



Full wwPDB EM Validation Report ⓘ

Apr 7, 2025 – 05:22 pm BST

PDB ID : 9GMA / pdb_00009gma
EMDB ID : EMD-51446
Title : MukBEF in a DNA capture state (dimer)
Authors : Burmann, F.; Lowe, J.
Deposited on : 2024-08-28
Resolution : 9.10 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.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

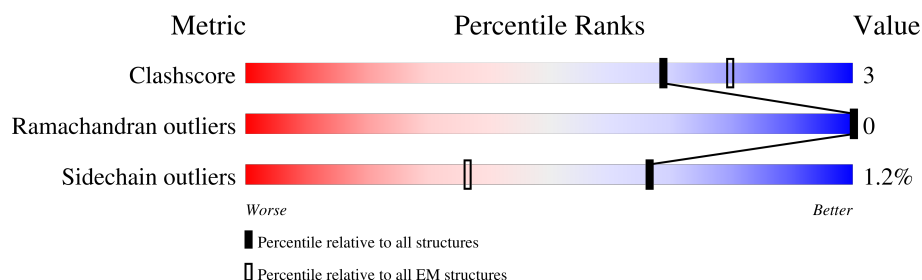
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1482	
1	B	1482	
1	O	1482	
1	P	1482	
2	C	440	
2	D	440	
3	E	240	
3	F	240	

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Mol	Chain	Length	Quality of chain
3	Q	240	
3	R	240	
4	G	78	
4	I	78	
4	M	78	
4	S	78	
5	K	2124	
6	L	2124	

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
4	4HH	G	36	-	-	X	-
4	4HH	S	36	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 130919 atoms, of which 64362 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 Chromosome partition protein MukB.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1467	Total	C	H	N	O	S	0	0
			23547	7298	11707	2188	2314	40		
1	B	1467	Total	C	H	N	O	S	0	0
			23546	7298	11706	2188	2314	40		
1	O	1467	Total	C	H	N	O	S	0	0
			23547	7298	11707	2188	2314	40		
1	P	1467	Total	C	H	N	O	S	0	0
			23546	7298	11706	2188	2314	40		

- Molecule 2 is a protein called Chromosome partition protein MukF.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	440	Total	C	H	N	O	S	0	0
			6982	2218	3451	614	686	13		
2	D	440	Total	C	H	N	O	S	0	0
			6982	2218	3451	614	686	13		

- Molecule 3 is a protein called Chromosome partition protein MukE.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	212	Total	C	H	N	O	S	0	0
			3441	1090	1719	301	322	9		
3	F	198	Total	C	H	N	O	S	0	0
			3246	1029	1627	284	298	8		
3	Q	212	Total	C	H	N	O	S	0	0
			3441	1090	1719	301	322	9		
3	R	198	Total	C	H	N	O	S	0	0
			3246	1029	1627	284	298	8		

- Molecule 4 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms							AltConf	Trace
4	G	72	Total	C	H	N	O	P	S	0	0
			1147	360	564	87	133	1	2		
4	I	72	Total	C	H	N	O	P	S	0	0
			1147	360	564	87	133	1	2		
4	S	72	Total	C	H	N	O	P	S	0	0
			1147	360	564	87	133	1	2		
4	M	72	Total	C	H	N	O	P	S	0	0
			1147	360	564	87	133	1	2		

- Molecule 5 is a DNA chain called pFB526.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	K	73	Total	C	H	N	O	P	0	0
			2311	708	815	285	430	73		

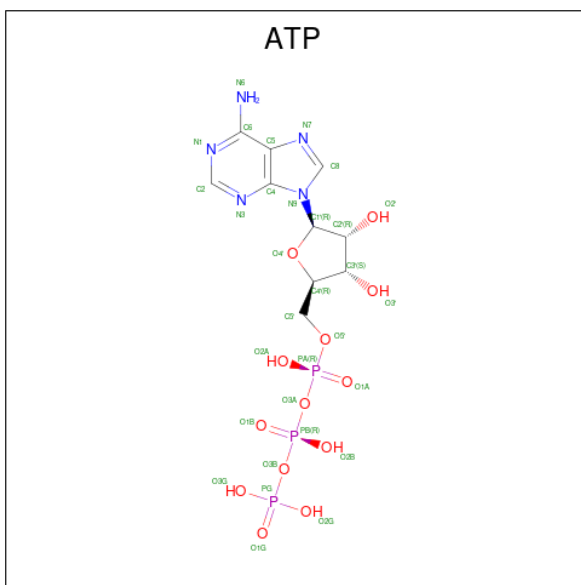
- Molecule 6 is a DNA chain called pFB526.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	L	73	Total	C	H	N	O	P	0	0
			2320	711	823	267	446	73		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Mg	0
			1	1	
7	B	1	Total	Mg	0
			1	1	
7	O	1	Total	Mg	0
			1	1	
7	P	1	Total	Mg	0
			1	1	

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

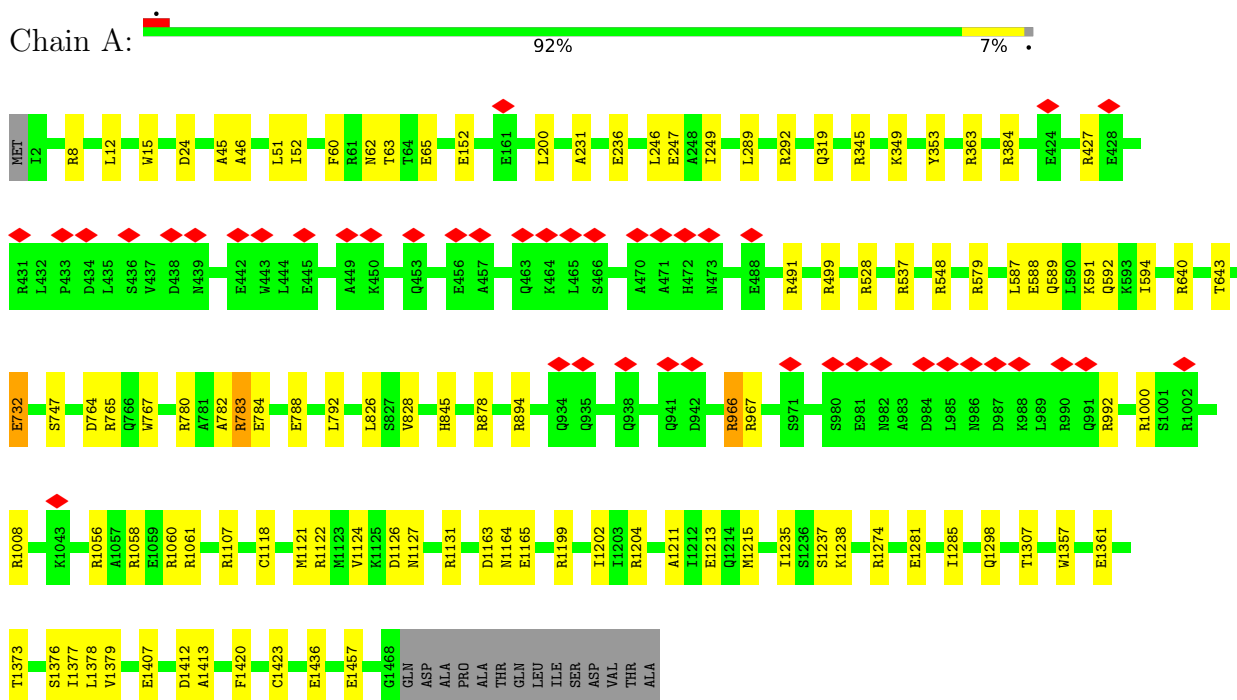


Mol	Chain	Residues	Atoms						AltConf
8	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
8	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
8	O	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
8	P	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

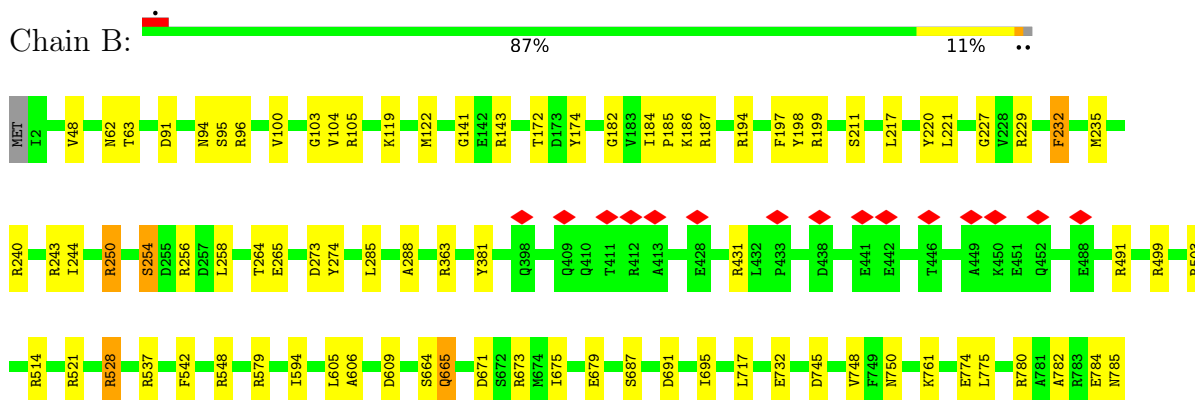
3 Residue-property plots

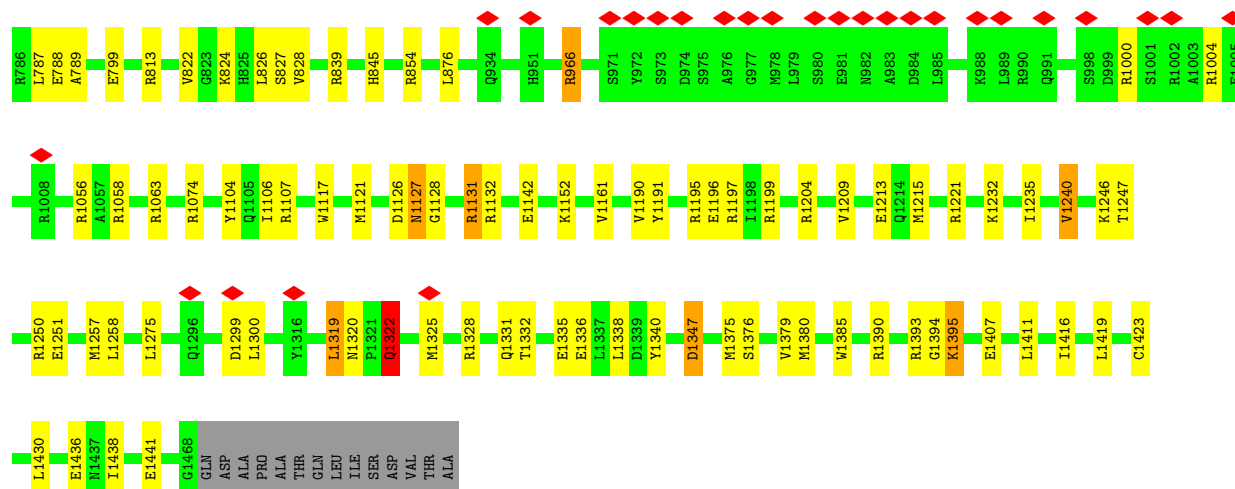
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Chromosome partition protein MukB

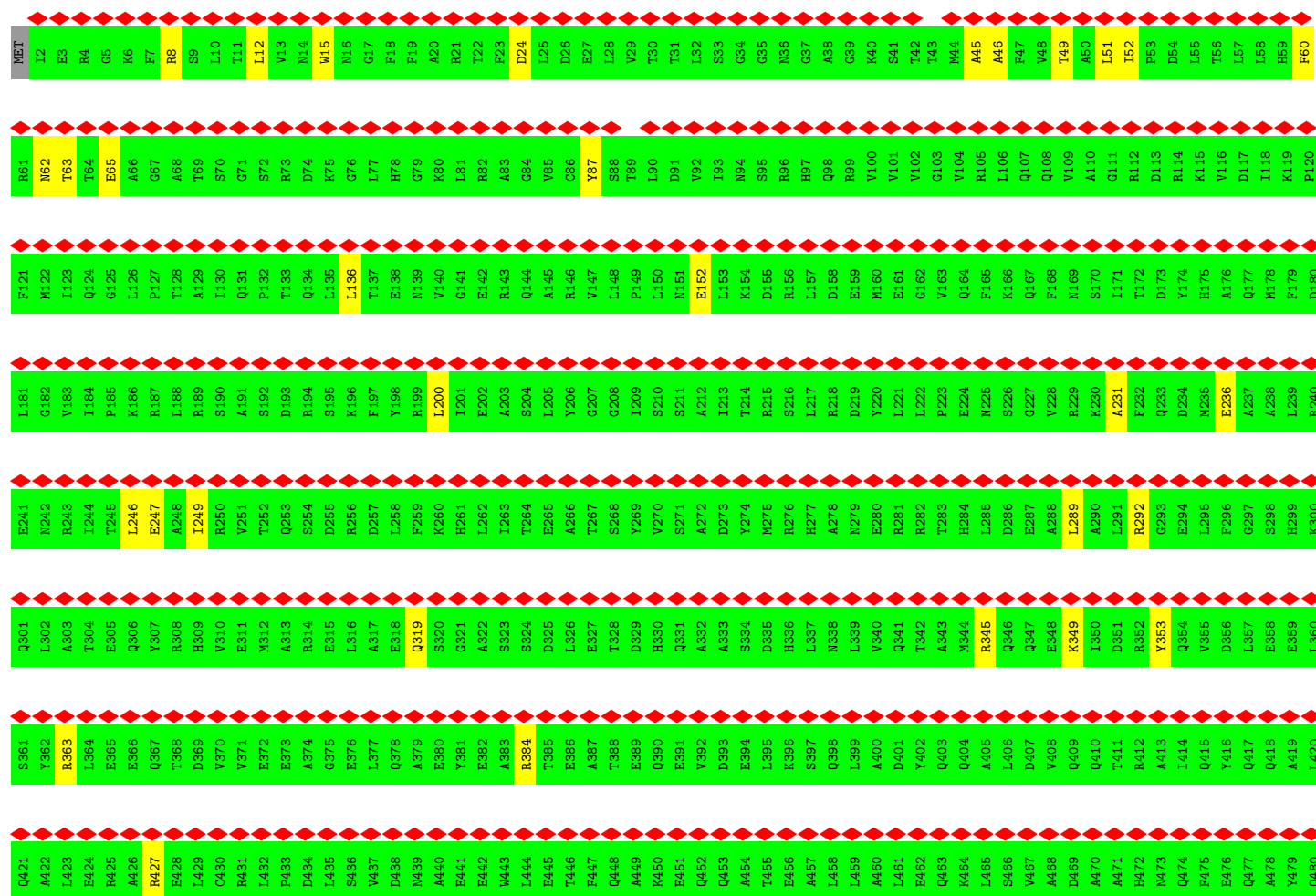
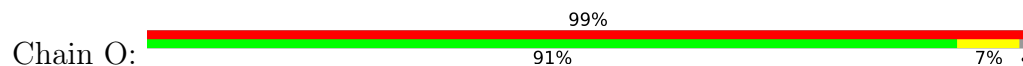


• Molecule 1: Chromosome partition protein MukB





• Molecule 1: Chromosome partition protein MukB



L481	V482	K483	N484	I485	V486	G487	E488	T489	S490	R491	S492	E493	A494	W495	Q496	S497	A498	R499	E500	L501	L502	R503	D504	W505	P506	S507	Q508	R509	H510	L511	A512	D513	R514	V515	Q516	P517	L518	R519	M520	R521	L522	S523	E524	L525	E526	Q527	R528	L529	N530	N531	Q532	Q533	A535	E536	R537	L538	L539	S540		
E541	F542	C543	K544	R545	Q546	G547	R548	Q549	Y550	Q551	A552	E553	D554	L555	E556	A557	L558	Q559	N560	E561	L562	E563	A564	R565	Q566	E567	A568	L569	S570	L571	S572	V573	E574	E575	G576	G577	E578	R579	R580	M581	E582	M583	R584	Q585	E586	L587	E588	Q589	L590	K591	Q592	K593	I594	Q595	S596	L597	T598	A599	R600	
A601	P602	V603	W604	L605	A606	A607	Q608	D609	T610	L611	N612	R613	L614	C615	E616	A617	S618	G619	E620	T621	L622	A623	S624	R625	N626	D627	V628	T629	E630	Y631	M632	Q633	Q634	L635	L636	E637	R638	E639	R640	E641	A642	T643	V644	E645	Q646	D647	E648	V649	A650	A651	G711	Q652	K653	R654	E655	L656	E657	K658	Q659	I660
E661	R662	L663	S664	Q665	P666	S667	Q668	A669	E670	D671	S672	R673	M674	I675	A676	L677	A678	E679	R680	F681	G682	G683	V684	L685	L686	S687	E688	I689	Y690	D691	D692	L693	T694	I695	D696	D697	A698	P699	Y700	F701	S702	A703	L704	W705	G706	F707	A708	R709	H710	G711	I712	V713	V714	F715	D716	L717	L718	L719	V720	
R721	P722	H723	L724	E725	T726	L727	E728	D729	C730	F731	E732	D733	L734	Y735	L736	I737	E738	G739	D740	F741	L742	S743	F744	S825	D746	S747	V748	F749	N750	A751	E752	E753	Q754	T755	L756	A757	V758	L759	V760	K761	S762	S763	D764	R765	Q766	L767	R768	Y769	S770	R771	V772	F773	E774	L775	P776	L777	F778	G779	R780	
A781	A782	R783	E784	M785	R786	L787	E788	A789	L790	M791	L792	E793	R794	D795	A796	L797	A798	E799	R800	F801	G802	T803	L804	S805	F806	D807	V808	Q809	K810	I811	Q812	R813	A814	H815	Q816	A817	F818	S819	Q820	F821	V822	G823	K824	H825	L826	S827	V828	A829	F830	D831	T832	D833	P834	E835	A836	E837	R838	R839	E840	
L841	R842	Q843	R844	H845	T846	E847	L848	E849	R850	E851	V852	S853	R854	F855	E856	D857	Q858	T859	Q860	Q861	Q862	R863	Q864	Q865	Y866	A867	Q868	A869	K870	E871	S872	L873	T874	T875	L876	R877	R878	L879	I880	P881	Q882	V883	T884	L885	L886	L887	D888	E889	T890	L891	I892	D893	R894	V895	E896	E897	V898	R899	E900	
E901	M902	D903	E904	A905	Q906	E907	A908	A909	R910	F911	L912	Q913	Q914	H915	G916	S917	A918	L919	T920	K921	L922	E923	P924	M925	V926	A927	V928	L929	Q930	S931	D932	P933	Q934	Q935	H936	E937	Q938	L939	Q940	Q941	D942	Y943	E944	T945	A946	K947	H948	S949	Q950	H951	Q952	A953	K954	Q955	Q956	A957	F958	A959	L960	
V961	E962	I963	V964	Q965	R966	R967	V968	H969	F970	S971	Y972	S973	D974	S975	A976	G977	M978	L979	S980	E981	N982	A983	D984	L985	N986	D987	K988	L989	R990	Q991	R992	L993	E994	H995	A996	E997	S998	D999	R1000	S1001	R1002	A1003	R1004	E1005	Q1006	L1007	R1008	Q1009	Q1010	Q1011	A1012	Q1013	Y1014	S1015	Q1016	F1017	L1018	Q1019	V1020	
L1021	A1022	S1023	L1024	K1025	S1026	S1027	Y1028	E1029	T1030	K1031	Q1032	D1033	M1034	L1035	K1036	E1037	L1038	L1039	Q1040	E1041	M1042	K1043	D1044	I1045	G1046	V1047	Q1048	A1049	D1050	A1051	M1052	A1053	E1054	M1055	R1056	A1057	L1058	E1059	R1060	L1061	D1062	R1063	L1064	H1065	E1066	A1067	L1068	S1069	V1070	M1071	L1072	S1073	R1074	V1075	M1076	Q1077	L1078	E1079	K1080	
Q1081	I1082	A1083	F1084	C1085	E1086	A1087	E1088	M1089	E1090	N1091	V1092	Q1093	K1094	K1095	L1096	R1097	K1098	L1099	E1100	R1101	D1102	Y1103	Y1104	Q1105	I1106	R1107	E1108	Q1109	V1110	V1111	S1112	A1113	K1114	A1115	G1116	W1117	C1118	A1119	V1120	M1121	R1122	M1123	V1124	K1125	D1126	N1127	G1128	V1129	E1130	R1131	R1132	L1133	H1134	R1135	R1136	E1137	L1138	A1139	Y1140	
M141	E142	G143	G144	L145	L146	R147	S148	M149	S1150	D1151	K1152	L1153	L1154	G1155	A1156	L1157	R1158	L1159	A1160	V1161	A1162	D1163	M1164	E1165	H1166	L1167	R1168	L1169	A1170	L1171	R1172	S1173	L1174	E1175	D1176	P1177	K1178	R1179	P1180	E1181	R1182	K1183	V1184	Q1185	F1186	F1187	I1188	A1189	V1190	Y1191	Q1192	H1193	L1194	R1195	E1196	L1197	I1198	R1199	Q1200	
D1201	I1202	I1203	R1204	T1205	D1206	L1207	P1208	V1209	D1210	A1211	I1212	E1213	Q1214	M1215	E1216	I1217	E1218	L1219	A1220	R1221	L1222	T1223	E1224	E1225	L1226	T1227	A1228	R1229	E1230	Q1231	K1232	L1233	A1234	I1235	S1236	L1237	K1238	S1239	V1240	A1241	N1242	I1243	T1244	R1245	K1246	T1247	T1248	Q1249	R1250	E1251	Q1252	N1253	R1254	I1255	R1256	M1257	L1258	N1259	Q1260	

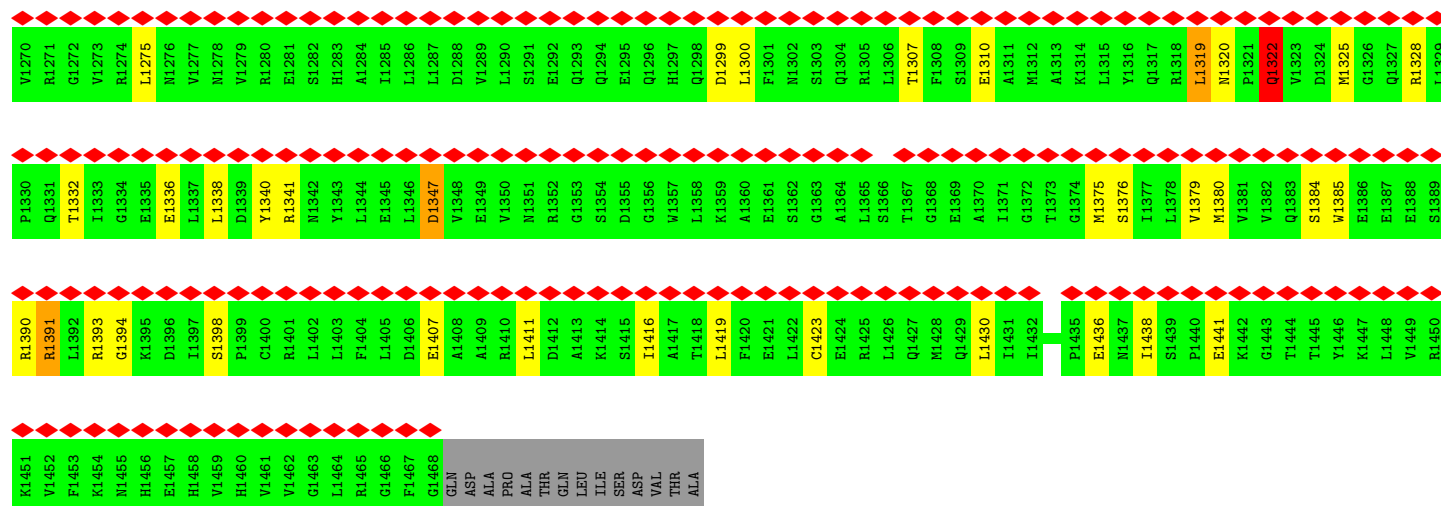
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V1381	V1382	G1383	S1384	V1385	E1386	E1387	E1388	S1389	R1390	R1391	L1392	R1393	G1394	K1395	D1396	I1397	S1398	P1399	C1400	R1401	L1402	L1403	F1404	L1405	D1406	E1407	A1408	A1409	R1410	L1411	D1412	A1413	K1414	S1415	I1416	A1417	T1418	L1419	F1420	E1421	L1422	C1423	E1424	R1425	L1426	Q1427	M1428	Q1429	L1430	I1431	I1432	A1433	A1434	P1435	E1436	N1437	I1438	S1439	P1440
P1321	Q1322	G1323	D1324	M1325	G1326	Q1327	R1328	Q1329	P1330	Q1331	T1332	L1333	G1334	E1335	E1336	L1337	D1338	D1339	C1400	R1401	L1402	L1403	F1404	L1405	D1406	E1407	A1408	A1409	R1410	L1411	D1412	A1413	K1414	S1415	I1416	G1417	T1418	L1419	F1420	E1421	L1422	C1423	E1424	R1425	L1426	Q1427	M1428	Q1429	L1430	I1431	I1432	A1433	A1434	P1435	E1436	N1437	I1438	S1439	P1440
G1261	L1262	Q1263	A1264	S1265	S1266	F1267	G1268	Q1269	V1270	R1271	G1272	V1273	R1274	L1275	N1276	V1277	N1278	V1279	R1280	E1281	S1282	H1283	A1284	I1285	L1286	L1287	D1288	L1289	L1290	S1291	E1292	Q1293	Q1294	E1295	Q1296	H1297	Q1298	D1299	L1300	F1301	M1302	S1303	Q1304	R1305	L1306	T1307	F1308	S1309	E1310	A1311	M1312	A1313	K1314	L1315	Y1316	Q1317	R1318	L1319	N1320

