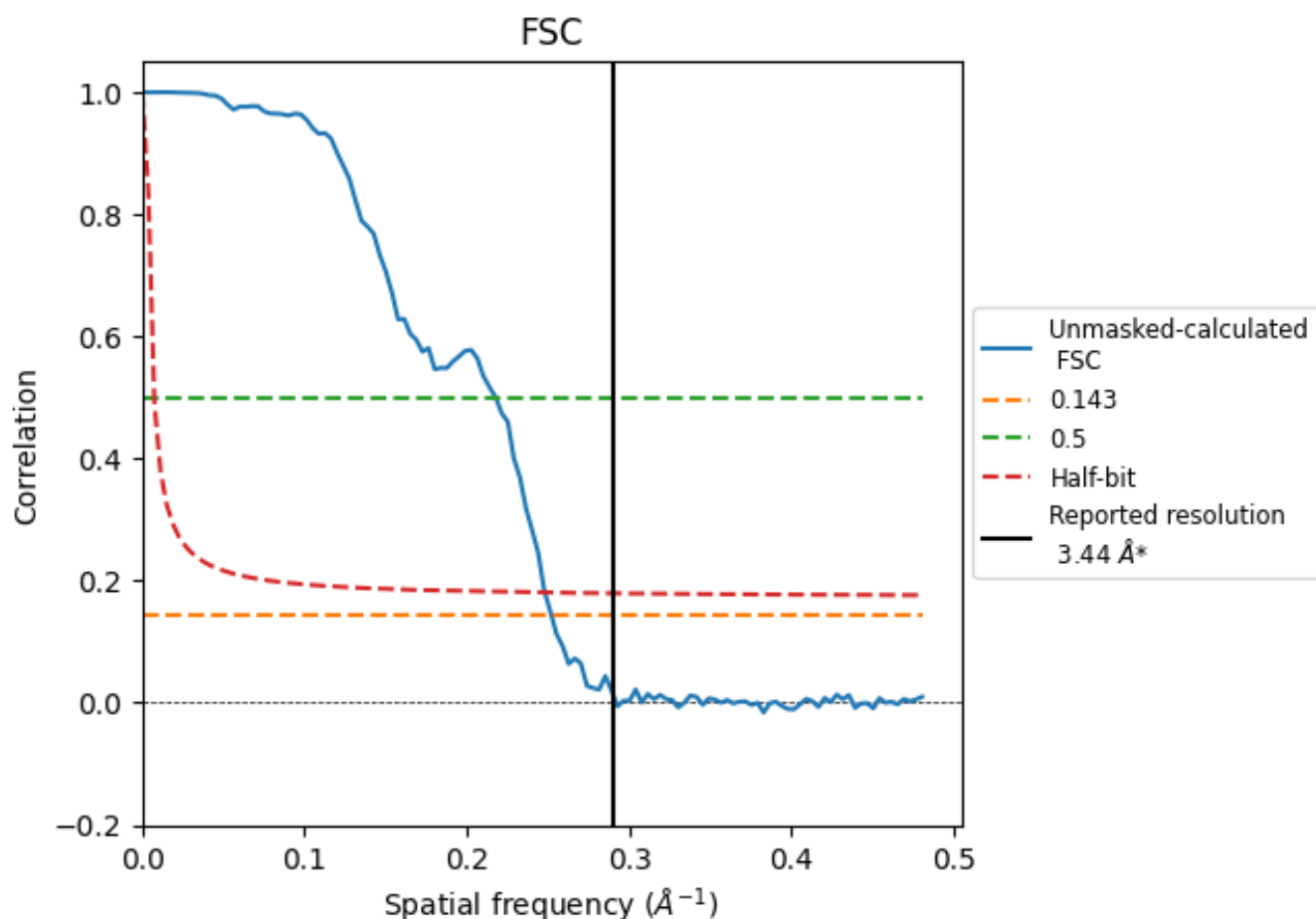


*Reported resolution corresponds to spatial frequency of 0.291 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.291 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

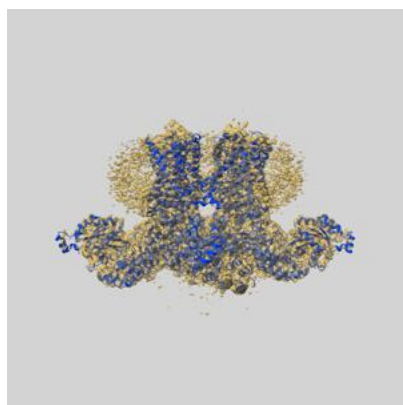
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.44	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.97	4.59	4.03

