



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:45 PM UTC

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:

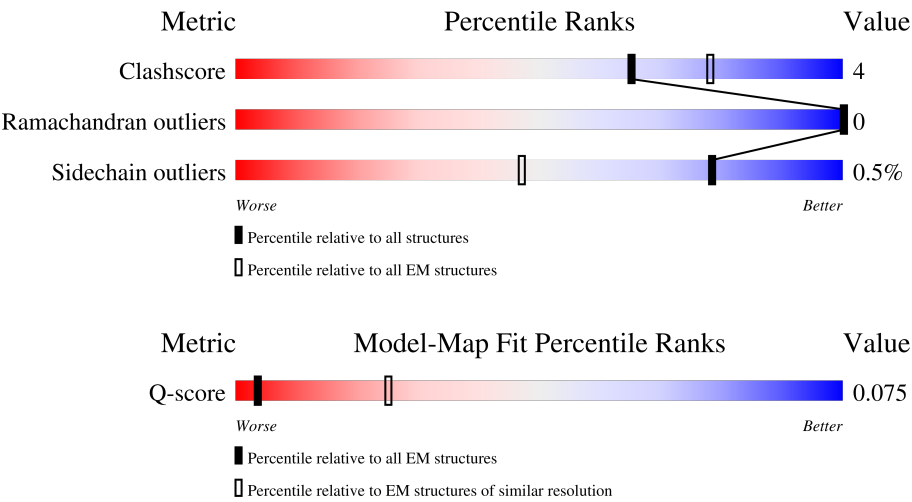
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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.



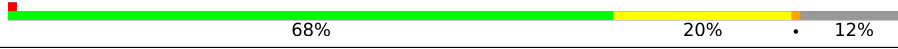
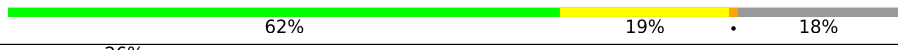
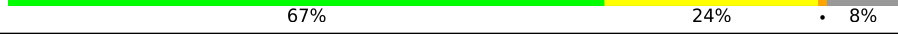
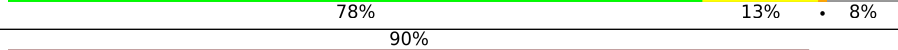
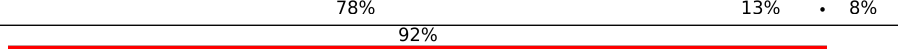
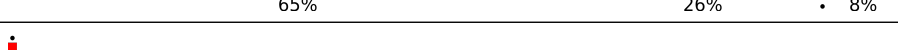
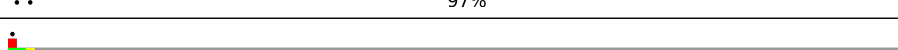
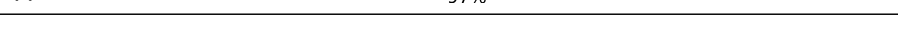
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	244 (8.60 - 9.60)

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	92%7%.
1	B	1482	85%13%..
1	O	1482	99%92%7%.
1	P	1482	96%84%15%..

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Mol	Chain	Length	Quality of chain
2	C	440	
2	D	440	
3	E	240	
3	F	240	
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			

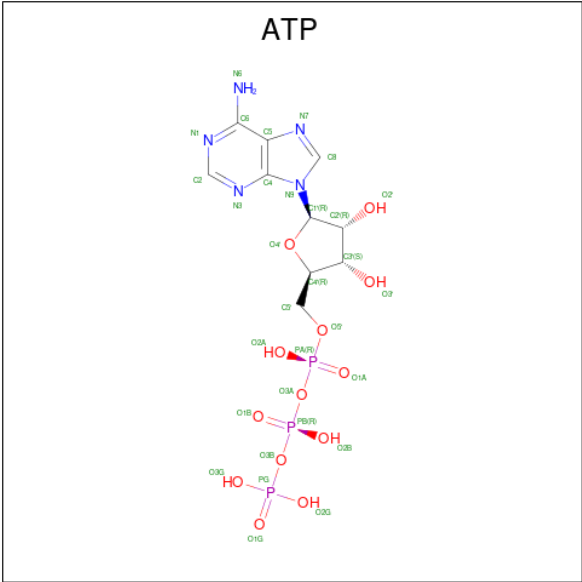
- Molecule 6 is a DNA chain called pFB526.

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).

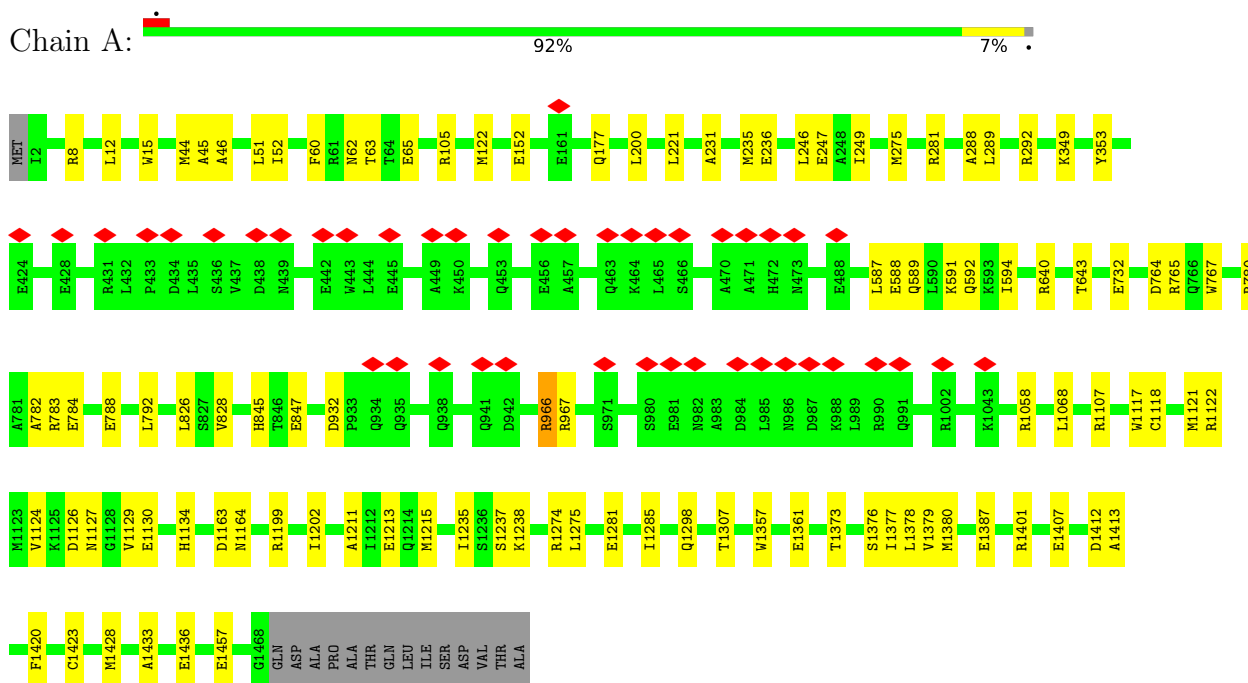


Mol	Chain	Residues	Atoms						AltConf
8	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
8	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
8	O	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
8	P	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

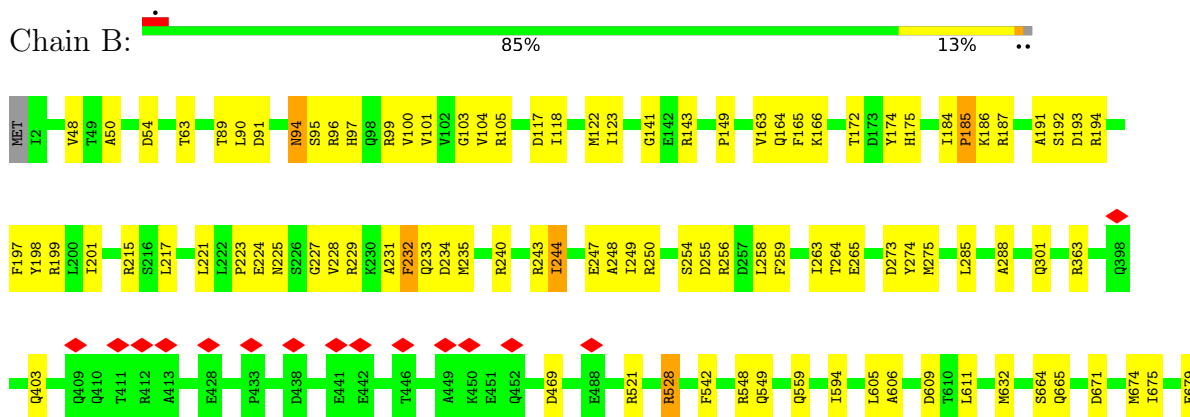
3 Residue-property plots

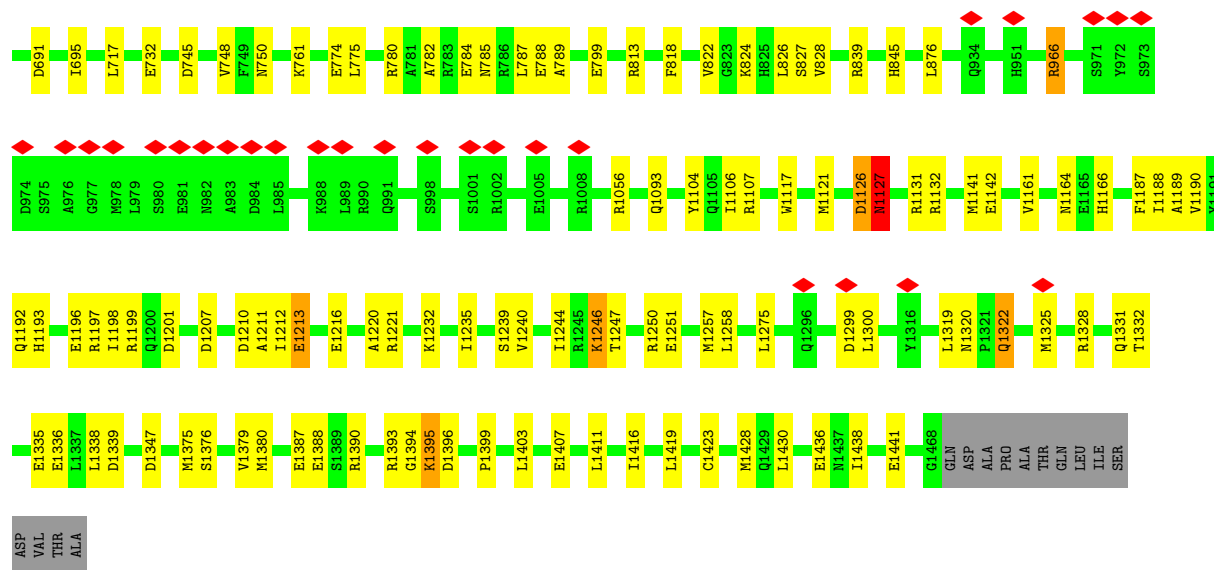
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

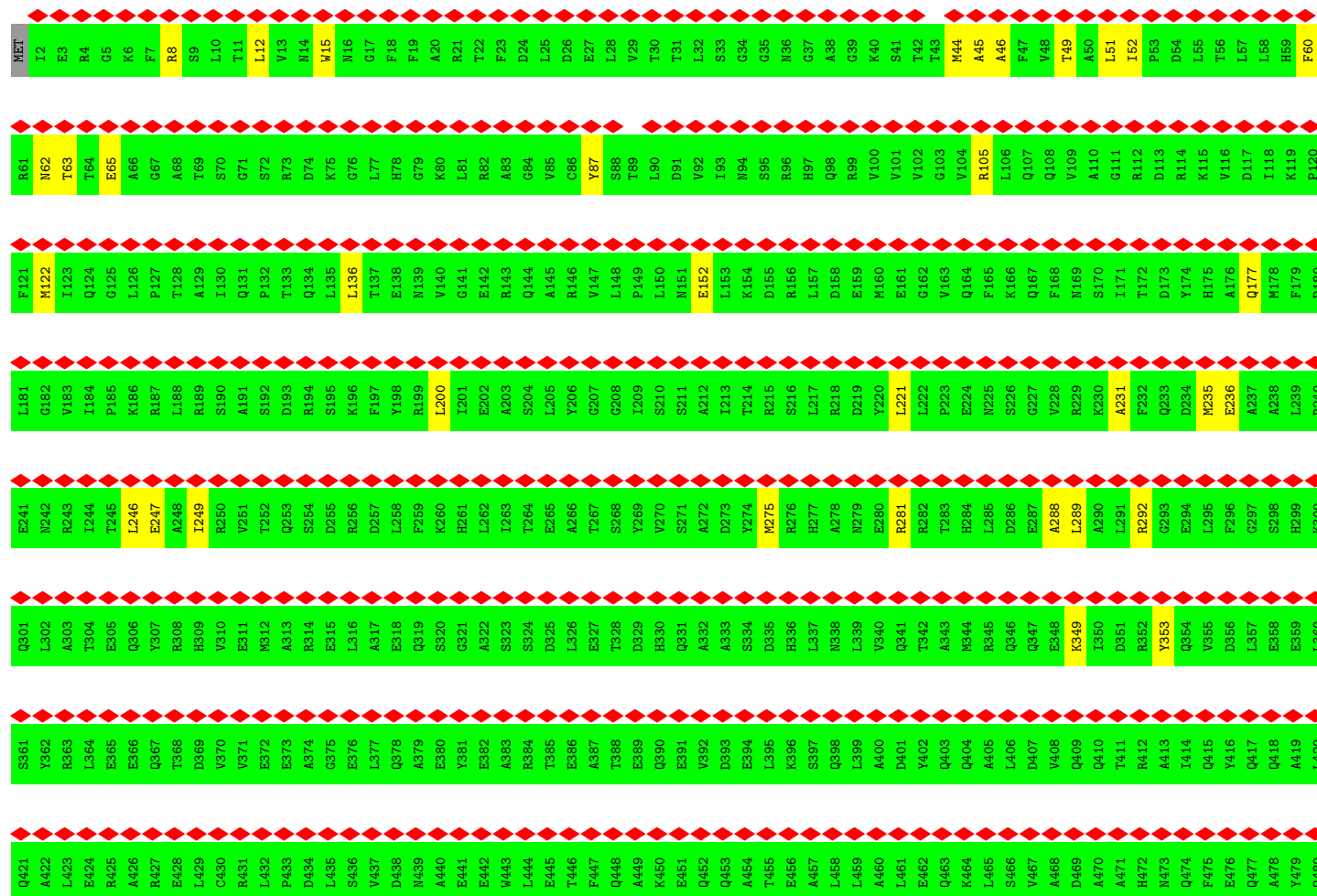
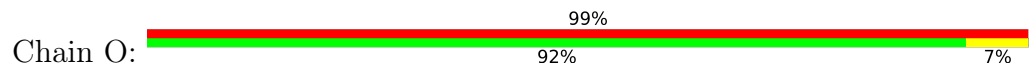


• Molecule 1: Chromosome partition protein MukB



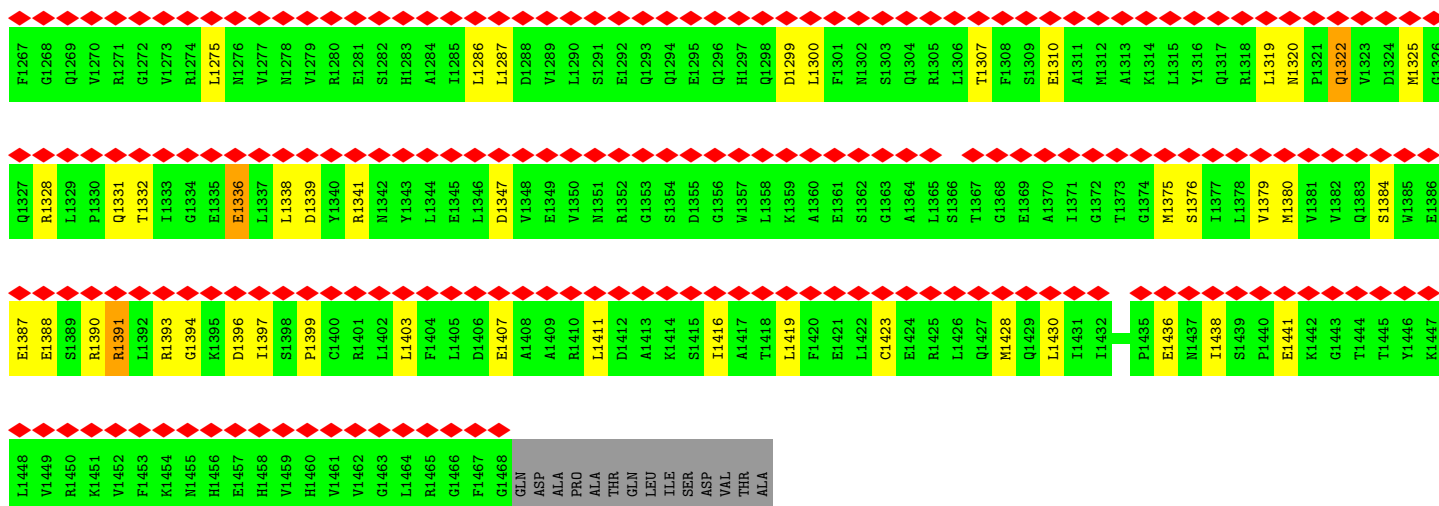


• Molecule 1: Chromosome partition protein MukB

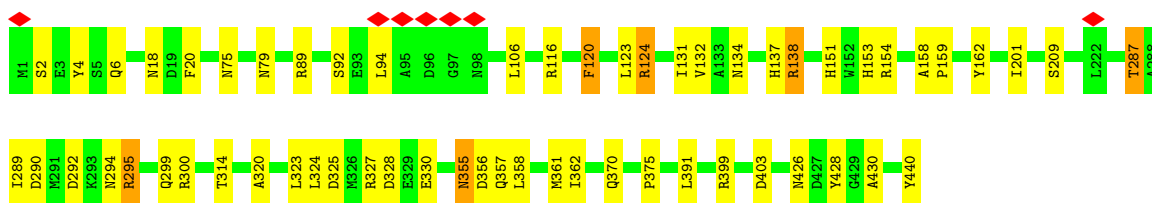
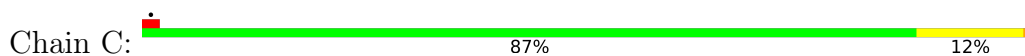