● Molecule 1: Chromosome partition protein MukB

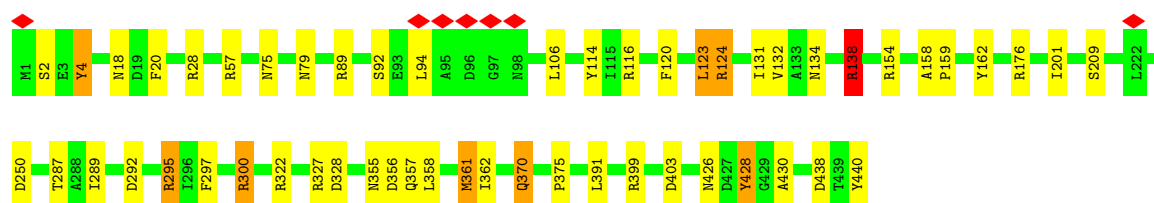
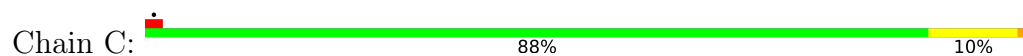


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R243	L244	T245	L246	L249	R250	Q253	S254	D255	R256	D257	L258	F259	K260	H261	L262	L263	T264	E265	A266	T267	S268	Y269	V270	S271	A272	D273	Y274	M275	R276	H277	A278	N279	E280	R281	R282	T283	H284	L285	D286	E287	A288	L289	A290	L291	R292	G293	E294	L295	F296	G297	S298	H299	K300	Q301	L302	A303	T304			
V183	I184	P185	K186	R187	L188	E189	S190	A191	S192	D193	R194	S195	K196	F197	Y198	R199	L200	I201	E202	A203	S204	L205	Y206	G207	G208	I209	S210	S211	A212	I213	T214	R215	S216	L217	R218	D219	Y220	L221	L222	E224	N225	S226	G227	V228	R229	K230	A231	F232	Q233	D234	M235	E236	A237	A238	L239	R240	E241	N242		
M122	I123	Q124	G125	L126	P127	T128	A129	S130	Q131	P132	T133	Q134	L135	L136	T137	E138	N139	V140	G141	E142	R143	Q144	L145	G207	V147	L148	P149	L150	N151	I152	T153	L154	K155	D156	R157	D158	E159	M160	E161	G162	V163	Q164	F165	K166	Q167	F168	R169	N170	S171	I172	D173	Y174	Q177	M178	F179	L181	G182			
N62	T63	T64	E65	A66	G67	T68	T69	S70	G71	S72	R73	D74	K75	G76	L77	H78	G79	K80	L81	R82	A83	G84	V85	C86	Y87	S88	T89	L90	D91	V92	I93	N94	S95	R96	H97	Q98	R99	V100	V101	V102	G103	V104	R105	L106	Q107	Q108	V109	A110	G111	R112	D113	R114	K115	V116	D117	I118	K119	P120	F121	
MET	I2	E3	R4	G5	K6	F7	R8	S9	L10	T11	V13	N14	W15	N16	G17	F18	F19	A20	R21	T22	F23	D24	L25	D26	E27	L28	V29	T30	T31	L32	S33	G34	G35	N36	G37	A38	G39	K40	S41	T42	T43	M44	A45	A46	F47	V48	T49	A50	L51	D54	L55	T56	L57	L58	H59	F60	R61			

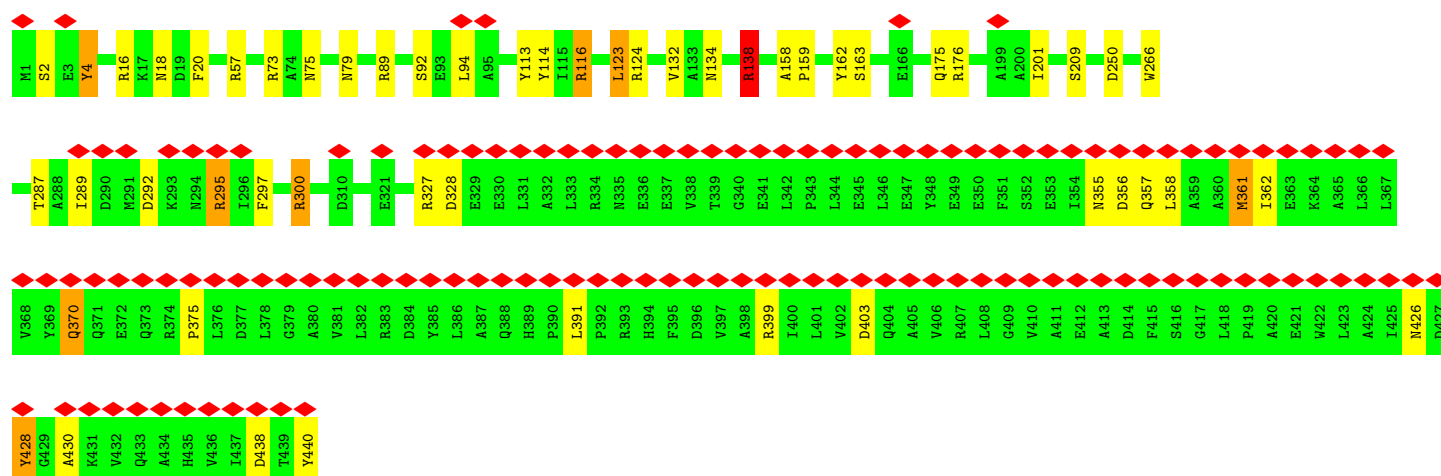
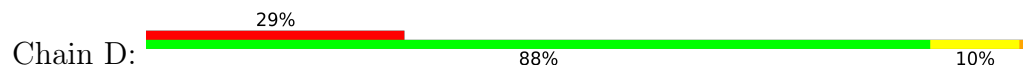
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R545	Q546	G547	R548	Q549	Y550	Q551	A552	E553	D554	L555	E556	A557	L558	Q559	N560	E561	L562	E563	A564	R565	Q566	E567	A568	L569	T569	E570	L571	S572	Q573	N574	E575	G576	E577	E578	R579	R580	E581	E582	M583	R584	Q585	E586	L587	E588	Q589	N590	K591	Q592	K593	I594	Q595	S596	L597	L598	A599	R600	A601	P602	V603	W604
L605	A606	A607	Q608	D609	T610	L611	N612	Q613	L614	C615	E616	Q617	S618	G619	E620	T621	L622	E623	S624	S625	Q626	D627	V628	T629	E630	Y631	D632	Q633	Q634	L635	L636	E637	R638	E639	R640	E641	E642	T643	V644	E645	R646	D647	E648	V649	A650	A651	Q652	K653	R654	E655	L656	E657	K658	Q659	I660	E661	L662	L663	S664	
Q665	P666	S667	G668	A669	E670	D671	S672	R673	M674	I675	A676	L677	A678	E679	R680	F681	G682	G683	V684	L685	Q686	S687	E688	I689	Y690	D691	I692	I693	T694	I695	D696	D697	A698	P699	T700	F701	S702	A703	L704	Y705	G706	F707	A708	R709	H710	G711	I712	V713	F714	F715	D716	L717	S718	L719	V720	R721	P722	H723	L724	
E725	T726	L727	E728	D729	C730	F731	E732	D733	L734	Y735	L736	I737	E738	G739	D740	F741	G742	S743	E744	D745	S746	E747	V748	F749	A751	E752	E753	Q754	T755	H756	A757	V758	L759	V760	K761	S762	S763	D764	R765	Q766	F767	R768	Y769	S770	R771	Y772	F773	E774	L775	P776	L777	G778	G779	R780	A781	R782	R783	E784		
N785	R786	L787	E788	A789	L790	N791	L792	E793	R794	D795	A796	L797	A798	E799	R800	Y801	A802	T803	L804	S805	F806	D807	V808	Q809	K810	I811	Q812	R813	A814	H815	Q816	A817	F818	S819	Q820	F821	V822	G823	K824	H825	L826	S827	V828	A829	F830	D831	T832	D833	E835	A836	E837	I838	R839	E840	L841	R842	Q843	R844		
H845	T846	E847	L848	E849	R850	E851	V852	S853	R854	F855	E856	D857	Q858	T859	Q860	Q861	R862	R863	Q864	Q865	Y866	A867	Q868	A869	K870	E871	S872	L873	T874	T875	L876	N877	R878	L879	I880	P881	Q882	V883	T884	L885	L886	L887	D888	E889	T890	L891	I892	D893	R894	V895	E896	E897	V898	R899	E900	E901	N902	D903	E904	
A905	Q906	E907	A908	A909	R910	F911	L912	Q913	Q914	H915	G916	S917	A918	L919	T920	K921	L922	E923	P924	N925	V926	A927	V928	L929	Q930	S931	D932	P933	Q934	Q935	H936	E937	Q938	L939	Q940	Q941	D942	Y943	E944	T945	A946	K947	H948	S949	Q950	H951	Q952	A953	K954	Q955	Q956	A957	F958	A959	L960	V961	E962	I963	V964	
Q965	R966	R967	V968	H969	F970	S971	Y972	S973	D974	S975	A976	G977	M978	L979	S980	E981	N982	A983	D984	L985	N986	D987	K988	L989	R990	Q991	R992	L993	E994	H995	A996	E997	S998	D999	R1000	S1001	R1002	A1003	R1004	E1005	Q1006	L1007	R1008	Q1009	Q1010	Q1011	A1012	Q1013	Y1014	S1015	Q1016	F1017	N1018	Q1019	V1020	L1021	A1022	S1023	L1024	
K1025	S1026	S1027	Y1028	E1029	T1030	K1031	Q1032	M1033	M1034	L1035	K1036	E1037	L1038	L1039	Q1040	E1041	M1042	K1043	D1044	L1045	G1046	V1047	Q1048	A1049	D1050	A1051	M1052	A1053	E1054	M1055	R1056	A1057	L1058	E1059	R1060	R1061	D1062	R1063	L1064	H1065	A1066	A1067	L1068	S1069	V1070	M1071	R1072	S1073	R1074	V1075	Q1076	Q1077	L1078	E1079	K1080	Q1081	A1083	F1084		
C1085	E1086	A1087	E1088	M1089	E1090	N1091	V1092	Q1093	K1094	K1095	L1096	R1097	K1098	L1099	E1100	R1101	D1102	Y1103	Y1104	Q1105	I1106	R1107	E1108	Q1109	V1110	V1111	S1112	A1113	K1114	A1115	G1116	Y1117	C1118	A1119	Q1120	M1121	R1122	M1123	V1124	K1125	D1126	N1127	G1128	V1129	E1130	R1131	R1132	L1133	H1134	R1135	L1136	E1137	L1138	A1139	Y1140	M1141	E1142	G1143	G1144	
A1145	L1146	R1147	S1148	M1149	S1150	D1151	K1152	L1153	L1154	G1155	A1156	L1157	R1158	L1159	A1160	V1161	E1165	H1166	L1167	R1168	D1169	R1172	E1175	D1176	P1177	K1178	R1179	P1180	E1181	R1182	K1183	V1184	Q1185	F1186	F1187	I1188	A1189	Y1190	Q1192	H1193	L1194	R1195	E1196	I1197	R1198	R1199	I1202	I1203	R1204	T1205	D1206	D1207	P1208	V1209						
D1210	A1211	I1212	E1213	Q1214	M1215	E1216	I1217	E1218	L1219	A1220	R1221	L1222	T1223	E1224	E1225	L1226	A1228	R1229	E1230	Q1231	K1232	L1233	A1234	I1235	S1236	S1237	K1238	S1239	V1240	A1241	N1242	I1243	I1244	R1245	K1246	T1247	I1248	Q1249	R1250	E1251	Q1252	N1253	R1254	I1255	R1256	M1257	L1258	N1259	Q1260	G1261	L1262	Q1263	A1264	V1265	S1266	G1267	Q1268			



• Molecule 2: Chromosome partition protein MukF



• Molecule 2: Chromosome partition protein MukF



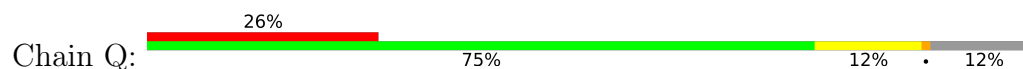
• Molecule 3: Chromosome partition protein MukE



- Molecule 3: Chromosome partition protein MukE



- Molecule 3: Chromosome partition protein MukE



- Molecule 3: Chromosome partition protein MukE



- Molecule 4: Acyl carrier protein



[illegible]

- Molecule 6: pFB526

Chain L:  97%

[illegible]



DG DT DG DA DT DA DC DG DC DC DT DA DT DT DT DT DT DA DT DA DG DG DT DT

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3754	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.346	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.07	Depositor
Map size (\AA)	720.7206, 720.7206, 720.7206	wwPDB
Map dimensions	166, 166, 166	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	4.34169, 4.34169, 4.34169	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4HH, MG, ATP

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	0.47	1/11999 (0.0%)	0.79	21/16166 (0.1%)
1	B	0.96	59/11999 (0.5%)	1.05	57/16166 (0.4%)
1	O	0.47	1/11999 (0.0%)	0.79	22/16166 (0.1%)
1	P	1.01	72/11999 (0.6%)	1.08	60/16166 (0.4%)
2	C	0.68	1/3592 (0.0%)	0.99	13/4862 (0.3%)
2	D	0.68	1/3592 (0.0%)	1.01	13/4862 (0.3%)
3	E	1.32	16/1753 (0.9%)	1.37	17/2361 (0.7%)
3	F	1.41	19/1648 (1.2%)	1.24	5/2218 (0.2%)
3	Q	1.32	16/1753 (0.9%)	1.36	17/2361 (0.7%)
3	R	1.42	25/1648 (1.5%)	1.26	10/2218 (0.5%)
4	G	0.25	0/558	0.42	0/754
4	I	0.25	0/558	0.41	0/754
4	M	0.25	0/558	0.41	0/754
4	S	0.25	0/558	0.42	0/754
5	K	1.61	1/1680 (0.1%)	2.66	199/2589 (7.7%)
6	L	1.59	3/1676 (0.2%)	2.55	174/2586 (6.7%)
All	All	0.89	215/67570 (0.3%)	1.13	608/91737 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	O	0	3
1	P	0	3
2	C	0	6
2	D	0	6
3	E	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	Q	0	2
5	K	0	19
6	L	0	17
All	All	0	65

All (215) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	295	ARG	C-N	-13.11	1.03	1.34
2	D	295	ARG	C-N	-13.07	1.03	1.34
1	A	589	GLN	C-N	7.64	1.51	1.34
1	O	589	GLN	C-N	7.60	1.51	1.34
3	R	85	ARG	CZ-NH2	-7.48	1.23	1.33
1	P	1341	ARG	CZ-NH2	-7.46	1.23	1.33
1	P	1250	ARG	CZ-NH2	-7.43	1.23	1.33
1	P	1393	ARG	CZ-NH2	-7.42	1.23	1.33
1	P	1245	ARG	CZ-NH2	-7.41	1.23	1.33
3	Q	203	ARG	CZ-NH2	-7.41	1.23	1.33
1	B	1131	ARG	CZ-NH2	-7.40	1.23	1.33
1	P	96	ARG	CZ-NH2	-7.40	1.23	1.33
3	R	34	ARG	CZ-NH2	-7.38	1.23	1.33
1	P	1131	ARG	CZ-NH2	-7.37	1.23	1.33
3	R	161	ARG	CZ-NH2	-7.37	1.23	1.33
3	E	206	ARG	CZ-NH2	-7.36	1.23	1.33
1	P	199	ARG	CZ-NH2	-7.36	1.23	1.33
3	R	156	ARG	CZ-NH2	-7.36	1.23	1.33
1	P	1328	ARG	CZ-NH2	-7.35	1.23	1.33
3	F	31	ARG	CZ-NH2	-7.33	1.23	1.33
3	Q	206	ARG	CZ-NH2	-7.33	1.23	1.33
1	B	1221	ARG	CZ-NH2	-7.31	1.23	1.33
3	E	31	ARG	CZ-NH2	-7.31	1.23	1.33
1	P	1132	ARG	CZ-NH2	-7.31	1.23	1.33
1	P	1254	ARG	CZ-NH2	-7.30	1.23	1.33
1	B	1197	ARG	CZ-NH2	-7.27	1.23	1.33
3	R	31	ARG	CZ-NH2	-7.25	1.23	1.33
1	B	1199	ARG	CZ-NH2	-7.25	1.23	1.33
1	B	240	ARG	CZ-NH2	-7.24	1.23	1.33
1	P	1221	ARG	CZ-NH2	-7.24	1.23	1.33
1	P	1197	ARG	CZ-NH2	-7.24	1.23	1.33
3	Q	31	ARG	CZ-NH2	-7.23	1.23	1.33
3	E	203	ARG	CZ-NH2	-7.22	1.23	1.33
1	B	1132	ARG	CZ-NH2	-7.22	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	250	ARG	CZ-NH2	-7.18	1.23	1.33
1	P	1199	ARG	CZ-NH2	-7.17	1.23	1.33
3	F	164	ARG	CZ-NH2	-7.17	1.23	1.33
1	P	240	ARG	CZ-NH2	-7.17	1.23	1.33
3	E	67	ARG	CZ-NH2	-7.15	1.23	1.33
3	Q	67	ARG	CZ-NH2	-7.15	1.23	1.33
1	B	199	ARG	CZ-NH2	-7.14	1.23	1.33
1	P	250	ARG	CZ-NH2	-7.13	1.23	1.33
3	R	164	ARG	CZ-NH2	-7.13	1.23	1.33
1	B	243	ARG	CZ-NH2	-7.12	1.23	1.33
3	F	85	ARG	CZ-NH2	-7.11	1.23	1.33
1	B	1328	ARG	CZ-NH2	-7.09	1.23	1.33
1	B	1393	ARG	CZ-NH2	-7.09	1.23	1.33
1	P	243	ARG	CZ-NH2	-7.08	1.23	1.33
1	B	229	ARG	CZ-NH2	-7.07	1.23	1.33
3	F	34	ARG	CZ-NH2	-7.07	1.23	1.33
3	F	161	ARG	CZ-NH2	-7.05	1.23	1.33
3	Q	60	ARG	CZ-NH2	-7.04	1.23	1.33
1	B	105	ARG	CZ-NH2	-7.02	1.24	1.33
3	E	60	ARG	CZ-NH2	-7.02	1.24	1.33
1	B	1250	ARG	CZ-NH2	-7.01	1.24	1.33
3	R	34	ARG	CZ-NH1	-7.01	1.24	1.33
1	P	1250	ARG	CZ-NH1	-7.00	1.24	1.33
3	R	161	ARG	CZ-NH1	-6.99	1.24	1.33
1	B	96	ARG	CZ-NH2	-6.99	1.24	1.33
3	F	156	ARG	CZ-NH2	-6.98	1.24	1.33
1	P	1341	ARG	CZ-NH1	-6.96	1.24	1.33
1	P	1393	ARG	CZ-NH1	-6.96	1.24	1.33
1	P	96	ARG	CZ-NH1	-6.94	1.24	1.33
1	B	250	ARG	CZ-NH1	-6.92	1.24	1.33
3	R	156	ARG	CZ-NH1	-6.92	1.24	1.33
1	P	1254	ARG	CZ-NH1	-6.92	1.24	1.33
1	P	1328	ARG	CZ-NH1	-6.92	1.24	1.33
1	B	1390	ARG	CZ-NH2	-6.91	1.24	1.33
1	P	250	ARG	CZ-NH1	-6.87	1.24	1.33
1	P	1245	ARG	CZ-NH1	-6.86	1.24	1.33
3	Q	67	ARG	CZ-NH1	-6.83	1.24	1.33
3	Q	31	ARG	CZ-NH1	-6.82	1.24	1.33
1	P	199	ARG	CZ-NH1	-6.82	1.24	1.33
1	B	1199	ARG	CZ-NH1	-6.81	1.24	1.33
3	E	67	ARG	CZ-NH1	-6.80	1.24	1.33
3	E	31	ARG	CZ-NH1	-6.79	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	203	ARG	CZ-NH1	-6.79	1.24	1.33
1	B	240	ARG	CZ-NH1	-6.78	1.24	1.33
3	R	31	ARG	CZ-NH1	-6.78	1.24	1.33
3	Q	203	ARG	CZ-NH1	-6.78	1.24	1.33
3	E	206	ARG	CZ-NH1	-6.76	1.24	1.33
1	P	240	ARG	CZ-NH1	-6.76	1.24	1.33
3	R	164	ARG	CZ-NH1	-6.76	1.24	1.33
3	F	31	ARG	CZ-NH1	-6.76	1.24	1.33
3	F	164	ARG	CZ-NH1	-6.75	1.24	1.33
1	P	1199	ARG	CZ-NH1	-6.75	1.24	1.33
1	B	105	ARG	CZ-NH1	-6.75	1.24	1.33
1	P	243	ARG	CZ-NH1	-6.74	1.24	1.33
3	Q	206	ARG	CZ-NH1	-6.73	1.24	1.33
1	B	243	ARG	CZ-NH1	-6.70	1.24	1.33
1	B	1221	ARG	CZ-NH1	-6.68	1.24	1.33
3	R	85	ARG	CZ-NH1	-6.67	1.24	1.33
3	E	60	ARG	CZ-NH1	-6.66	1.24	1.33
3	F	34	ARG	CZ-NH1	-6.65	1.24	1.33
1	B	1132	ARG	CZ-NH1	-6.65	1.24	1.33
3	Q	60	ARG	CZ-NH1	-6.62	1.24	1.33
1	P	1132	ARG	CZ-NH1	-6.62	1.24	1.33
1	P	1191	TYR	CD2-CE2	-6.62	1.29	1.39
1	B	1191	TYR	CD2-CE2	-6.61	1.29	1.39
1	P	1131	ARG	CZ-NH1	-6.61	1.24	1.33
1	B	1131	ARG	CZ-NH1	-6.61	1.24	1.33
1	P	1197	ARG	CZ-NH1	-6.60	1.24	1.33
1	P	1221	ARG	CZ-NH1	-6.60	1.24	1.33
1	B	96	ARG	CZ-NH1	-6.60	1.24	1.33
1	B	1328	ARG	CZ-NH1	-6.54	1.24	1.33
1	B	229	ARG	CZ-NH1	-6.54	1.24	1.33
3	F	156	ARG	CZ-NH1	-6.52	1.24	1.33
3	F	85	ARG	CZ-NH1	-6.51	1.24	1.33
1	P	174	TYR	CD2-CE2	-6.50	1.29	1.39
1	B	1250	ARG	CZ-NH1	-6.49	1.24	1.33
1	B	199	ARG	CZ-NH1	-6.47	1.24	1.33
1	B	1197	ARG	CZ-NH1	-6.47	1.24	1.33
3	F	161	ARG	CZ-NH1	-6.45	1.24	1.33
1	B	1393	ARG	CZ-NH1	-6.44	1.24	1.33
1	B	1390	ARG	CZ-NH1	-6.39	1.24	1.33
5	K	63	DG	C4'-O4'	-6.39	1.38	1.45
1	P	198	TYR	CD1-CE1	-6.39	1.29	1.39
1	B	198	TYR	CD1-CE1	-6.38	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	1240	VAL	CB-CG1	-6.36	1.39	1.52
1	B	174	TYR	CD2-CE2	-6.32	1.29	1.39
1	B	174	TYR	CD1-CE1	-6.32	1.29	1.39
1	B	220	TYR	CD2-CE2	-6.28	1.29	1.39
3	E	58	TYR	CD1-CE1	-6.28	1.29	1.39
1	P	220	TYR	CD2-CE2	-6.27	1.29	1.39
1	P	174	TYR	CD1-CE1	-6.26	1.29	1.39
1	P	1340	TYR	CD2-CE2	-6.24	1.29	1.39
3	Q	58	TYR	CD1-CE1	-6.24	1.29	1.39
1	P	198	TYR	CD2-CE2	-6.19	1.30	1.39
3	Q	61	TYR	CD2-CE2	-6.19	1.30	1.39
1	B	1340	TYR	CD2-CE2	-6.15	1.30	1.39
3	E	61	TYR	CD2-CE2	-6.10	1.30	1.39
1	B	1340	TYR	CD1-CE1	-6.07	1.30	1.39
3	Q	61	TYR	CD1-CE1	-6.06	1.30	1.39
1	B	1240	VAL	CB-CG1	-6.06	1.40	1.52
1	B	198	TYR	CD2-CE2	-6.04	1.30	1.39
3	E	61	TYR	CD1-CE1	-6.03	1.30	1.39
1	P	1340	TYR	CD1-CE1	-6.01	1.30	1.39
3	E	58	TYR	CD2-CE2	-6.00	1.30	1.39
1	B	1191	TYR	CD1-CE1	-5.94	1.30	1.39
1	P	220	TYR	CD1-CE1	-5.92	1.30	1.39
3	Q	58	TYR	CD2-CE2	-5.92	1.30	1.39
1	P	1191	TYR	CD1-CE1	-5.85	1.30	1.39
1	B	220	TYR	CD1-CE1	-5.83	1.30	1.39
1	P	1394	GLY	N-CA	-5.79	1.37	1.46
3	F	121	TYR	CD2-CE2	-5.77	1.30	1.39
3	R	121	TYR	CD2-CE2	-5.73	1.30	1.39
1	B	1394	GLY	N-CA	-5.72	1.37	1.46
1	P	1385	TRP	CD1-NE1	-5.71	1.28	1.38
1	B	1385	TRP	CD1-NE1	-5.67	1.28	1.38
3	F	121	TYR	CD1-CE1	-5.61	1.30	1.39
1	B	48	VAL	CB-CG1	-5.60	1.41	1.52
3	R	121	TYR	CD1-CE1	-5.60	1.30	1.39
1	P	104	VAL	CB-CG1	-5.57	1.41	1.52
1	P	48	VAL	CB-CG1	-5.56	1.41	1.52
1	P	100	VAL	CB-CG2	-5.51	1.41	1.52
1	P	1128	GLY	N-CA	-5.48	1.37	1.46
1	P	119	LYS	CE-NZ	-5.40	1.35	1.49
1	B	1190	VAL	CB-CG2	-5.38	1.41	1.52
1	B	1128	GLY	N-CA	-5.38	1.38	1.46
3	R	95	VAL	CB-CG1	-5.35	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	104	VAL	CB-CG2	-5.34	1.41	1.52
1	P	1190	VAL	CB-CG2	-5.33	1.41	1.52
1	P	163	VAL	CB-CG1	-5.32	1.41	1.52
1	B	104	VAL	CB-CG1	-5.31	1.41	1.52
3	Q	63	VAL	CB-CG1	-5.30	1.41	1.52
1	P	102	VAL	CB-CG1	-5.29	1.41	1.52
3	R	33	GLY	N-CA	-5.29	1.38	1.46
3	R	95	VAL	CB-CG2	-5.28	1.41	1.52
3	E	63	VAL	CB-CG1	-5.27	1.41	1.52
1	P	196	LYS	CE-NZ	-5.26	1.35	1.49
1	P	101	VAL	CB-CG2	-5.25	1.41	1.52
6	L	63	DG	C2-N2	-5.24	1.29	1.34
1	P	182	GLY	N-CA	-5.23	1.38	1.46
1	B	48	VAL	CB-CG2	-5.22	1.41	1.52
1	P	154	LYS	CE-NZ	-5.21	1.36	1.49
3	R	155	VAL	CB-CG2	-5.20	1.42	1.52
3	F	33	GLY	N-CA	-5.18	1.38	1.46
1	P	48	VAL	CB-CG2	-5.18	1.42	1.52
1	P	101	VAL	CB-CG1	-5.18	1.42	1.52
1	P	227	GLY	N-CA	-5.18	1.38	1.46
1	P	100	VAL	CB-CG1	-5.16	1.42	1.52
3	R	131	GLY	N-CA	-5.16	1.38	1.46
1	P	186	LYS	CE-NZ	-5.14	1.36	1.49
1	B	100	VAL	CB-CG2	-5.13	1.42	1.52
1	P	1398	SER	CB-OG	-5.12	1.35	1.42
3	R	132	LYS	CE-NZ	-5.12	1.36	1.49
1	B	227	GLY	N-CA	-5.12	1.38	1.46
3	R	79	SER	CB-OG	-5.11	1.35	1.42
3	F	86	SER	CB-OG	-5.11	1.35	1.42
3	R	142	SER	CB-OG	-5.09	1.35	1.42
1	B	103	GLY	N-CA	-5.09	1.38	1.46
1	P	228	VAL	CB-CG1	-5.09	1.42	1.52
3	Q	63	VAL	CB-CG2	-5.09	1.42	1.52
1	B	104	VAL	CB-CG2	-5.08	1.42	1.52
3	R	97	LYS	CE-NZ	-5.08	1.36	1.49
3	R	96	GLY	N-CA	-5.08	1.38	1.46
1	B	182	GLY	N-CA	-5.08	1.38	1.46
1	B	1209	VAL	CB-CG2	-5.07	1.42	1.52
1	B	119	LYS	CE-NZ	-5.06	1.36	1.49
3	F	95	VAL	CB-CG2	-5.06	1.42	1.52
1	P	183	VAL	CB-CG1	-5.06	1.42	1.52
1	P	1384	SER	CB-OG	-5.06	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	63	VAL	CB-CG2	-5.05	1.42	1.52
1	P	195	SER	CB-OG	-5.04	1.35	1.42
3	F	95	VAL	CB-CG1	-5.03	1.42	1.52
1	P	254	SER	CB-OG	-5.02	1.35	1.42
3	R	148	LYS	CE-NZ	-5.02	1.36	1.49
6	L	55	DG	C2-N2	-5.02	1.29	1.34
1	P	102	VAL	CB-CG2	-5.02	1.42	1.52
1	P	103	GLY	N-CA	-5.02	1.38	1.46
1	B	254	SER	CB-OG	-5.01	1.35	1.42
1	P	1209	VAL	CB-CG1	-5.01	1.42	1.52
1	B	1209	VAL	CB-CG1	-5.01	1.42	1.52
3	F	96	GLY	N-CA	-5.01	1.38	1.46
6	L	65	DG	C2-N2	-5.01	1.29	1.34