*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 3.97 differs from the reported value 3.44 by more than 10 %

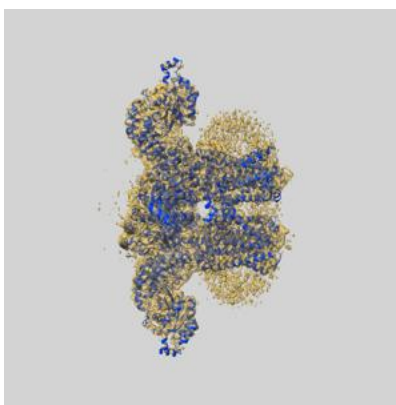
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36676 and PDB model 8JVJ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

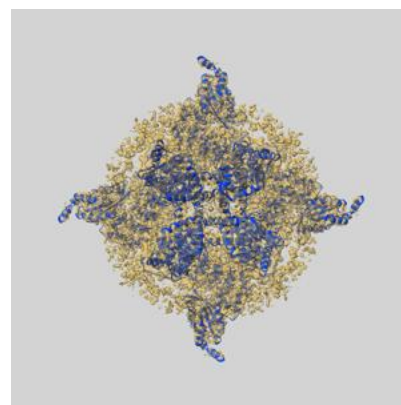
9.1 Map-model overlay [i](#)



X



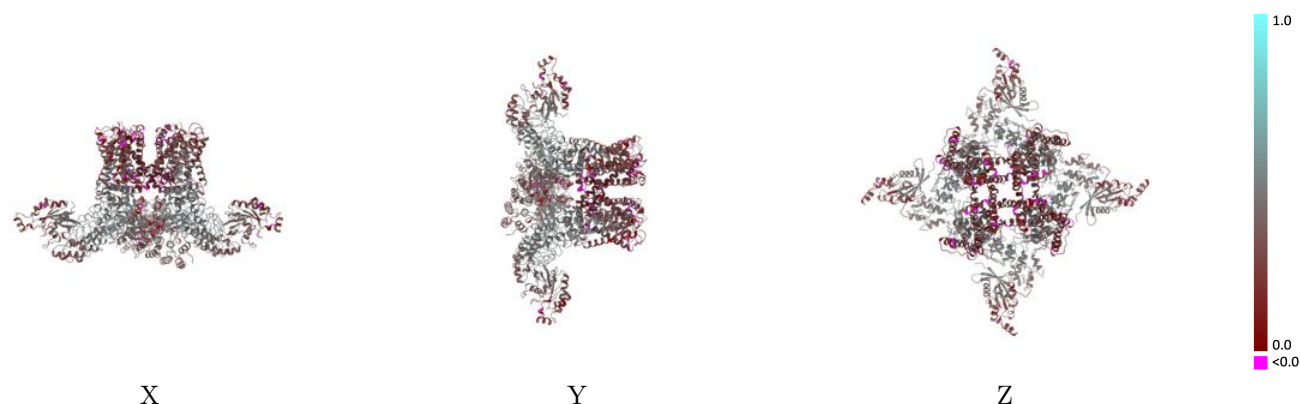
Y



Z

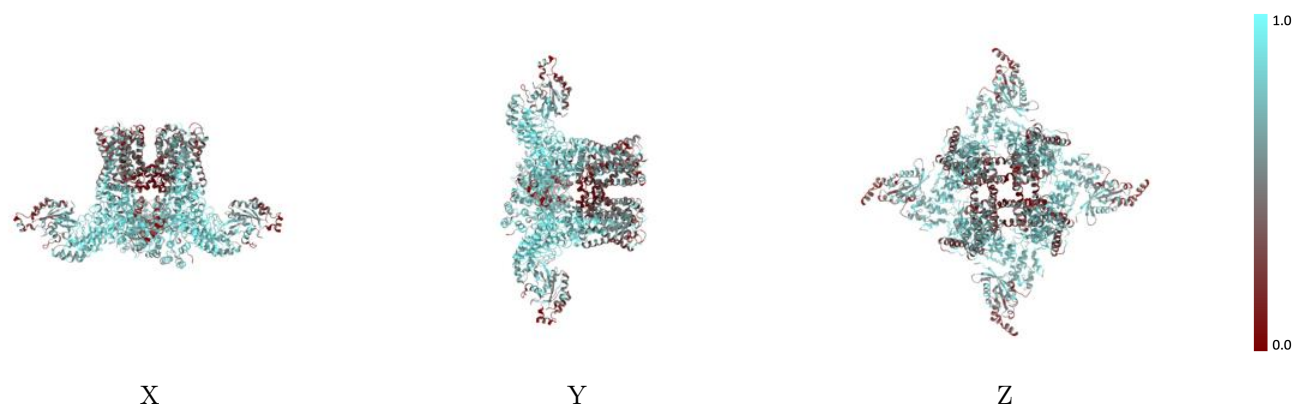
The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