L481	E541	A601	E661	R721	A781	L841	E901	V961	L1021	Q1081	M141	D1201
V482	F642	P602	R662	P722	A782	R642	M902	E962	A1022	I1082	E1142	I1202
K483	C642	V603	L662	H723	R783	Q643	D903	I963	S1023	A1083	G1143	I1203
N484	K644	W604	S664	L724	E784	R644	E904	V964	L1024	F1084	G1144	R1204
I485	R645	L605	Q665	T725	M785	H645	Q905	Q965	K1025	C1085	A1145	T1205
V486	Q646	A606	P666	T726	R786	T646	Q906	R966	S1026	E1086	L1146	T1206
G487	G647	A607	S667	L727	L787	E647	E907	R967	S1027	A1087	R1147	D1207
E488	R648	Q608	Q668	E728	E788	L448	A908	V968	Y1028	E1088	S1148	P1208
T489	Q649	D609	A669	T729	A789	E649	A909	H969	E1029	M1089	M1149	V1209
S490	Y650	T610	E670	C730	L790	R650	R910	F970	T1030	E1090	S1150	D1210
R491	Q651	L611	D671	F731	M791	E651	F911	S971	K1031	N1091	D1151	A1211
S492	A652	N612	S672	E732	L792	V652	L912	Y972	Q1032	V1092	K1152	I1212
E493	E653	Q613	R673	D733	E793	S653	Q913	S973	D1033	Q1093	A1153	E1213
A494	D654	L614	M674	L734	R794	R654	Q914	D974	M1034	K1094	L1154	Q1214
W495	L655	C615	I675	Y735	D795	F655	H915	S975	L1035	K1095	G1155	M1215
Q496	E656	E616	A676	L736	A796	E656	G916	A976	K1036	L1096	A1156	E1216
S497	A657	Q617	L677	I737	L797	D657	S917	G977	E1037	R1097	L1157	I1217
A498	L658	S618	A678	E738	A798	Q658	A918	M978	L1038	K1098	R1158	E1218
R499	Q659	G619	E679	G739	E799	T659	L919	L979	L1039	L1099	L1159	L1219
E500	N660	E620	R680	D740	R800	Q660	T920	S980	Q1040	E1100	A1160	A1220
L501	E661	T621	F681	F741	Y601	Q661	K921	E981	E1041	R1101	V1161	R1221
S502	L662	L622	G682	Q742	A602	Q662	L922	N982	M1042	D1102	A1162	L1222
R503	E663	A623	G683	S743	T903	R663	E923	A983	K1043	Y1103	D1163	T1223
D504	A664	S624	V684	F744	L804	Q664	P924	D984	D1044	Y1104	M1164	E1224
W505	R665	S625	L686	D745	S905	Q665	M925	L985	I1045	Q1105	E1165	E1225
P506	Q666	N626	I686	T746	F906	Y666	V926	N986	G1046	I1106	H1166	L1226
S507	E667	D627	S687	S747	D607	A667	A927	D987	V1047	R1107	L1167	T1227
Q508	A668	V628	E688	V748	V608	Q668	V928	K988	Q1048	E1108	R1168	A1228
R509	L669	T629	I689	F749	Q909	A669	L929	L989	A1049	Q1109	D1169	R1229
H510	S670	E630	Y690	N750	K810	K670	Q930	R990	D1050	V1110	A1170	E1230
L511	L671	Y631	D691	A751	I811	E671	S931	Q991	A1051	V1111	L1171	Q1231
A512	S672	M632	D692	E752	Q812	S672	D932	R992	M1052	S1112	R1172	K1232
D513	V673	Q633	I693	E753	R813	L873	P933	E993	A1053	A1113	L1173	L1233
R514	N674	Q634	T694	Q754	A814	T674	Q934	E994	E1054	K1114	S1174	A1234
V515	E675	L635	I695	T755	H815	T675	Q935	H995	M1055	A1115	E1175	I1235
Q516	G576	L636	D696	N756	Q816	L876	H936	A996	L1056	G1116	D1176	S1236
P517	E677	E637	D697	A757	A917	N677	E937	E997	A1057	W1117	P1177	S1237
L518	S678	R638	A698	V758	F818	R678	Q938	S998	R1058	C1118	K1178	K1238
R519	R679	E639	P699	L759	S819	L879	L939	D999	E1059	A1119	R1179	S1239
M520	R680	R640	Y700	V760	Q820	T880	Q940	R1000	R1060	V1120	P1180	V1240
E521	M681	E641	F701	K761	F821	P681	Q941	S1001	R1061	M1121	E1181	A1241
L522	E682	A642	S702	S762	V822	Q682	D942	R1002	D1062	R1122	R1182	N1242
S523	M683	T643	A703	S763	G823	V683	Y943	A1003	R1063	M1123	K1183	I1243
E524	R684	V644	L704	D764	K824	T684	E944	R1004	L1064	V1124	L1184	T1244
L525	Q685	E645	Y705	R765	H825	L885	T945	E1005	H1065	K1125	Q1185	R1245
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Q527	L687	D647	P707	W767	S827	L867	K947	L1007	A1067	N1127	F1187	T1247
R528	E688	E648	A708	R768	V828	D688	H948	R1008	L1068	G1128	I1188	T1248
L529	Q689	V649	R709	Y769	A829	E689	S949	Q1009	S1069	V1129	A1189	Q1249
N530	E690	A650	H710	S770	F830	T690	Q950	Q1010	V1070	E1130	V1190	R1250
M531	K591	A651	G711	R771	D831	L691	H951	Q1011	M1071	R1131	Y1191	E1251
Q532	Q592	Q652	I712	Y772	T832	T892	Q952	A1012	R1072	Q1132	Q1192	Q1252
E533	K593	K653	V713	F773	D833	D693	A953	Q1013	S1073	L1133	H1193	N1253
N534	I594	R654	V714	E774	P834	R694	K954	Y1014	R1074	H1134	L1194	R1254
A535	Q595	E655	F715	L775	E635	V695	Q955	S1015	V1075	R1135	R1195	I1255
E536	S596	L656	D716	P776	A836	E696	Q956	Q1016	N1076	R1136	E1196	R1256
R537	L597	E657	L717	L777	E637	E697	A957	F1017	Q1077	E1137	L1197	M1257
L538	T598	K658	S718	F778	I838	V698	F958	L1018	L1078	L1138	I1198	L1258
L539	A599	Q659	L719	G779	R639	R699	A959	Q1019	E1079	A1139	R1199	N1259
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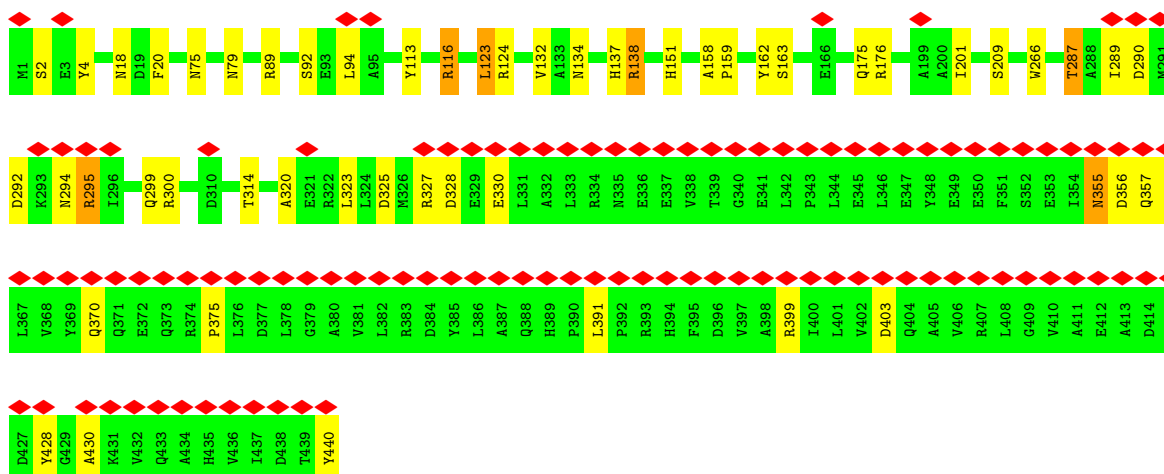
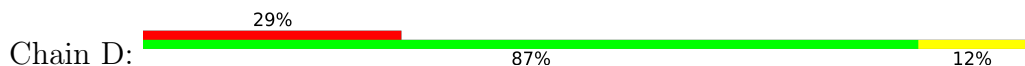
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V1209	E1086	S1026	R966	Q906	T646	R786	T726	P666	A06	Q646	V486
D1210	A1087	S1027	R967	E907	E647	L787	L727	G667	A607	G647	G487
I1211	E1088	E1028	H968	A908	L848	E788	E728	G668	Q608	E488	E488
A1212	M1089	E1029	H969	A909	E649	A789	E729	Q669	D609	Q549	T489
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Q1214	N1091	K1031	S971	F911	E651	N791	P731	D671	L611	Q651	R491
M1215	V1092	Q1032	S972	L912	V652	L792	E732	S672	N612	A552	S492
A1216	Q1093	D1033	S973	Q913	S653	E793	D733	R673	Q613	E553	E493
I1217	K1094	M1034	D974	Q914	R654	R794	L734	M674	L614	D554	A494
E1218	K1095	L1035	S975	H915	F655	D795	V735	I675	C615	L555	V495
E1219	L1096	K1036	A976	G916	E656	A796	L736	A676	E616	E556	Q496
L1220	R1097	E1037	G977	S917	D657	L797	L737	A677	Q617	A557	Q497
R1221	K1098	L1038	M978	A918	Q658	A798	E738	A678	S618	L558	A498
L1222	L1099	L1039	L979	L919	T659	E799	G739	E679	G619	Q559	R499
E1223	E1100	Q1040	S980	T920	Q660	R600	D740	R680	E620	N560	E500
E1224	R1101	E1041	E981	K921	Q661	Y601	P741	F681	T621	E561	L501
E1225	D1102	M1042	N982	L922	Q662	A902	Q742	G682	L622	L562	L502
L1226	Y1103	K1043	A983	E923	R663	T903	S743	G683	A623	E563	R503
T1227	Y1104	D1044	D984	P924	Q664	L904	F744	V684	S624	A564	D504
E1228	Q1105	L1045	L985	M925	Q665	S905	D745	L685	S625	R565	W505
R1229	I1106	G1046	N986	V926	Y666	F906	D746	L686	N626	Q566	P506
E1230	R1107	V1047	D987	A927	A667	D907	S747	S687	D627	E567	S507
Q1231	E1108	Q1048	K988	V928	Q668	V908	V748	E688	V628	A568	Q508
L1232	L1109	A1049	L989	L929	A669	Q909	F749	E689	T629	L569	R509
A1234	V1110	D1050	R990	Q930	K670	K910	N750	Y690	E630	S570	H510
I1235	V1111	A1051	Q991	S931	E671	E611	A751	D691	Y631	L571	L511
S1236	S1112	M1052	R992	D932	S672	Q612	E752	D692	M632	S572	A512
S1237	A1113	A1053	L993	P933	L673	A914	Q754	I693	Q633	V573	D513
S1238	K1114	E1054	E994	Q934	T674	L615	T755	T694	Q634	N574	R514
E1239	A1115	M1055	H995	Q935	T675	H815	T756	I695	L635	E575	V515
V1240	G1116	R1056	A996	H936	L676	Q616	N756	D696	L636	G576	Q516
A1241	W1117	A1057	E997	E937	N677	A617	A757	D697	E637	G577	P517
I1242	C1118	R1058	S998	Q938	R678	F918	V758	A698	R638	E578	L518
T1243	A1119	E1059	D999	L939	L679	S919	L759	P699	E639	R579	R519
E1244	V1120	R1060	R1000	Q940	I680	Q920	V760	Y700	R640	M520	M520
R1245	M1121	R1061	S1001	Q941	P681	F921	K761	F701	E641	M581	R521
L1246	R1122	D1062	R1002	D942	Q682	V622	S762	S702	A642	E582	L522
T1247	M1123	R1063	A1003	Y943	V683	G823	S763	A703	T643	M583	S523
I1248	V1124	L1064	R1004	E944	T684	K924	D764	L704	V644	Q584	E524
E1249	K1125	H1065	E1005	T945	L685	H825	R765	V705	E645	Q585	L525
R1250	D1126	E1066	Q1006	A946	L686	L626	Q766	G706	R646	E586	E526
E1251	M1127	A1067	L1007	K947	L687	S927	V767	P707	D647	L587	Q527
Q1252	G1128	L1068	R1008	H948	D688	V628	R768	A708	E648	E588	R528
N1253	V1129	S1069	Q1009	S949	E689	A629	V769	R709	V649	Q589	L529
R1254	R1130	V1070	Q1010	Q950	T690	F930	S770	H710	A650	L590	N530
I1255	R1131	M1071	Q1011	H951	L691	D831	T771	G711	A651	K591	N531
E1256	R1132	L1072	A1012	Q952	I692	T932	Y772	I712	Q652	Q592	Q532
M1257	L1133	S1073	Q1013	A953	D693	D833	P773	V713	K593	K593	Q533
L1258	H1134	R1074	Y1014	K954	R694	P634	E774	V714	R654	L594	N534
N1259	R1135	V1075	S1015	Q955	V695	E635	L775	P715	E655	Q595	A535
E1260	R1136	Q1076	Q1016	Q956	E696	A636	F776	D716	L656	S596	E536
G1261	E1137	L1077	F1017	A957	E697	E637	L777	L717	E657	L597	R537
L1262	L1138	L1078	N1018	F958	V698	I638	F778	S718	K658	T598	L538
Q1263	A1139	E1079	Q1019	A959	R699	R639	G779	L719	Q659	A599	L539
A1264	Y1140	K1080	V1020	L960	E900	E940	R780	V720	I660	R600	S540
V1265	M1141	Q1081	L1021	E961	E901	L841	A781	R721	E661	A601	E541
S1266	G1143	I1082	A1022	E962	M902	R642	A782	P722	R662	P602	F542
											C543



• Molecule 2: Chromosome partition protein MukF

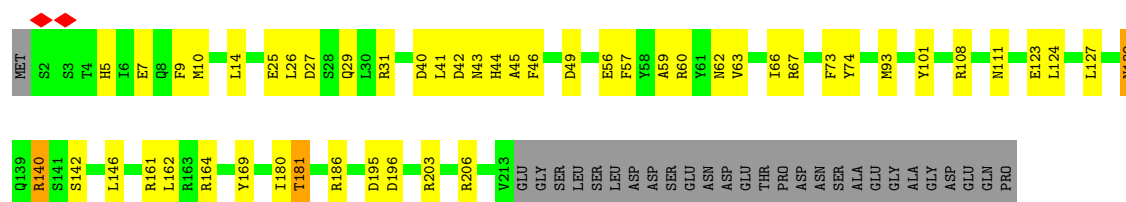


• Molecule 2: Chromosome partition protein MukF

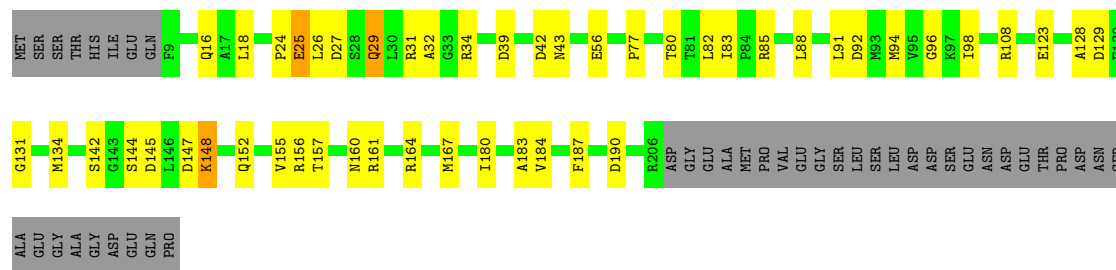


• Molecule 3: Chromosome partition protein MukE

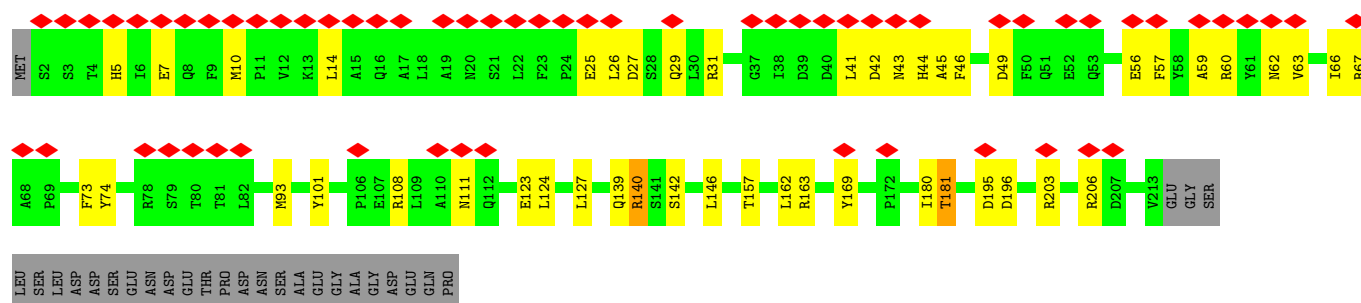




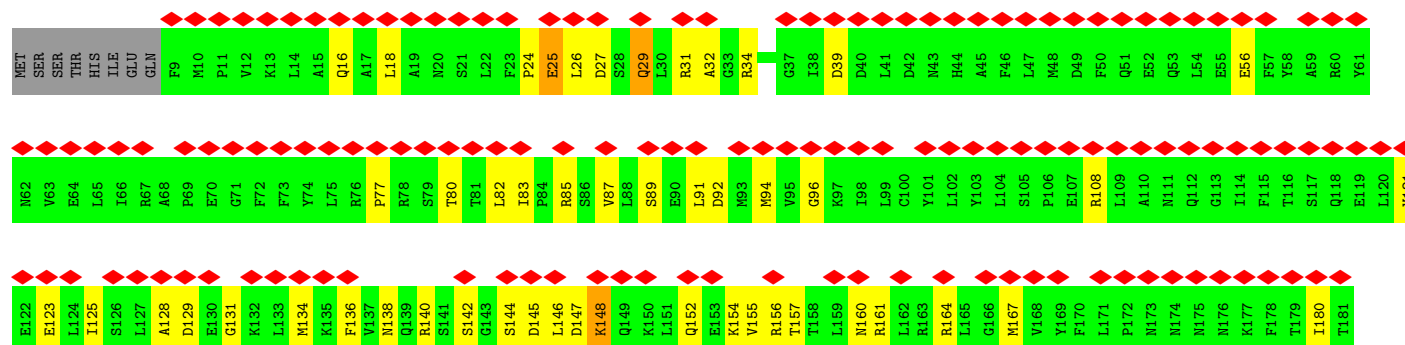
• Molecule 3: Chromosome partition protein MukE



• Molecule 3: Chromosome partition protein MukE



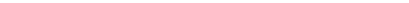
• Molecule 3: Chromosome partition protein MukE





[illegible]

- Molecule 6: pFB526

Chain L:  97%

[illegible]





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 (Å)	720.7206, 720.7206, 720.7206	wwPDB
Map dimensions	166, 166, 166	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: ATP, 4HH, MG

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	0.53	2/11999 (0.0%)	0.98	5/16166 (0.0%)
1	B	1.09	64/11999 (0.5%)	1.35	147/16166 (0.9%)
1	O	0.53	2/11999 (0.0%)	0.98	5/16166 (0.0%)
1	P	1.14	63/11999 (0.5%)	1.39	165/16166 (1.0%)
2	C	0.83	2/3592 (0.1%)	1.31	23/4862 (0.5%)
2	D	0.84	2/3592 (0.1%)	1.31	22/4862 (0.5%)
3	E	1.50	19/1753 (1.1%)	1.71	45/2361 (1.9%)
3	F	1.64	24/1648 (1.5%)	1.68	50/2218 (2.3%)
3	Q	1.50	19/1753 (1.1%)	1.70	43/2361 (1.8%)
3	R	1.63	23/1648 (1.4%)	1.68	57/2218 (2.6%)
4	G	0.13	0/558	0.28	0/754
4	I	0.13	0/558	0.27	0/754
4	M	0.14	0/558	0.27	0/754
4	S	0.13	0/558	0.28	0/754
5	K	0.69	0/1680	1.66	16/2589 (0.6%)
6	L	0.70	0/1676	1.60	11/2586 (0.4%)
All	All	0.94	220/67570 (0.3%)	1.27	589/91737 (0.6%)