All (608) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	187	ARG	NE-CZ-NH2	11.30	125.95	120.30
6	L	29	DA	N1-C6-N6	-11.16	111.90	118.60
2	C	295	ARG	C-N-CA	10.48	147.90	121.70
2	D	295	ARG	C-N-CA	10.43	147.77	121.70
5	K	46	DA	N1-C6-N6	-10.34	112.39	118.60
6	L	37	DA	N1-C6-N6	-10.13	112.52	118.60
5	K	35	DA	N1-C6-N6	-9.56	112.86	118.60
2	D	123	LEU	CB-CG-CD2	-9.50	94.84	111.00
5	K	66	DA	N1-C6-N6	-9.47	112.92	118.60
5	K	41	DA	N1-C6-N6	-9.42	112.95	118.60
1	B	966	ARG	NE-CZ-NH2	9.36	124.98	120.30
5	K	64	DG	O4'-C1'-N9	9.18	114.42	108.00
1	P	966	ARG	NE-CZ-NH2	9.14	124.87	120.30
1	B	187	ARG	NE-CZ-NH2	9.13	124.87	120.30
6	L	43	DG	O4'-C1'-N9	9.05	114.33	108.00
6	L	46	DA	N1-C6-N6	-8.92	113.25	118.60
1	B	1056	ARG	NE-CZ-NH2	8.69	124.65	120.30
6	L	18	DA	N1-C6-N6	-8.68	113.39	118.60
1	P	1056	ARG	NE-CZ-NH2	8.56	124.58	120.30
5	K	8	DA	N1-C6-N6	-8.45	113.53	118.60
1	P	1390	ARG	NE-CZ-NH2	8.43	124.52	120.30
5	K	65	DA	N1-C6-N6	-8.34	113.59	118.60
5	K	46	DA	C4-C5-C6	-8.33	112.84	117.00
3	Q	58	TYR	CB-CG-CD2	8.23	125.94	121.00
5	K	23	DA	N1-C6-N6	-8.18	113.69	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	9	DA	N1-C6-N6	-8.17	113.70	118.60
5	K	25	DA	C5-C6-N1	8.15	121.78	117.70
5	K	43	DG	O4'-C1'-N9	8.14	113.70	108.00
5	K	57	DC	N3-C2-O2	-8.10	116.23	121.90
3	E	58	TYR	CB-CG-CD2	8.08	125.85	121.00
6	L	38	DC	N3-C2-O2	-8.06	116.26	121.90
6	L	52	DA	C4-C5-C6	-8.01	113.00	117.00
5	K	10	DG	O4'-C1'-N9	7.99	113.59	108.00
5	K	40	DA	N1-C6-N6	-7.96	113.82	118.60
1	P	528	ARG	NE-CZ-NH2	7.95	124.27	120.30
6	L	47	DT	O4'-C1'-N1	7.92	113.54	108.00
3	R	136	PHE	CB-CG-CD2	7.91	126.34	120.80
5	K	61	DC	N3-C2-O2	-7.89	116.38	121.90
5	K	32	DA	C4-C5-C6	-7.84	113.08	117.00
5	K	52	DC	N3-C2-O2	-7.84	116.41	121.90
5	K	40	DA	C4-C5-C6	-7.84	113.08	117.00
5	K	35	DA	C4-C5-C6	-7.82	113.09	117.00
1	B	528	ARG	NE-CZ-NH2	7.81	124.20	120.30
5	K	32	DA	C5-C6-N1	7.78	121.59	117.70
6	L	36	DA	C5-C6-N1	7.76	121.58	117.70
5	K	24	DA	C5-C6-N1	7.72	121.56	117.70
5	K	30	DA	C4-C5-C6	-7.71	113.14	117.00
6	L	35	DA	C5-C6-N1	7.70	121.55	117.70
6	L	22	DA	C5-C6-N1	7.67	121.53	117.70
6	L	54	DA	C5-C6-N1	7.67	121.54	117.70
6	L	38	DC	O4'-C1'-N1	7.67	113.37	108.00
5	K	16	DG	O4'-C1'-N9	7.66	113.36	108.00
6	L	85	DA	N1-C6-N6	-7.66	114.01	118.60
5	K	41	DA	C4-C5-C6	-7.65	113.18	117.00
5	K	51	DG	O4'-C1'-N9	7.65	113.35	108.00
5	K	7	DC	N3-C2-O2	-7.59	116.58	121.90
2	C	116	ARG	NE-CZ-NH2	7.55	124.07	120.30
6	L	76	DT	O4'-C1'-N1	7.54	113.28	108.00
6	L	22	DA	N1-C6-N6	-7.54	114.08	118.60
6	L	37	DA	C5-C6-N1	7.50	121.45	117.70
5	K	62	DT	N3-C2-O2	-7.48	117.81	122.30
5	K	21	DC	N3-C2-O2	-7.48	116.66	121.90
5	K	36	DC	N3-C2-O2	-7.47	116.67	121.90
1	B	363	ARG	NE-CZ-NH2	7.45	124.03	120.30
5	K	42	DA	C4-C5-C6	-7.43	113.28	117.00
1	B	194	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	P	363	ARG	NE-CZ-NH2	7.41	124.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	37	DA	C4-C5-C6	-7.38	113.31	117.00
5	K	49	DA	C4-C5-C6	-7.37	113.31	117.00
5	K	44	DA	O4'-C1'-N9	7.34	113.14	108.00
5	K	42	DA	N1-C6-N6	-7.32	114.21	118.60
5	K	44	DA	N1-C6-N6	-7.31	114.22	118.60
5	K	70	DC	N3-C2-O2	-7.30	116.79	121.90
5	K	25	DA	C4-C5-C6	-7.29	113.36	117.00
6	L	87	DC	N3-C2-O2	-7.27	116.81	121.90
2	D	116	ARG	NE-CZ-NH2	7.26	123.93	120.30
5	K	3	DC	N3-C2-O2	-7.25	116.82	121.90
1	P	232	PHE	CB-CG-CD2	7.25	125.88	120.80
6	L	85	DA	O4'-C1'-N9	7.24	113.07	108.00
6	L	48	DC	O4'-C1'-N1	7.24	113.07	108.00
1	A	966	ARG	NE-CZ-NH2	7.23	123.91	120.30
6	L	73	DA	C5-C6-N1	7.20	121.30	117.70
1	B	232	PHE	CB-CG-CD2	7.15	125.81	120.80
5	K	23	DA	C4-C5-C6	-7.15	113.42	117.00
6	L	39	DG	O4'-C1'-N9	7.14	113.00	108.00
5	K	15	DA	N1-C6-N6	-7.13	114.32	118.60
5	K	29	DG	C1'-O4'-C4'	-7.13	102.97	110.10
5	K	60	DC	N3-C2-O2	-7.10	116.93	121.90
5	K	2	DA	C5-C6-N1	7.09	121.25	117.70
6	L	90	DC	N3-C2-O2	-7.09	116.94	121.90
5	K	13	DA	C5-C6-N1	7.07	121.23	117.70
5	K	66	DA	C5-C6-N1	7.06	121.23	117.70
6	L	75	DC	N3-C2-O2	-7.06	116.96	121.90
1	O	966	ARG	NE-CZ-NH2	7.06	123.83	120.30
5	K	65	DA	C5-C6-N1	7.05	121.22	117.70
1	P	521	ARG	NE-CZ-NH2	7.00	123.80	120.30
5	K	30	DA	C5-C6-N1	7.00	121.20	117.70
1	B	521	ARG	NE-CZ-NH2	7.00	123.80	120.30
5	K	49	DA	C5-C6-N1	6.99	121.20	117.70
5	K	2	DA	N1-C6-N6	-6.98	114.41	118.60
5	K	25	DA	N1-C6-N6	-6.97	114.42	118.60
6	L	85	DA	C5-C6-N1	6.97	121.19	117.70
6	L	80	DA	N1-C6-N6	-6.96	114.43	118.60
5	K	49	DA	N1-C6-N6	-6.90	114.46	118.60
5	K	66	DA	C4-C5-C6	-6.88	113.56	117.00
6	L	48	DC	N3-C2-O2	-6.88	117.08	121.90
2	D	114	TYR	CB-CG-CD1	-6.87	116.88	121.00
1	B	1131	ARG	CD-NE-CZ	6.85	133.19	123.60
1	P	1131	ARG	CD-NE-CZ	6.85	133.19	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	186	ARG	NE-CZ-NH2	6.84	123.72	120.30
5	K	22	DG	O4'-C1'-N9	6.84	112.79	108.00
5	K	38	DA	C4-C5-C6	-6.83	113.58	117.00
3	Q	163	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	P	548	ARG	NE-CZ-NH2	6.81	123.70	120.30
6	L	29	DA	C4-C5-C6	-6.80	113.60	117.00
5	K	9	DA	C5-C6-N1	6.80	121.10	117.70
5	K	38	DA	C5-C6-N1	6.80	121.10	117.70
5	K	44	DA	C4-C5-C6	-6.79	113.60	117.00
3	Q	186	ARG	NE-CZ-NH2	6.79	123.70	120.30
5	K	47	DC	N3-C2-O2	-6.78	117.16	121.90
5	K	28	DC	N3-C2-O2	-6.77	117.16	121.90
1	P	579	ARG	NE-CZ-NH2	6.77	123.69	120.30
6	L	69	DC	N3-C2-O2	-6.77	117.16	121.90
6	L	36	DA	N1-C6-N6	-6.76	114.54	118.60
6	L	72	DC	N3-C2-O2	-6.76	117.17	121.90
6	L	30	DG	N1-C6-O6	-6.76	115.84	119.90
1	B	1195	ARG	NE-CZ-NH2	6.76	123.68	120.30
5	K	14	DG	O4'-C1'-N9	6.75	112.73	108.00
1	B	499	ARG	NE-CZ-NH2	6.75	123.67	120.30
2	D	16	ARG	NE-CZ-NH2	6.74	123.67	120.30
5	K	5	DC	N3-C2-O2	-6.73	117.19	121.90
1	B	1132	ARG	CD-NE-CZ	6.72	133.01	123.60
6	L	24	DC	N3-C2-O2	-6.71	117.20	121.90
1	B	1221	ARG	CD-NE-CZ	6.71	133.00	123.60
1	P	189	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	P	1221	ARG	CD-NE-CZ	6.71	132.99	123.60
6	L	52	DA	N1-C6-N6	-6.69	114.59	118.60
5	K	58	DC	N3-C2-O2	-6.68	117.22	121.90
6	L	47	DT	N3-C2-O2	-6.67	118.30	122.30
1	P	1132	ARG	CD-NE-CZ	6.67	132.94	123.60
1	P	194	ARG	NE-CZ-NH2	6.67	123.63	120.30
1	B	579	ARG	NE-CZ-NH2	6.66	123.63	120.30
5	K	46	DA	C5-C6-N1	6.66	121.03	117.70
5	K	23	DA	C5-C6-N1	6.66	121.03	117.70
1	P	1328	ARG	CD-NE-CZ	6.65	132.90	123.60
1	B	431	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	B	548	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	P	1195	ARG	NE-CZ-NH2	6.64	123.62	120.30
6	L	81	DC	N3-C2-O2	-6.63	117.26	121.90
1	B	229	ARG	CD-NE-CZ	6.63	132.89	123.60
6	L	52	DA	C5-C6-N1	6.63	121.02	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1328	ARG	CD-NE-CZ	6.62	132.87	123.60
1	P	431	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	B	105	ARG	CD-NE-CZ	6.61	132.86	123.60
5	K	13	DA	C4-C5-C6	-6.61	113.69	117.00
5	K	71	DC	N3-C2-O2	-6.61	117.28	121.90
5	K	12	DC	N3-C2-O2	-6.60	117.28	121.90
6	L	36	DA	O4'-C1'-N9	6.60	112.62	108.00
6	L	46	DA	C4-C5-C6	-6.60	113.70	117.00
3	R	156	ARG	CD-NE-CZ	6.60	132.84	123.60
6	L	62	DC	N3-C2-O2	-6.59	117.28	121.90
6	L	57	DC	N3-C2-O2	-6.59	117.29	121.90
1	P	499	ARG	NE-CZ-NH2	6.58	123.59	120.30
6	L	80	DA	C4-C5-C6	-6.58	113.71	117.00
1	P	1063	ARG	NE-CZ-NH2	6.57	123.58	120.30
5	K	31	DC	N3-C2-O2	-6.55	117.31	121.90
6	L	27	DC	N3-C2-O2	-6.55	117.31	121.90
5	K	55	DT	O4'-C1'-N1	6.54	112.58	108.00
1	P	1341	ARG	CD-NE-CZ	6.54	132.76	123.60
3	F	156	ARG	CD-NE-CZ	6.54	132.75	123.60
1	B	1191	TYR	CB-CG-CD2	6.53	124.92	121.00
6	L	77	DC	N3-C2-O2	-6.53	117.33	121.90
2	D	4	TYR	CB-CG-CD2	-6.53	117.08	121.00
1	P	96	ARG	CD-NE-CZ	6.53	132.74	123.60
5	K	25	DA	O4'-C1'-N9	6.52	112.56	108.00
1	B	1063	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	P	1191	TYR	CB-CG-CD2	6.51	124.91	121.00
5	K	24	DA	C4-C5-C6	-6.50	113.75	117.00
6	L	22	DA	C4-C5-C6	-6.50	113.75	117.00
1	O	1056	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	B	96	ARG	CD-NE-CZ	6.50	132.70	123.60
3	E	60	ARG	CD-NE-CZ	6.49	132.68	123.60
5	K	18	DT	C6-C5-C7	-6.49	119.01	122.90
3	Q	60	ARG	CD-NE-CZ	6.48	132.67	123.60
3	R	31	ARG	CD-NE-CZ	6.48	132.67	123.60
1	P	1250	ARG	CD-NE-CZ	6.46	132.64	123.60
5	K	67	DG	N1-C6-O6	-6.46	116.03	119.90
1	P	243	ARG	CG-CD-NE	6.45	125.35	111.80
6	L	74	DC	N3-C2-O2	-6.44	117.39	121.90
3	F	31	ARG	CD-NE-CZ	6.43	132.61	123.60
1	B	243	ARG	CG-CD-NE	6.43	125.30	111.80
3	Q	31	ARG	CD-NE-CZ	6.42	132.59	123.60
6	L	83	DT	O4'-C1'-N1	6.40	112.48	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	28	DC	N3-C2-O2	-6.39	117.43	121.90
6	L	29	DA	C5-C6-N1	6.39	120.90	117.70
5	K	72	DC	N3-C2-O2	-6.39	117.43	121.90
5	K	62	DT	C6-C5-C7	-6.38	119.07	122.90
3	E	31	ARG	CD-NE-CZ	6.38	132.53	123.60
6	L	35	DA	O4'-C1'-N9	6.38	112.47	108.00
5	K	68	DC	N3-C2-O2	-6.37	117.44	121.90
6	L	18	DA	C4-C5-C6	-6.37	113.82	117.00
1	P	1074	ARG	NE-CZ-NH2	6.36	123.48	120.30
1	B	1250	ARG	CD-NE-CZ	6.35	132.49	123.60
5	K	35	DA	C5-C6-N1	6.34	120.87	117.70
1	B	491	ARG	NE-CZ-NH2	6.33	123.47	120.30
1	P	491	ARG	NE-CZ-NH2	6.33	123.47	120.30
5	K	26	DC	N3-C2-O2	-6.33	117.47	121.90
5	K	2	DA	C4-C5-C6	-6.32	113.84	117.00
1	A	537	ARG	NE-CZ-NH2	6.31	123.45	120.30
5	K	59	DC	N3-C2-O2	-6.30	117.49	121.90
6	L	54	DA	C4-C5-C6	-6.30	113.85	117.00
5	K	37	DT	N3-C2-O2	-6.30	118.52	122.30
1	A	1056	ARG	NE-CZ-NH2	6.29	123.45	120.30
1	A	992	ARG	NE-CZ-NH2	6.29	123.44	120.30
2	C	123	LEU	CB-CG-CD2	-6.28	100.32	111.00
2	C	176	ARG	NE-CZ-NH1	-6.28	117.16	120.30
5	K	33	DG	C1'-O4'-C4'	-6.28	103.82	110.10
6	L	47	DT	O4'-C1'-C2'	-6.28	100.88	105.90
5	K	42	DA	C5-C6-N1	6.27	120.83	117.70
6	L	25	DT	C6-C5-C7	-6.27	119.14	122.90
1	O	537	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	O	992	ARG	NE-CZ-NH2	6.26	123.43	120.30
5	K	65	DA	O4'-C1'-N9	6.26	112.38	108.00
5	K	69	DT	C6-C5-C7	-6.26	119.15	122.90
1	P	1319	LEU	CA-CB-CG	6.25	129.68	115.30
5	K	37	DT	C6-C5-C7	-6.25	119.15	122.90
1	B	1319	LEU	CA-CB-CG	6.23	129.63	115.30
3	E	108	ARG	NE-CZ-NH2	6.23	123.42	120.30
6	L	67	DT	N3-C2-O2	-6.23	118.56	122.30
5	K	16	DG	C1'-O4'-C4'	-6.23	103.87	110.10
6	L	46	DA	C5-C6-N1	6.23	120.81	117.70
1	A	878	ARG	NE-CZ-NH2	6.23	123.41	120.30
5	K	8	DA	C4-C5-C6	-6.22	113.89	117.00
6	L	40	DC	N3-C2-O2	-6.22	117.55	121.90
6	L	55	DG	O4'-C1'-N9	6.22	112.35	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	42	DA	O4'-C1'-N9	6.21	112.35	108.00
6	L	48	DC	C1'-O4'-C4'	-6.21	103.89	110.10
1	O	878	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	P	256	ARG	CD-NE-CZ	6.19	132.26	123.60
1	B	256	ARG	CD-NE-CZ	6.19	132.26	123.60
1	B	1074	ARG	NE-CZ-NH2	6.18	123.39	120.30
5	K	9	DA	C4-C5-C6	-6.17	113.91	117.00
5	K	46	DA	O4'-C1'-N9	6.17	112.32	108.00
5	K	15	DA	C4-C5-C6	-6.17	113.92	117.00
5	K	48	DC	N3-C2-O2	-6.16	117.59	121.90
6	L	55	DG	N3-C2-N2	-6.16	115.59	119.90
3	F	121	TYR	CB-CG-CD2	6.15	124.69	121.00
3	R	121	TYR	CB-CG-CD2	6.15	124.69	121.00
6	L	43	DG	C1'-O4'-C4'	-6.15	103.95	110.10
6	L	45	DT	N3-C2-O2	-6.15	118.61	122.30
6	L	73	DA	C4-C5-C6	-6.14	113.93	117.00
5	K	57	DC	P-O3'-C3'	6.13	127.06	119.70
6	L	66	DT	C6-C5-C7	-6.12	119.23	122.90
6	L	18	DA	C5-C6-N1	6.12	120.76	117.70
3	Q	108	ARG	NE-CZ-NH2	6.12	123.36	120.30
5	K	13	DA	N1-C6-N6	-6.09	114.94	118.60
5	K	30	DA	N1-C6-N6	-6.09	114.95	118.60
5	K	56	DT	N3-C2-O2	-6.08	118.65	122.30
6	L	71	DC	N3-C2-O2	-6.07	117.65	121.90
5	K	38	DA	O4'-C1'-N9	6.07	112.25	108.00
2	C	297	PHE	CB-CG-CD2	-6.06	116.56	120.80
2	D	297	PHE	CB-CG-CD2	-6.06	116.56	120.80
1	O	548	ARG	NE-CZ-NH2	6.06	123.33	120.30
6	L	46	DA	O4'-C1'-N9	6.06	112.24	108.00
1	B	1197	ARG	CD-NE-CZ	6.05	132.07	123.60
1	O	589	GLN	O-C-N	6.05	132.38	122.70
5	K	7	DC	O4'-C1'-N1	6.04	112.23	108.00
5	K	42	DA	C1'-O4'-C4'	-6.04	104.06	110.10
1	A	589	GLN	O-C-N	6.03	132.35	122.70
1	B	1058	ARG	NE-CZ-NH2	6.03	123.31	120.30
3	E	156	ARG	NE-CZ-NH2	6.02	123.31	120.30
6	L	36	DA	C4-C5-C6	-6.01	113.99	117.00
5	K	38	DA	N1-C6-N6	-6.01	114.99	118.60
5	K	63	DG	O4'-C1'-N9	-6.01	103.79	108.00
5	K	54	DT	N3-C2-O2	-6.00	118.70	122.30
6	L	66	DT	O4'-C1'-N1	6.00	112.20	108.00
3	E	67	ARG	CG-CD-NE	6.00	124.40	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	36	DC	O4'-C1'-N1	5.99	112.19	108.00
3	Q	67	ARG	CG-CD-NE	5.99	124.38	111.80
5	K	55	DT	C6-C5-C7	-5.98	119.31	122.90
1	A	548	ARG	NE-CZ-NH2	5.97	123.29	120.30
1	P	1197	ARG	CD-NE-CZ	5.97	131.95	123.60
2	C	4	TYR	CB-CG-CD2	-5.96	117.42	121.00
6	L	76	DT	C6-C5-C7	-5.96	119.33	122.90
5	K	28	DC	C3'-C2'-C1'	-5.94	95.37	102.50
5	K	52	DC	O4'-C1'-N1	5.94	112.16	108.00
1	P	1058	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	P	243	ARG	CD-NE-CZ	5.93	131.91	123.60
6	L	59	DT	N3-C2-O2	-5.93	118.74	122.30
1	P	243	ARG	CA-CB-CG	5.93	126.44	113.40
1	B	243	ARG	CA-CB-CG	5.93	126.44	113.40
1	P	122	MET	CA-CB-CG	5.92	123.37	113.30
6	L	35	DA	C4-C5-C6	-5.92	114.04	117.00
6	L	80	DA	C5-C6-N1	5.91	120.65	117.70
1	A	499	ARG	NE-CZ-NH2	5.91	123.25	120.30
1	B	243	ARG	CD-NE-CZ	5.90	131.87	123.60
6	L	78	DT	C6-C5-C7	-5.89	119.36	122.90
5	K	65	DA	C4-C5-C6	-5.89	114.05	117.00
6	L	23	DG	O4'-C1'-N9	5.89	112.12	108.00
6	L	68	DT	C1'-O4'-C4'	-5.89	104.21	110.10
6	L	82	DT	O4'-C1'-N1	5.88	112.12	108.00
1	P	174	TYR	CB-CG-CD2	5.88	124.53	121.00
3	Q	67	ARG	CD-NE-CZ	5.88	131.84	123.60
6	L	25	DT	O4'-C1'-N1	5.88	112.12	108.00
5	K	45	DT	N3-C2-O2	-5.87	118.78	122.30
5	K	19	DG	C1'-O4'-C4'	-5.86	104.24	110.10
5	K	62	DT	N1-C2-N3	5.86	118.12	114.60
3	E	67	ARG	CD-NE-CZ	5.86	131.80	123.60
5	K	24	DA	N1-C6-N6	-5.86	115.08	118.60
6	L	59	DT	O4'-C1'-N1	5.86	112.10	108.00
5	K	64	DG	N1-C6-O6	-5.84	116.40	119.90
5	K	6	DT	N3-C2-O2	-5.83	118.80	122.30
6	L	56	DT	N3-C2-O2	-5.83	118.80	122.30
5	K	37	DT	O4'-C1'-C2'	-5.82	101.24	105.90
2	D	176	ARG	CB-CG-CD	5.82	126.74	111.60
6	L	42	DT	C6-C5-C7	-5.82	119.41	122.90
3	Q	76	ARG	NE-CZ-NH2	5.81	123.21	120.30
5	K	56	DT	C6-C5-C7	-5.80	119.42	122.90
6	L	84	DG	O4'-C1'-N9	5.80	112.06	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	76	ARG	NE-CZ-NH2	5.80	123.20	120.30
5	K	41	DA	O4'-C1'-N9	5.79	112.06	108.00
6	L	65	DG	O4'-C1'-N9	5.77	112.04	108.00
1	O	499	ARG	NE-CZ-NH2	5.76	123.18	120.30
2	C	124	ARG	NE-CZ-NH2	5.76	123.18	120.30
5	K	55	DT	N3-C2-O2	-5.76	118.84	122.30
5	K	32	DA	N1-C6-N6	-5.76	115.15	118.60
5	K	44	DA	C5-C6-N1	5.75	120.58	117.70
1	B	174	TYR	CB-CG-CD2	5.75	124.45	121.00
1	B	122	MET	CA-CB-CG	5.75	123.07	113.30
6	L	64	DG	O4'-C1'-N9	5.75	112.02	108.00
6	L	21	DG	N1-C6-O6	-5.74	116.45	119.90
5	K	57	DC	N1-C2-O2	5.74	122.34	118.90
1	O	363	ARG	NE-CZ-NH2	5.73	123.17	120.30
5	K	36	DC	C1'-O4'-C4'	-5.73	104.37	110.10
6	L	50	DT	C5-C6-N1	-5.73	120.26	123.70
2	D	73	ARG	NE-CZ-NH2	5.72	123.16	120.30
6	L	67	DT	C6-C5-C7	-5.72	119.47	122.90
1	P	1391	ARG	CD-NE-CZ	5.72	131.61	123.60
5	K	66	DA	O4'-C1'-N9	5.71	112.00	108.00
6	L	49	DT	C5-C6-N1	-5.71	120.28	123.70
1	P	1204	ARG	NE-CZ-NH2	5.71	123.15	120.30
5	K	11	DT	C6-C5-C7	-5.70	119.48	122.90
6	L	49	DT	N3-C2-O2	-5.70	118.88	122.30
5	K	24	DA	C1'-O4'-C4'	-5.70	104.40	110.10
6	L	50	DT	C1'-O4'-C4'	-5.70	104.40	110.10
6	L	73	DA	O4'-C1'-N9	5.69	111.98	108.00
1	B	1204	ARG	NE-CZ-NH2	5.69	123.14	120.30
2	C	124	ARG	CA-CB-CG	5.69	125.92	113.40
6	L	26	DT	C6-C5-C7	-5.69	119.49	122.90
3	Q	78	ARG	NE-CZ-NH2	5.69	123.14	120.30
5	K	47	DC	O3'-P-O5'	-5.68	93.22	104.00
3	Q	163	ARG	NE-CZ-NH1	-5.68	117.46	120.30
6	L	41	DC	N3-C2-O2	-5.67	117.93	121.90
5	K	37	DT	C1'-O4'-C4'	-5.67	104.43	110.10
6	L	68	DT	C6-C5-C7	-5.67	119.50	122.90
6	L	35	DA	N1-C6-N6	-5.67	115.20	118.60
6	L	86	DG	N1-C6-O6	-5.67	116.50	119.90
5	K	63	DG	C4-N9-C1'	-5.67	119.14	126.50
6	L	50	DT	C6-C5-C7	-5.67	119.50	122.90
5	K	57	DC	O4'-C1'-N1	5.66	111.96	108.00
6	L	59	DT	C6-C5-C7	-5.66	119.50	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	46	DA	C6-C5-N7	5.65	136.26	132.30
6	L	59	DT	C1'-O4'-C4'	-5.65	104.45	110.10
5	K	31	DC	N1-C2-O2	5.65	122.29	118.90
6	L	51	DT	C5-C6-N1	-5.65	120.31	123.70
5	K	26	DC	C1'-O4'-C4'	-5.64	104.46	110.10
5	K	28	DC	O4'-C1'-N1	5.64	111.95	108.00
6	L	38	DC	O4'-C1'-C2'	-5.64	101.39	105.90
5	K	32	DA	C1'-O4'-C4'	-5.64	104.46	110.10
6	L	19	DG	N1-C6-O6	-5.64	116.52	119.90
1	P	537	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	A	363	ARG	NE-CZ-NH2	5.63	123.12	120.30
2	C	114	TYR	CB-CG-CD1	-5.63	117.62	121.00
6	L	39	DG	O4'-C1'-C2'	-5.63	101.39	105.90
6	L	50	DT	N3-C2-O2	-5.63	118.92	122.30
5	K	63	DG	O4'-C1'-C2'	5.62	110.40	105.90
1	A	894	ARG	NE-CZ-NH1	-5.61	117.49	120.30
5	K	73	DT	C6-C5-C7	-5.61	119.53	122.90
6	L	85	DA	C4-C5-C6	-5.61	114.20	117.00
1	P	197	PHE	CB-CG-CD2	5.60	124.72	120.80
5	K	21	DC	N1-C2-O2	5.60	122.26	118.90
1	B	1395	LYS	CA-CB-CG	5.59	125.71	113.40
5	K	54	DT	C6-C5-C7	-5.59	119.54	122.90
6	L	64	DG	C1'-O4'-C4'	-5.59	104.51	110.10
6	L	19	DG	N3-C2-N2	-5.58	115.99	119.90
1	O	894	ARG	NE-CZ-NH1	-5.58	117.51	120.30
3	F	85	ARG	CD-NE-CZ	5.58	131.41	123.60
6	L	57	DC	C3'-C2'-C1'	-5.57	95.81	102.50
3	R	85	ARG	CD-NE-CZ	5.57	131.40	123.60
6	L	57	DC	N1-C2-O2	5.57	122.24	118.90
5	K	6	DT	C6-C5-C7	-5.57	119.56	122.90
6	L	78	DT	N3-C2-O2	-5.57	118.96	122.30
5	K	39	DT	O4'-C1'-N1	5.56	111.89	108.00
6	L	54	DA	C1'-O4'-C4'	-5.56	104.54	110.10
5	K	63	DG	N1-C6-O6	-5.54	116.57	119.90
6	L	49	DT	C1'-O4'-C4'	-5.54	104.56	110.10
5	K	64	DG	O4'-C1'-C2'	-5.54	101.47	105.90
5	K	70	DC	N1-C2-O2	5.54	122.22	118.90
6	L	62	DC	C1'-O4'-C4'	-5.53	104.57	110.10
6	L	64	DG	N1-C6-O6	-5.53	116.58	119.90
1	A	491	ARG	NE-CZ-NH2	5.53	123.07	120.30
5	K	18	DT	C1'-O4'-C4'	-5.52	104.58	110.10
1	P	194	ARG	NE-CZ-NH1	-5.52	117.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1056	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	A	894	ARG	NE-CZ-NH2	5.51	123.06	120.30
6	L	49	DT	C6-C5-C7	-5.51	119.59	122.90
3	E	192	ARG	NE-CZ-NH2	5.51	123.05	120.30
6	L	58	DC	N3-C2-O2	-5.50	118.05	121.90
3	E	163	ARG	NE-CZ-NH2	5.50	123.05	120.30
6	L	66	DT	N3-C2-O2	-5.50	119.00	122.30
1	B	537	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	O	1056	ARG	NE-CZ-NH1	-5.49	117.56	120.30
5	K	56	DT	O4'-C1'-C2'	-5.48	101.52	105.90
6	L	82	DT	N3-C2-O2	-5.48	119.01	122.30
6	L	61	DT	C6-C5-C7	-5.47	119.62	122.90
1	B	1340	TYR	CB-CG-CD1	5.47	124.28	121.00
1	A	579	ARG	NE-CZ-NH2	5.47	123.03	120.30
3	R	164	ARG	CD-NE-CZ	5.47	131.25	123.60
6	L	37	DA	O4'-C1'-N9	5.47	111.83	108.00
3	E	78	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	O	1008	ARG	NE-CZ-NH2	5.46	123.03	120.30
3	Q	192	ARG	NE-CZ-NH2	5.46	123.03	120.30
2	C	28	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	P	198	TYR	CB-CG-CD2	5.46	124.27	121.00
6	L	60	DG	C3'-C2'-C1'	-5.45	95.95	102.50
5	K	48	DC	N1-C2-O2	5.45	122.17	118.90
6	L	30	DG	P-O3'-C3'	5.45	126.24	119.70
3	F	164	ARG	CD-NE-CZ	5.45	131.23	123.60
5	K	63	DG	C6-C5-N7	5.45	133.67	130.40
1	P	235	MET	CA-CB-CG	5.45	122.56	113.30
2	D	57	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	A	345	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	B	197	PHE	CB-CG-CD2	5.44	124.61	120.80
6	L	56	DT	C6-C5-C7	-5.44	119.64	122.90
6	L	86	DG	O4'-C1'-N9	5.44	111.81	108.00
1	B	1393	ARG	CD-NE-CZ	5.44	131.21	123.60
1	O	579	ARG	NE-CZ-NH2	5.43	123.02	120.30
6	L	25	DT	N3-C2-O2	-5.43	119.04	122.30
6	L	53	DT	N3-C2-O2	-5.42	119.05	122.30
1	O	491	ARG	NE-CZ-NH2	5.42	123.01	120.30
5	K	15	DA	C5-C6-N1	5.42	120.41	117.70
6	L	54	DA	O4'-C1'-N9	5.42	111.79	108.00
1	P	1393	ARG	CD-NE-CZ	5.40	131.16	123.60
1	B	1000	ARG	NE-CZ-NH2	5.39	123.00	120.30
5	K	53	DG	O4'-C1'-N9	5.39	111.77	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	84	DG	N1-C6-O6	-5.39	116.67	119.90
5	K	7	DC	N1-C2-O2	5.38	122.13	118.90
5	K	48	DC	N3-C4-C5	5.38	124.05	121.90
6	L	42	DT	N3-C2-O2	-5.38	119.07	122.30
1	P	1000	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	A	1008	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	P	1215	MET	CA-CB-CG	5.38	122.44	113.30
5	K	30	DA	O4'-C1'-N9	5.37	111.76	108.00
5	K	19	DG	C3'-C2'-C1'	-5.37	96.06	102.50
6	L	57	DC	N3-C4-C5	5.37	124.05	121.90
1	P	186	LYS	CA-CB-CG	5.36	125.19	113.40
5	K	27	DC	C1'-O4'-C4'	-5.36	104.75	110.10
1	P	1340	TYR	CB-CG-CD1	5.36	124.21	121.00
1	B	1215	MET	CA-CB-CG	5.35	122.40	113.30
5	K	37	DT	O4'-C1'-N1	5.35	111.74	108.00
5	K	63	DG	N3-C2-N2	-5.35	116.16	119.90
6	L	47	DT	C6-C5-C7	-5.35	119.69	122.90
1	B	198	TYR	CB-CG-CD2	5.34	124.21	121.00
6	L	61	DT	C5-C6-N1	-5.34	120.50	123.70
1	B	854	ARG	NE-CZ-NH2	5.34	122.97	120.30
6	L	83	DT	C6-C5-C7	-5.33	119.70	122.90
6	L	51	DT	C3'-C2'-C1'	-5.33	96.10	102.50
1	P	229	ARG	NE-CZ-NH2	5.33	122.97	120.30
5	K	8	DA	C5-C6-N1	5.33	120.36	117.70
6	L	83	DT	N3-C2-O2	-5.32	119.11	122.30
6	L	45	DT	C6-C5-C7	-5.32	119.71	122.90
5	K	22	DG	C1'-O4'-C4'	-5.31	104.79	110.10
6	L	34	DG	P-O3'-C3'	5.31	126.07	119.70
2	D	138	ARG	NE-CZ-NH2	5.30	122.95	120.30
3	E	61	TYR	CB-CG-CD2	5.30	124.18	121.00
5	K	54	DT	O4'-C1'-N1	5.30	111.71	108.00
6	L	89	DT	C6-C5-C7	-5.29	119.72	122.90
1	B	1390	ARG	CD-NE-CZ	5.29	131.01	123.60
5	K	17	DG	C1'-O4'-C4'	-5.29	104.81	110.10
6	L	51	DT	C6-C5-C7	-5.29	119.73	122.90
6	L	82	DT	C6-C5-C7	-5.28	119.73	122.90
6	L	29	DA	C6-C5-N7	5.27	135.99	132.30
6	L	68	DT	C5-C6-N1	-5.27	120.54	123.70
5	K	27	DC	N3-C2-O2	-5.26	118.22	121.90
5	K	41	DA	C5-C6-N1	5.26	120.33	117.70
5	K	11	DT	N3-C2-O2	-5.26	119.14	122.30
5	K	20	DG	O4'-C1'-N9	5.26	111.68	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	6	DT	O4'-C1'-N1	5.26	111.68	108.00
1	B	381	TYR	CB-CG-CD2	-5.25	117.85	121.00
6	L	63	DG	C1'-O4'-C4'	-5.25	104.85	110.10
6	L	76	DT	C1'-O4'-C4'	-5.25	104.85	110.10
6	L	90	DC	N1-C2-O2	5.25	122.05	118.90
1	O	345	ARG	NE-CZ-NH2	5.24	122.92	120.30
6	L	66	DT	O4'-C1'-C2'	-5.24	101.71	105.90
5	K	40	DA	C5-C6-N1	5.24	120.32	117.70
1	B	235	MET	CA-CB-CG	5.23	122.19	113.30
3	E	58	TYR	CD1-CG-CD2	-5.23	112.15	117.90
2	C	138	ARG	NE-CZ-NH2	5.23	122.91	120.30
6	L	38	DC	N1-C2-O2	5.23	122.04	118.90
1	P	187	ARG	CG-CD-NE	5.22	122.77	111.80
1	O	427	ARG	NE-CZ-NH2	5.22	122.91	120.30
6	L	67	DT	C5-C6-N1	-5.22	120.57	123.70
1	B	1221	ARG	CA-CB-CG	5.21	124.87	113.40
1	P	1221	ARG	CA-CB-CG	5.21	124.86	113.40
5	K	60	DC	N1-C2-O2	5.21	122.03	118.90
6	L	39	DG	C1'-O4'-C4'	-5.21	104.89	110.10
1	P	1322	GLN	CA-CB-CG	5.21	124.86	113.40
5	K	58	DC	N1-C2-O2	5.21	122.02	118.90
6	L	65	DG	O4'-C1'-C2'	-5.21	101.74	105.90
5	K	29	DG	C3'-C2'-C1'	-5.20	96.26	102.50
1	A	1061	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	O	1000	ARG	NE-CZ-NH2	5.20	122.90	120.30
2	C	57	ARG	NE-CZ-NH2	5.20	122.90	120.30
6	L	26	DT	N3-C2-O2	-5.20	119.18	122.30
1	B	1322	GLN	CA-CB-CG	5.19	124.83	113.40
1	O	894	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	P	854	ARG	NE-CZ-NH2	5.19	122.90	120.30
5	K	56	DT	O4'-C1'-N1	5.19	111.63	108.00
3	Q	61	TYR	CB-CG-CD2	5.19	124.11	121.00
3	Q	58	TYR	CD1-CG-CD2	-5.19	112.19	117.90
2	C	322	ARG	NE-CZ-NH2	5.19	122.89	120.30
6	L	48	DC	O4'-C1'-C2'	-5.18	101.75	105.90
1	A	528	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	B	514	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	B	1004	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	O	1061	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	B	186	LYS	CA-CB-CG	5.17	124.78	113.40
3	R	140	ARG	NE-CZ-NH2	5.17	122.89	120.30
6	L	53	DT	C6-C5-C7	-5.17	119.80	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	528	ARG	NE-CZ-NH2	5.17	122.88	120.30
6	L	76	DT	N3-C2-O2	-5.16	119.20	122.30
1	P	381	TYR	CB-CG-CD2	-5.16	117.90	121.00
5	K	64	DG	C5'-C4'-O4'	5.16	119.10	109.30
6	L	83	DT	C5-C6-N1	-5.16	120.61	123.70
6	L	57	DC	C1'-O4'-C4'	-5.15	104.95	110.10
5	K	37	DT	C5-C6-N1	-5.15	120.61	123.70
5	K	46	DA	C1'-O4'-C4'	-5.14	104.96	110.10
6	L	61	DT	C1'-O4'-C4'	-5.14	104.96	110.10
1	A	427	ARG	NE-CZ-NH2	5.14	122.87	120.30
3	E	67	ARG	CA-CB-CG	5.14	124.71	113.40
5	K	21	DC	N3-C4-C5	5.14	123.96	121.90
5	K	18	DT	N3-C2-O2	-5.13	119.22	122.30
1	P	1245	ARG	CD-NE-CZ	5.13	130.78	123.60
5	K	45	DT	C6-C5-C7	-5.13	119.82	122.90
6	L	52	DA	C1'-O4'-C4'	-5.13	104.97	110.10
5	K	39	DT	C5-C6-N1	-5.13	120.62	123.70
1	A	1000	ARG	NE-CZ-NH2	5.12	122.86	120.30
3	E	138	ASN	CB-CA-C	5.12	120.64	110.40
2	D	176	ARG	CD-NE-CZ	5.12	130.77	123.60
5	K	56	DT	C4-C5-C6	5.12	121.07	118.00
1	P	503	ARG	NE-CZ-NH2	5.12	122.86	120.30
2	D	176	ARG	NE-CZ-NH2	5.12	122.86	120.30
5	K	35	DA	O4'-C1'-N9	5.12	111.58	108.00
3	R	85	ARG	CA-CB-CG	5.12	124.65	113.40
5	K	47	DC	N1-C2-O2	5.11	121.97	118.90
5	K	66	DA	C6-C5-N7	5.11	135.88	132.30
6	L	27	DC	O4'-C1'-N1	5.11	111.58	108.00
1	A	384	ARG	NE-CZ-NH2	5.11	122.85	120.30
5	K	50	DG	O4'-C1'-N9	5.11	111.58	108.00
6	L	88	DG	N1-C6-O6	-5.11	116.83	119.90
5	K	17	DG	O4'-C1'-N9	5.11	111.58	108.00
6	L	66	DT	C1'-O4'-C4'	-5.10	105.00	110.10
3	E	61	TYR	CD1-CG-CD2	-5.10	112.29	117.90
5	K	41	DA	C1'-O4'-C4'	-5.09	105.01	110.10
6	L	31	DG	N1-C6-O6	-5.09	116.85	119.90
3	Q	67	ARG	CA-CB-CG	5.09	124.59	113.40
1	B	1191	TYR	CD1-CG-CD2	-5.08	112.31	117.90
5	K	62	DT	P-O3'-C3'	5.08	125.79	119.70
1	O	384	ARG	NE-CZ-NH2	5.08	122.84	120.30
6	L	27	DC	N1-C2-O2	5.07	121.94	118.90
6	L	62	DC	N3-C4-C5	5.07	123.93	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	124	LEU	CA-CB-CG	5.07	126.97	115.30
6	L	63	DG	N1-C6-O6	-5.07	116.86	119.90
1	P	1191	TYR	CD1-CG-CD2	-5.07	112.32	117.90
5	K	54	DT	C4-C5-C6	5.06	121.04	118.00
6	L	56	DT	C1'-O4'-C4'	-5.06	105.04	110.10
5	K	18	DT	C5-C6-N1	-5.06	120.67	123.70
1	P	174	TYR	CA-CB-CG	5.06	123.01	113.40
6	L	20	DG	N3-C2-N2	-5.05	116.36	119.90
6	L	23	DG	N1-C6-O6	-5.05	116.87	119.90
6	L	68	DT	N3-C2-O2	-5.05	119.27	122.30
1	B	1340	TYR	CD1-CG-CD2	-5.05	112.35	117.90
5	K	39	DT	N3-C2-O2	-5.05	119.27	122.30
6	L	69	DC	N3-C4-C5	5.04	123.92	121.90
1	B	220	TYR	CB-CG-CD2	5.04	124.03	121.00
3	R	134	MET	CA-CB-CG	5.04	121.87	113.30
1	P	187	ARG	CD-NE-CZ	5.04	130.66	123.60
1	P	1199	ARG	CD-NE-CZ	5.04	130.66	123.60
5	K	20	DG	N3-C2-N2	-5.04	116.37	119.90
5	K	47	DC	N3-C4-C5	5.04	123.91	121.90
3	Q	61	TYR	CD1-CG-CD2	-5.04	112.36	117.90
5	K	39	DT	C6-C5-C7	-5.03	119.88	122.90
5	K	64	DG	N3-C4-C5	-5.03	126.08	128.60
3	Q	198	ARG	NE-CZ-NH2	5.03	122.82	120.30
5	K	5	DC	O4'-C1'-N1	5.02	111.52	108.00
1	B	503	ARG	NE-CZ-NH2	5.02	122.81	120.30
5	K	31	DC	N3-C4-C5	5.02	123.91	121.90
5	K	73	DT	N3-C2-O2	-5.02	119.29	122.30
6	L	19	DG	N9-C4-C5	5.02	107.41	105.40
5	K	35	DA	C6-C5-N7	5.02	135.81	132.30
1	P	1004	ARG	NE-CZ-NH2	5.01	122.81	120.30
5	K	52	DC	N1-C2-O2	5.01	121.91	118.90
1	B	1199	ARG	CD-NE-CZ	5.01	130.61	123.60
6	L	79	DG	O4'-C1'-N9	5.01	111.50	108.00
1	O	972	TYR	CB-CG-CD2	-5.01	118.00	121.00
6	L	26	DT	O4'-C1'-N1	5.00	111.50	108.00
5	K	45	DT	C5-C6-N1	-5.00	120.70	123.70
5	K	55	DT	C4-C5-C6	5.00	121.00	118.00