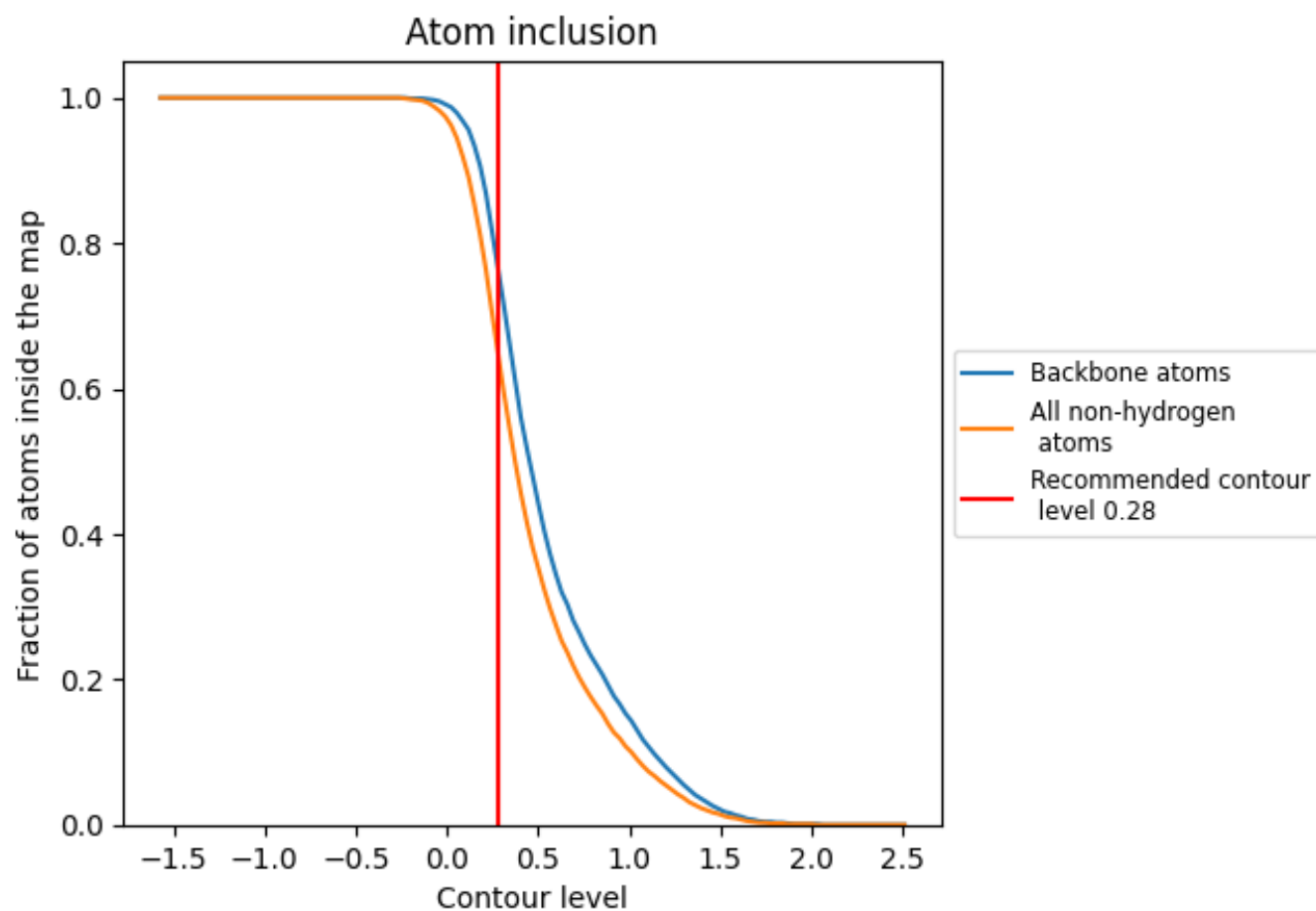
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.28).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 65% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6490	0.3780
A	0.6830	0.3880
B	0.6830	0.3860
C	0.6830	0.3880
D	0.6870	0.3910
E	0.5120	0.3380
F	0.5100	0.3380
G	0.5210	0.3400
H	0.5160	0.3440

1.0

0.0

<0.0