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 (220) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	295	ARG	C-N	-24.37	1.03	1.33
2	D	295	ARG	C-N	-24.30	1.03	1.33
1	A	589	GLN	C-N	13.59	1.51	1.33
1	O	589	GLN	C-N	13.52	1.51	1.33
3	E	44	HIS	CE1-NE2	-8.96	1.23	1.32
3	Q	44	HIS	CE1-NE2	-8.90	1.23	1.32
1	B	1166	HIS	CE1-NE2	-8.86	1.23	1.32
1	B	1193	HIS	CE1-NE2	-8.86	1.23	1.32
1	P	1193	HIS	CE1-NE2	-8.84	1.23	1.32
1	P	1166	HIS	CE1-NE2	-8.82	1.23	1.32
1	B	175	HIS	CE1-NE2	-8.79	1.23	1.32
1	B	1193	HIS	CD2-NE2	-8.02	1.29	1.37
3	Q	44	HIS	CD2-NE2	-8.00	1.29	1.37
1	P	1166	HIS	CD2-NE2	-7.97	1.29	1.37
1	P	1193	HIS	CD2-NE2	-7.95	1.29	1.37
1	B	175	HIS	CD2-NE2	-7.93	1.29	1.37
1	B	1166	HIS	CD2-NE2	-7.93	1.29	1.37
3	E	44	HIS	CD2-NE2	-7.85	1.29	1.37
3	R	85	ARG	CZ-NH2	-7.79	1.23	1.33
1	P	1341	ARG	CZ-NH2	-7.77	1.23	1.33
1	P	1250	ARG	CZ-NH2	-7.74	1.23	1.33
1	P	1393	ARG	CZ-NH2	-7.72	1.23	1.33
1	P	1245	ARG	CZ-NH2	-7.72	1.23	1.33
3	Q	203	ARG	CZ-NH2	-7.71	1.23	1.33
1	B	1131	ARG	CZ-NH2	-7.71	1.23	1.33
1	P	96	ARG	CZ-NH2	-7.71	1.23	1.33
3	R	34	ARG	CZ-NH2	-7.69	1.23	1.33
1	P	1131	ARG	CZ-NH2	-7.68	1.23	1.33
3	R	161	ARG	CZ-NH2	-7.68	1.23	1.33
1	P	199	ARG	CZ-NH2	-7.67	1.23	1.33
3	E	206	ARG	CZ-NH2	-7.67	1.23	1.33
3	R	156	ARG	CZ-NH2	-7.67	1.23	1.33
1	P	1328	ARG	CZ-NH2	-7.66	1.23	1.33
3	F	31	ARG	CZ-NH2	-7.64	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	206	ARG	CZ-NH2	-7.63	1.23	1.33
1	P	1093	GLN	C-N	7.63	1.44	1.33
1	B	1221	ARG	CZ-NH2	-7.62	1.23	1.33
3	E	31	ARG	CZ-NH2	-7.62	1.23	1.33
1	P	1132	ARG	CZ-NH2	-7.61	1.23	1.33
1	P	1254	ARG	CZ-NH2	-7.61	1.23	1.33
1	B	1197	ARG	CZ-NH2	-7.58	1.23	1.33
3	R	31	ARG	CZ-NH2	-7.56	1.23	1.33
1	B	1199	ARG	CZ-NH2	-7.55	1.23	1.33
1	B	240	ARG	CZ-NH2	-7.55	1.23	1.33
1	P	1221	ARG	CZ-NH2	-7.55	1.23	1.33
1	P	1197	ARG	CZ-NH2	-7.54	1.23	1.33
3	Q	31	ARG	CZ-NH2	-7.54	1.23	1.33
1	B	1093	GLN	C-N	7.53	1.44	1.33
3	E	203	ARG	CZ-NH2	-7.53	1.23	1.33
1	B	1132	ARG	CZ-NH2	-7.53	1.23	1.33
1	B	250	ARG	CZ-NH2	-7.49	1.23	1.33
1	P	1199	ARG	CZ-NH2	-7.48	1.23	1.33
3	F	164	ARG	CZ-NH2	-7.48	1.23	1.33
1	P	240	ARG	CZ-NH2	-7.47	1.23	1.33
3	E	67	ARG	CZ-NH2	-7.45	1.23	1.33
3	Q	67	ARG	CZ-NH2	-7.45	1.23	1.33
1	B	199	ARG	CZ-NH2	-7.45	1.23	1.33
1	P	250	ARG	CZ-NH2	-7.44	1.23	1.33
3	R	164	ARG	CZ-NH2	-7.44	1.23	1.33
1	B	243	ARG	CZ-NH2	-7.42	1.23	1.33
3	F	85	ARG	CZ-NH2	-7.42	1.23	1.33
1	B	1328	ARG	CZ-NH2	-7.40	1.23	1.33
1	B	1393	ARG	CZ-NH2	-7.40	1.23	1.33
1	P	243	ARG	CZ-NH2	-7.38	1.23	1.33
1	B	229	ARG	CZ-NH2	-7.38	1.23	1.33
3	F	34	ARG	CZ-NH2	-7.38	1.23	1.33
3	F	161	ARG	CZ-NH2	-7.36	1.23	1.33
3	Q	60	ARG	CZ-NH2	-7.35	1.23	1.33
1	B	105	ARG	CZ-NH2	-7.33	1.24	1.33
3	E	60	ARG	CZ-NH2	-7.33	1.24	1.33
1	B	1250	ARG	CZ-NH2	-7.32	1.24	1.33
1	B	96	ARG	CZ-NH2	-7.30	1.24	1.33
3	F	156	ARG	CZ-NH2	-7.29	1.24	1.33
1	P	301	GLN	C-N	7.25	1.44	1.34
1	B	1390	ARG	CZ-NH2	-7.22	1.24	1.33
1	B	301	GLN	C-N	7.10	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	1394	GLY	N-CA	-6.80	1.37	1.45
1	B	1394	GLY	N-CA	-6.71	1.37	1.45
1	P	1189	ALA	CA-CB	-6.66	1.43	1.53
1	P	231	ALA	CA-CB	-6.62	1.43	1.53
1	B	1189	ALA	CA-CB	-6.61	1.43	1.53
1	P	248	ALA	CA-CB	-6.58	1.43	1.53
1	A	847	GLU	C-N	6.55	1.42	1.33
1	B	248	ALA	CA-CB	-6.54	1.43	1.53
1	P	237	ALA	CA-CB	-6.50	1.43	1.53
1	O	847	GLU	C-N	6.47	1.42	1.33
1	P	103	GLY	N-CA	-6.40	1.38	1.45
1	P	50	ALA	CA-CB	-6.34	1.43	1.53
3	E	45	ALA	CA-CB	-6.30	1.43	1.53
1	B	103	GLY	N-CA	-6.30	1.38	1.45
3	Q	45	ALA	CA-CB	-6.29	1.43	1.53
3	R	34	ARG	CZ-NH1	-6.29	1.24	1.32
1	P	1250	ARG	CZ-NH1	-6.29	1.24	1.32
1	B	231	ALA	CA-CB	-6.28	1.43	1.53
3	R	161	ARG	CZ-NH1	-6.28	1.24	1.32
1	P	1241	ALA	CA-CB	-6.28	1.43	1.53
1	P	1341	ARG	CZ-NH1	-6.25	1.24	1.32
1	P	1393	ARG	CZ-NH1	-6.25	1.24	1.32
2	C	320	ALA	CA-CB	-6.24	1.43	1.53
1	P	96	ARG	CZ-NH1	-6.23	1.24	1.32
1	B	250	ARG	CZ-NH1	-6.22	1.24	1.32
3	R	156	ARG	CZ-NH1	-6.21	1.24	1.32
1	P	1254	ARG	CZ-NH1	-6.21	1.24	1.32
1	P	1328	ARG	CZ-NH1	-6.21	1.24	1.32
2	D	320	ALA	CA-CB	-6.20	1.43	1.53
1	P	250	ARG	CZ-NH1	-6.16	1.24	1.32
1	B	191	ALA	CA-CB	-6.16	1.43	1.53
1	P	1245	ARG	CZ-NH1	-6.16	1.24	1.32
3	Q	67	ARG	CZ-NH1	-6.13	1.24	1.32
3	Q	31	ARG	CZ-NH1	-6.12	1.24	1.32
1	P	199	ARG	CZ-NH1	-6.11	1.24	1.32
1	B	1199	ARG	CZ-NH1	-6.11	1.24	1.32
3	E	67	ARG	CZ-NH1	-6.10	1.24	1.32
3	R	131	GLY	N-CA	-6.09	1.38	1.45
3	E	31	ARG	CZ-NH1	-6.09	1.24	1.32
3	E	203	ARG	CZ-NH1	-6.09	1.24	1.32
1	B	240	ARG	CZ-NH1	-6.08	1.24	1.32
3	R	31	ARG	CZ-NH1	-6.08	1.24	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	203	ARG	CZ-NH1	-6.08	1.24	1.32
3	E	206	ARG	CZ-NH1	-6.07	1.24	1.32
1	P	240	ARG	CZ-NH1	-6.07	1.24	1.32
3	R	164	ARG	CZ-NH1	-6.06	1.24	1.32
3	F	31	ARG	CZ-NH1	-6.06	1.24	1.32
3	F	164	ARG	CZ-NH1	-6.06	1.24	1.32
1	P	1199	ARG	CZ-NH1	-6.06	1.24	1.32
1	B	105	ARG	CZ-NH1	-6.05	1.24	1.32
1	P	243	ARG	CZ-NH1	-6.04	1.24	1.32
3	Q	206	ARG	CZ-NH1	-6.03	1.24	1.32
1	B	50	ALA	CA-CB	-6.03	1.43	1.53
1	B	243	ARG	CZ-NH1	-6.01	1.24	1.32
3	R	96	GLY	N-CA	-6.00	1.38	1.45
3	F	128	ALA	CA-CB	-6.00	1.43	1.53
1	B	1211	ALA	CA-CB	-5.99	1.43	1.53
1	B	1221	ARG	CZ-NH1	-5.99	1.24	1.32
1	P	1211	ALA	CA-CB	-5.98	1.43	1.53
3	R	85	ARG	CZ-NH1	-5.98	1.24	1.32
3	E	60	ARG	CZ-NH1	-5.97	1.24	1.32
3	F	34	ARG	CZ-NH1	-5.96	1.24	1.32
1	B	1132	ARG	CZ-NH1	-5.96	1.24	1.32
1	P	1132	ARG	CZ-NH1	-5.93	1.24	1.32
3	Q	60	ARG	CZ-NH1	-5.93	1.24	1.32
1	P	1131	ARG	CZ-NH1	-5.92	1.24	1.32
1	B	1131	ARG	CZ-NH1	-5.92	1.24	1.32
1	P	1197	ARG	CZ-NH1	-5.91	1.24	1.32
1	P	1221	ARG	CZ-NH1	-5.91	1.24	1.32
3	F	96	GLY	N-CA	-5.91	1.38	1.45
1	B	96	ARG	CZ-NH1	-5.91	1.24	1.32
3	Q	59	ALA	CA-CB	-5.88	1.43	1.53
1	B	1328	ARG	CZ-NH1	-5.86	1.24	1.32
1	B	229	ARG	CZ-NH1	-5.86	1.24	1.32
3	F	156	ARG	CZ-NH1	-5.84	1.24	1.32
1	P	227	GLY	N-CA	-5.83	1.38	1.45
3	F	85	ARG	CZ-NH1	-5.83	1.24	1.32
1	B	1250	ARG	CZ-NH1	-5.81	1.24	1.32
1	B	199	ARG	CZ-NH1	-5.80	1.24	1.32
1	B	1197	ARG	CZ-NH1	-5.79	1.24	1.32
3	F	161	ARG	CZ-NH1	-5.77	1.24	1.32
1	B	1393	ARG	CZ-NH1	-5.77	1.24	1.32
3	F	131	GLY	N-CA	-5.77	1.38	1.45
1	B	227	GLY	N-CA	-5.76	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	83	ILE	N-CA	-5.76	1.42	1.46
3	E	59	ALA	CA-CB	-5.75	1.43	1.53
3	F	83	ILE	N-CA	-5.74	1.42	1.46
3	R	32	ALA	CA-CB	-5.73	1.43	1.53
1	B	1390	ARG	CZ-NH1	-5.72	1.24	1.32
3	F	32	ALA	CA-CB	-5.66	1.43	1.53
3	R	85	ARG	CD-NE	-5.56	1.38	1.46
1	P	199	ARG	CD-NE	-5.55	1.38	1.46
1	P	1245	ARG	CD-NE	-5.51	1.38	1.46
1	B	199	ARG	CD-NE	-5.51	1.38	1.46
1	P	223	PRO	CA-CB	-5.47	1.46	1.53
1	P	240	ARG	CD-NE	-5.44	1.38	1.46
1	B	240	ARG	CD-NE	-5.42	1.38	1.46
1	P	1254	ARG	CD-NE	-5.42	1.38	1.46
3	F	85	ARG	CD-NE	-5.40	1.38	1.46
3	R	34	ARG	CD-NE	-5.36	1.38	1.46
1	P	1250	ARG	CD-NE	-5.35	1.38	1.46
3	R	161	ARG	CD-NE	-5.34	1.38	1.46
3	Q	203	ARG	CD-NE	-5.32	1.38	1.46
1	B	223	PRO	CA-CB	-5.32	1.46	1.53
1	B	1132	ARG	CD-NE	-5.31	1.38	1.46
1	P	250	ARG	CD-NE	-5.31	1.38	1.46
1	P	1132	ARG	CD-NE	-5.31	1.38	1.46
3	R	142	SER	CA-CB	-5.30	1.45	1.52
3	E	203	ARG	CD-NE	-5.29	1.38	1.46
3	F	34	ARG	CD-NE	-5.29	1.38	1.46
1	B	1199	ARG	CD-NE	-5.27	1.38	1.46
3	R	77	PRO	CA-CB	-5.25	1.47	1.53
3	Q	60	ARG	CD-NE	-5.25	1.39	1.46
3	R	164	ARG	CD-NE	-5.24	1.39	1.46
1	P	1341	ARG	CD-NE	-5.23	1.39	1.46
1	P	1199	ARG	CD-NE	-5.22	1.39	1.46
1	B	250	ARG	CD-NE	-5.20	1.39	1.46
1	P	243	ARG	CD-NE	-5.18	1.39	1.46
1	P	1393	ARG	CD-NE	-5.18	1.39	1.46
3	F	164	ARG	CD-NE	-5.17	1.39	1.46
1	B	1221	ARG	CD-NE	-5.16	1.39	1.46
3	F	161	ARG	CD-NE	-5.16	1.39	1.46
1	P	96	ARG	CD-NE	-5.15	1.39	1.46
1	B	1390	ARG	CD-NE	-5.14	1.39	1.46
3	E	60	ARG	CD-NE	-5.13	1.39	1.46
3	E	67	ARG	CD-NE	-5.13	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	105	ARG	CD-NE	-5.13	1.39	1.46
1	B	1393	ARG	CD-NE	-5.13	1.39	1.46
1	B	96	ARG	CD-NE	-5.13	1.39	1.46
3	F	31	ARG	CD-NE	-5.11	1.39	1.46
1	P	1221	ARG	CD-NE	-5.09	1.39	1.46
3	Q	31	ARG	CD-NE	-5.09	1.39	1.46
3	Q	67	ARG	CD-NE	-5.09	1.39	1.46
1	B	243	ARG	CD-NE	-5.08	1.39	1.46
3	R	31	ARG	CD-NE	-5.08	1.39	1.46
1	B	1250	ARG	CD-NE	-5.08	1.39	1.46
3	F	142	SER	CA-CB	-5.07	1.46	1.52
1	B	229	ARG	CD-NE	-5.07	1.39	1.46
3	Q	206	ARG	CD-NE	-5.06	1.39	1.46
3	E	31	ARG	CD-NE	-5.06	1.39	1.46
1	B	1131	ARG	CD-NE	-5.05	1.39	1.46
1	P	1131	ARG	CD-NE	-5.05	1.39	1.46
3	F	77	PRO	CA-CB	-5.04	1.47	1.53
3	E	206	ARG	CD-NE	-5.03	1.39	1.46