There are no chirality outliers.

All (65) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1058	ARG	Sidechain
1	A	966	ARG	Sidechain
1	A	967	ARG	Sidechain
1	B	528	ARG	Sidechain
1	B	966	ARG	Sidechain
2	C	120	PHE	Sidechain
2	C	138	ARG	Sidechain
2	C	300	ARG	Sidechain
2	C	327	ARG	Sidechain
2	C	4	TYR	Sidechain
2	C	89	ARG	Sidechain
2	D	116	ARG	Sidechain
2	D	138	ARG	Sidechain
2	D	300	ARG	Sidechain
2	D	327	ARG	Sidechain
2	D	4	TYR	Sidechain
2	D	89	ARG	Sidechain
3	E	101	TYR	Sidechain
3	E	140	ARG	Sidechain
3	E	161	ARG	Sidechain
3	E	164	ARG	Sidechain
5	K	11	DT	Sidechain
5	K	12	DC	Sidechain
5	K	14	DG	Sidechain
5	K	18	DT	Sidechain
5	K	28	DC	Sidechain
5	K	29	DG	Sidechain
5	K	36	DC	Sidechain
5	K	4	DG	Sidechain
5	K	44	DA	Sidechain
5	K	45	DT	Sidechain
5	K	46	DA	Sidechain
5	K	49	DA	Sidechain
5	K	52	DC	Sidechain
5	K	54	DT	Sidechain
5	K	58	DC	Sidechain
5	K	63	DG	Sidechain
5	K	66	DA	Sidechain
5	K	71	DC	Sidechain
5	K	8	DA	Sidechain
6	L	29	DA	Sidechain
6	L	30	DG	Sidechain
6	L	31	DG	Sidechain

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Mol	Chain	Res	Type	Group
6	L	37	DA	Sidechain
6	L	38	DC	Sidechain
6	L	39	DG	Sidechain
6	L	46	DA	Sidechain
6	L	47	DT	Sidechain
6	L	49	DT	Sidechain
6	L	50	DT	Sidechain
6	L	51	DT	Sidechain
6	L	56	DT	Sidechain
6	L	59	DT	Sidechain
6	L	68	DT	Sidechain
6	L	76	DT	Sidechain
6	L	83	DT	Sidechain
6	L	86	DG	Sidechain
1	O	1058	ARG	Sidechain
1	O	966	ARG	Sidechain
1	O	967	ARG	Sidechain
1	P	189	ARG	Sidechain
1	P	528	ARG	Sidechain
1	P	966	ARG	Sidechain
3	Q	101	TYR	Sidechain
3	Q	140	ARG	Sidechain

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	11840	11707	11705	58	0
1	B	11840	11706	11705	82	0
1	O	11840	11707	11705	61	0
1	P	11840	11706	11705	90	0
2	C	3531	3451	3450	69	0
2	D	3531	3451	3450	69	0
3	E	1722	1719	1718	12	0
3	F	1619	1627	1626	13	0
3	Q	1722	1719	1718	13	0
3	R	1619	1627	1626	12	0
4	G	583	564	563	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	583	564	563	8	0
4	M	583	564	563	9	0
4	S	583	564	563	26	0
5	K	1496	815	816	13	0
6	L	1497	823	822	6	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	O	1	0	0	0	0
7	P	1	0	0	0	0
8	A	31	12	12	0	0
8	B	31	12	12	0	0
8	O	31	12	12	0	0
8	P	31	12	12	0	0
All	All	66557	64362	64346	455	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 3.

All (455) 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)
2:C:158:ALA:HB1	2:D:123:LEU:HG	1.19	1.18
2:C:162:TYR:HB3	2:D:124:ARG:HG3	1.23	1.15
2:C:158:ALA:CB	2:D:123:LEU:HG	1.82	1.10
2:C:131:ILE:HD11	2:D:163:SER:OG	1.56	1.06
4:S:36:4HH:CL3	4:S:40:VAL:HG21	1.87	1.05
4:G:36:4HH:CL3	4:G:40:VAL:HG21	1.87	1.04
1:B:1127:ASN:O	1:B:1127:ASN:ND2	1.91	1.03
1:P:1127:ASN:O	1:P:1127:ASN:ND2	1.91	1.03
2:C:138:ARG:NH1	2:D:134:ASN:ND2	2.10	0.99
2:C:162:TYR:HB3	2:D:124:ARG:CG	1.93	0.98
2:C:134:ASN:HD21	2:D:138:ARG:HH12	1.12	0.93
2:C:131:ILE:CD1	2:D:163:SER:OG	2.18	0.91
1:B:1107:ARG:NE	4:I:48:GLU:OE1	2.04	0.90
1:P:1107:ARG:NE	4:M:48:GLU:OE1	2.04	0.89
1:A:292:ARG:HD3	4:G:36:4HH:SU	2.14	0.88
1:O:292:ARG:HD3	4:S:36:4HH:SU	2.13	0.88
2:C:138:ARG:NH1	2:D:134:ASN:HD21	1.70	0.87
2:C:138:ARG:HH12	2:D:134:ASN:ND2	1.70	0.86
2:C:158:ALA:CB	2:D:123:LEU:CG	2.51	0.86
2:C:162:TYR:CB	2:D:124:ARG:HG3	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:162:TYR:CG	2:D:124:ARG:HB2	2.12	0.85
1:P:665:GLN:NE2	1:P:671:ASP:OD2	2.11	0.84
1:B:665:GLN:NE2	1:B:671:ASP:OD2	2.11	0.82
2:C:123:LEU:HG	2:D:158:ALA:HB1	1.61	0.82
2:C:158:ALA:HB2	2:D:123:LEU:CD2	2.13	0.79
2:C:134:ASN:HD21	2:D:138:ARG:NH1	1.80	0.78
2:C:123:LEU:HD21	2:D:158:ALA:HB2	1.67	0.77
4:G:36:4HH:HT3	4:G:56:ASP:OD1	1.85	0.76
1:P:1127:ASN:HD22	1:P:1127:ASN:C	1.88	0.76
4:S:36:4HH:HT3	4:S:56:ASP:OD1	1.85	0.76
1:A:1412:ASP:OD1	1:A:1413:ALA:N	2.20	0.75
1:O:1412:ASP:OD1	1:O:1413:ALA:N	2.20	0.74
4:G:23:THR:OG1	4:G:25:ASN:OD1	2.04	0.73
2:C:131:ILE:HD11	2:D:163:SER:CB	2.18	0.73
1:B:172:THR:HG21	5:K:21:DC:H5''	1.71	0.72
2:C:124:ARG:HA	2:D:162:TYR:CB	2.20	0.72
4:S:36:4HH:CL3	4:S:40:VAL:CG2	2.68	0.71
2:C:124:ARG:HA	2:D:162:TYR:HB3	1.73	0.71
4:G:36:4HH:HB2	4:G:36:4HH:HJ2	1.74	0.70
4:S:23:THR:OG1	4:S:25:ASN:OD1	2.04	0.69
4:G:36:4HH:CL3	4:G:40:VAL:CG2	2.68	0.69
4:S:36:4HH:HJ2	4:S:36:4HH:HB2	1.74	0.69
1:P:273:ASP:OD1	1:P:274:TYR:N	2.26	0.69
1:B:273:ASP:OD1	1:B:274:TYR:N	2.26	0.68
1:O:826:LEU:HD21	1:P:827:SER:HA	1.75	0.68
1:A:1298:GLN:N	1:A:1298:GLN:OE1	2.26	0.68
1:A:826:LEU:HD21	1:B:827:SER:HA	1.75	0.67
1:A:784:GLU:OE1	1:A:784:GLU:N	2.28	0.67
1:A:1436:GLU:O	1:A:1436:GLU:OE1	2.13	0.67
4:S:36:4HH:HJ2	4:S:36:4HH:CB	2.25	0.67
5:K:63:DG:C3'	1:P:187:ARG:HD3	2.24	0.67
1:O:1436:GLU:O	1:O:1436:GLU:OE1	2.12	0.67
1:O:1298:GLN:N	1:O:1298:GLN:OE1	2.27	0.67
5:K:63:DG:H3'	1:P:187:ARG:HD3	1.77	0.66
1:O:784:GLU:N	1:O:784:GLU:OE1	2.28	0.66
4:S:46:LEU:HD21	4:S:72:ILE:HD11	1.78	0.65
2:C:158:ALA:HB2	2:D:123:LEU:HD21	1.77	0.65
1:B:1332:THR:O	1:B:1336:GLU:N	2.30	0.65
2:C:123:LEU:HG	2:D:158:ALA:CB	2.26	0.65
1:P:1332:THR:O	1:P:1336:GLU:N	2.30	0.65
4:G:46:LEU:HD21	4:G:72:ILE:HD11	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1457:GLU:OE1	1:O:1457:GLU:N	2.28	0.63
4:G:36:4HH:HJ2	4:G:36:4HH:CB	2.25	0.63
4:G:36:4HH:ON	4:G:40:VAL:CG2	2.47	0.62
2:C:162:TYR:HB3	2:D:124:ARG:CB	2.29	0.62
4:S:36:4HH:ON	4:S:40:VAL:CG2	2.47	0.62
1:O:231:ALA:HB2	1:P:665:GLN:CB	2.30	0.62
1:A:1457:GLU:OE1	1:A:1457:GLU:N	2.28	0.61
1:P:254:SER:O	1:P:258:LEU:HD22	2.00	0.61
1:A:231:ALA:HB2	1:B:665:GLN:CB	2.30	0.61
2:C:124:ARG:HB2	2:D:162:TYR:CD1	2.35	0.61
1:B:254:SER:O	1:B:258:LEU:HD22	2.01	0.61
1:O:289:LEU:HD22	4:S:36:4HH:HS3	1.83	0.60
2:C:138:ARG:NH1	2:D:134:ASN:HD22	2.00	0.60
2:C:123:LEU:CG	2:D:158:ALA:CB	2.79	0.60
1:P:788:GLU:OE1	1:P:789:ALA:N	2.35	0.60
1:A:289:LEU:HD22	4:G:36:4HH:HS3	1.83	0.59
4:M:24:ASN:O	4:M:66:GLN:N	2.35	0.59
1:B:788:GLU:OE1	1:B:789:ALA:N	2.35	0.59
2:C:123:LEU:CG	2:D:158:ALA:HB1	2.30	0.59
2:C:162:TYR:CG	2:D:124:ARG:CB	2.85	0.59
5:K:63:DG:C2'	1:P:187:ARG:HD3	2.33	0.59
2:C:158:ALA:HB3	2:C:159:PRO:HD3	1.85	0.59
3:E:10:MET:SD	3:F:18:LEU:HD11	2.43	0.58
4:I:24:ASN:O	4:I:66:GLN:N	2.35	0.58
3:Q:10:MET:SD	3:R:18:LEU:HD11	2.43	0.58
1:B:1142:GLU:OE1	1:B:1142:GLU:N	2.36	0.58
1:P:1322:GLN:O	1:P:1322:GLN:CD	2.43	0.57
1:P:1142:GLU:N	1:P:1142:GLU:OE1	2.36	0.57
1:B:1322:GLN:O	1:B:1322:GLN:CD	2.43	0.57
2:C:124:ARG:HA	2:D:162:TYR:CG	2.41	0.56
2:C:131:ILE:CD1	2:D:163:SER:CB	2.83	0.55
4:G:36:4HH:HJ3	4:G:37:LEU:N	2.22	0.55
1:O:231:ALA:HB2	1:P:665:GLN:HB2	1.89	0.55
1:A:231:ALA:HB2	1:B:665:GLN:HB2	1.89	0.55
2:C:123:LEU:CD2	2:D:158:ALA:HB2	2.36	0.55
2:D:328:ASP:OD1	2:D:328:ASP:O	2.25	0.55
1:P:822:VAL:HA	1:P:826:LEU:HD23	1.88	0.55
1:O:764:ASP:N	1:O:764:ASP:OD1	2.40	0.55
4:S:36:4HH:HJ3	4:S:37:LEU:N	2.22	0.54
1:A:828:VAL:HG12	1:A:828:VAL:O	2.08	0.54
3:F:148:LYS:HD3	3:F:148:LYS:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:236:GLU:OE2	1:O:1307:THR:HG21	2.08	0.54
1:O:828:VAL:O	1:O:828:VAL:HG12	2.08	0.54
1:A:764:ASP:N	1:A:764:ASP:OD1	2.40	0.54
1:B:822:VAL:HA	1:B:826:LEU:HD23	1.88	0.54
1:B:1423:CYS:SG	1:B:1430:LEU:HD11	2.48	0.54
1:P:1423:CYS:SG	1:P:1430:LEU:HD11	2.48	0.54
3:E:7:GLU:OE1	3:E:7:GLU:N	2.38	0.54
1:O:1281:GLU:O	1:O:1285:ILE:HD12	2.08	0.54
1:A:1420:PHE:HA	1:A:1423:CYS:SG	2.48	0.53
1:B:1299:ASP:OD1	1:B:1300:LEU:N	2.42	0.53
2:C:328:ASP:OD1	2:C:328:ASP:O	2.25	0.53
1:A:236:GLU:OE2	1:A:1307:THR:HG21	2.08	0.53
1:B:1395:LYS:O	1:B:1395:LYS:HD3	2.09	0.53
3:R:148:LYS:HD3	3:R:148:LYS:N	2.23	0.53
1:A:289:LEU:HD22	4:G:36:4HH:CS	2.39	0.53
1:A:1281:GLU:O	1:A:1285:ILE:HD12	2.08	0.53
1:P:1299:ASP:OD1	1:P:1300:LEU:N	2.42	0.53
1:O:65:GLU:O	1:O:65:GLU:HG3	2.08	0.53
1:O:1420:PHE:HA	1:O:1423:CYS:SG	2.48	0.53
2:C:123:LEU:HD11	2:D:158:ALA:CB	2.39	0.53
1:O:289:LEU:HD22	4:S:36:4HH:CS	2.39	0.53
1:O:1126:ASP:O	1:O:1127:ASN:OD1	2.27	0.53
1:P:1107:ARG:HE	4:M:48:GLU:CD	2.12	0.53
1:A:65:GLU:O	1:A:65:GLU:HG3	2.08	0.53
1:B:1441:GLU:OE1	1:B:1441:GLU:N	2.37	0.52
1:P:1258:LEU:HD21	1:P:1380:MET:HG2	1.90	0.52
1:P:1441:GLU:OE1	1:P:1441:GLU:N	2.37	0.52
1:A:1126:ASP:O	1:A:1127:ASN:OD1	2.27	0.52
1:B:1258:LEU:HD21	1:B:1380:MET:HG2	1.90	0.52
2:C:158:ALA:HB2	2:D:123:LEU:CG	2.31	0.52
3:Q:7:GLU:OE1	3:Q:7:GLU:N	2.38	0.52
1:P:217:LEU:HG	1:P:221:LEU:HD12	1.91	0.52
1:B:828:VAL:HG12	1:B:828:VAL:O	2.10	0.52
1:B:1107:ARG:HE	4:I:48:GLU:CD	2.12	0.52
2:D:158:ALA:HB3	2:D:159:PRO:HD3	1.91	0.52
1:P:63:THR:HG21	1:P:1407:GLU:HG3	1.92	0.52
1:P:1161:VAL:HG12	1:P:1161:VAL:O	2.10	0.51
1:B:1246:LYS:HD2	1:B:1246:LYS:O	2.11	0.51
1:B:63:THR:HG21	1:B:1407:GLU:HG3	1.92	0.51
4:G:62:ILE:HG22	4:G:62:ILE:O	2.10	0.51
1:P:828:VAL:HG12	1:P:828:VAL:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:124:ARG:HB2	2:D:162:TYR:CG	2.46	0.51
2:C:134:ASN:ND2	2:D:138:ARG:NH1	2.57	0.51
1:P:1319:LEU:HD12	1:P:1320:ASN:N	2.26	0.51
1:B:217:LEU:HG	1:B:221:LEU:HD12	1.91	0.51
5:K:63:DG:H4'	1:P:189:ARG:HG3	1.93	0.51
6:L:39:DG:H3'	3:Q:157:THR:HG23	1.93	0.51
1:P:273:ASP:OD1	1:P:273:ASP:C	2.49	0.51
1:B:1161:VAL:HG12	1:B:1161:VAL:O	2.09	0.50
1:B:1319:LEU:HD12	1:B:1320:ASN:N	2.26	0.50
2:D:370:GLN:OE1	2:D:370:GLN:O	2.29	0.50
4:S:62:ILE:HG22	4:S:62:ILE:O	2.10	0.50
2:D:358:LEU:HG	2:D:362:ILE:HD11	1.94	0.50
1:O:200:LEU:HD12	1:O:1378:LEU:HD22	1.94	0.50
1:B:273:ASP:OD1	1:B:273:ASP:C	2.49	0.50
2:C:370:GLN:OE1	2:C:370:GLN:O	2.29	0.50
1:P:1196:GLU:N	1:P:1196:GLU:OE1	2.45	0.50
1:B:1107:ARG:CZ	4:I:48:GLU:OE1	2.59	0.50
1:A:1361:GLU:OE1	1:A:1361:GLU:HA	2.12	0.50
1:A:200:LEU:HD12	1:A:1378:LEU:HD22	1.94	0.50
2:C:162:TYR:CD1	2:D:124:ARG:HD2	2.47	0.50
1:O:1361:GLU:OE1	1:O:1361:GLU:HA	2.12	0.50
1:P:1107:ARG:CZ	4:M:48:GLU:OE1	2.60	0.50
2:C:134:ASN:ND2	2:D:138:ARG:HH12	1.95	0.49
1:A:1163:ASP:OD1	1:A:1164:ASN:N	2.45	0.49
2:C:358:LEU:HG	2:C:362:ILE:HD11	1.94	0.49
5:K:63:DG:H3'	1:P:187:ARG:CD	2.41	0.49
1:O:1163:ASP:OD1	1:O:1164:ASN:N	2.45	0.49
1:A:1237:SER:OG	1:A:1238:LYS:N	2.45	0.49
1:A:1376:SER:O	1:A:1379:VAL:HG22	2.12	0.49
1:B:1196:GLU:N	1:B:1196:GLU:OE1	2.45	0.49
4:G:36:4HH:CB	4:G:36:4HH:CJ	2.90	0.49
1:P:244:ILE:HD13	3:Q:41:LEU:HD21	1.94	0.49
2:D:75:ASN:HD21	3:E:146:LEU:HB2	1.78	0.49
1:O:732:GLU:N	1:O:732:GLU:OE1	2.46	0.49
4:S:2:THR:OG1	4:S:3:ILE:N	2.45	0.49
5:K:63:DG:H1'	5:K:64:DG:C8	2.48	0.49
1:A:732:GLU:OE1	1:A:732:GLU:N	2.46	0.49
2:C:124:ARG:CB	2:D:162:TYR:CG	2.96	0.49
4:I:36:4HH:O	4:I:40:VAL:HG23	2.12	0.49
4:M:36:4HH:O	4:M:40:VAL:HG23	2.11	0.49
1:O:1376:SER:O	1:O:1379:VAL:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:79:ASN:CG	3:Q:142:SER:HB3	2.34	0.48
1:P:799:GLU:OE1	1:P:799:GLU:C	2.52	0.48
4:S:36:4HH:ON	4:S:40:VAL:HG21	2.06	0.48
1:A:1211:ALA:O	1:A:1215:MET:HG2	2.13	0.48
4:G:36:4HH:ON	4:G:40:VAL:HG23	2.14	0.48
3:R:56:GLU:OE1	3:R:56:GLU:HA	2.13	0.48
1:B:1376:SER:O	1:B:1379:VAL:HG22	2.13	0.48
2:C:123:LEU:CG	2:D:158:ALA:HB2	2.44	0.48
2:D:79:ASN:CG	3:E:142:SER:HB3	2.34	0.48
1:O:1237:SER:OG	1:O:1238:LYS:N	2.45	0.48
1:P:782:ALA:O	1:P:785:ASN:N	2.47	0.48
1:B:244:ILE:HD13	3:E:41:LEU:HD21	1.94	0.48
2:C:391:LEU:HD13	2:C:428:TYR:CE2	2.49	0.48
4:G:2:THR:OG1	4:G:3:ILE:N	2.45	0.48
2:C:75:ASN:HD21	3:Q:146:LEU:HB2	1.78	0.48
2:C:106:LEU:HB2	2:D:113:TYR:CD1	2.49	0.48
1:O:1211:ALA:O	1:O:1215:MET:HG2	2.13	0.48
1:P:1376:SER:O	1:P:1379:VAL:HG22	2.13	0.48
3:F:56:GLU:OE1	3:F:56:GLU:HA	2.13	0.48
3:E:124:LEU:C	3:E:124:LEU:HD23	2.34	0.48
3:Q:124:LEU:C	3:Q:124:LEU:HD23	2.34	0.48
4:S:11:ILE:HG23	4:S:12:GLY:N	2.29	0.48
1:B:1161:VAL:O	1:B:1161:VAL:CG1	2.62	0.47
4:S:36:4HH:ON	4:S:40:VAL:HG23	2.13	0.47
1:B:799:GLU:C	1:B:799:GLU:OE1	2.52	0.47
1:P:1161:VAL:O	1:P:1161:VAL:CG1	2.62	0.47
1:B:1275:LEU:HD12	1:B:1347:ASP:O	2.14	0.47
4:G:11:ILE:HG23	4:G:12:GLY:N	2.29	0.47
1:B:94:ASN:OD1	1:B:95:SER:N	2.47	0.47
1:B:1322:GLN:O	1:B:1322:GLN:OE1	2.32	0.47
2:D:375:PRO:HA	2:D:440:TYR:OH	2.15	0.47
2:D:391:LEU:HD13	2:D:428:TYR:CE2	2.49	0.47
1:A:62:ASN:OD1	1:A:63:THR:N	2.48	0.47
1:B:184:ILE:HG23	1:B:185:PRO:HD2	1.97	0.47
1:B:285:LEU:HD13	4:I:41:GLU:OE2	2.15	0.47
1:B:774:GLU:N	1:B:774:GLU:OE1	2.48	0.47
1:P:665:GLN:OE1	1:P:665:GLN:C	2.53	0.47
1:P:732:GLU:H	1:P:732:GLU:CD	2.18	0.47
1:P:774:GLU:N	1:P:774:GLU:OE1	2.48	0.47
1:P:1322:GLN:O	1:P:1322:GLN:OE1	2.31	0.47
1:B:665:GLN:C	1:B:665:GLN:OE1	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:782:ALA:O	1:B:785:ASN:N	2.47	0.47
2:C:162:TYR:CB	2:D:124:ARG:CB	2.93	0.47
2:C:375:PRO:HA	2:C:440:TYR:OH	2.15	0.47
1:P:184:ILE:HG23	1:P:185:PRO:HD2	1.97	0.47
3:R:180:ILE:HG23	3:R:184:VAL:HG21	1.96	0.47
2:D:391:LEU:HD13	2:D:428:TYR:CD2	2.50	0.47
1:O:588:GLU:O	1:O:592:GLN:HG3	2.15	0.47
1:A:588:GLU:O	1:A:592:GLN:HG3	2.15	0.46
1:B:824:LYS:HG2	1:B:824:LYS:O	2.15	0.46
1:P:91:ASP:C	1:P:91:ASP:OD1	2.54	0.46
1:P:1117:TRP:O	1:P:1121:MET:HG2	2.14	0.46
1:P:1320:ASN:ND2	3:Q:49:ASP:OD2	2.49	0.46
1:O:62:ASN:OD1	1:O:63:THR:N	2.48	0.46
1:P:1275:LEU:HD12	1:P:1347:ASP:O	2.15	0.46
4:S:28:PHE:CE1	4:S:65:VAL:HG22	2.51	0.46
3:E:5:HIS:CD2	3:E:7:GLU:OE1	2.69	0.46
1:A:12:LEU:HD21	1:A:46:ALA:HB2	1.97	0.46
3:F:39:ASP:OD1	3:F:39:ASP:N	2.49	0.46
3:F:180:ILE:HG23	3:F:184:VAL:HG21	1.96	0.46
4:G:28:PHE:CE1	4:G:65:VAL:HG22	2.51	0.46
1:P:824:LYS:O	1:P:824:LYS:HG2	2.15	0.46
3:Q:140:ARG:HD2	3:Q:140:ARG:O	2.15	0.46
2:C:138:ARG:HH11	2:D:134:ASN:HD21	1.56	0.46
1:P:285:LEU:HD13	4:M:41:GLU:OE2	2.15	0.46
1:B:1117:TRP:O	1:B:1121:MET:HG2	2.14	0.46
1:P:1391:ARG:HA	1:P:1391:ARG:NE	2.30	0.46
4:S:57:GLU:OE1	4:S:57:GLU:N	2.45	0.46
1:O:1285:ILE:HD12	1:O:1285:ILE:H	1.81	0.46
1:B:542:PHE:CD2	1:B:876:LEU:HD21	2.51	0.46
1:B:782:ALA:O	1:B:785:ASN:CB	2.64	0.46
2:C:426:ASN:OD1	2:C:430:ALA:HB3	2.16	0.46
2:D:426:ASN:OD1	2:D:430:ALA:HB3	2.16	0.46
4:G:57:GLU:OE1	4:G:57:GLU:N	2.46	0.46
1:O:349:LYS:HE3	1:O:353:TYR:CZ	2.51	0.46
1:A:8:ARG:HH21	1:A:8:ARG:HG3	1.80	0.46
1:B:664:SER:OG	1:B:665:GLN:HG3	2.15	0.46
1:B:1257:MET:SD	1:B:1257:MET:C	2.95	0.46
2:C:391:LEU:HD13	2:C:428:TYR:CD2	2.50	0.46
3:Q:5:HIS:CD2	3:Q:7:GLU:OE1	2.69	0.46
1:B:1320:ASN:ND2	3:E:49:ASP:OD2	2.49	0.45
1:P:664:SER:OG	1:P:665:GLN:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:679:GLU:OE1	1:P:679:GLU:HA	2.16	0.45
1:A:1285:ILE:HD12	1:A:1285:ILE:H	1.81	0.45
2:C:355:ASN:OD1	2:C:355:ASN:N	2.49	0.45
4:G:36:4HH:OM	4:G:37:LEU:HA	2.17	0.45
1:B:679:GLU:OE1	1:B:679:GLU:HA	2.16	0.45
2:C:356:ASP:C	2:C:356:ASP:OD1	2.55	0.45
1:P:1257:MET:C	1:P:1257:MET:SD	2.95	0.45
3:R:39:ASP:OD1	3:R:39:ASP:N	2.49	0.45
2:C:106:LEU:HD13	2:D:113:TYR:CG	2.51	0.45
2:D:356:ASP:OD1	2:D:356:ASP:C	2.55	0.45
3:R:121:TYR:CZ	3:R:125:ILE:HD11	2.52	0.45
1:B:91:ASP:C	1:B:91:ASP:OD1	2.54	0.45
1:B:1375:MET:HG2	1:B:1419:LEU:HD11	1.98	0.45
1:O:247:GLU:OE1	1:O:247:GLU:HA	2.17	0.45
1:O:765:ARG:HH11	1:P:748:VAL:HG23	1.81	0.45
1:P:782:ALA:O	1:P:785:ASN:CB	2.65	0.45
1:A:349:LYS:HE3	1:A:353:TYR:CZ	2.51	0.45
5:K:38:DA:C2	6:L:54:DA:C2	3.05	0.45
1:A:247:GLU:HA	1:A:247:GLU:OE1	2.17	0.45
3:F:16:GLN:C	3:F:16:GLN:OE1	2.55	0.45
1:O:1213:GLU:OE1	1:P:813:ARG:NE	2.49	0.45
1:P:542:PHE:CD2	1:P:876:LEU:HD21	2.51	0.45
1:O:8:ARG:HH21	1:O:8:ARG:HG3	1.80	0.45
1:A:640:ARG:O	1:A:643:THR:HG22	2.17	0.45
1:A:1213:GLU:OE1	1:B:813:ARG:NE	2.49	0.45
1:B:784:GLU:HA	1:B:787:LEU:HG	1.99	0.45
1:O:12:LEU:HD21	1:O:46:ALA:HB2	1.97	0.45
2:D:355:ASN:N	2:D:355:ASN:OD1	2.48	0.44
1:O:640:ARG:O	1:O:643:THR:HG22	2.17	0.44
1:A:765:ARG:HH11	1:B:748:VAL:HG23	1.81	0.44
3:R:16:GLN:C	3:R:16:GLN:OE1	2.55	0.44
1:B:232:PHE:CZ	1:B:1240:VAL:HG11	2.53	0.44
1:P:1375:MET:HG2	1:P:1419:LEU:HD11	1.98	0.44
1:B:750:ASN:HB3	1:B:761:LYS:HB3	2.00	0.44
1:B:839:ARG:HG2	1:B:839:ARG:HH21	1.82	0.44
1:P:691:ASP:OD1	1:P:780:ARG:HB3	2.17	0.44
1:B:1104:TYR:CE1	1:B:1107:ARG:NH1	2.86	0.44
5:K:40:DA:C2	6:L:52:DA:C2	3.05	0.44
1:O:51:LEU:O	1:O:52:ILE:HD13	2.18	0.44
1:P:784:GLU:HA	1:P:787:LEU:HG	1.98	0.44
4:S:36:4HH:OM	4:S:37:LEU:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:152:GLU:OE1	1:O:152:GLU:N	2.51	0.44
1:A:1121:MET:HA	1:A:1124:VAL:HG12	1.99	0.44
1:P:750:ASN:HB3	1:P:761:LYS:HB3	2.00	0.44
2:D:399:ARG:O	2:D:403:ASP:OD2	2.36	0.44
4:I:64:THR:HG22	4:I:65:VAL:N	2.33	0.44
3:Q:180:ILE:HG22	3:Q:181:THR:N	2.33	0.44
1:O:1274:ARG:HG3	1:O:1357:TRP:CZ3	2.53	0.43
1:A:51:LEU:O	1:A:52:ILE:HD13	2.18	0.43
1:B:732:GLU:H	1:B:732:GLU:CD	2.18	0.43
1:B:782:ALA:O	1:B:785:ASN:HB3	2.18	0.43
4:S:36:4HH:CB	4:S:36:4HH:CJ	2.90	0.43
1:B:691:ASP:OD1	1:B:780:ARG:HB3	2.17	0.43
2:D:358:LEU:HA	2:D:361:MET:SD	2.59	0.43
1:P:1104:TYR:CE1	1:P:1107:ARG:NH1	2.86	0.43
1:P:1338:LEU:N	1:P:1338:LEU:HD23	2.32	0.43
4:M:64:THR:HG22	4:M:65:VAL:N	2.33	0.43
3:E:180:ILE:HG22	3:E:181:THR:N	2.33	0.43
5:K:63:DG:C5'	1:P:189:ARG:HG3	2.49	0.43
1:O:1121:MET:HA	1:O:1124:VAL:HG12	1.99	0.43
1:P:839:ARG:HG2	1:P:839:ARG:HH21	1.82	0.43
1:A:1285:ILE:HD11	3:F:108:ARG:NH1	2.34	0.43
1:O:1285:ILE:HD11	3:R:108:ARG:NH1	2.34	0.43
2:C:124:ARG:CA	2:D:162:TYR:CG	3.01	0.43
2:C:358:LEU:HA	2:C:361:MET:SD	2.59	0.43
2:D:292:ASP:CG	2:D:295:ARG:HA	2.39	0.43
1:O:1107:ARG:NH2	4:S:47:GLU:OE2	2.50	0.43
2:C:292:ASP:CG	2:C:295:ARG:HA	2.39	0.43
2:C:399:ARG:O	2:C:403:ASP:OD2	2.36	0.43
1:O:1235:ILE:HG21	1:P:675:ILE:HD13	2.01	0.43
1:P:1436:GLU:O	1:P:1438:ILE:HG23	2.19	0.43
1:P:232:PHE:CZ	1:P:1240:VAL:HG11	2.53	0.43
1:P:775:LEU:HD22	1:P:775:LEU:N	2.34	0.43
2:C:18:ASN:HB3	2:C:20:PHE:CZ	2.53	0.43
2:C:154:ARG:HA	2:D:123:LEU:HD21	2.00	0.43
1:O:782:ALA:O	1:O:783:ARG:HD3	2.19	0.43
1:P:782:ALA:O	1:P:785:ASN:HB3	2.18	0.42
3:R:25:GLU:O	3:R:29:GLN:HG3	2.19	0.42
1:A:1274:ARG:HG3	1:A:1357:TRP:CZ3	2.53	0.42
1:B:1436:GLU:O	1:B:1438:ILE:HG23	2.19	0.42
2:D:175:GLN:HB3	2:D:266:TRP:CE2	2.55	0.42
1:P:594:ILE:HD12	1:P:845:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1247:THR:O	1:P:1251:GLU:OE1	2.37	0.42
4:I:40:VAL:O	4:I:43:VAL:HG12	2.20	0.42
1:O:1118:CYS:SG	1:O:1122:ARG:NH1	2.92	0.42
1:O:1199:ARG:O	1:O:1199:ARG:HG2	2.19	0.42
1:P:605:LEU:O	1:P:609:ASP:OD2	2.37	0.42
1:P:745:ASP:OD1	1:P:745:ASP:N	2.51	0.42
1:B:594:ILE:HD12	1:B:845:HIS:CE1	2.55	0.42
1:B:606:ALA:HA	1:B:609:ASP:OD2	2.20	0.42
2:C:158:ALA:CB	2:D:123:LEU:CD2	2.85	0.42
1:O:1202:ILE:HG22	1:O:1202:ILE:O	2.20	0.42
1:P:606:ALA:HA	1:P:609:ASP:OD2	2.20	0.42
1:A:292:ARG:HD3	4:G:36:4HH:CT	2.49	0.42
1:A:1373:THR:O	1:A:1377:ILE:HG12	2.19	0.42
1:A:1199:ARG:O	1:A:1199:ARG:HG2	2.19	0.42
1:P:1325:MET:SD	1:P:1325:MET:N	2.90	0.42
1:A:767:TRP:CE3	1:B:717:LEU:HD13	2.55	0.42
1:A:782:ALA:O	1:A:783:ARG:HD3	2.19	0.42
1:B:605:LEU:O	1:B:609:ASP:OD2	2.37	0.42
1:B:1247:THR:O	1:B:1251:GLU:OE1	2.37	0.42
2:C:131:ILE:HD13	2:D:163:SER:OG	2.15	0.42
2:D:18:ASN:HB3	2:D:20:PHE:CZ	2.55	0.42
1:O:12:LEU:HD22	1:O:15:TRP:CG	2.55	0.42
1:O:1373:THR:O	1:O:1377:ILE:HG12	2.19	0.42
1:P:695:ILE:N	1:P:695:ILE:HD12	2.35	0.42
4:M:40:VAL:O	4:M:43:VAL:HG12	2.20	0.42
1:A:152:GLU:OE1	1:A:152:GLU:N	2.51	0.42
1:A:1235:ILE:HG21	1:B:675:ILE:HD13	2.01	0.42
3:F:25:GLU:CD	3:F:25:GLU:H	2.23	0.42
3:F:167:MET:HE2	3:F:167:MET:HA	2.01	0.42
1:O:292:ARG:HD3	4:S:36:4HH:CT	2.49	0.42
1:O:1331:GLN:NE2	1:O:1335:GLU:OE2	2.48	0.42
4:S:64:THR:HG23	4:S:67:ALA:H	1.85	0.42
1:A:45:ALA:HB1	1:A:60:PHE:CE2	2.55	0.42
1:A:780:ARG:O	1:A:783:ARG:N	2.46	0.42
1:B:775:LEU:N	1:B:775:LEU:HD22	2.34	0.42
5:K:63:DG:C3'	1:P:187:ARG:CD	2.94	0.42
1:P:94:ASN:OD1	1:P:95:SER:N	2.53	0.42
1:A:12:LEU:HD22	1:A:15:TRP:CG	2.55	0.41
1:B:695:ILE:HD12	1:B:695:ILE:N	2.35	0.41
2:C:131:ILE:HD11	2:D:163:SER:HB2	1.99	0.41
1:B:288:ALA:HB2	1:B:1106:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:55:DG:H2''	6:L:56:DT:C6	2.56	0.41
1:A:12:LEU:HD21	1:A:46:ALA:CB	2.50	0.41
1:B:264:THR:HG23	1:B:265:GLU:N	2.36	0.41
1:B:1331:GLN:OE1	1:B:1331:GLN:N	2.54	0.41
1:O:1407:GLU:OE1	1:O:1407:GLU:HA	2.21	0.41
1:B:141:GLY:O	1:B:143:ARG:NH1	2.54	0.41
2:C:357:GLN:O	2:C:361:MET:SD	2.78	0.41
5:K:13:DA:C2	6:L:79:DG:C2	3.08	0.41
1:O:767:TRP:CE3	1:P:717:LEU:HD13	2.55	0.41
3:R:25:GLU:CD	3:R:25:GLU:H	2.23	0.41
1:A:587:LEU:HD11	1:A:591:LYS:HE2	2.03	0.41
1:B:745:ASP:OD1	1:B:745:ASP:N	2.51	0.41
1:B:1126:ASP:O	1:B:1127:ASN:HB3	2.21	0.41
3:F:25:GLU:O	3:F:29:GLN:HG3	2.19	0.41
1:P:244:ILE:CD1	3:Q:41:LEU:HD21	2.51	0.41
3:F:89:SER:O	3:F:93:MET:HE2	2.21	0.41
1:P:141:GLY:O	1:P:143:ARG:NH1	2.54	0.41
1:P:674:MET:HE3	1:P:674:MET:HA	2.03	0.41
1:A:246:LEU:O	1:A:249:ILE:CG2	2.69	0.41
1:B:232:PHE:CZ	1:B:1338:LEU:HA	2.56	0.41
1:B:1411:LEU:HB2	1:B:1416:ILE:HD11	2.03	0.41
6:L:44:DG:H5''	3:R:140:ARG:CZ	2.51	0.41
1:O:12:LEU:HD21	1:O:46:ALA:CB	2.50	0.41
1:O:46:ALA:O	1:O:49:THR:HG22	2.21	0.41
1:P:264:THR:HG23	1:P:265:GLU:N	2.36	0.41
4:S:7:VAL:O	4:S:11:ILE:HG22	2.21	0.41
1:A:1118:CYS:SG	1:A:1122:ARG:NH1	2.92	0.41
1:B:1232:LYS:O	1:B:1235:ILE:HG22	2.21	0.41
4:G:64:THR:HG23	4:G:67:ALA:H	1.85	0.41
5:K:63:DG:C4'	1:P:189:ARG:HG3	2.51	0.41
1:O:45:ALA:HB1	1:O:60:PHE:CE2	2.55	0.41
1:P:288:ALA:HB2	1:P:1106:ILE:HG22	2.02	0.41
1:P:1227:THR:O	1:P:1230:GLU:HG3	2.21	0.41
3:Q:108:ARG:NH1	3:Q:111:ASN:HD21	2.19	0.41
1:A:1407:GLU:HA	1:A:1407:GLU:OE1	2.21	0.41
1:B:1335:GLU:HA	1:B:1338:LEU:HG	2.03	0.41
1:B:1338:LEU:HD23	1:B:1338:LEU:N	2.36	0.41
3:E:108:ARG:NH1	3:E:111:ASN:HD21	2.19	0.41
1:P:604:TRP:CH2	1:P:608:GLN:HG3	2.56	0.41
4:S:36:4HH:O	4:S:40:VAL:HG23	2.21	0.41
2:D:357:GLN:O	2:D:361:MET:SD	2.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:140:ARG:HD2	3:E:140:ARG:O	2.22	0.40
4:G:36:4HH:O	4:G:40:VAL:HG23	2.21	0.40
1:P:1126:ASP:O	1:P:1127:ASN:HB3	2.21	0.40
4:M:29:VAL:HG13	4:M:30:GLU:N	2.36	0.40
1:A:788:GLU:O	1:A:792:LEU:HD13	2.21	0.40
1:A:1202:ILE:O	1:A:1202:ILE:HG22	2.20	0.40
2:D:201:ILE:HD13	2:D:289:ILE:HD11	2.02	0.40
1:P:1411:LEU:HB2	1:P:1416:ILE:HD11	2.03	0.40
3:R:190:ASP:OD1	3:R:190:ASP:C	2.59	0.40
1:A:1107:ARG:NH2	4:G:47:GLU:OE2	2.50	0.40
2:C:162:TYR:CD2	2:D:124:ARG:HB2	2.54	0.40
2:C:440:TYR:CD1	2:C:440:TYR:N	2.90	0.40
1:O:246:LEU:O	1:O:249:ILE:CG2	2.69	0.40
1:O:1213:GLU:OE1	1:O:1213:GLU:HA	2.22	0.40
1:O:1387:GLU:OE1	1:O:1388:GLU:N	2.54	0.40
1:B:1325:MET:SD	1:B:1325:MET:N	2.90	0.40
2:C:124:ARG:CB	2:D:162:TYR:CD1	3.04	0.40
2:C:201:ILE:HD13	2:C:289:ILE:HD11	2.02	0.40
3:E:9:PHE:CE1	3:F:16:GLN:HG2	2.57	0.40
3:F:42:ASP:OD1	3:F:43:ASN:N	2.54	0.40
1:O:87:TYR:CG	1:O:136:LEU:HD23	2.56	0.40
1:O:587:LEU:HD11	1:O:591:LYS:HE2	2.03	0.40
1:O:788:GLU:O	1:O:792:LEU:HD13	2.21	0.40
1:A:594:ILE:HD12	1:A:845:HIS:CE1	2.56	0.40
1:P:1307:THR:OG1	1:P:1310:GLU:HG3	2.22	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	1465/1482 (99%)	1423 (97%)	42 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1465/1482 (99%)	1413 (96%)	52 (4%)	0	100	100
1	O	1465/1482 (99%)	1423 (97%)	42 (3%)	0	100	100
1	P	1465/1482 (99%)	1413 (96%)	52 (4%)	0	100	100
2	C	438/440 (100%)	426 (97%)	12 (3%)	0	100	100
2	D	438/440 (100%)	426 (97%)	12 (3%)	0	100	100
3	E	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
3	F	196/240 (82%)	191 (97%)	5 (3%)	0	100	100
3	Q	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
3	R	196/240 (82%)	191 (97%)	5 (3%)	0	100	100
4	G	69/78 (88%)	68 (99%)	1 (1%)	0	100	100
4	I	69/78 (88%)	67 (97%)	2 (3%)	0	100	100
4	M	69/78 (88%)	66 (96%)	3 (4%)	0	100	100
4	S	69/78 (88%)	68 (99%)	1 (1%)	0	100	100
All	All	7824/8080 (97%)	7587 (97%)	237 (3%)	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	1269/1281 (99%)	1260 (99%)	9 (1%)	81	87
1	B	1269/1281 (99%)	1257 (99%)	12 (1%)	75	83
1	O	1269/1281 (99%)	1260 (99%)	9 (1%)	81	87
1	P	1269/1281 (99%)	1257 (99%)	12 (1%)	75	83
2	C	376/376 (100%)	364 (97%)	12 (3%)	34	53
2	D	376/376 (100%)	364 (97%)	12 (3%)	34	53
3	E	189/212 (89%)	185 (98%)	4 (2%)	48	66
3	F	177/212 (84%)	174 (98%)	3 (2%)	56	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	189/212 (89%)	186 (98%)	3 (2%)	58	73
3	R	177/212 (84%)	174 (98%)	3 (2%)	56	72
4	G	62/66 (94%)	62 (100%)	0	100	100
4	I	62/66 (94%)	62 (100%)	0	100	100
4	M	62/66 (94%)	62 (100%)	0	100	100
4	S	62/66 (94%)	62 (100%)	0	100	100
All	All	6808/6988 (97%)	6729 (99%)	79 (1%)	66	78