All (589) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	295	ARG	CA-C-N	22.15	147.90	120.88
2	C	295	ARG	C-N-CA	22.15	147.90	120.88
2	D	295	ARG	CA-C-N	22.04	147.77	120.88
2	D	295	ARG	C-N-CA	22.04	147.77	120.88
1	O	589	GLN	O-C-N	10.01	132.38	122.07
1	A	589	GLN	O-C-N	9.99	132.35	122.07
3	R	82	LEU	CA-C-N	9.46	129.40	122.59
3	R	82	LEU	C-N-CA	9.46	129.40	122.59
3	F	82	LEU	CA-C-N	9.42	129.37	122.59
3	F	82	LEU	C-N-CA	9.42	129.37	122.59
1	P	469	ASP	CA-CB-CG	8.88	121.48	112.60
1	B	469	ASP	CA-CB-CG	8.79	121.39	112.60
1	B	1127	ASN	CA-CB-CG	8.41	121.01	112.60
1	P	1127	ASN	CA-CB-CG	8.38	120.98	112.60
1	A	589	GLN	CA-C-N	-7.85	109.63	120.38
1	A	589	GLN	C-N-CA	-7.85	109.63	120.38
1	B	259	PHE	CA-CB-CG	7.84	121.64	113.80
1	O	589	GLN	CA-C-N	-7.83	109.66	120.38
1	O	589	GLN	C-N-CA	-7.83	109.66	120.38
1	P	259	PHE	CA-CB-CG	7.81	121.61	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	63	DG	C4'-C3'-O3'	7.72	121.58	110.00
2	C	120	PHE	CA-CB-CG	-7.54	106.26	113.80
1	P	187	ARG	NE-CZ-NH2	7.50	125.95	119.20
1	P	232	PHE	CA-CB-CG	7.44	121.24	113.80
1	B	232	PHE	CA-CB-CG	7.20	121.00	113.80
5	K	47	DC	O3'-P-O5'	-7.19	93.22	104.00
5	K	64	DG	O5'-C5'-C4'	7.05	121.37	110.80
2	D	294	ASN	N-CA-C	-7.04	103.65	111.82
2	C	294	ASN	N-CA-C	-7.00	103.70	111.82
3	R	160	ASN	CA-CB-CG	6.92	119.52	112.60
3	R	89	SER	CA-C-N	6.91	129.87	120.54
3	R	89	SER	C-N-CA	6.91	129.87	120.54
5	K	62	DT	C4'-C3'-O3'	-6.85	99.72	110.00
1	P	197	PHE	CA-CB-CG	6.81	120.61	113.80
1	P	219	ASP	CA-CB-CG	6.75	119.35	112.60
1	P	225	ASN	CA-CB-CG	6.74	119.34	112.60
1	P	301	GLN	O-C-N	-6.72	115.00	122.12
2	D	176	ARG	CB-CG-CD	6.71	126.74	111.30
3	F	160	ASN	CA-CB-CG	6.71	119.31	112.60
1	P	94	ASN	CA-CB-CG	6.70	119.30	112.60
1	P	1253	ASN	CA-CB-CG	6.68	119.28	112.60
3	R	187	PHE	CA-CB-CG	6.68	120.48	113.80
1	B	197	PHE	CA-CB-CG	6.67	120.47	113.80
1	B	301	GLN	O-C-N	-6.65	115.07	122.12
3	Q	44	HIS	CA-CB-CG	6.65	120.45	113.80
3	E	44	HIS	CA-CB-CG	6.64	120.44	113.80
1	P	158	ASP	CA-CB-CG	6.63	119.23	112.60
3	E	195	ASP	CA-CB-CG	6.60	119.20	112.60
1	B	225	ASN	CA-CB-CG	6.59	119.19	112.60
3	Q	195	ASP	CA-CB-CG	6.55	119.15	112.60
3	E	73	PHE	CA-CB-CG	6.54	120.34	113.80
1	P	1187	PHE	CA-CB-CG	6.51	120.31	113.80
1	P	54	ASP	CA-CB-CG	6.49	119.09	112.60
3	Q	73	PHE	CA-CB-CG	6.49	120.29	113.80
1	B	94	ASN	CA-CB-CG	6.48	119.08	112.60
1	B	1187	PHE	CA-CB-CG	6.48	120.28	113.80
5	K	64	DG	C5'-C4'-O4'	6.47	119.10	109.40
3	Q	43	ASN	CA-CB-CG	6.47	119.07	112.60
3	E	196	ASP	CA-CB-CG	6.47	119.07	112.60
1	P	1207	ASP	CA-CB-CG	6.47	119.07	112.60
3	Q	196	ASP	CA-CB-CG	6.47	119.07	112.60
3	F	187	PHE	CA-CB-CG	6.45	120.25	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	1164	ASN	CA-CB-CG	6.45	119.05	112.60
3	E	43	ASN	CA-CB-CG	6.43	119.03	112.60
1	B	1164	ASN	CA-CB-CG	6.43	119.03	112.60
1	B	966	ARG	NE-CZ-NH2	6.42	124.98	119.20
1	B	1207	ASP	CA-CB-CG	6.41	119.01	112.60
2	D	325	ASP	CA-CB-CG	6.39	118.99	112.60
6	L	43	DG	C2'-C3'-O3'	-6.38	101.93	111.50
1	B	175	HIS	CA-CB-CG	6.36	120.16	113.80
1	B	1210	ASP	CA-CB-CG	6.33	118.93	112.60
1	P	1201	ASP	N-CA-C	6.33	118.70	111.11
1	B	54	ASP	CA-CB-CG	6.32	118.92	112.60
1	P	1210	ASP	CA-CB-CG	6.32	118.92	112.60
1	P	966	ARG	NE-CZ-NH2	6.30	124.87	119.20
1	B	187	ARG	NE-CZ-NH2	6.30	124.87	119.20
1	B	1201	ASP	N-CA-C	6.30	118.67	111.11
1	B	1193	HIS	CA-CB-CG	6.29	120.09	113.80
1	B	255	ASP	CA-CB-CG	6.28	118.88	112.60
1	B	1131	ARG	CD-NE-CZ	6.28	133.19	124.40
1	P	1131	ARG	CD-NE-CZ	6.28	133.19	124.40
3	R	145	ASP	CA-CB-CG	6.26	118.86	112.60
1	P	1193	HIS	CA-CB-CG	6.25	120.05	113.80
1	P	234	ASP	CA-CB-CG	6.24	118.84	112.60
2	C	325	ASP	CA-CB-CG	6.23	118.83	112.60
1	B	97	HIS	CA-C-N	6.23	131.59	123.00
1	B	97	HIS	C-N-CA	6.23	131.59	123.00
1	P	168	PHE	CA-CB-CG	6.21	120.01	113.80
3	Q	57	PHE	CA-CB-CG	6.21	120.01	113.80
3	E	57	PHE	CA-CB-CG	6.21	120.01	113.80
1	P	255	ASP	CA-CB-CG	6.19	118.79	112.60
5	K	47	DC	C2'-C3'-O3'	-6.19	102.21	111.50
3	R	136	PHE	CA-CB-CG	6.18	119.98	113.80
5	K	46	DA	O3'-P-O5'	6.18	113.27	104.00
1	P	243	ARG	CA-CB-CG	6.17	126.44	114.10
1	P	1242	ASN	CA-CB-CG	6.17	118.77	112.60
1	B	243	ARG	CA-CB-CG	6.17	126.44	114.10
1	B	1132	ARG	CD-NE-CZ	6.15	133.01	124.40
1	B	1221	ARG	CD-NE-CZ	6.14	133.00	124.40
1	P	1221	ARG	CD-NE-CZ	6.14	132.99	124.40
1	B	164	GLN	CA-C-N	6.13	131.46	123.00
1	B	164	GLN	C-N-CA	6.13	131.46	123.00
1	B	234	ASP	CA-CB-CG	6.12	118.72	112.60
1	P	198	TYR	N-CA-CB	6.11	118.87	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	1132	ARG	CD-NE-CZ	6.10	132.94	124.40
1	P	97	HIS	CA-C-N	6.09	131.41	123.00
1	P	97	HIS	C-N-CA	6.09	131.41	123.00
1	P	1339	ASP	CA-CB-CG	6.08	118.68	112.60
3	E	62	ASN	CA-CB-CG	6.08	118.67	112.60
1	P	164	GLN	CA-C-N	6.08	131.38	123.00
1	P	164	GLN	C-N-CA	6.08	131.38	123.00
1	P	1328	ARG	CD-NE-CZ	6.07	132.90	124.40
1	P	1331	GLN	N-CA-C	6.07	123.73	110.80
1	P	201	ILE	N-CA-CB	6.07	117.65	110.55
1	P	243	ARG	CG-CD-NE	6.07	125.35	112.00
1	B	229	ARG	CD-NE-CZ	6.06	132.89	124.40
1	B	201	ILE	N-CA-CB	6.06	117.64	110.55
3	R	27	ASP	CA-CB-CG	6.05	118.66	112.60
1	B	1056	ARG	NE-CZ-NH2	6.05	124.65	119.20
1	B	1328	ARG	CD-NE-CZ	6.05	132.87	124.40
3	Q	62	ASN	CA-CB-CG	6.05	118.65	112.60
1	B	243	ARG	CG-CD-NE	6.04	125.30	112.00
3	R	147	ASP	CA-CB-CG	6.04	118.64	112.60
1	B	105	ARG	CD-NE-CZ	6.04	132.86	124.40
1	B	224	GLU	CA-C-N	6.03	131.50	123.00
1	B	224	GLU	C-N-CA	6.03	131.50	123.00
3	R	156	ARG	CD-NE-CZ	6.03	132.84	124.40
1	P	224	GLU	CA-C-N	6.02	131.48	123.00
1	P	224	GLU	C-N-CA	6.02	131.48	123.00
3	E	138	ASN	CA-CB-CG	6.00	118.61	112.60
1	B	198	TYR	N-CA-CB	6.00	118.71	110.01
3	F	145	ASP	CA-CB-CG	6.00	118.60	112.60
3	E	138	ASN	CB-CA-C	5.99	120.64	109.86
1	B	263	ILE	N-CA-CB	5.98	117.14	110.62
1	P	1056	ARG	NE-CZ-NH2	5.98	124.58	119.20
3	E	42	ASP	CA-C-N	5.97	128.21	120.44
3	E	42	ASP	C-N-CA	5.97	128.21	120.44
1	P	1341	ARG	CD-NE-CZ	5.97	132.76	124.40
1	P	118	ILE	CA-C-N	5.96	130.85	122.74
1	P	118	ILE	C-N-CA	5.96	130.85	122.74
3	F	156	ARG	CD-NE-CZ	5.96	132.75	124.40
3	Q	66	ILE	CA-C-N	5.96	131.78	123.07
3	Q	66	ILE	C-N-CA	5.96	131.78	123.07
1	P	263	ILE	N-CA-CB	5.96	117.12	110.62
3	Q	42	ASP	CA-C-N	5.96	128.19	120.44
3	Q	42	ASP	C-N-CA	5.96	128.19	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	96	ARG	CD-NE-CZ	5.96	132.74	124.40
3	Q	42	ASP	CA-CB-CG	5.95	118.55	112.60
1	P	103	GLY	N-CA-C	5.95	119.44	110.75
3	E	66	ILE	CA-C-N	5.95	131.75	123.07
3	E	66	ILE	C-N-CA	5.95	131.75	123.07
3	E	42	ASP	CA-CB-CG	5.95	118.55	112.60
1	B	122	MET	CA-C-N	5.94	131.25	122.99
1	B	122	MET	C-N-CA	5.94	131.25	122.99
3	F	27	ASP	CA-CB-CG	5.94	118.54	112.60
1	P	165	PHE	CA-CB-CG	5.93	119.73	113.80
1	B	96	ARG	CD-NE-CZ	5.93	132.70	124.40
1	B	118	ILE	CA-C-N	5.92	130.79	122.74
1	B	118	ILE	C-N-CA	5.92	130.79	122.74
3	E	60	ARG	CD-NE-CZ	5.92	132.68	124.40
3	Q	63	VAL	CA-C-N	5.92	130.29	122.30
3	Q	63	VAL	C-N-CA	5.92	130.29	122.30
1	P	122	MET	CA-C-N	5.91	131.21	122.99
1	P	122	MET	C-N-CA	5.91	131.21	122.99
1	P	1339	ASP	CA-C-N	5.91	128.20	120.28
1	P	1339	ASP	C-N-CA	5.91	128.20	120.28
3	Q	60	ARG	CD-NE-CZ	5.91	132.67	124.40
2	C	124	ARG	CA-CB-CG	5.91	125.92	114.10
3	R	31	ARG	CD-NE-CZ	5.91	132.67	124.40
1	P	1390	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	P	1244	ILE	N-CA-CB	5.90	117.45	110.55
1	P	1250	ARG	CD-NE-CZ	5.89	132.64	124.40
1	B	1339	ASP	CA-C-N	5.88	128.16	120.28
1	B	1339	ASP	C-N-CA	5.88	128.16	120.28
1	B	103	GLY	N-CA-C	5.87	119.16	110.42
3	E	63	VAL	CA-C-N	5.87	130.22	122.30
3	E	63	VAL	C-N-CA	5.87	130.22	122.30
5	K	32	DA	C5'-C4'-C3'	-5.87	106.10	114.90
3	F	31	ARG	CD-NE-CZ	5.86	132.61	124.40
1	B	1244	ILE	N-CA-CB	5.85	117.40	110.55
3	Q	31	ARG	CD-NE-CZ	5.85	132.59	124.40
6	L	30	DG	C4'-C3'-O3'	-5.84	101.24	110.00
1	B	548	ARG	CA-C-N	5.82	130.54	121.76
1	B	548	ARG	C-N-CA	5.82	130.54	121.76
6	L	47	DT	C5'-C4'-O4'	5.81	118.12	109.40
3	E	31	ARG	CD-NE-CZ	5.81	132.53	124.40
3	F	147	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	166	LYS	CA-C-N	5.80	131.18	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	LYS	C-N-CA	5.80	131.18	122.99
1	B	1395	LYS	CA-CB-CG	5.80	125.71	114.10
1	B	1192	GLN	CA-C-N	5.80	128.37	120.54
1	B	1192	GLN	C-N-CA	5.80	128.37	120.54
1	P	548	ARG	CA-C-N	5.80	130.52	121.76
1	P	548	ARG	C-N-CA	5.80	130.52	121.76
3	Q	74	TYR	CA-C-N	5.79	130.71	122.72
3	Q	74	TYR	C-N-CA	5.79	130.71	122.72
2	C	294	ASN	CA-C-N	5.79	130.79	122.40
2	C	294	ASN	C-N-CA	5.79	130.79	122.40
6	L	56	DT	O3'-P-O5'	-5.78	95.33	104.00
1	B	1250	ARG	CD-NE-CZ	5.78	132.49	124.40
1	B	235	MET	CA-C-N	5.77	127.94	120.44
1	B	235	MET	C-N-CA	5.77	127.94	120.44
3	Q	25	GLU	CA-C-N	5.77	127.94	120.44
3	Q	25	GLU	C-N-CA	5.77	127.94	120.44
3	E	25	GLU	CA-C-N	5.77	127.94	120.44
3	E	25	GLU	C-N-CA	5.77	127.94	120.44
3	R	92	ASP	CA-CB-CG	5.76	118.36	112.60
1	B	1197	ARG	CA-C-N	5.76	128.22	120.50
1	B	1197	ARG	C-N-CA	5.76	128.22	120.50
3	F	129	ASP	CA-C-N	5.76	127.99	120.28
3	F	129	ASP	C-N-CA	5.76	127.99	120.28
1	P	153	LEU	CA-C-N	5.75	127.92	120.44
1	P	153	LEU	C-N-CA	5.75	127.92	120.44
1	P	1197	ARG	CA-C-N	5.75	128.20	120.50
1	P	1197	ARG	C-N-CA	5.75	128.20	120.50
1	P	235	MET	CA-C-N	5.75	127.91	120.44
1	P	235	MET	C-N-CA	5.75	127.91	120.44
2	D	294	ASN	CA-C-N	5.74	130.73	122.40
2	D	294	ASN	C-N-CA	5.74	130.73	122.40
1	B	165	PHE	CA-CB-CG	5.73	119.53	113.80
1	P	1192	GLN	CA-C-N	5.72	128.26	120.54
1	P	1192	GLN	C-N-CA	5.72	128.26	120.54
3	E	27	ASP	CA-CB-CG	5.70	118.30	112.60
3	R	161	ARG	N-CA-CB	5.70	118.43	109.94
3	E	74	TYR	CA-C-N	5.70	130.58	122.72
3	E	74	TYR	C-N-CA	5.70	130.58	122.72
3	R	129	ASP	CA-C-N	5.69	127.90	120.28
3	R	129	ASP	C-N-CA	5.69	127.90	120.28
2	C	137	HIS	CB-CG-CD2	-5.68	123.82	131.20
1	B	100	VAL	CA-C-N	5.68	131.05	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	VAL	C-N-CA	5.68	131.05	123.10
3	Q	27	ASP	CA-CB-CG	5.68	118.28	112.60
1	B	103	GLY	CA-C-N	5.67	130.97	122.58
1	B	103	GLY	C-N-CA	5.67	130.97	122.58
3	F	161	ARG	N-CA-CB	5.67	118.39	109.94
3	Q	56	GLU	CA-C-N	5.67	128.13	120.65
3	Q	56	GLU	C-N-CA	5.67	128.13	120.65
1	P	100	VAL	CA-C-N	5.66	131.02	123.10
1	P	100	VAL	C-N-CA	5.66	131.02	123.10
2	C	330	GLU	N-CA-CB	5.66	118.25	109.48
1	P	163	VAL	CA-C-N	5.65	130.97	123.05
1	P	163	VAL	C-N-CA	5.65	130.97	123.05
2	D	330	GLU	N-CA-CB	5.65	118.24	109.48
3	F	26	LEU	CA-C-N	5.65	127.78	120.44
3	F	26	LEU	C-N-CA	5.65	127.78	120.44
1	B	249	ILE	N-CA-CB	5.65	117.16	110.55
1	B	244	ILE	N-CA-CB	5.64	116.55	110.62
1	P	1387	GLU	N-CA-CB	5.64	118.42	110.12
1	P	101	VAL	CA-C-N	5.64	130.18	122.34
1	P	101	VAL	C-N-CA	5.64	130.18	122.34
1	P	1287	LEU	N-CA-CB	5.64	118.19	110.01
1	P	528	ARG	NE-CZ-NH2	5.64	124.27	119.20
1	B	1188	ILE	N-CA-CB	5.63	116.77	110.51
3	E	67	ARG	CG-CD-NE	5.63	124.40	112.00
1	P	244	ILE	N-CA-CB	5.63	116.53	110.62
6	L	33	DG	C4'-C3'-O3'	-5.63	101.56	110.00
3	Q	67	ARG	CG-CD-NE	5.62	124.38	112.00
3	Q	46	PHE	N-CA-CB	5.62	118.32	109.94
3	R	26	LEU	CA-C-N	5.62	127.75	120.44
3	R	26	LEU	C-N-CA	5.62	127.75	120.44
3	E	56	GLU	CA-C-N	5.62	128.07	120.65
3	E	56	GLU	C-N-CA	5.62	128.07	120.65
2	D	137	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	P	256	ARG	CD-NE-CZ	5.62	132.26	124.40
1	B	256	ARG	CD-NE-CZ	5.61	132.26	124.40
3	F	92	ASP	CA-CB-CG	5.61	118.20	112.60
1	B	163	VAL	CA-C-N	5.60	130.90	123.05
1	B	163	VAL	C-N-CA	5.60	130.90	123.05
1	P	1126	ASP	CA-CB-CG	5.60	118.20	112.60
1	B	101	VAL	CA-C-N	5.60	130.13	122.34
1	B	101	VAL	C-N-CA	5.60	130.13	122.34
1	P	249	ILE	N-CA-CB	5.60	117.10	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1387	GLU	N-CA-CB	5.60	118.35	110.12
1	P	1188	ILE	N-CA-CB	5.59	116.72	110.51
3	E	46	PHE	N-CA-CB	5.59	118.27	109.94
3	F	88	LEU	CA-C-N	5.59	130.67	121.39
3	F	88	LEU	C-N-CA	5.59	130.67	121.39
6	L	39	DG	C4'-C3'-O3'	-5.59	101.62	110.00
1	P	103	GLY	CA-C-N	5.58	130.84	122.58
1	P	103	GLY	C-N-CA	5.58	130.84	122.58
5	K	57	DC	C4'-C3'-O3'	-5.57	101.64	110.00
1	B	1126	ASP	CA-CB-CG	5.56	118.16	112.60
1	P	149	PRO	CA-C-N	5.56	127.67	120.44
1	P	149	PRO	C-N-CA	5.56	127.67	120.44
3	F	24	PRO	CA-C-N	5.56	127.67	120.44
3	F	24	PRO	C-N-CA	5.56	127.67	120.44
1	B	104	VAL	CA-C-N	5.56	130.16	122.77
1	B	104	VAL	C-N-CA	5.56	130.16	122.77
1	B	528	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	B	193	ASP	CA-CB-CG	5.56	118.16	112.60
2	D	287	THR	CA-CB-OG1	5.56	117.94	109.60
3	R	148	LYS	CG-CD-CE	5.55	124.08	111.30
2	C	287	THR	CA-CB-OG1	5.55	117.93	109.60
2	C	295	ARG	CB-CA-C	5.55	120.28	111.51