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	A	319	GLN
1	A	732	GLU
1	A	747	SER
1	A	783	ARG
1	A	1060	ARG
1	A	1131	ARG
1	A	1165	GLU
1	A	1204	ARG
1	B	62	ASN
1	B	211	SER
1	B	250	ARG
1	B	665	GLN
1	B	673	ARG
1	B	687	SER
1	B	1127	ASN
1	B	1131	ARG
1	B	1152	LYS
1	B	1213	GLU
1	B	1322	GLN
1	B	1347	ASP
2	C	2	SER
2	C	92	SER
2	C	94	LEU
2	C	132	VAL
2	C	209	SER
2	C	250	ASP
2	C	287	THR
2	C	300	ARG

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Mol	Chain	Res	Type
2	C	361	MET
2	C	370	GLN
2	C	428	TYR
2	C	438	ASP
2	D	2	SER
2	D	92	SER
2	D	94	LEU
2	D	132	VAL
2	D	209	SER
2	D	250	ASP
2	D	287	THR
2	D	300	ARG
2	D	361	MET
2	D	370	GLN
2	D	428	TYR
2	D	438	ASP
3	E	138	ASN
3	E	147	ASP
3	E	169	TYR
3	E	181	THR
3	F	39	ASP
3	F	152	GLN
3	F	190	ASP
1	O	24	ASP
1	O	319	GLN
1	O	732	GLU
1	O	747	SER
1	O	783	ARG
1	O	1060	ARG
1	O	1131	ARG
1	O	1165	GLU
1	O	1204	ARG
1	P	62	ASN
1	P	211	SER
1	P	250	ARG
1	P	665	GLN
1	P	673	ARG
1	P	687	SER
1	P	1127	ASN
1	P	1131	ARG
1	P	1152	LYS
1	P	1213	GLU

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Mol	Chain	Res	Type
1	P	1322	GLN
1	P	1347	ASP
3	Q	147	ASP
3	Q	169	TYR
3	Q	181	THR
3	R	39	ASP
3	R	152	GLN
3	R	190	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	75	ASN
2	C	128	GLN
2	C	134	ASN
2	C	198	GLN
2	D	75	ASN
2	D	134	ASN
2	D	198	GLN
3	E	111	ASN
3	Q	111	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
4	4HH	S	36	4	21,26,27	0.45	0	27,35,37	3.13	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	4HH	I	36	4	21,26,27	0.46	0	27,35,37	1.72	3 (11%)
4	4HH	G	36	4	21,26,27	0.45	0	27,35,37	3.13	4 (14%)
4	4HH	M	36	4	21,26,27	0.47	0	27,35,37	1.73	3 (11%)

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	4HH	S	36	4	-	5/32/35/37	-
4	4HH	I	36	4	-	6/32/35/37	-
4	4HH	G	36	4	-	5/32/35/37	-
4	4HH	M	36	4	-	6/32/35/37	-

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	36	4HH	O1P-P-OG	11.65	161.86	107.75
4	S	36	4HH	O1P-P-OG	11.64	161.82	107.75
4	S	36	4HH	OG-P-O2P	-8.87	74.39	109.07
4	G	36	4HH	OG-P-O2P	-8.86	74.46	109.07
4	G	36	4HH	P-OG-CB	6.13	157.62	121.68
4	S	36	4HH	P-OG-CB	6.11	157.50	121.68
4	I	36	4HH	P-OG-CB	-5.41	89.97	121.68
4	M	36	4HH	P-OG-CB	-5.39	90.07	121.68
4	M	36	4HH	O1P-P-OG	4.65	129.33	107.75
4	I	36	4HH	O1P-P-OG	4.64	129.28	107.75
4	M	36	4HH	OG-CB-CA	4.42	112.45	108.14
4	I	36	4HH	OG-CB-CA	4.35	112.38	108.14
4	G	36	4HH	OG-CB-CA	2.86	110.93	108.14
4	S	36	4HH	OG-CB-CA	2.80	110.87	108.14

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	36	4HH	N-CA-CB-OG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	I	36	4HH	CB-OG-P-O1P
4	M	36	4HH	N-CA-CB-OG
4	M	36	4HH	CB-OG-P-O1P
4	G	36	4HH	CJ-O3P-P-OG
4	S	36	4HH	CJ-O3P-P-OG
4	S	36	4HH	CB-OG-P-O3P
4	G	36	4HH	CB-OG-P-O3P
4	I	36	4HH	CO-CP-CQ-NR
4	M	36	4HH	CO-CP-CQ-NR
4	I	36	4HH	CO-CP-CQ-OR
4	M	36	4HH	CO-CP-CQ-OR
4	I	36	4HH	CB-OG-P-O3P
4	M	36	4HH	CB-OG-P-O3P
4	G	36	4HH	ON-CL3-CM-OM
4	I	36	4HH	ON-CL3-CM-OM
4	S	36	4HH	ON-CL3-CM-OM
4	M	36	4HH	ON-CL3-CM-OM
4	G	36	4HH	CT-CS-NR-CQ
4	S	36	4HH	CT-CS-NR-CQ
4	G	36	4HH	CB-OG-P-O2P
4	S	36	4HH	CB-OG-P-O2P

There are no ring outliers.

4 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	36	4HH	16	0
4	I	36	4HH	1	0
4	G	36	4HH	15	0
4	M	36	4HH	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
8	ATP	O	1502	7	26,33,33	0.61	0	31,52,52	1.13	3 (9%)
8	ATP	A	1502	7	26,33,33	0.61	0	31,52,52	1.13	3 (9%)
8	ATP	B	1502	7	26,33,33	0.63	0	31,52,52	1.12	3 (9%)
8	ATP	P	1502	7	26,33,33	0.63	0	31,52,52	1.12	3 (9%)

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
8	ATP	O	1502	7	-	1/18/38/38	0/3/3/3
8	ATP	A	1502	7	-	1/18/38/38	0/3/3/3
8	ATP	B	1502	7	-	2/18/38/38	0/3/3/3
8	ATP	P	1502	7	-	2/18/38/38	0/3/3/3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	1502	ATP	C5-C6-N6	2.39	123.99	120.35
8	B	1502	ATP	C5-C6-N6	2.37	123.96	120.35
8	A	1502	ATP	C5-C6-N6	2.35	123.92	120.35
8	A	1502	ATP	O2'-C2'-C3'	-2.32	104.30	111.82
8	O	1502	ATP	O2'-C2'-C3'	-2.31	104.36	111.82
8	O	1502	ATP	C5-C6-N6	2.30	123.85	120.35
8	P	1502	ATP	O2'-C2'-C3'	-2.20	104.72	111.82
8	B	1502	ATP	O2'-C2'-C3'	-2.18	104.77	111.82
8	B	1502	ATP	O3'-C3'-C2'	-2.14	104.90	111.82
8	P	1502	ATP	O3'-C3'-C2'	-2.13	104.93	111.82
8	O	1502	ATP	O3'-C3'-C2'	-2.08	105.10	111.82
8	A	1502	ATP	O3'-C3'-C2'	-2.07	105.12	111.82

There are no chirality outliers.

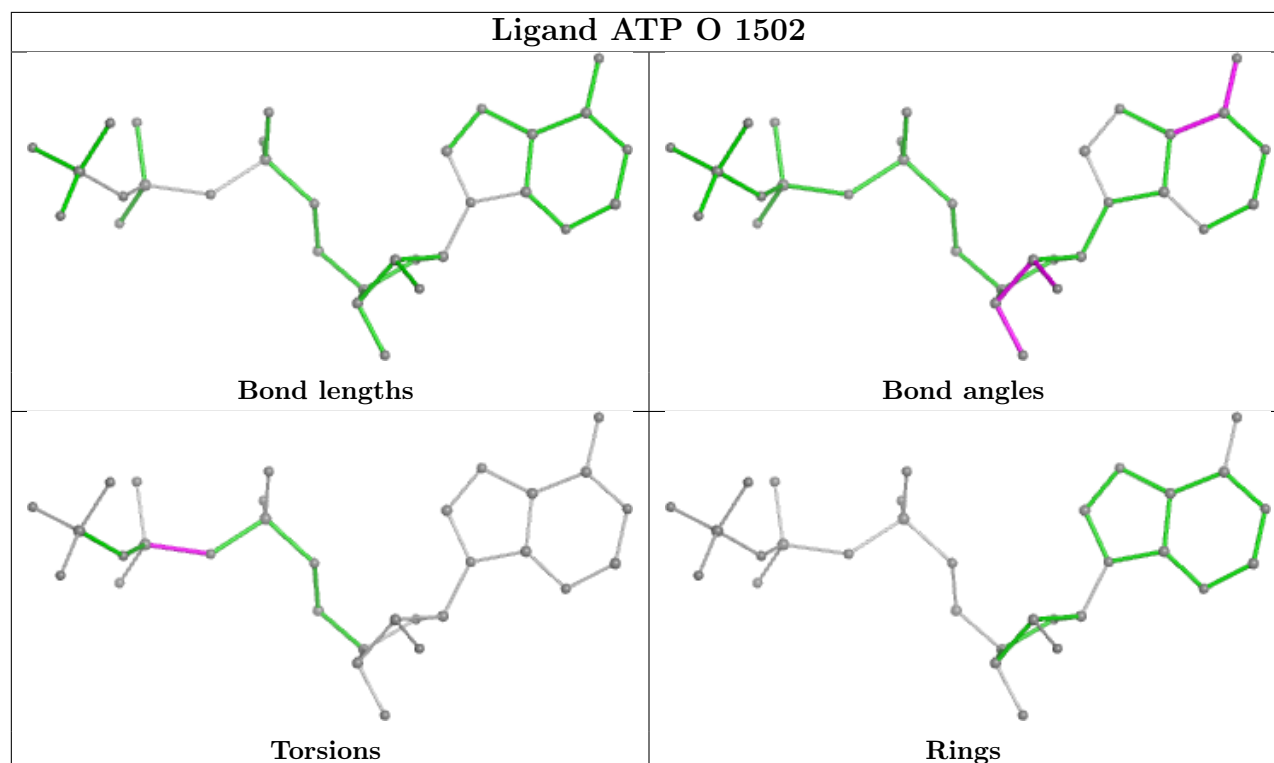
All (6) torsion outliers are listed below:

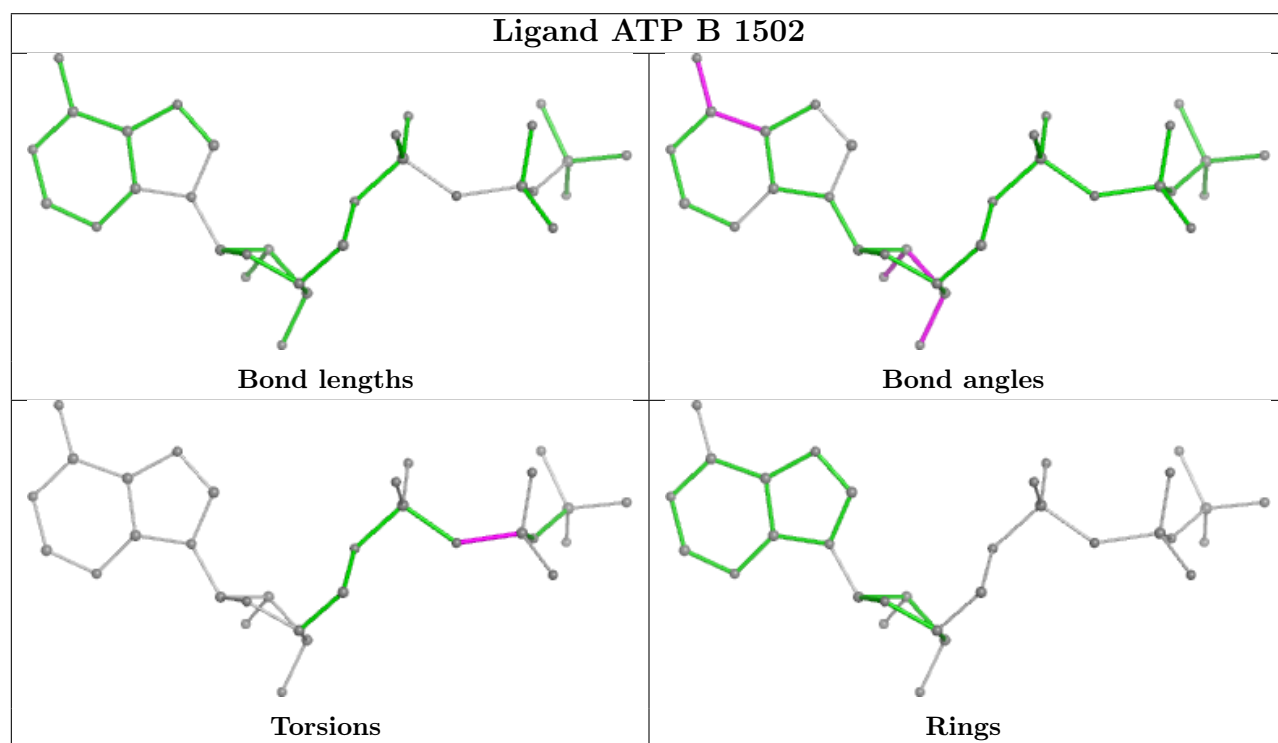
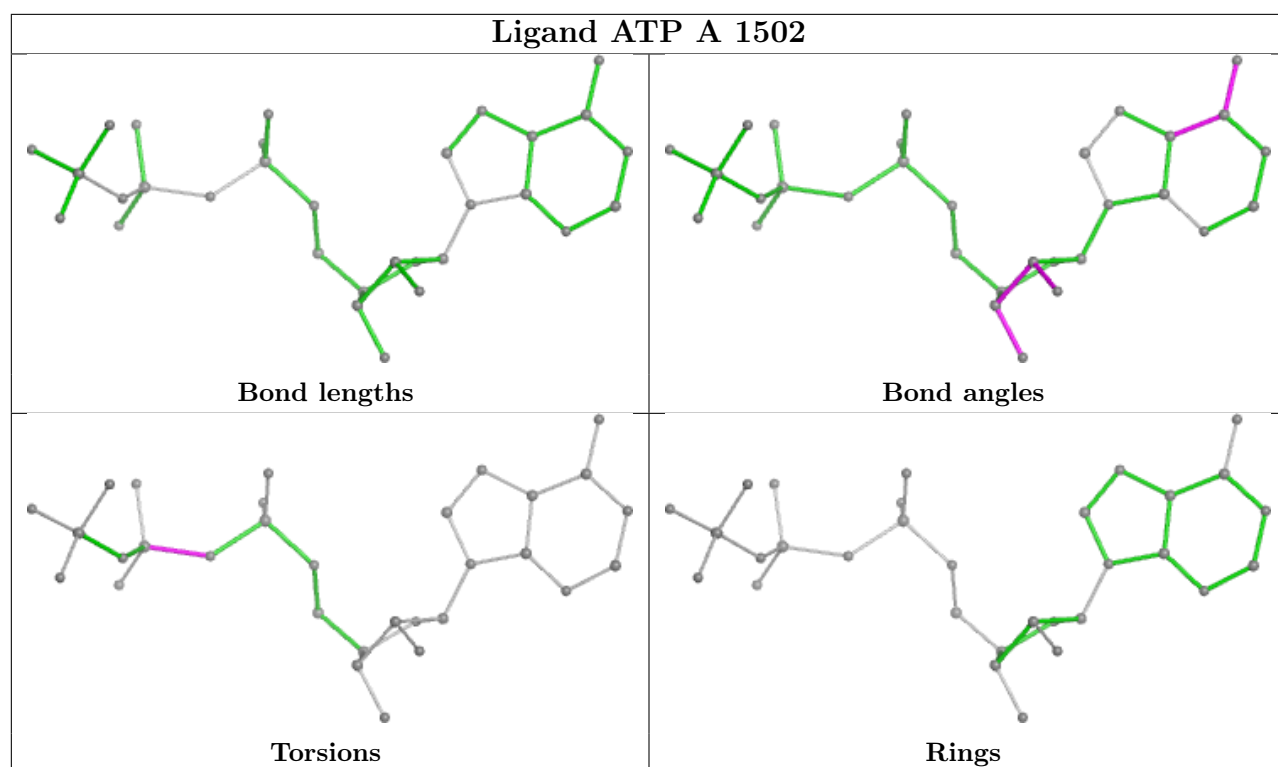
Mol	Chain	Res	Type	Atoms
8	A	1502	ATP	PA-O3A-PB-O2B
8	O	1502	ATP	PA-O3A-PB-O2B
8	B	1502	ATP	PA-O3A-PB-O1B
8	B	1502	ATP	PA-O3A-PB-O2B
8	P	1502	ATP	PA-O3A-PB-O1B
8	P	1502	ATP	PA-O3A-PB-O2B

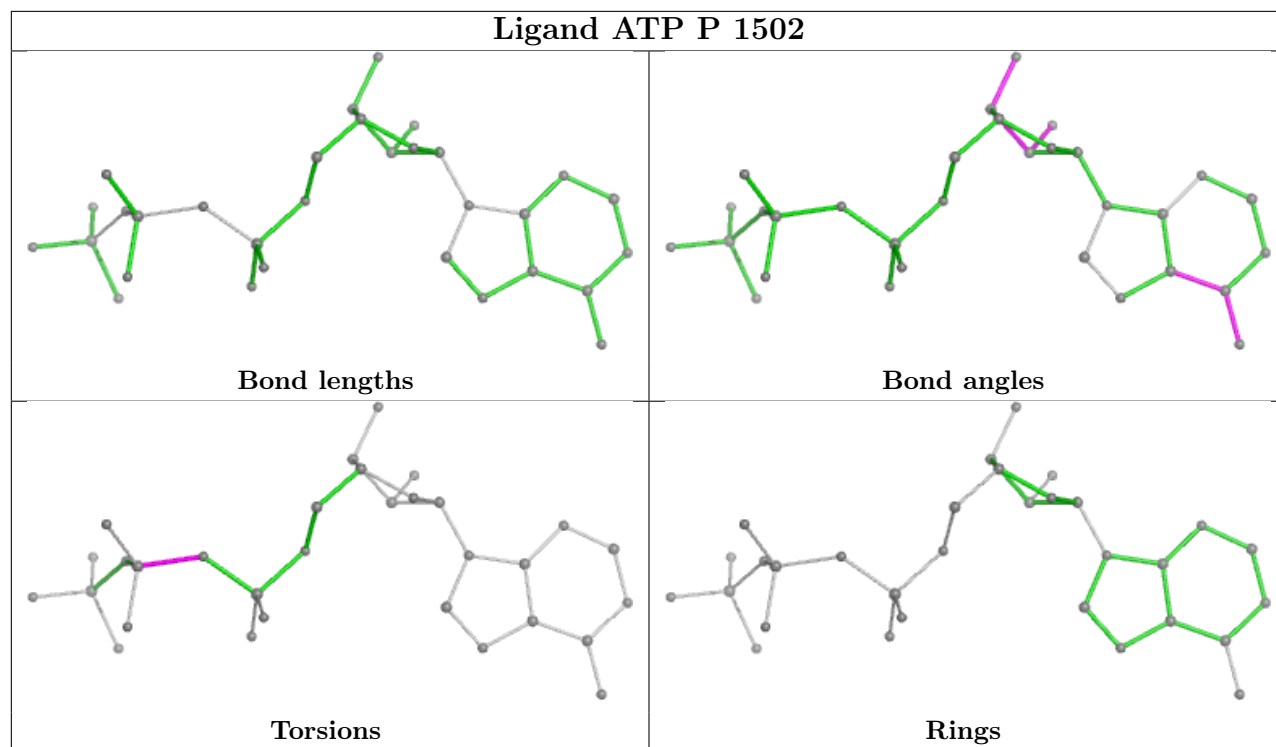
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	295:ARG	C	296:ILE	N	1.04
1	C	295:ARG	C	296:ILE	N	1.03

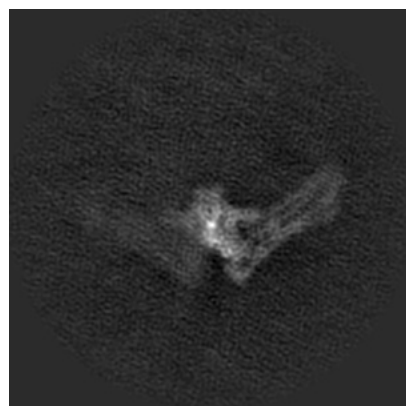
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51446. These allow visual inspection of the internal detail of the map and identification of artifacts.

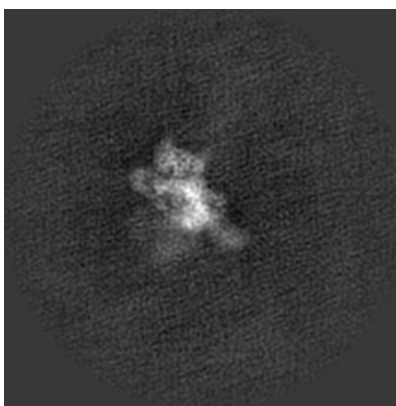
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

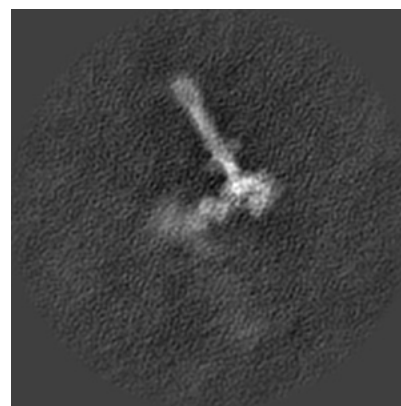
6.1.1 Primary map



X

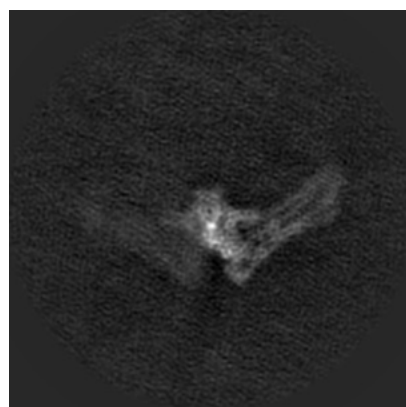


Y

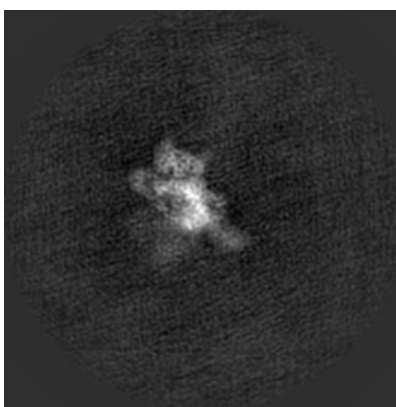


Z

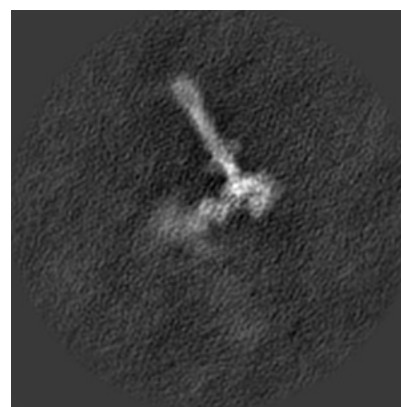
6.1.2 Raw map



X



Y

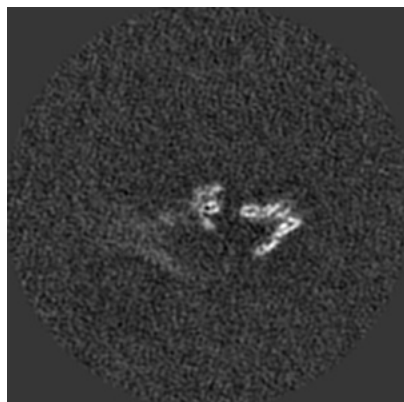


Z

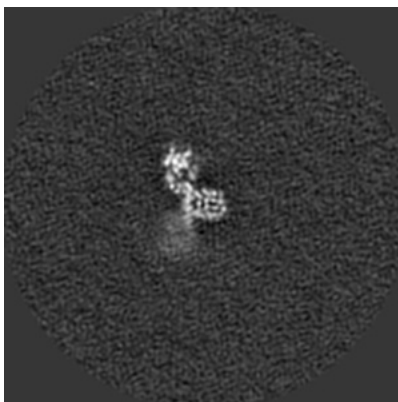
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

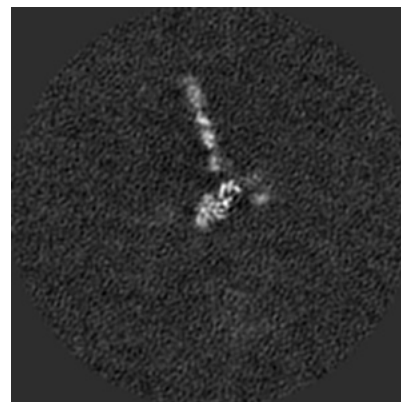
6.2.1 Primary map



X Index: 83

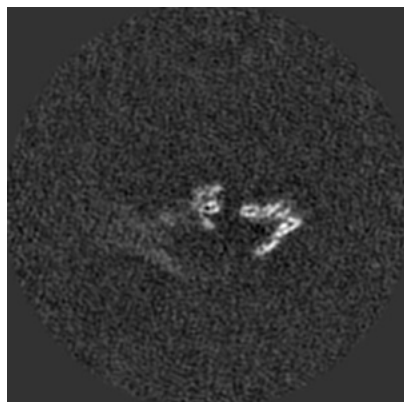


Y Index: 83

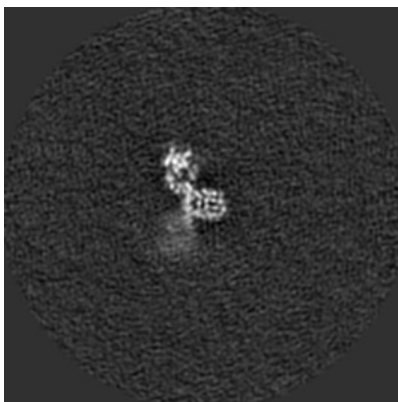


Z Index: 83

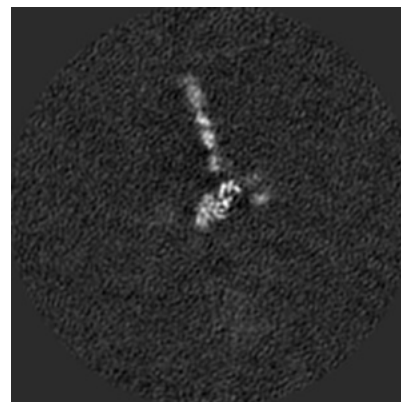
6.2.2 Raw map



X Index: 83



Y Index: 83

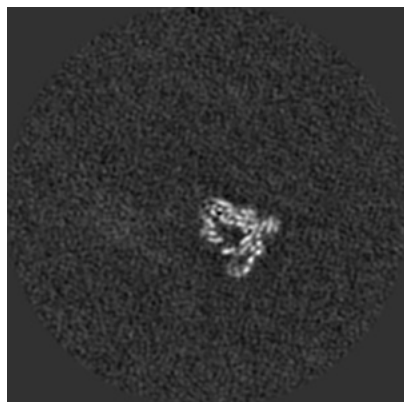


Z Index: 83

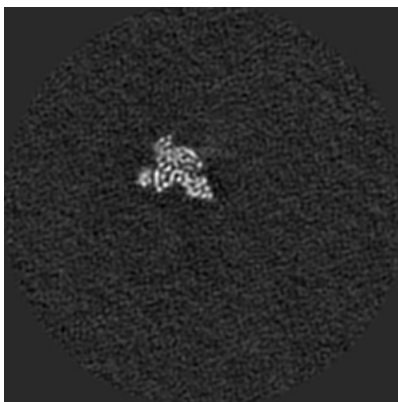
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

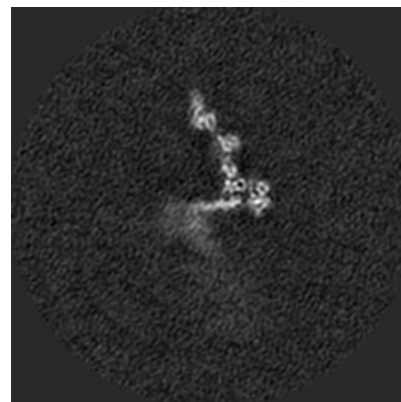
6.3.1 Primary map



X Index: 90

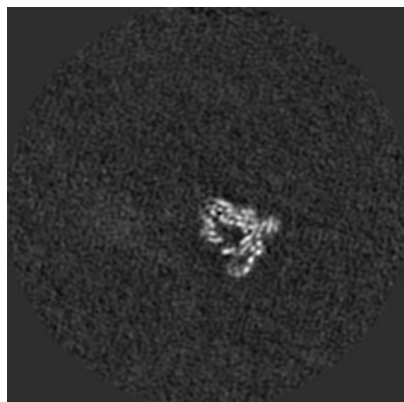


Y Index: 90

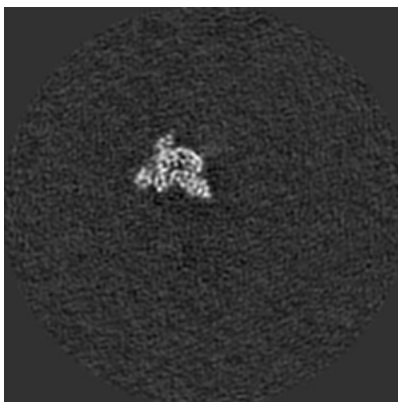


Z Index: 76

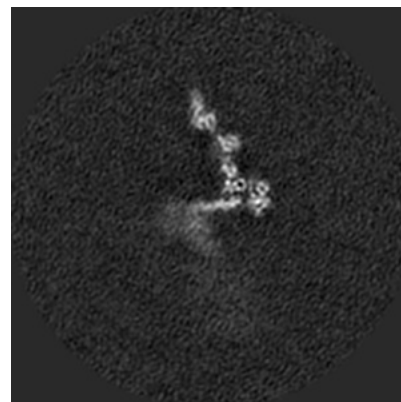
6.3.2 Raw map



X Index: 90



Y Index: 91

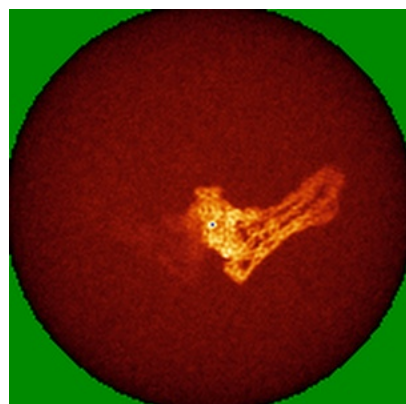


Z Index: 76

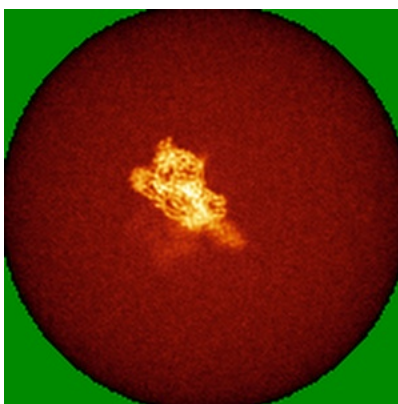
The images above show the largest variance slices of the map in three orthogonal directions.

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

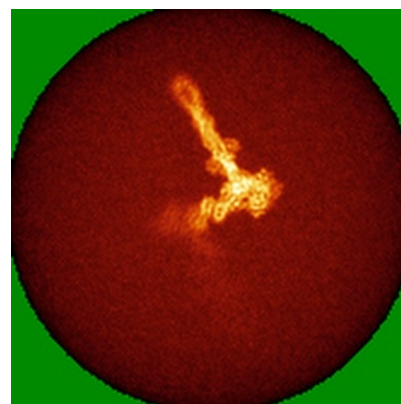
6.4.1 Primary map



X

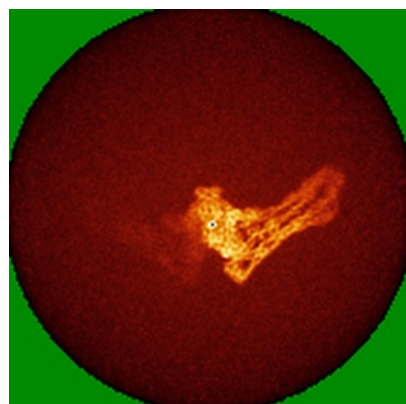


Y

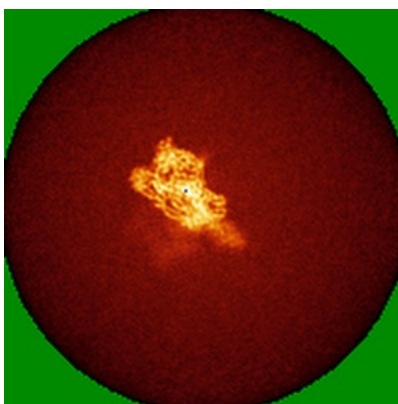


Z

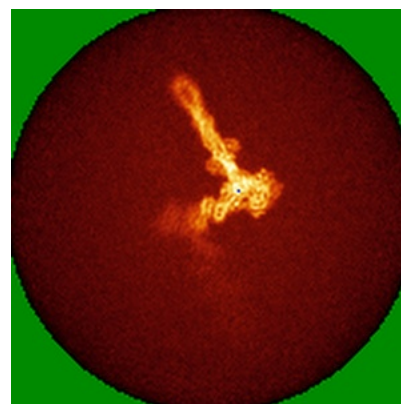
6.4.2 Raw map



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.