1	P	99	ARG	CA-C-N	5.55	130.71	122.99
1	P	99	ARG	C-N-CA	5.55	130.71	122.99
1	P	186	LYS	CA-CB-CG	5.54	125.19	114.10
3	R	129	ASP	CA-CB-CG	5.54	118.14	112.60
6	L	43	DG	O3'-P-O5'	-5.54	95.69	104.00
1	B	1216	GLU	CA-C-N	5.53	127.53	120.56
1	B	1216	GLU	C-N-CA	5.53	127.53	120.56
1	P	1216	GLU	CA-C-N	5.51	127.51	120.56
1	P	1216	GLU	C-N-CA	5.51	127.51	120.56
1	P	1328	ARG	CB-CG-CD	5.51	123.97	111.30
1	B	99	ARG	CA-C-N	5.50	130.64	122.99
1	B	99	ARG	C-N-CA	5.50	130.64	122.99
1	B	228	VAL	CA-C-N	5.50	127.59	120.44
1	B	228	VAL	C-N-CA	5.50	127.59	120.44
1	B	149	PRO	CA-C-N	5.50	127.59	120.44
1	B	149	PRO	C-N-CA	5.50	127.59	120.44
1	P	167	GLN	CA-C-N	5.50	130.31	122.72
1	P	167	GLN	C-N-CA	5.50	130.31	122.72
1	P	1396	ASP	CA-C-N	5.50	130.26	123.12
1	P	1396	ASP	C-N-CA	5.50	130.26	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	295	ARG	CB-CA-C	5.49	120.19	111.51
1	B	1399	PRO	CA-C-N	5.49	129.04	120.75
1	B	1399	PRO	C-N-CA	5.49	129.04	120.75
1	B	403	GLN	OE1-CD-NE2	-5.49	117.11	122.60
3	R	128	ALA	CA-C-N	5.48	129.26	121.42
3	R	128	ALA	C-N-CA	5.48	129.26	121.42
1	P	117	ASP	CA-C-N	5.48	130.61	122.99
1	P	117	ASP	C-N-CA	5.48	130.61	122.99
1	B	1197	ARG	CD-NE-CZ	5.48	132.07	124.40
1	B	1396	ASP	CA-C-N	5.47	130.23	123.12
1	B	1396	ASP	C-N-CA	5.47	130.23	123.12
3	F	128	ALA	CA-C-N	5.47	129.24	121.42
3	F	128	ALA	C-N-CA	5.47	129.24	121.42
3	Q	44	HIS	CA-C-N	5.46	127.54	120.44
3	Q	44	HIS	C-N-CA	5.46	127.54	120.44
1	B	1212	ILE	N-CA-CB	5.46	116.35	110.62
3	E	44	HIS	CA-C-N	5.46	127.54	120.44
3	E	44	HIS	C-N-CA	5.46	127.54	120.44
1	P	1212	ILE	N-CA-CB	5.46	116.35	110.62
3	E	43	ASN	CA-C-N	5.45	127.53	120.44
3	E	43	ASN	C-N-CA	5.45	127.53	120.44
3	Q	43	ASN	CA-C-N	5.45	127.53	120.44
3	Q	43	ASN	C-N-CA	5.45	127.53	120.44
2	D	323	LEU	CA-C-N	5.45	128.50	120.82
2	D	323	LEU	C-N-CA	5.45	128.50	120.82
1	P	227	GLY	CA-C-N	5.45	127.42	120.56
1	P	227	GLY	C-N-CA	5.45	127.42	120.56
3	R	155	VAL	N-CA-CB	5.45	116.92	110.55
5	K	56	DT	C2'-C3'-O3'	5.44	119.66	111.50
3	Q	46	PHE	CA-CB-CG	5.44	119.24	113.80
1	P	403	GLN	OE1-CD-NE2	-5.43	117.17	122.60
3	E	46	PHE	CA-CB-CG	5.43	119.23	113.80
3	R	24	PRO	CA-C-N	5.43	127.50	120.44
3	R	24	PRO	C-N-CA	5.43	127.50	120.44
3	F	155	VAL	N-CA-CB	5.42	116.90	110.55
1	P	1399	PRO	CA-C-N	5.42	128.94	120.75
1	P	1399	PRO	C-N-CA	5.42	128.94	120.75
2	C	116	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	B	117	ASP	CA-C-N	5.41	130.51	122.99
1	B	117	ASP	C-N-CA	5.41	130.51	122.99
1	P	218	ARG	CA-C-N	5.40	127.52	120.28
1	P	218	ARG	C-N-CA	5.40	127.52	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	1197	ARG	CD-NE-CZ	5.40	131.95	124.40
1	P	1384	SER	N-CA-CB	5.39	117.83	110.01
1	B	1221	ARG	CA-CB-CG	5.38	124.87	114.10
2	C	323	LEU	CA-C-N	5.38	128.41	120.82
2	C	323	LEU	C-N-CA	5.38	128.41	120.82
1	P	1221	ARG	CA-CB-CG	5.38	124.86	114.10
1	P	1322	GLN	CA-CB-CG	5.38	124.86	114.10
3	Q	139	GLN	CB-CG-CD	5.38	121.74	112.60
1	B	227	GLY	CA-C-N	5.38	127.33	120.56
1	B	227	GLY	C-N-CA	5.38	127.33	120.56
3	F	91	LEU	CA-C-N	5.37	127.42	120.44
3	F	91	LEU	C-N-CA	5.37	127.42	120.44
1	B	48	VAL	N-CA-CB	5.37	117.84	110.54
1	B	363	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	B	1322	GLN	CA-CB-CG	5.36	124.83	114.10
3	F	129	ASP	CA-CB-CG	5.36	117.96	112.60
1	P	243	ARG	CD-NE-CZ	5.36	131.91	124.40
1	B	250	ARG	CA-C-N	5.36	127.26	120.72
1	B	250	ARG	C-N-CA	5.36	127.26	120.72
3	Q	62	ASN	CA-C-N	5.35	130.41	122.71
3	Q	62	ASN	C-N-CA	5.35	130.41	122.71
1	B	233	GLN	CA-C-N	5.35	127.71	120.65
1	B	233	GLN	C-N-CA	5.35	127.71	120.65
3	R	91	LEU	CA-C-N	5.35	127.39	120.44
3	R	91	LEU	C-N-CA	5.35	127.39	120.44
1	B	194	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	B	186	LYS	CA-CB-CG	5.34	124.78	114.10
1	P	363	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	P	1241	ALA	CA-C-N	5.34	127.70	120.65
1	P	1241	ALA	C-N-CA	5.34	127.70	120.65
1	B	194	ARG	N-CA-CB	-5.34	102.28	110.12
2	C	299	GLN	CA-C-N	5.33	127.74	120.54
2	C	299	GLN	C-N-CA	5.33	127.74	120.54
1	B	243	ARG	CD-NE-CZ	5.33	131.87	124.40
3	F	98	ILE	N-CA-CB	5.33	116.79	110.55
2	D	299	GLN	CA-C-N	5.32	127.72	120.54
2	D	299	GLN	C-N-CA	5.32	127.72	120.54
1	P	233	GLN	CA-C-N	5.32	127.67	120.65
1	P	233	GLN	C-N-CA	5.32	127.67	120.65
3	R	123	GLU	CA-C-N	5.32	127.72	120.54
3	R	123	GLU	C-N-CA	5.32	127.72	120.54
1	P	156	ARG	CA-C-N	5.31	127.67	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	156	ARG	C-N-CA	5.31	127.67	120.44
3	R	34	ARG	N-CA-CB	5.31	117.85	109.83
3	F	148	LYS	CG-CD-CE	5.31	123.52	111.30
3	Q	67	ARG	CD-NE-CZ	5.31	131.84	124.40
1	P	48	VAL	N-CA-CB	5.31	117.76	110.54
3	R	138	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	B	1328	ARG	CB-CG-CD	5.31	123.50	111.30
3	E	67	ARG	CA-CB-CG	5.30	124.71	114.10
3	F	123	GLU	CA-C-N	5.30	127.70	120.54
3	F	123	GLU	C-N-CA	5.30	127.70	120.54
5	K	56	DT	C4'-C3'-O3'	-5.30	102.05	110.00
3	R	144	SER	CA-C-N	5.30	127.69	120.54
3	R	144	SER	C-N-CA	5.30	127.69	120.54
3	F	161	ARG	CA-C-N	5.29	127.37	120.28
3	F	161	ARG	C-N-CA	5.29	127.37	120.28
1	P	162	GLY	CA-C-N	5.29	128.96	121.66
1	P	162	GLY	C-N-CA	5.29	128.96	121.66
1	B	1220	ALA	CA-C-N	5.29	127.68	120.54
1	B	1220	ALA	C-N-CA	5.29	127.68	120.54
1	P	250	ARG	CA-C-N	5.29	127.17	120.72
1	P	250	ARG	C-N-CA	5.29	127.17	120.72
3	E	67	ARG	CD-NE-CZ	5.29	131.80	124.40
1	B	1188	ILE	CA-C-N	5.29	127.31	120.44
1	B	1188	ILE	C-N-CA	5.29	127.31	120.44
2	D	123	LEU	CB-CG-CD2	-5.29	94.84	110.70
2	C	290	ASP	N-CA-C	5.28	118.88	112.23
1	P	1188	ILE	CA-C-N	5.28	127.30	120.44
1	P	1188	ILE	C-N-CA	5.28	127.30	120.44
2	D	290	ASP	N-CA-C	5.28	118.88	112.23
3	R	85	ARG	CA-CB-CG	5.28	124.65	114.10
3	F	144	SER	CA-C-N	5.27	127.66	120.54
3	F	144	SER	C-N-CA	5.27	127.66	120.54
3	E	62	ASN	CA-C-N	5.27	130.30	122.71
3	E	62	ASN	C-N-CA	5.27	130.30	122.71
3	F	34	ARG	N-CA-CB	5.27	117.79	109.83
3	R	161	ARG	CA-C-N	5.27	127.34	120.28
3	R	161	ARG	C-N-CA	5.27	127.34	120.28
1	P	1248	ILE	N-CA-CB	5.26	117.70	110.54
2	D	116	ARG	NE-CZ-NH2	5.26	123.93	119.20
3	F	94	MET	CA-C-N	5.26	127.19	120.56
3	F	94	MET	C-N-CA	5.26	127.19	120.56
1	P	1164	ASN	N-CA-CB	5.25	117.73	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	147	ASP	CA-C-N	5.25	127.31	120.28
3	F	147	ASP	C-N-CA	5.25	127.31	120.28
3	R	156	ARG	CA-C-N	5.25	127.58	120.65
3	R	156	ARG	C-N-CA	5.25	127.58	120.65
3	Q	67	ARG	CA-CB-CG	5.25	124.59	114.10
3	F	29	GLN	CA-C-N	5.24	127.26	120.44
3	F	29	GLN	C-N-CA	5.24	127.26	120.44
5	K	26	DC	C5'-C4'-O4'	5.24	117.26	109.40
5	K	63	DG	C4-N9-C1'	-5.24	119.14	127.00
3	R	147	ASP	CA-C-N	5.24	127.31	120.28
3	R	147	ASP	C-N-CA	5.24	127.31	120.28
1	P	1254	ARG	N-CA-CB	5.24	117.61	110.01
3	R	29	GLN	CA-C-N	5.24	127.25	120.44
3	R	29	GLN	C-N-CA	5.24	127.25	120.44
1	A	966	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	B	191	ALA	CA-C-N	5.24	127.30	120.28
1	B	191	ALA	C-N-CA	5.24	127.30	120.28
1	P	1220	ALA	CA-C-N	5.24	127.61	120.54
1	P	1220	ALA	C-N-CA	5.24	127.61	120.54
6	L	48	DC	C5'-C4'-O4'	5.23	117.24	109.40
2	C	151	HIS	CB-CG-CD2	-5.23	124.41	131.20
1	P	1397	ILE	CA-C-N	5.22	131.36	122.06
1	P	1397	ILE	C-N-CA	5.22	131.36	122.06
1	B	234	ASP	CA-C-N	5.22	127.27	120.28
1	B	234	ASP	C-N-CA	5.22	127.27	120.28
3	R	94	MET	CA-C-N	5.22	127.13	120.56
3	R	94	MET	C-N-CA	5.22	127.13	120.56
3	E	29	GLN	CA-C-N	5.21	127.21	120.44
3	E	29	GLN	C-N-CA	5.21	127.21	120.44
2	D	320	ALA	CA-C-N	5.20	128.26	120.87
2	D	320	ALA	C-N-CA	5.20	128.26	120.87
1	B	194	ARG	CA-C-N	5.20	127.20	120.44
1	B	194	ARG	C-N-CA	5.20	127.20	120.44
5	K	62	DT	C2'-C3'-O3'	5.20	119.30	111.50
3	F	156	ARG	CA-C-N	5.20	127.51	120.65
3	F	156	ARG	C-N-CA	5.20	127.51	120.65
1	P	173	ASP	CA-C-N	5.20	127.19	120.44
1	P	173	ASP	C-N-CA	5.20	127.19	120.44
1	B	1187	PHE	CA-C-N	5.19	127.30	120.60
1	B	1187	PHE	C-N-CA	5.19	127.30	120.60
3	Q	29	GLN	CA-C-N	5.19	127.18	120.44
3	Q	29	GLN	C-N-CA	5.19	127.18	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	234	ASP	CA-C-N	5.18	127.23	120.28
1	P	234	ASP	C-N-CA	5.18	127.23	120.28
3	F	80	THR	CA-C-N	5.18	128.46	121.05
3	F	80	THR	C-N-CA	5.18	128.46	121.05
1	P	240	ARG	N-CA-CB	5.18	117.52	110.01
1	B	1164	ASN	N-CA-CB	5.18	117.62	110.17
1	P	1250	ARG	N-CA-CB	5.17	117.65	109.94
3	E	206	ARG	N-CA-CB	5.17	117.72	110.12
3	Q	26	LEU	CA-C-N	5.17	127.16	120.44
3	Q	26	LEU	C-N-CA	5.17	127.16	120.44
3	E	26	LEU	CA-C-N	5.17	127.16	120.44
3	E	26	LEU	C-N-CA	5.17	127.16	120.44
2	D	151	HIS	CB-CG-CD2	-5.17	124.48	131.20
1	P	559	GLN	OE1-CD-NE2	-5.17	117.44	122.60
3	Q	206	ARG	N-CA-CB	5.17	117.71	110.12
1	B	1246	LYS	CA-C-N	5.16	127.15	120.44
1	B	1246	LYS	C-N-CA	5.16	127.15	120.44
2	C	6	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	P	1388	GLU	N-CA-CB	5.16	117.50	110.01
1	P	1286	LEU	CA-C-N	5.16	127.15	120.44
1	P	1286	LEU	C-N-CA	5.16	127.15	120.44
3	R	80	THR	CA-C-N	5.16	128.43	121.05
3	R	80	THR	C-N-CA	5.16	128.43	121.05
1	P	1391	ARG	CD-NE-CZ	5.15	131.61	124.40
3	R	154	LYS	CA-C-N	5.15	127.05	120.56
3	R	154	LYS	C-N-CA	5.15	127.05	120.56
1	O	932	ASP	CB-CA-C	5.14	115.64	109.31
1	O	966	ARG	NE-CZ-NH2	5.14	123.83	119.20
6	L	66	DT	C5'-C4'-O4'	5.13	117.10	109.40
6	L	59	DT	C5'-C4'-O4'	5.13	117.09	109.40
1	P	255	ASP	CA-C-N	5.13	127.11	120.44
1	P	255	ASP	C-N-CA	5.13	127.11	120.44
1	P	1187	PHE	CA-C-N	5.12	127.21	120.60
1	P	1187	PHE	C-N-CA	5.12	127.21	120.60
1	P	1190	VAL	N-CA-CB	5.12	116.54	110.55
1	B	192	SER	CA-C-N	5.12	127.09	120.44
1	B	192	SER	C-N-CA	5.12	127.09	120.44
1	P	521	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	B	240	ARG	N-CA-CB	5.11	117.42	110.01
1	B	521	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	B	559	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	B	1190	VAL	N-CA-CB	5.11	116.53	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	185	PRO	CA-C-N	5.10	131.07	122.87
1	P	185	PRO	C-N-CA	5.10	131.07	122.87
1	B	185	PRO	CA-C-N	5.09	131.06	122.87
1	B	185	PRO	C-N-CA	5.09	131.06	122.87
1	B	174	TYR	CA-C-N	5.09	127.10	120.28
1	B	174	TYR	C-N-CA	5.09	127.10	120.28
1	P	157	LEU	CA-C-N	5.08	127.09	120.28
1	P	157	LEU	C-N-CA	5.08	127.09	120.28
3	R	148	LYS	CA-C-N	5.08	127.05	120.44
3	R	148	LYS	C-N-CA	5.08	127.05	120.44
3	F	148	LYS	CA-C-N	5.08	127.04	120.44
3	F	148	LYS	C-N-CA	5.08	127.04	120.44
3	E	40	ASP	CA-C-N	5.08	127.39	120.54
3	E	40	ASP	C-N-CA	5.08	127.39	120.54
1	P	123	ILE	CA-C-N	5.08	130.55	122.94
1	P	123	ILE	C-N-CA	5.08	130.55	122.94
3	F	85	ARG	CA-CB-CG	5.07	124.25	114.10
1	P	1239	SER	CA-C-N	5.07	128.67	120.55
1	P	1239	SER	C-N-CA	5.07	128.67	120.55
3	Q	27	ASP	N-CA-CB	5.07	117.36	110.01
1	B	1388	GLU	N-CA-CB	5.07	117.36	110.01
3	E	27	ASP	N-CA-CB	5.07	117.36	110.01
5	K	18	DT	C5'-C4'-O4'	5.07	117.00	109.40
1	P	154	LYS	N-CA-CB	5.07	117.36	110.01
1	A	932	ASP	CB-CA-C	5.07	115.54	109.31
1	B	1250	ARG	N-CA-CB	5.07	117.49	109.94
1	P	174	TYR	CA-CB-CG	5.06	123.01	113.90
1	P	549	GLN	N-CA-C	-5.06	98.81	107.61
3	Q	139	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	B	1198	ILE	CA-C-N	5.05	128.47	120.89
1	B	1198	ILE	C-N-CA	5.05	128.47	120.89
6	L	68	DT	C5'-C4'-O4'	5.05	116.98	109.40
1	B	123	ILE	CA-C-N	5.04	130.51	122.94
1	B	123	ILE	C-N-CA	5.04	130.51	122.94
2	D	176	ARG	CA-CB-CG	-5.04	104.02	114.10
1	P	1198	ILE	CA-C-N	5.04	128.45	120.89
1	P	1198	ILE	C-N-CA	5.04	128.45	120.89
1	B	1239	SER	CA-C-N	5.04	128.61	120.55
1	B	1239	SER	C-N-CA	5.04	128.61	120.55
3	R	157	THR	CA-C-N	5.03	127.02	120.28
3	R	157	THR	C-N-CA	5.03	127.02	120.28
3	E	186	ARG	NE-CZ-NH2	5.03	123.72	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	31	ARG	CB-CG-CD	5.03	122.86	111.30
1	P	1336	GLU	CA-C-N	5.02	129.11	120.72
1	P	1336	GLU	C-N-CA	5.02	129.11	120.72
3	R	146	LEU	N-CA-CB	5.02	117.50	110.12
3	R	87	VAL	CA-C-N	5.02	128.82	120.94
3	R	87	VAL	C-N-CA	5.02	128.82	120.94
1	B	255	ASP	CA-C-N	5.02	126.97	120.44
1	B	255	ASP	C-N-CA	5.02	126.97	120.44
1	B	549	GLN	N-CA-C	-5.02	98.88	107.61
3	F	157	THR	CA-C-N	5.02	127.00	120.28
3	F	157	THR	C-N-CA	5.02	127.00	120.28
1	P	102	VAL	CA-C-N	5.02	128.55	120.97
1	P	102	VAL	C-N-CA	5.02	128.55	120.97
1	P	1207	ASP	N-CA-CB	5.02	117.45	110.07
3	Q	163	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	P	548	ARG	NE-CZ-NH2	5.00	123.70	119.20
1	B	247	GLU	N-CA-CB	5.00	117.48	110.12
2	C	324	LEU	CA-C-N	5.00	130.44	122.59
2	C	324	LEU	C-N-CA	5.00	130.44	122.59
3	F	85	ARG	CD-NE-CZ	5.00	131.41	124.40
3	R	85	ARG	CD-NE-CZ	5.00	131.40	124.40
2	C	153	HIS	CB-CG-CD2	-5.00	124.70	131.20
5	K	15	DA	C2'-C3'-O3'	-5.00	104.00	111.50

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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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	76	0
1	B	11840	11706	11705	95	0
1	O	11840	11707	11705	79	0
1	P	11840	11706	11705	99	0
2	C	3531	3451	3450	71	0
2	D	3531	3451	3450	71	0
3	E	1722	1719	1718	15	0
3	F	1619	1627	1626	15	0
3	Q	1722	1719	1718	16	0
3	R	1619	1627	1626	15	0
4	G	583	564	563	25	0
4	I	583	564	563	9	0
4	M	583	564	563	9	0
4	S	583	564	563	27	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	66557	64362	64346	526	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 4.

All (526) 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
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:131:ILE:HD11	2:D:163:SER:HG	1.42	0.82
2:C:123:LEU:HG	2:D:158:ALA:HB1	1.61	0.82
1:P:1127:ASN:HD22	1:P:1127:ASN:C	1.88	0.81
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:B:1127:ASN:HD22	1:B: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:288:ALA:HB1	4:G:44:MET:HE1	1.73	0.71
2:C:124:ARG:HA	2:D:162:TYR:HB3	1.73	0.71
1:O:288:ALA:HB1	4:S:44:MET:HE1	1.73	0.70
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
1:O:1457:GLU:OE1	1:O:1457:GLU:N	2.28	0.63
3:F:167:MET:HE2	3:F:167:MET:HA	1.79	0.63
3:R:167:MET:HE2	3:R:167:MET:HA	1.79	0.63
4:G:36:4HH:HJ2	4:G:36:4HH:CB	2.25	0.63
1:P:1141:MET:HA	1:P:1141:MET:HE3	1.81	0.63
2:D:314:THR:HA	3:Q:93:MET:HE2	1.81	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:231:ALA:HB2	1:P:665:GLN:CB	2.30	0.62
1:P:1322:GLN:O	1:P:1322:GLN:CD	2.43	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:B:1322:GLN:O	1:B:1322:GLN:CD	2.43	0.61
1:A:231:ALA:HB2	1:B:665:GLN:CB	2.30	0.61
1:B:1141:MET:HE3	1:B:1141:MET:HA	1.81	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
2:C:314:THR:HA	3:E:93:MET:HE2	1.81	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:674:MET:HE3	1:P:674:MET:HA	1.86	0.58
1:P:1107:ARG:HE	4:M:48:GLU:CD	2.12	0.57
1:B:674:MET:HE3	1:B:674:MET:HA	1.85	0.57
1:P:1142:GLU:N	1:P:1142:GLU:OE1	2.36	0.57
1:B:1107:ARG:HE	4:I:48:GLU:CD	2.12	0.56
2:C:124:ARG:HA	2:D:162:TYR:CG	2.41	0.56
1:P:273:ASP:OD1	1:P:273:ASP:C	2.49	0.55
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
1:B:273:ASP:OD1	1:B:273:ASP:C	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:36:HH:HJ3	4:S:37:LEU:N	2.22	0.54
3:F:148:LYS:HD3	3:F:148:LYS:N	2.23	0.54
1:O:236:GLU:OE2	1:O:1307:THR:HG21	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
2:C:79:ASN:CG	3:Q:142:SER:HB3	2.34	0.53
1:A:828:VAL:HG12	1:A:828:VAL:O	2.08	0.53
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:HH: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
1:P:799:GLU:OE1	1:P:799:GLU:C	2.52	0.53
2:C:123:LEU:HD11	2:D:158:ALA:CB	2.39	0.53
1:O:289:LEU:HD22	4:S:36:HH:CS	2.39	0.53
1:O:1126:ASP:O	1:O:1127:ASN:OD1	2.27	0.53
1:O:828:VAL:O	1:O:828:VAL:HG12	2.08	0.53
3:Q:124:LEU:C	3:Q:124:LEU:HD23	2.34	0.53
1:A:65:GLU:O	1:A:65:GLU:HG3	2.08	0.53
1:B:799:GLU:C	1:B:799:GLU:OE1	2.52	0.52
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
3:E:124:LEU:C	3:E:124:LEU:HD23	2.34	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
2:D:79:ASN:CG	3:E:142:SER:HB3	2.34	0.52
1:A:122:MET:HE1	1:A:177:GLN:HB3	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:828:VAL:HG12	1:B:828:VAL:O	2.10	0.52
1:B:665:GLN:C	1:B:665:GLN:OE1	2.53	0.52
1:O:122:MET:HE1	1:O:177:GLN:HB3	1.90	0.52
2:D:158:ALA:HB3	2:D:159:PRO:HD3	1.91	0.52
1:A:44:MET:HE3	1:A:1433:ALA:HB2	1.92	0.52
1:P:63:THR:HG21	1:P:1407:GLU:HG3	1.92	0.52
1:P:665:GLN:OE1	1:P:665:GLN:C	2.53	0.52
1:P:732:GLU:H	1:P:732:GLU:CD	2.18	0.52
3:E:10:MET:HE3	3:E:14:LEU:HD22	1.92	0.51
1:P:1161:VAL:HG12	1:P:1161:VAL:O	2.10	0.51
1:O:44:MET:HE3	1:O:1433:ALA:HB2	1.92	0.51
1:B:1246:LYS:HD2	1:B:1246:LYS:O	2.11	0.51
1:P:91:ASP:C	1:P:91:ASP:OD1	2.54	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
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
3:Q:10:MET:HE3	3:Q:14:LEU:HD22	1.92	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: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
1:B:1257:MET:SD	1:B:1257:MET:C	2.95	0.50
2:D:358:LEU:HG	2:D:362:ILE:HD11	1.94	0.50
1:B:732:GLU:CD	1:B:732:GLU:H	2.18	0.50
1:O:200:LEU:HD12	1:O:1378:LEU:HD22	1.94	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:P:1257:MET:C	1:P:1257:MET:SD	2.95	0.50
1:B:1107:ARG:CZ	4:I:48:GLU:OE1	2.59	0.50
2:C:356:ASP:C	2:C:356:ASP:OD1	2.55	0.50
1:A:1361:GLU:OE1	1:A:1361:GLU:HA	2.12	0.50
2:D:356:ASP:OD1	2:D:356:ASP:C	2.55	0.50
1:A:200:LEU:HD12	1:A:1378:LEU:HD22	1.94	0.50
1:B:91:ASP:C	1:B:91:ASP:OD1	2.54	0.50
2:C:162:TYR:CD1	2:D:124:ARG:HD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:16:GLN:C	3:F:16:GLN:OE1	2.55	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: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
1:A:235:MET:HA	1:A:235:MET:HE2	1.95	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
3:R:16:GLN:C	3:R:16:GLN:OE1	2.55	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
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
1:O:235:MET:HE2	1:O:235:MET:HA	1.95	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
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
4:S:11:ILE:HG23	4:S:12:GLY:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1237:SER:OG	1:A:1238:LYS:N	2.45	0.47
1:B:1161:VAL:O	1:B:1161:VAL:CG1	2.62	0.47
2:D:292:ASP:CG	2:D:295:ARG:HA	2.39	0.47
2:C:292:ASP:CG	2:C:295:ARG:HA	2.39	0.47
4:S:36:4HH:ON	4:S:40:VAL:HG23	2.13	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: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: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
3:F:25:GLU:CD	3:F:25:GLU:H	2.23	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: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
3:R:25:GLU:CD	3:R:25:GLU:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
1:O:1275:LEU:HD23	1:O:1380:MET:HE2	1.98	0.45
3:R:121:TYR:CZ	3:R:125:ILE:HD11	2.52	0.45
3:R:190:ASP:C	3:R:190:ASP:OD1	2.59	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
1:B:611:LEU:C	1:B:611:LEU:HD23	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:784:GLU:HA	1:B:787:LEU:HG	1.99	0.45
3:F:134:MET:N	3:F:134:MET:HE2	2.32	0.45
1:O:12:LEU:HD21	1:O:46:ALA:HB2	1.97	0.45
1:A:275:MET:HE1	1:A:1134:HIS:ND1	2.31	0.44
1:A:1127:ASN:OD1	1:A:1127:ASN:C	2.60	0.44
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:O:1127:ASN:OD1	1:O:1127:ASN:C	2.60	0.44
1:A:765:ARG:HH11	1:B:748:VAL:HG23	1.81	0.44
1:A:1275:LEU:HD23	1:A:1380:MET:HE2	1.98	0.44
1:B:232:PHE:CZ	1:B:1240:VAL:HG11	2.53	0.44
3:F:190:ASP:C	3:F:190:ASP:OD1	2.60	0.44
4:I:58:GLU:OE1	4:I:71:TYR:OH	2.31	0.44
1:O:275:MET:HE1	1:O:1134:HIS:CE1	2.52	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:632:MET:HE1	1:P:818:PHE:HB3	1.99	0.44
1:P:784:GLU:HA	1:P:787:LEU:HG	1.98	0.44
3:R:134:MET:N	3:R:134:MET:HE2	2.32	0.44
4:S:36:4HH:OM	4:S:37:LEU:HA	2.17	0.44
1:O:152:GLU:OE1	1:O:152:GLU:N	2.51	0.44
1:O:275:MET:HE1	1:O:1134:HIS:ND1	2.31	0.44
1:P:611:LEU:HD23	1:P:611:LEU:C	2.42	0.44
1:A:275:MET:HE1	1:A:1134:HIS:CE1	2.52	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
1:A:1387:GLU:C	1:A:1387:GLU:OE1	2.61	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
1:P:1213:GLU:H	1:P:1213:GLU:CD	2.26	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:O:1380:MET:HE3	1:O:1380:MET:HB3	1.96	0.43
1:A:51:LEU:O	1:A:52:ILE:HD13	2.18	0.43
1:B:782:ALA:O	1:B:785:ASN:HB3	2.18	0.43
1:O:1401:ARG:HB3	1:O:1428:MET:HE2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:36:4HH:CB	4:S:36:4HH:CJ	2.90	0.43
1:B:215:ARG:HG2	1:B:1325:MET:HE2	2.01	0.43
1:B:89:THR:C	1:B:90:LEU:HD12	2.43	0.43
1:B:632:MET:HE1	1:B:818:PHE:HB3	2.00	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:105:ARG:HD2	1:P:105:ARG:C	2.44	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
1:A:1401:ARG:HB3	1:A:1428:MET:HE2	1.99	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:1129:VAL:O	1:O:1130:GLU:C	2.61	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
1:O:782:ALA:C	1:O:783:ARG:HD3	2.43	0.43
1:O:1107:ARG:NH2	4:S:47:GLU:OE2	2.50	0.43
3:Q:127:LEU:HD23	3:Q:127:LEU:C	2.44	0.43
2:C:399:ARG:O	2:C:403:ASP:OD2	2.36	0.43
1:O:105:ARG:HD2	1:O:105:ARG:C	2.44	0.43
1:O:1235:ILE:HG21	1:P:675:ILE:HD13	2.01	0.43
1:P:89:THR:C	1:P:90:LEU:HD12	2.43	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:215:ARG:HG2	1:P:1325:MET:HE2	2.00	0.43
1:B:1213:GLU:H	1:B:1213:GLU:CD	2.26	0.42
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:782:ALA:C	1:A:783:ARG:HD3	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:594:ILE:HD12	1:P:845:HIS:CE1	2.54	0.42
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:1387:GLU:CD	1:O:1387:GLU:C	2.87	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:1387:GLU:C	1:A:1387:GLU:CD	2.87	0.42
1:O:1387:GLU:C	1:O:1387:GLU:OE1	2.61	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:A:1129:VAL:O	1:A:1130:GLU:C	2.61	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
3:E:127:LEU:C	3:E:127:LEU:HD23	2.44	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:105:ARG:HD2	1:A:105:ARG:C	2.44	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
1:B:1395:LYS:HD3	1:B:1395:LYS:C	2.45	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:O:782:ALA:O	1:O:783:ARG:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1068:LEU:C	1:A:1068:LEU:HD23	2.45	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
3:R:167:MET:HE1	3:R:183:ALA:HB1	2.01	0.41
3:F:167:MET:HE1	3:F:183:ALA:HB1	2.01	0.41
1:A:1199:ARG:O	1:A:1199:ARG:HG2	2.19	0.41
1:B:288:ALA:HB2	1:B:1106:ILE:HG22	2.03	0.41
1:B:1142:GLU:CD	1:B:1142:GLU:H	2.28	0.41
1:B:1246:LYS:HD2	1:B:1246:LYS:C	2.45	0.41
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:1068:LEU:C	1:O:1068:LEU:HD23	2.45	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
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:O:1199:ARG:O	1:O:1199:ARG:HG2	2.19	0.41
1:P:244:ILE:CD1	3:Q:41:LEU:HD21	2.51	0.41
1:P:141:GLY:O	1:P:143:ARG:NH1	2.54	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:1403:LEU:HD13	1:B:1428:MET:HE3	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:45:ALA:HB1	1:O:60:PHE:CE2	2.55	0.41
1:O:281:ARG:HD2	1:O:281:ARG:C	2.46	0.41
1:O:1117:TRP:CE3	1:O:1121:MET:HE1	2.56	0.41
1:P:288:ALA:HB2	1:P:1106:ILE:HG22	2.02	0.41
1:P:1142:GLU:H	1:P:1142:GLU:CD	2.28	0.41
1:P:1227:THR:O	1:P:1230:GLU:HG3	2.21	0.41
1:P:1403:LEU:HD13	1:P:1428:MET:HE3	2.03	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
1:A:281:ARG:C	1:A:281:ARG:HD2	2.46	0.40
2:D:357:GLN:O	2:D:361:MET:SD	2.78	0.40
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
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
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:1387:GLU:OE1	1:O:1388:GLU:N	2.54	0.40
1:P:275:MET:HA	1:P:275:MET:HE3	2.04	0.40
1:A:1117:TRP:CE3	1:A:1121:MET:HE1	2.56	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:A:782:ALA:O	1:A:783:ARG:C	2.63	0.40
1:B:275:MET:HE3	1:B:275:MET:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1307:THR:OG1	1:P:1310:GLU:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1465/1482 (99%)	1423 (97%)	42 (3%)	0	100	100
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%)	1268 (100%)	1 (0%)	88	89
1	B	1269/1281 (99%)	1267 (100%)	2 (0%)	87	87
1	O	1269/1281 (99%)	1268 (100%)	1 (0%)	88	89
1	P	1269/1281 (99%)	1266 (100%)	3 (0%)	87	87
2	C	376/376 (100%)	369 (98%)	7 (2%)	50	67
2	D	376/376 (100%)	369 (98%)	7 (2%)	50	67
3	E	189/212 (89%)	184 (97%)	5 (3%)	40	62
3	F	177/212 (84%)	175 (99%)	2 (1%)	65	76
3	Q	189/212 (89%)	185 (98%)	4 (2%)	47	65
3	R	177/212 (84%)	175 (99%)	2 (1%)	65	76
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%)	6774 (100%)	34 (0%)	78	83

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	LEU
1	B	1127	ASN
1	B	1213	GLU
2	C	2	SER
2	C	92	SER
2	C	94	LEU
2	C	132	VAL
2	C	209	SER
2	C	287	THR
2	C	355	ASN
2	D	2	SER

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Mol	Chain	Res	Type
2	D	92	SER
2	D	94	LEU
2	D	132	VAL
2	D	209	SER
2	D	287	THR
2	D	355	ASN
3	E	123	GLU
3	E	138	ASN
3	E	162	LEU
3	E	169	TYR
3	E	181	THR
3	F	25	GLU
3	F	152	GLN
1	O	221	LEU
1	P	189	ARG
1	P	1127	ASN
1	P	1213	GLU
3	Q	123	GLU
3	Q	162	LEU
3	Q	169	TYR
3	Q	181	THR
3	R	25	GLU
3	R	152	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	ASN
1	A	306	GLN
1	A	331	GLN
1	A	367	GLN
1	A	404	GLN
1	A	409	GLN
1	A	472	HIS
1	A	510	HIS
1	A	516	GLN
1	A	652	GLN
1	A	865	GLN
1	A	882	GLN
1	A	930	GLN
1	A	951	HIS
1	A	1077	GLN

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Mol	Chain	Res	Type
1	A	1105	GLN
1	A	1109	GLN
1	A	1242	ASN
1	A	1293	GLN
1	B	62	ASN
1	B	78	HIS
1	B	98	GLN
1	B	175	HIS
1	B	306	GLN
1	B	330	HIS
1	B	398	GLN
1	B	418	GLN
1	B	473	ASN
1	B	531	ASN
1	B	559	GLN
1	B	566	GLN
1	B	766	GLN
1	B	864	GLN
1	B	986	ASN
1	B	1006	GLN
1	B	1013	GLN
1	B	1032	GLN
1	B	1091	ASN
1	B	1166	HIS
1	B	1193	HIS
1	B	1342	ASN
1	B	1437	ASN
2	C	75	ASN
2	C	134	ASN
2	C	198	GLN
2	C	435	HIS
2	D	18	ASN
2	D	75	ASN
2	D	134	ASN
2	D	198	GLN
2	D	435	HIS
3	E	8	GLN
3	E	111	ASN
1	O	242	ASN
1	O	306	GLN
1	O	331	GLN
1	O	367	GLN

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Mol	Chain	Res	Type
1	O	378	GLN
1	O	404	GLN
1	O	409	GLN
1	O	472	HIS
1	O	480	GLN
1	O	510	HIS
1	O	516	GLN
1	O	865	GLN
1	O	882	GLN
1	O	930	GLN
1	O	951	HIS
1	O	1077	GLN
1	O	1105	GLN
1	O	1109	GLN
1	O	1242	ASN
1	O	1293	GLN
1	P	62	ASN
1	P	78	HIS
1	P	97	HIS
1	P	98	GLN
1	P	306	GLN
1	P	330	HIS
1	P	398	GLN
1	P	418	GLN
1	P	473	ASN
1	P	531	ASN
1	P	546	GLN
1	P	559	GLN
1	P	566	GLN
1	P	766	GLN
1	P	864	GLN
1	P	986	ASN
1	P	1006	GLN
1	P	1013	GLN
1	P	1091	ASN
1	P	1342	ASN
1	P	1437	ASN
3	Q	8	GLN
3	Q	111	ASN
3	Q	201	GLN
3	R	139	GLN

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	I	36	4	22,26,27	0.47	0	27,35,37	1.74	3 (11%)
4	4HH	M	36	4	22,26,27	0.47	0	27,35,37	1.75	3 (11%)
4	4HH	S	36	4	22,26,27	0.45	0	27,35,37	3.17	4 (14%)
4	4HH	G	36	4	22,26,27	0.45	0	27,35,37	3.17	4 (14%)

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	I	36	4	-	7/33/35/37	-
4	4HH	M	36	4	-	7/33/35/37	-
4	4HH	S	36	4	-	5/33/35/37	-
4	4HH	G	36	4	-	5/33/35/37	-

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	11.98	161.86	107.57
4	S	36	4HH	O1P-P-OG	11.97	161.82	107.57
4	S	36	4HH	OG-P-O2P	-8.72	74.39	108.94
4	G	36	4HH	OG-P-O2P	-8.70	74.46	108.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	36	4HH	P-OG-CB	6.33	157.62	121.35
4	S	36	4HH	P-OG-CB	6.31	157.50	121.35
4	I	36	4HH	P-OG-CB	-5.48	89.97	121.35
4	M	36	4HH	P-OG-CB	-5.46	90.07	121.35
4	M	36	4HH	O1P-P-OG	4.80	129.33	107.57
4	I	36	4HH	O1P-P-OG	4.79	129.28	107.57
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 (24) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	36	4HH	1	0
4	M	36	4HH	1	0
4	S	36	4HH	16	0
4	G	36	4HH	15	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	A	1502	7	32,33,33	0.58	1 (3%)	48,52,52	0.75	2 (4%)
8	ATP	O	1502	7	32,33,33	0.57	1 (3%)	48,52,52	0.75	2 (4%)
8	ATP	P	1502	7	32,33,33	0.56	1 (3%)	48,52,52	0.74	2 (4%)
8	ATP	B	1502	7	32,33,33	0.55	1 (3%)	48,52,52	0.74	2 (4%)