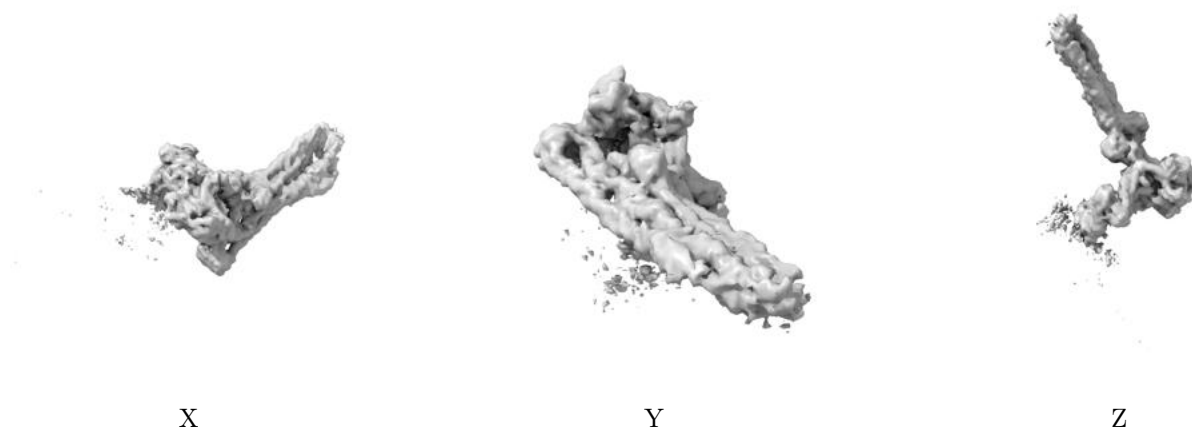
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

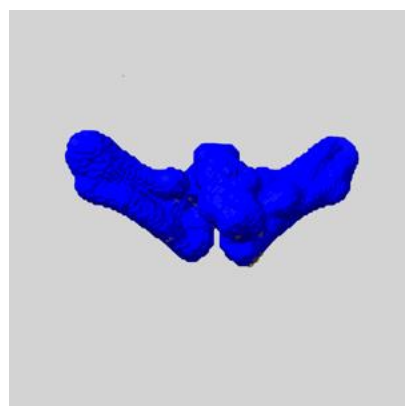
6.6 Mask visualisation [i](#)

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

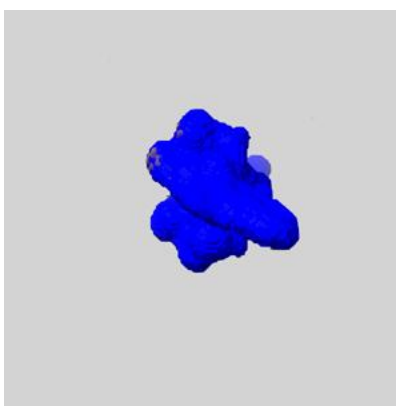
A mask typically either:

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

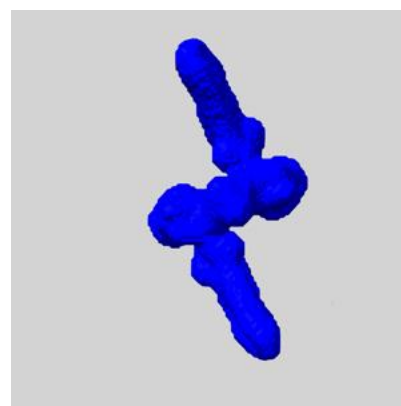
6.6.1 emd_51446_msk_1.map [i](#)



X



Y

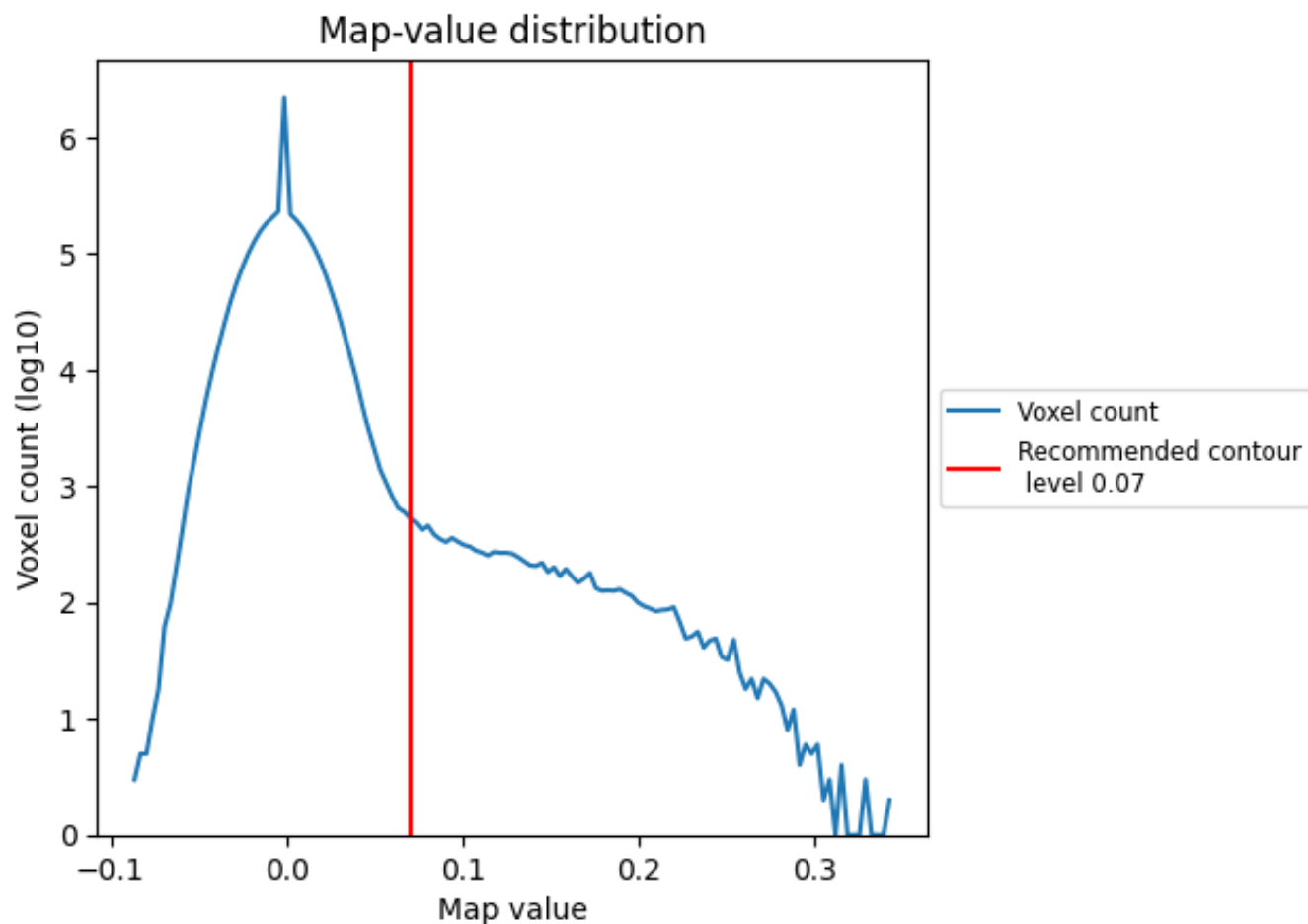


Z

7 Map analysis [i](#)

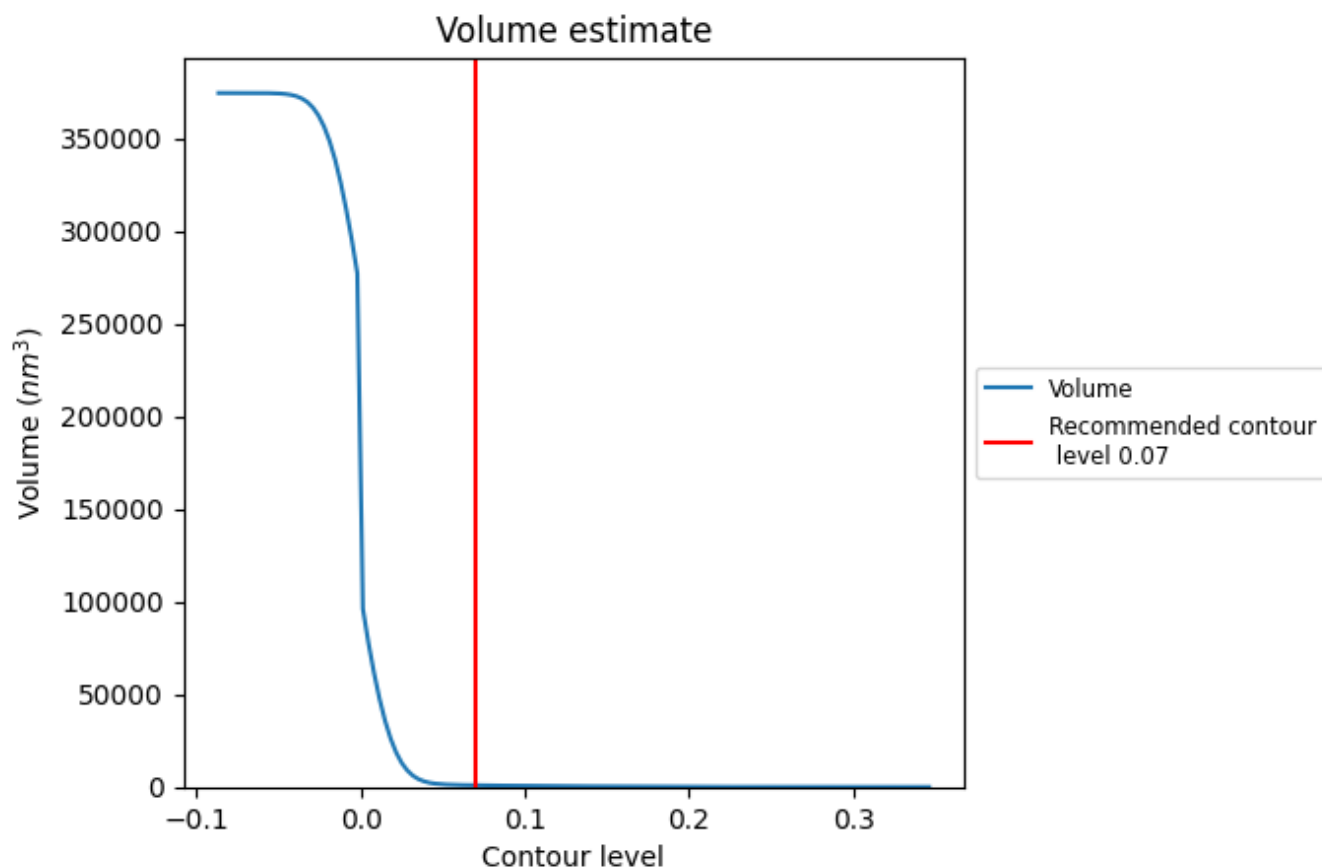
This section contains the results of statistical analysis of the map.

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.

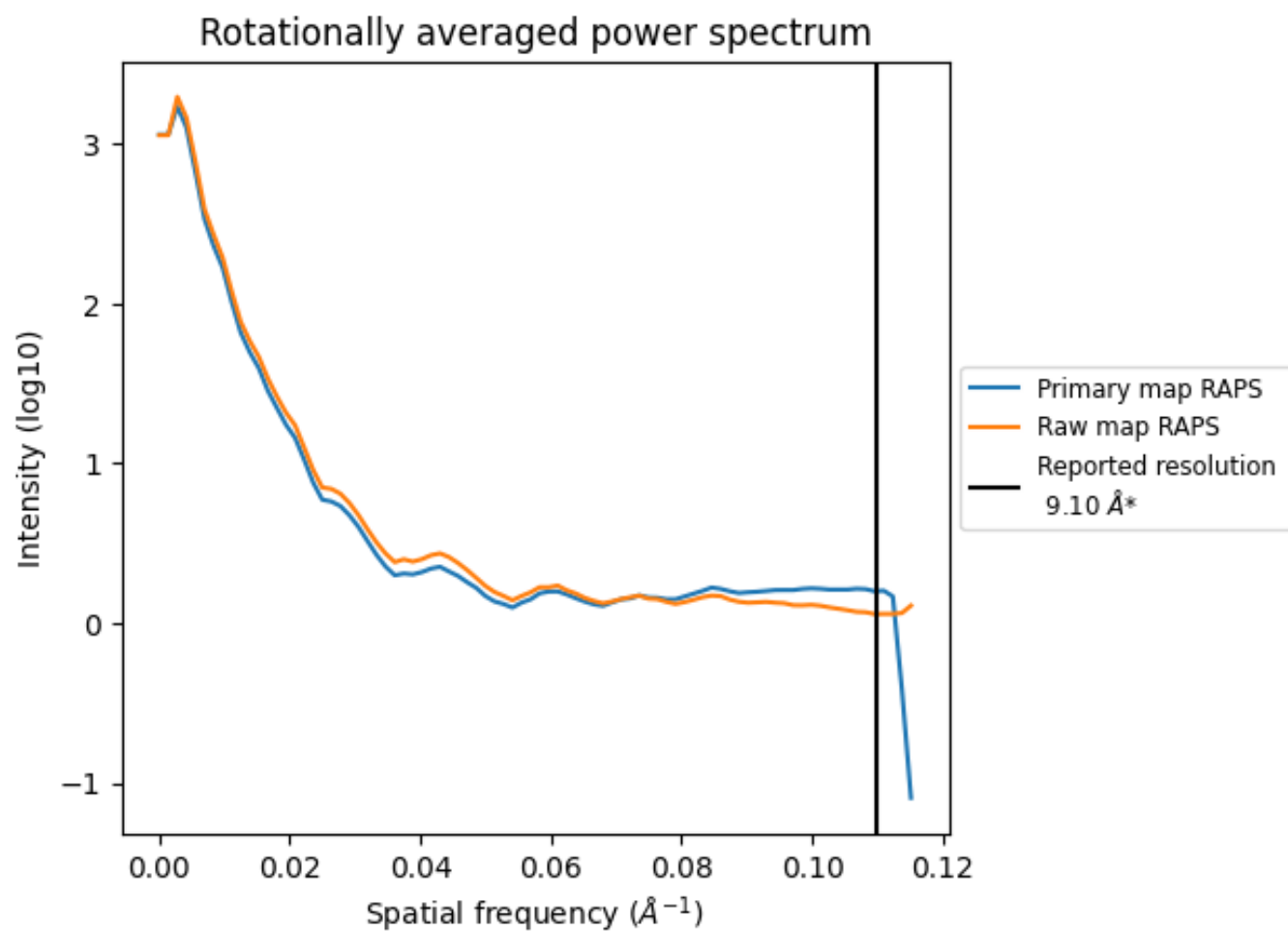
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 892 nm^3 ; this corresponds to an approximate mass of 806 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 [i](#)

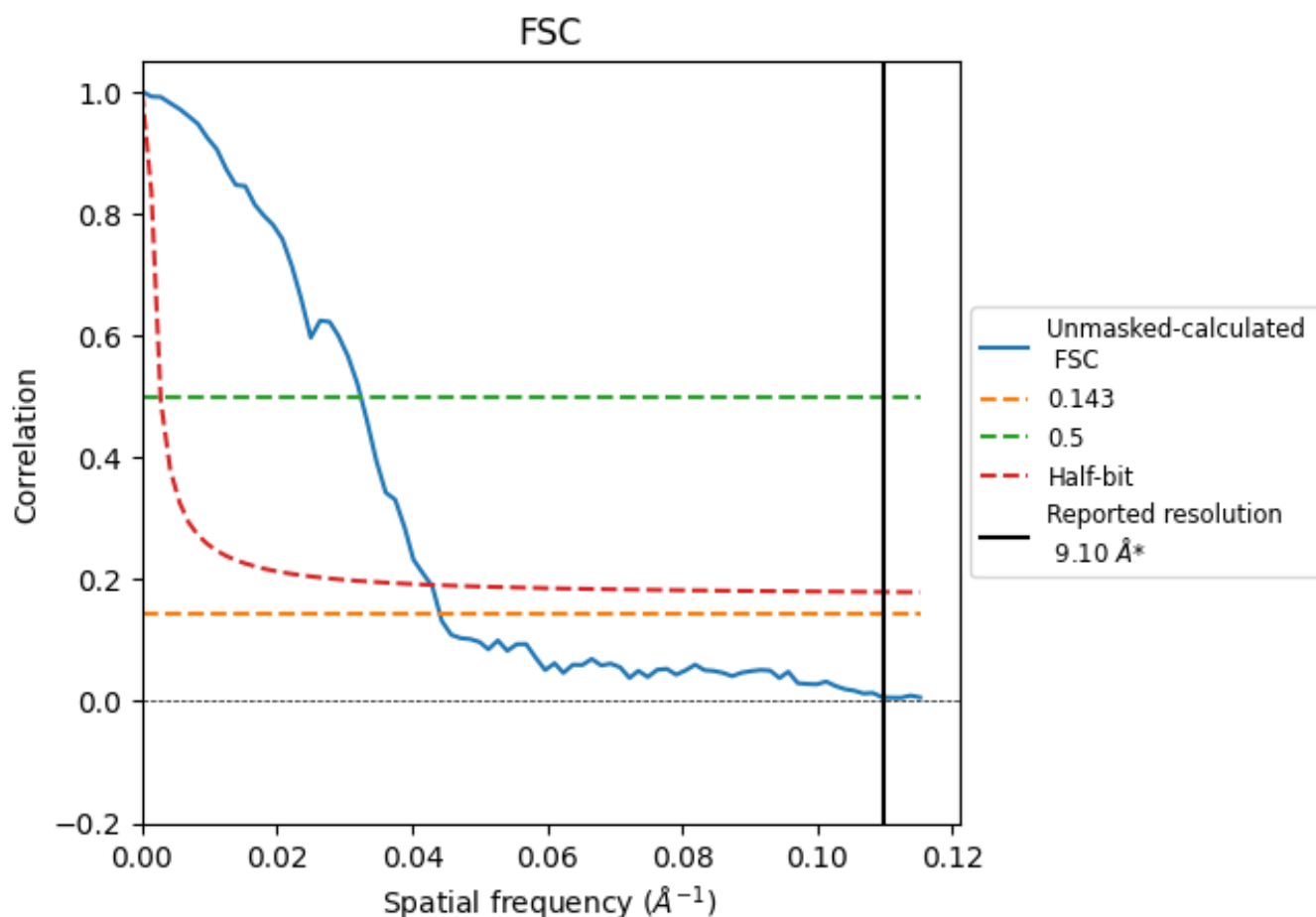


*Reported resolution corresponds to spatial frequency of 0.110 \AA^{-1}

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 0.110 \AA^{-1}

8.2 Resolution estimates [i](#)

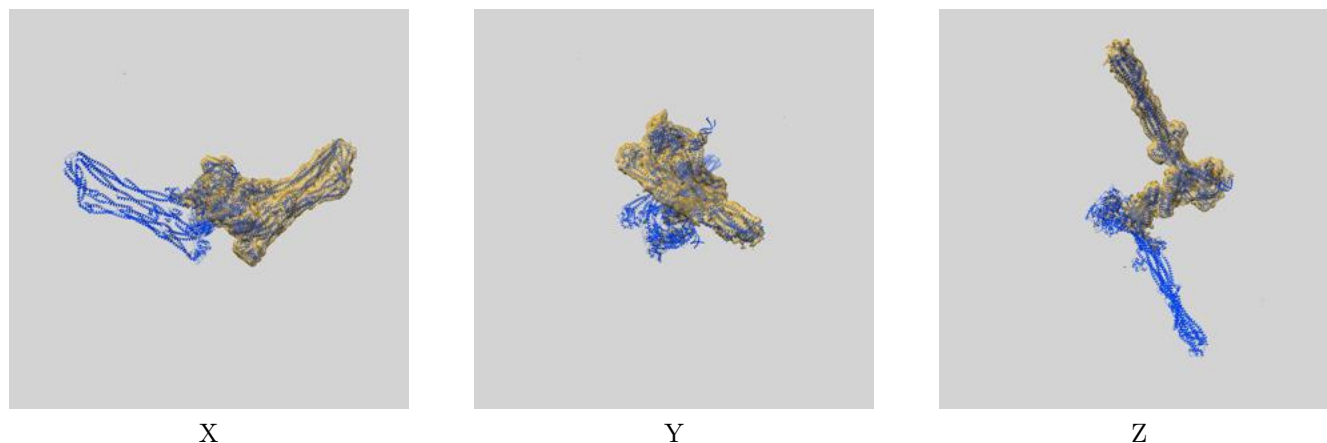
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	22.68	30.86	23.36

*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 22.68 differs from the reported value 9.1 by more than 10 %

9 Map-model fit [i](#)

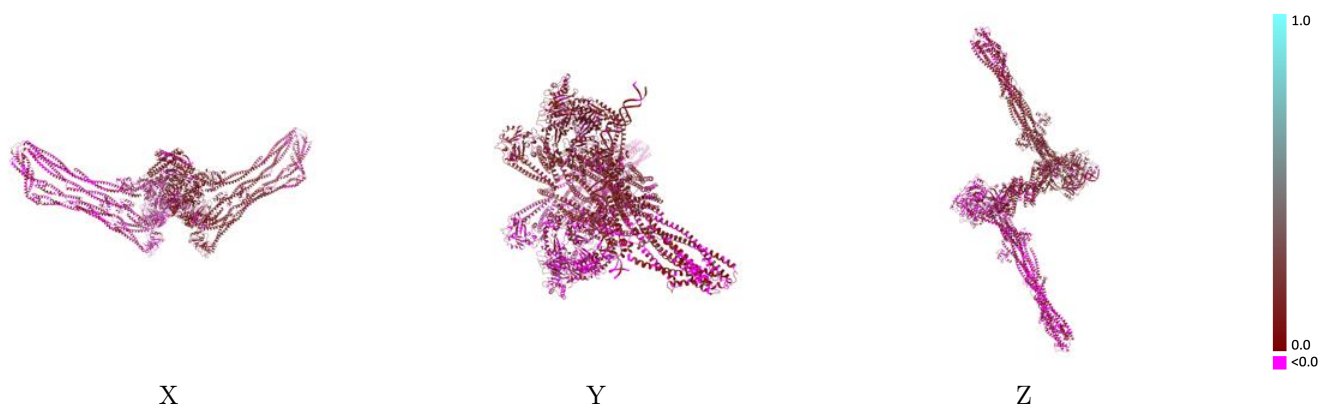
This section contains information regarding the fit between EMDB map EMD-51446 and PDB model 9GMA. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



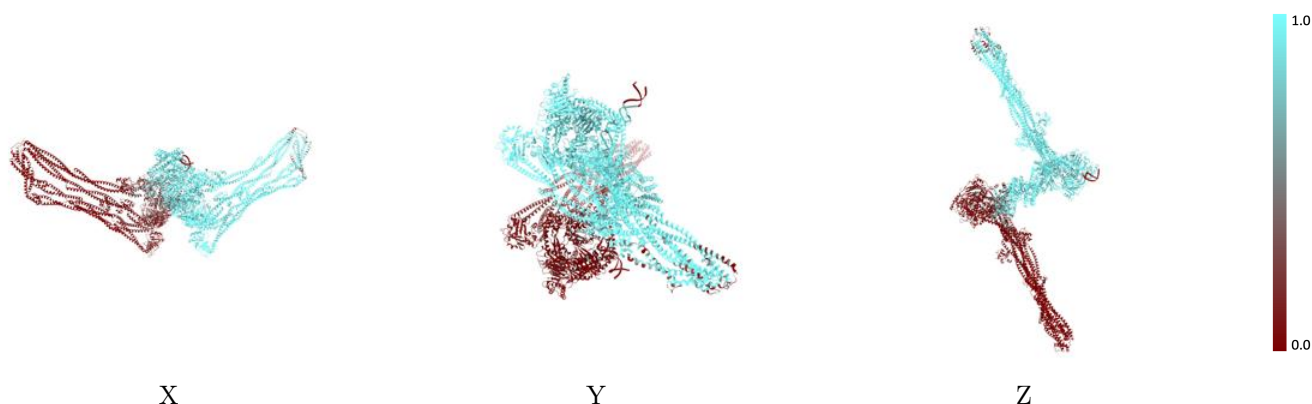
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



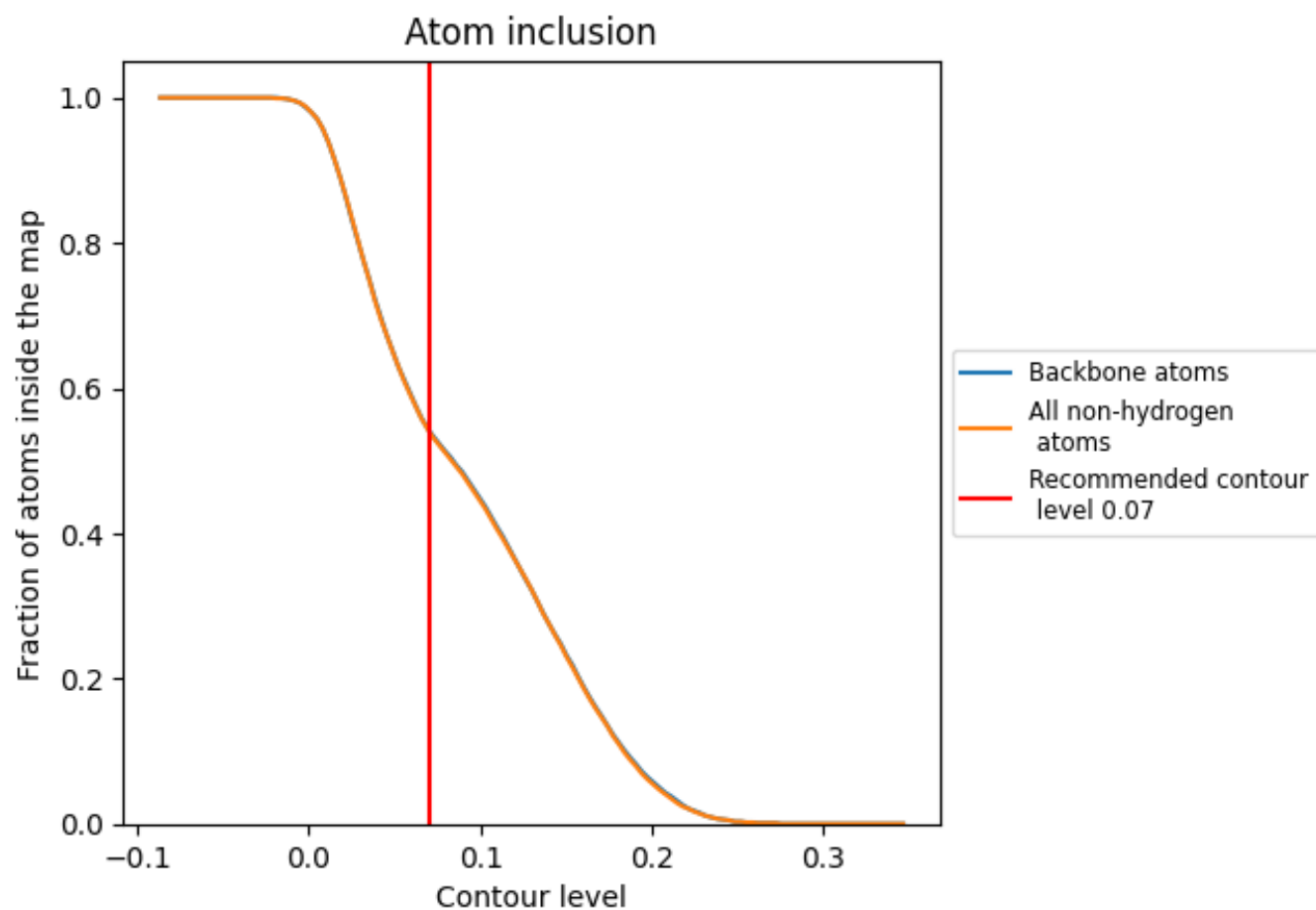
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 54% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5410	 0.0750
A	 0.9440	 0.1220
B	 0.9390	 0.1190
C	 0.9450	 0.1200
D	 0.6710	 0.0760
E	 0.9470	 0.1300
F	 0.9570	 0.1330
G	 0.9830	 0.1350
I	 0.9640	 0.1490
K	 0.6510	 0.1010
L	 0.6390	 0.0990
M	 0.0360	 0.0260
O	 0.0050	 0.0160
P	 0.0350	 0.0200
Q	 0.6600	 0.0450
R	 0.1760	 0.0320
S	 0.0000	 0.0030