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	A	1502	7	-	2/22/38/38	0/3/3/3
8	ATP	O	1502	7	-	2/22/38/38	0/3/3/3
8	ATP	P	1502	7	-	2/22/38/38	0/3/3/3
8	ATP	B	1502	7	-	2/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1502	ATP	PB-O3B	-2.37	1.56	1.59
8	O	1502	ATP	PB-O3B	-2.24	1.57	1.59
8	B	1502	ATP	PB-O3B	-2.04	1.57	1.59
8	P	1502	ATP	PB-O3B	-2.01	1.57	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1502	ATP	O2'-C2'-C3'	-2.34	104.30	111.82
8	O	1502	ATP	O2'-C2'-C3'	-2.33	104.36	111.82
8	P	1502	ATP	O2'-C2'-C3'	-2.21	104.72	111.82
8	B	1502	ATP	O2'-C2'-C3'	-2.20	104.77	111.82
8	B	1502	ATP	O3'-C3'-C2'	-2.16	104.90	111.82
8	P	1502	ATP	O3'-C3'-C2'	-2.15	104.93	111.82
8	O	1502	ATP	O3'-C3'-C2'	-2.10	105.10	111.82
8	A	1502	ATP	O3'-C3'-C2'	-2.09	105.12	111.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

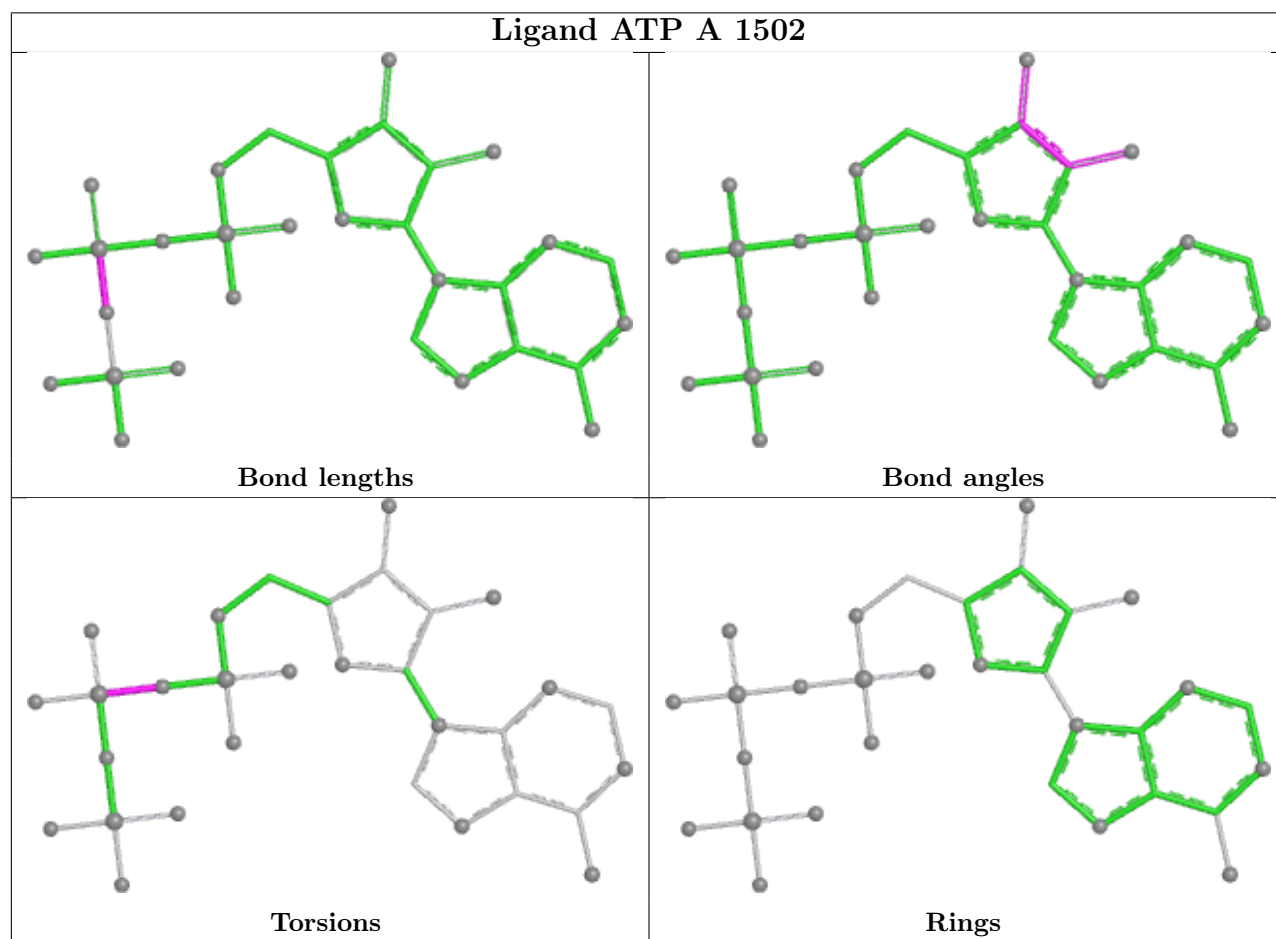
Mol	Chain	Res	Type	Atoms
8	A	1502	ATP	PA-O3A-PB-O2B
8	O	1502	ATP	PA-O3A-PB-O2B
8	B	1502	ATP	PA-O3A-PB-O1B
8	B	1502	ATP	PA-O3A-PB-O2B
8	P	1502	ATP	PA-O3A-PB-O1B
8	P	1502	ATP	PA-O3A-PB-O2B
8	A	1502	ATP	PA-O3A-PB-O1B
8	O	1502	ATP	PA-O3A-PB-O1B

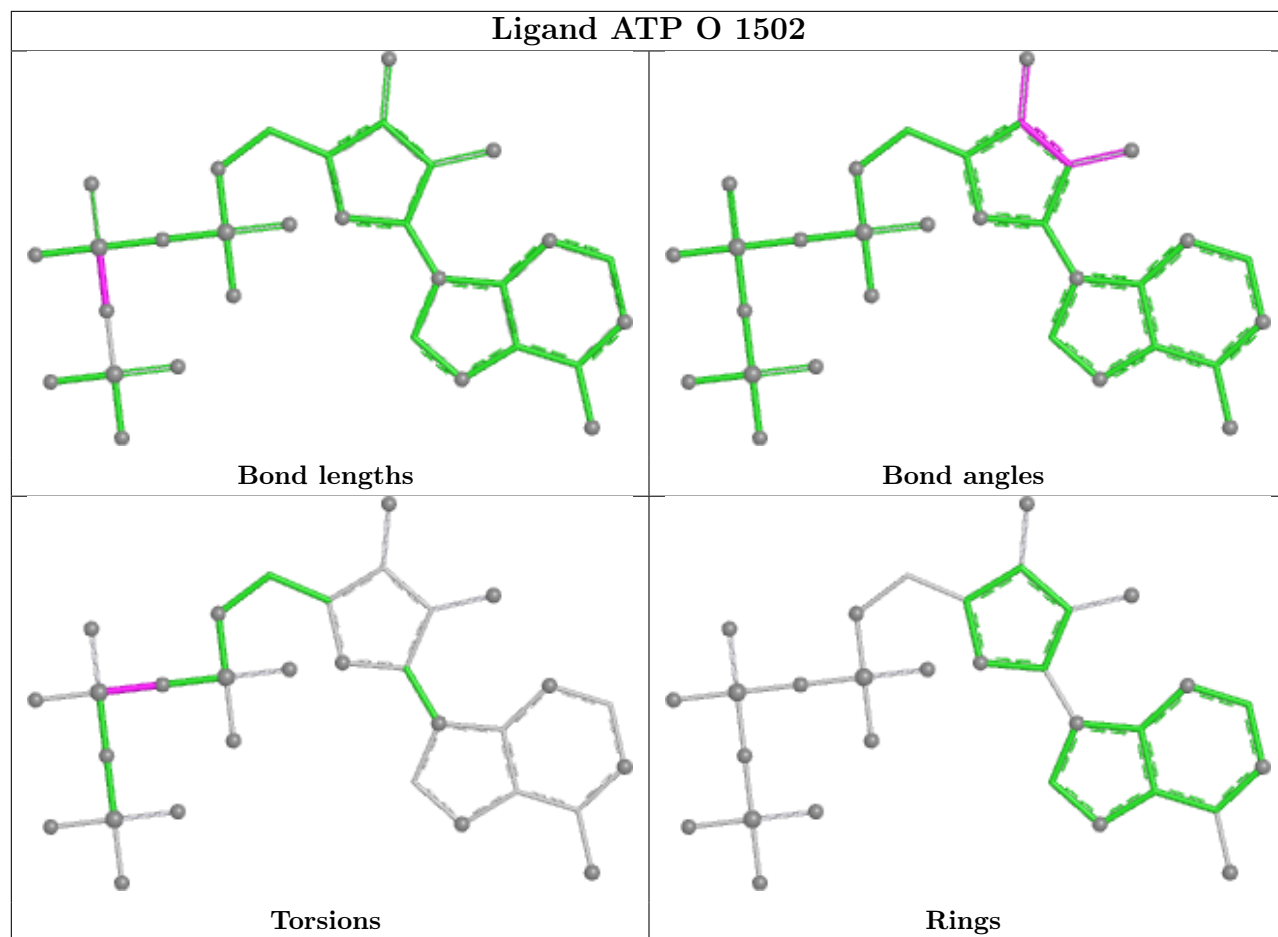
There are no ring outliers.

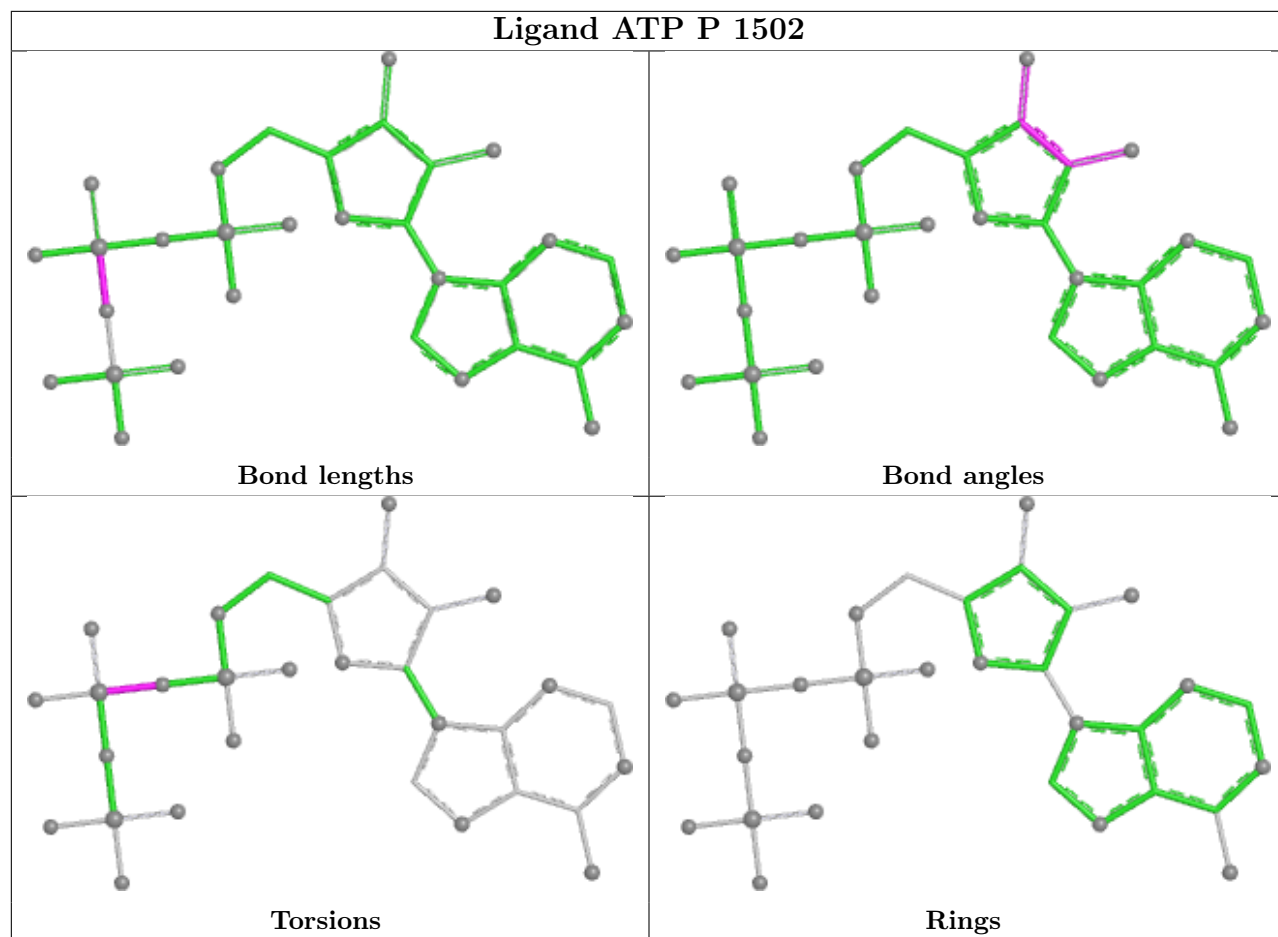
No monomer is involved in short contacts.

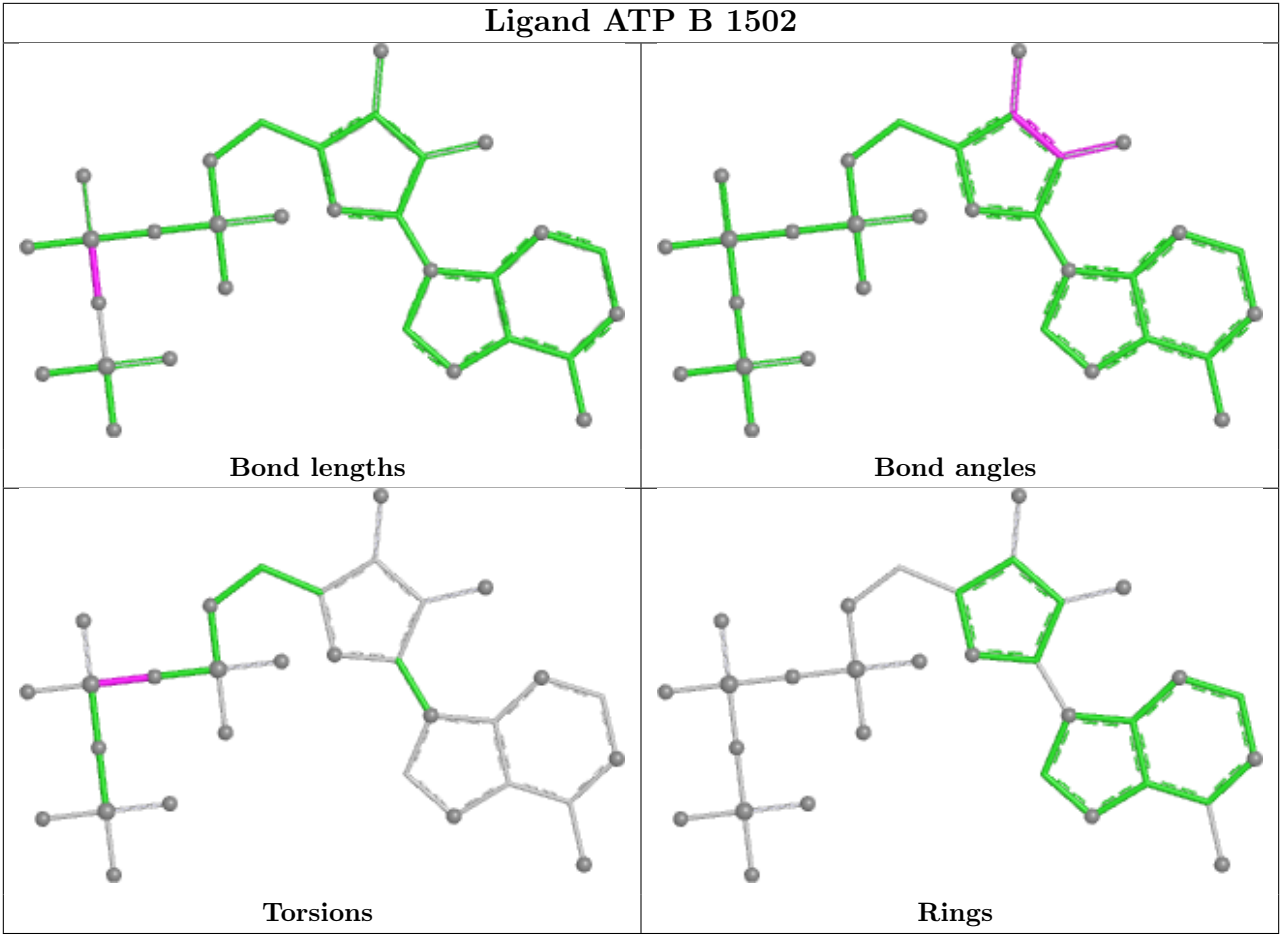
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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

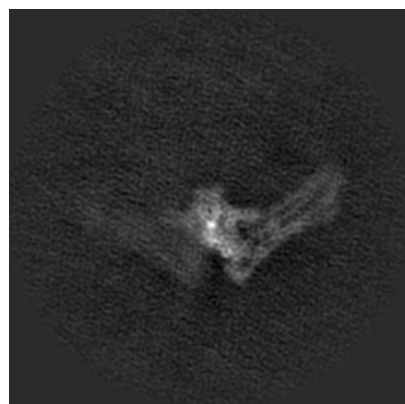
6 Map visualisation [i](#)

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.

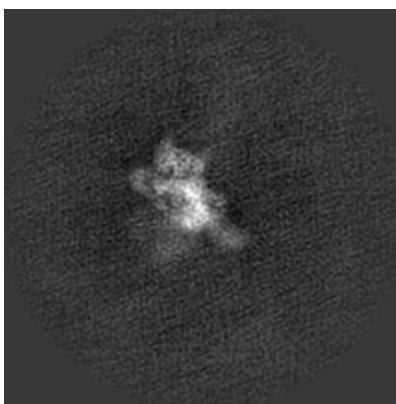
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

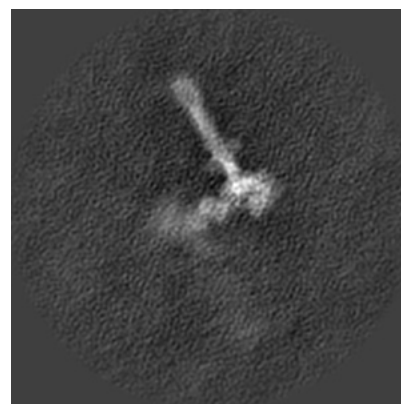
6.1.1 Primary map



X

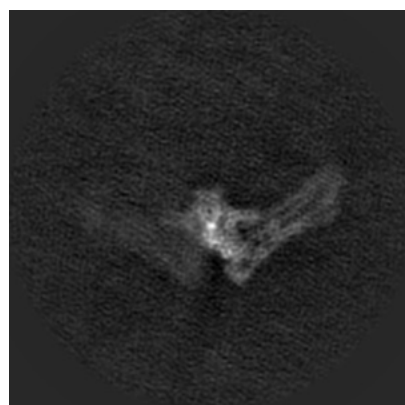


Y

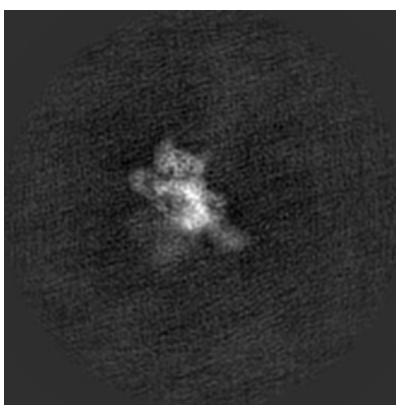


Z

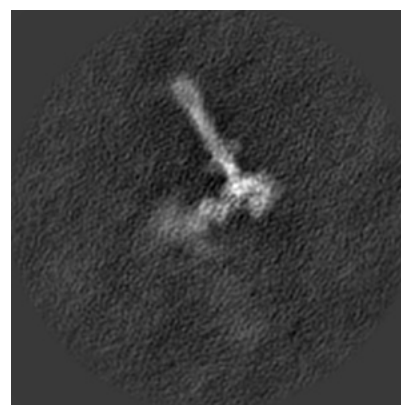
6.1.2 Raw map



X



Y

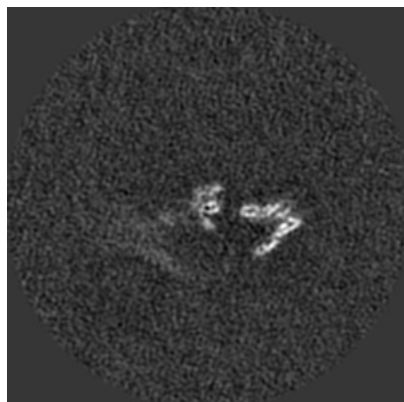


Z

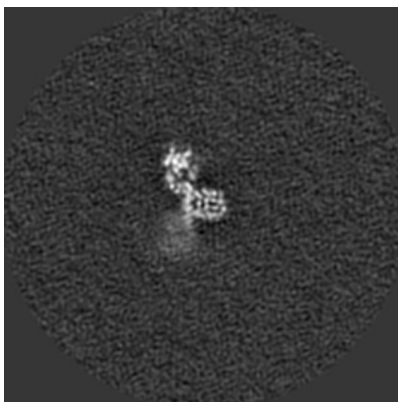
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

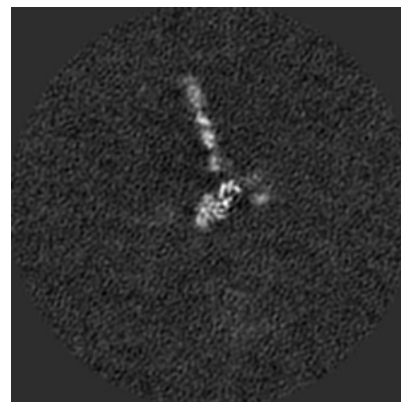
6.2.1 Primary map



X Index: 83

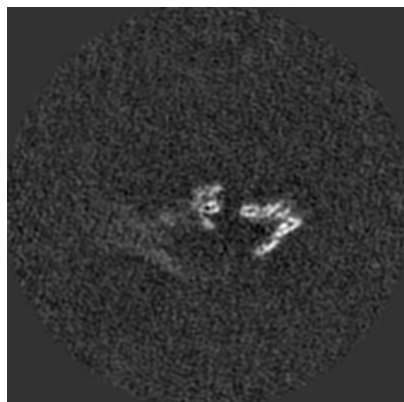


Y Index: 83

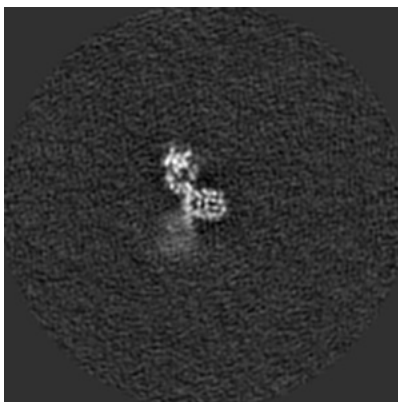


Z Index: 83

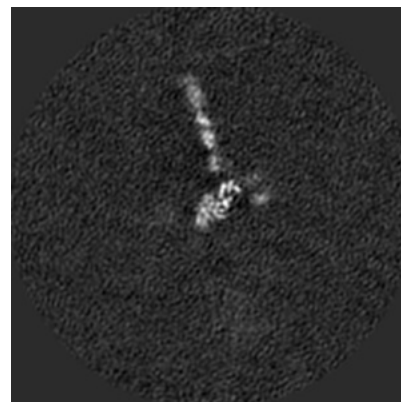
6.2.2 Raw map



X Index: 83



Y Index: 83

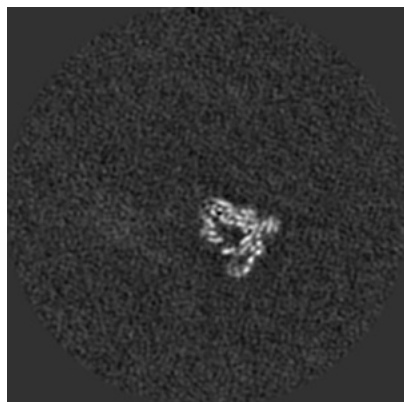


Z Index: 83

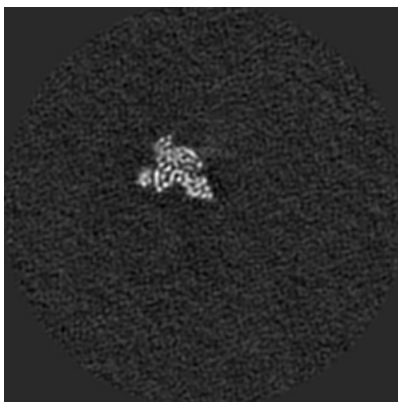
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

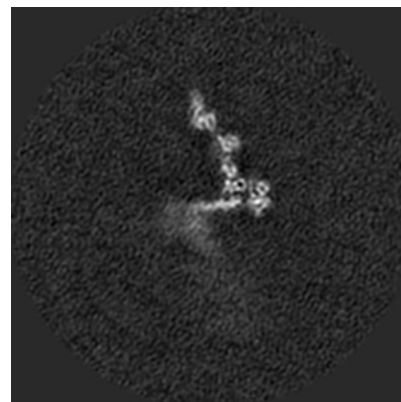
6.3.1 Primary map



X Index: 90

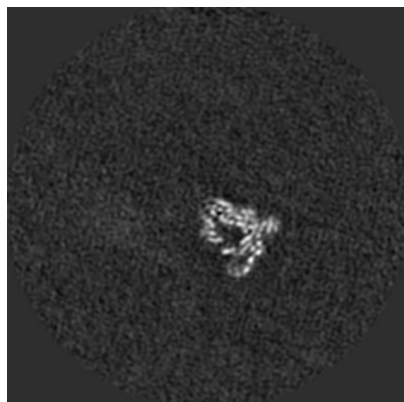


Y Index: 90

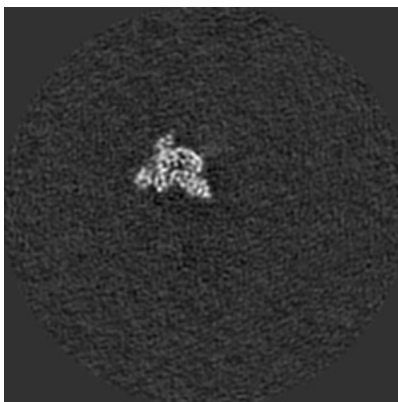


Z Index: 76

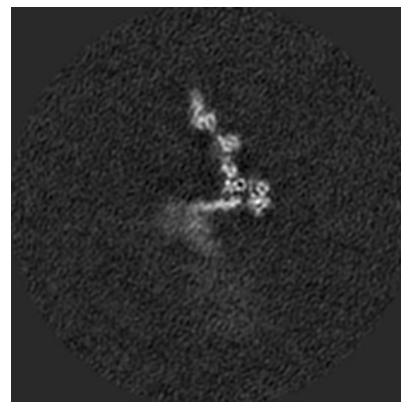
6.3.2 Raw map



X Index: 90



Y Index: 91

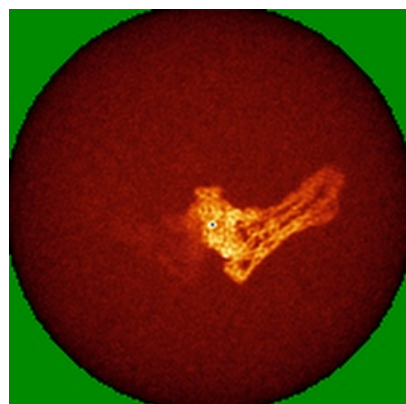


Z Index: 76

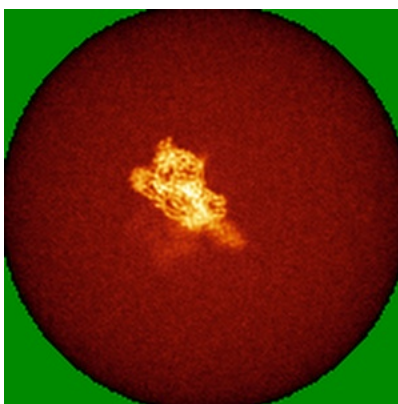
The images above show the largest variance slices of the map in three orthogonal directions.

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

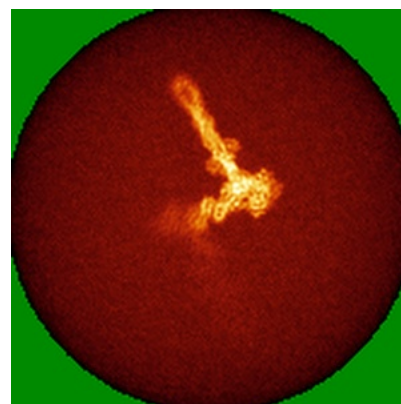
6.4.1 Primary map



X

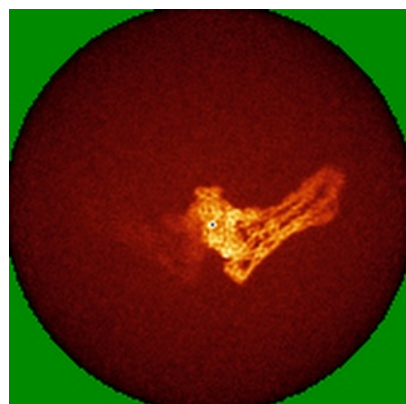


Y

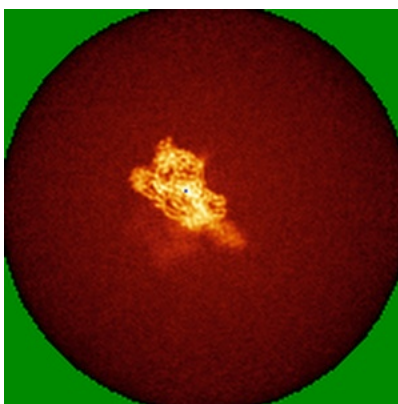


Z

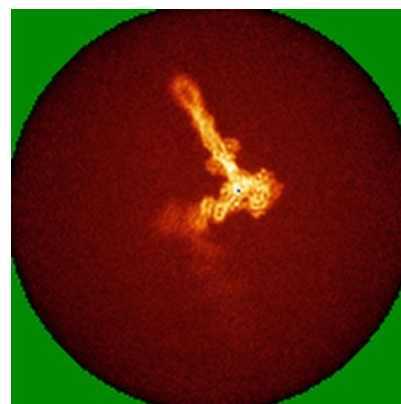
6.4.2 Raw map



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.

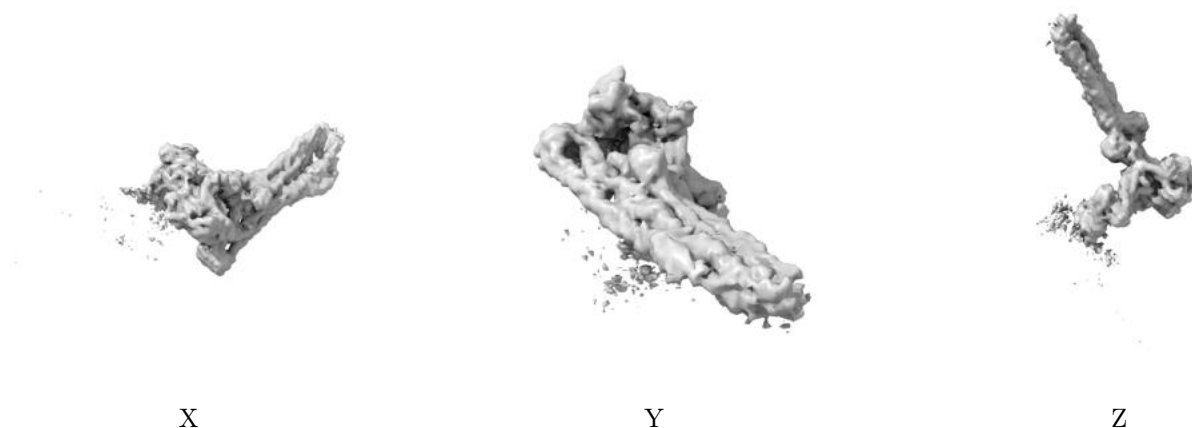
6.5 Orthogonal surface views [i](#)

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.

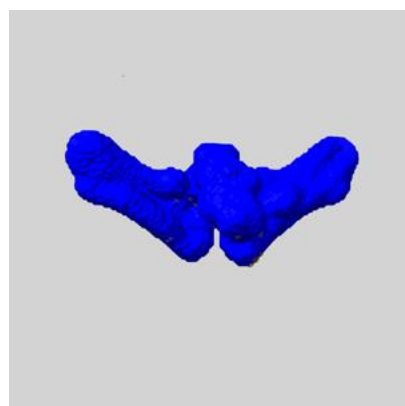
6.6 Mask visualisation [i](#)

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

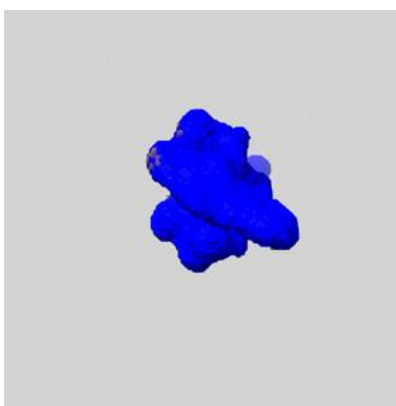
A mask typically either:

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

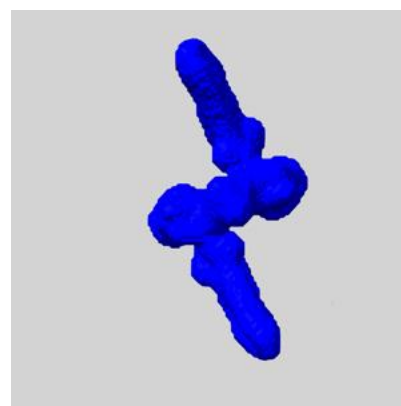
6.6.1 emd_51446_msk_1.map [i](#)



X



Y

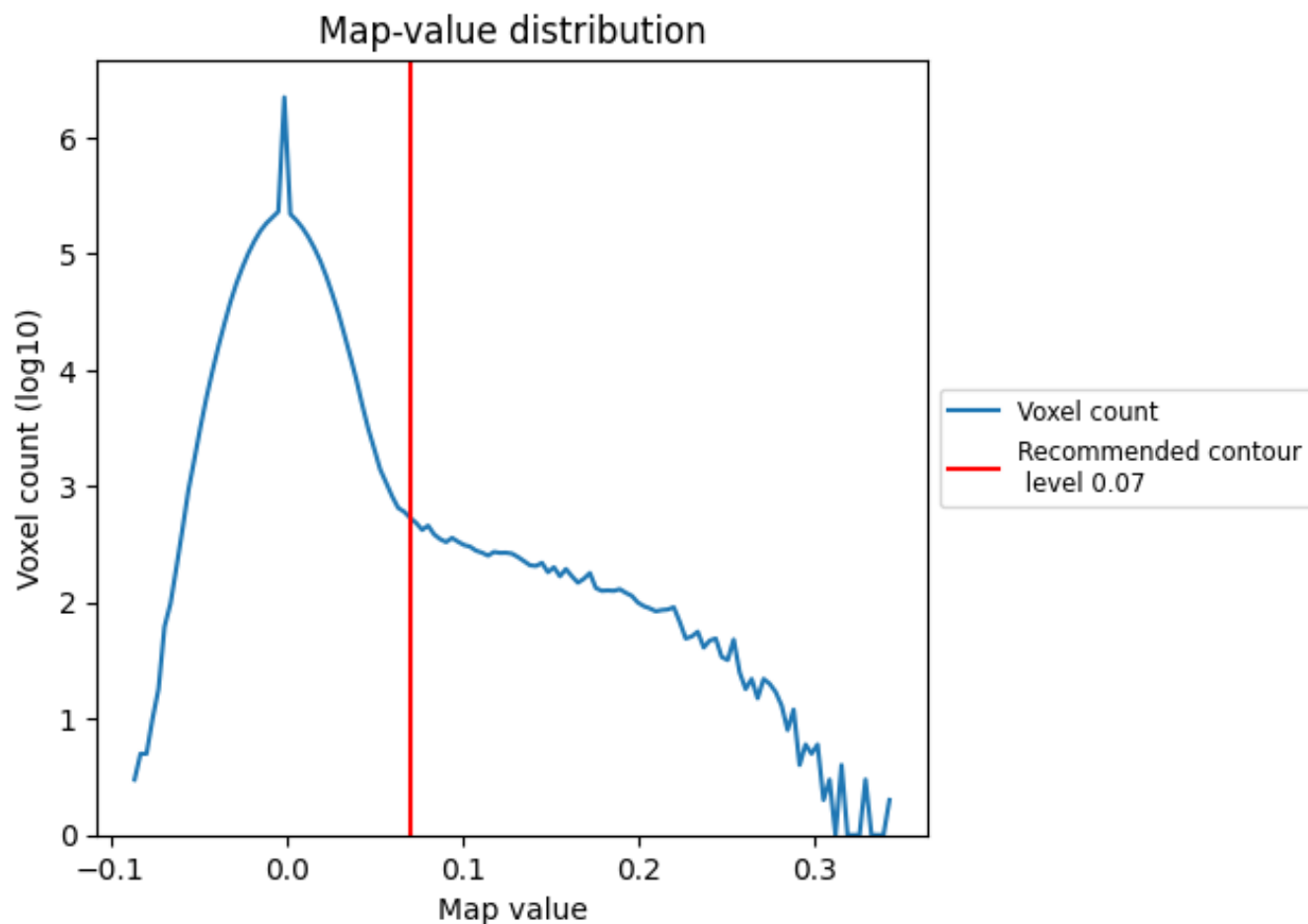


Z

7 Map analysis [i](#)

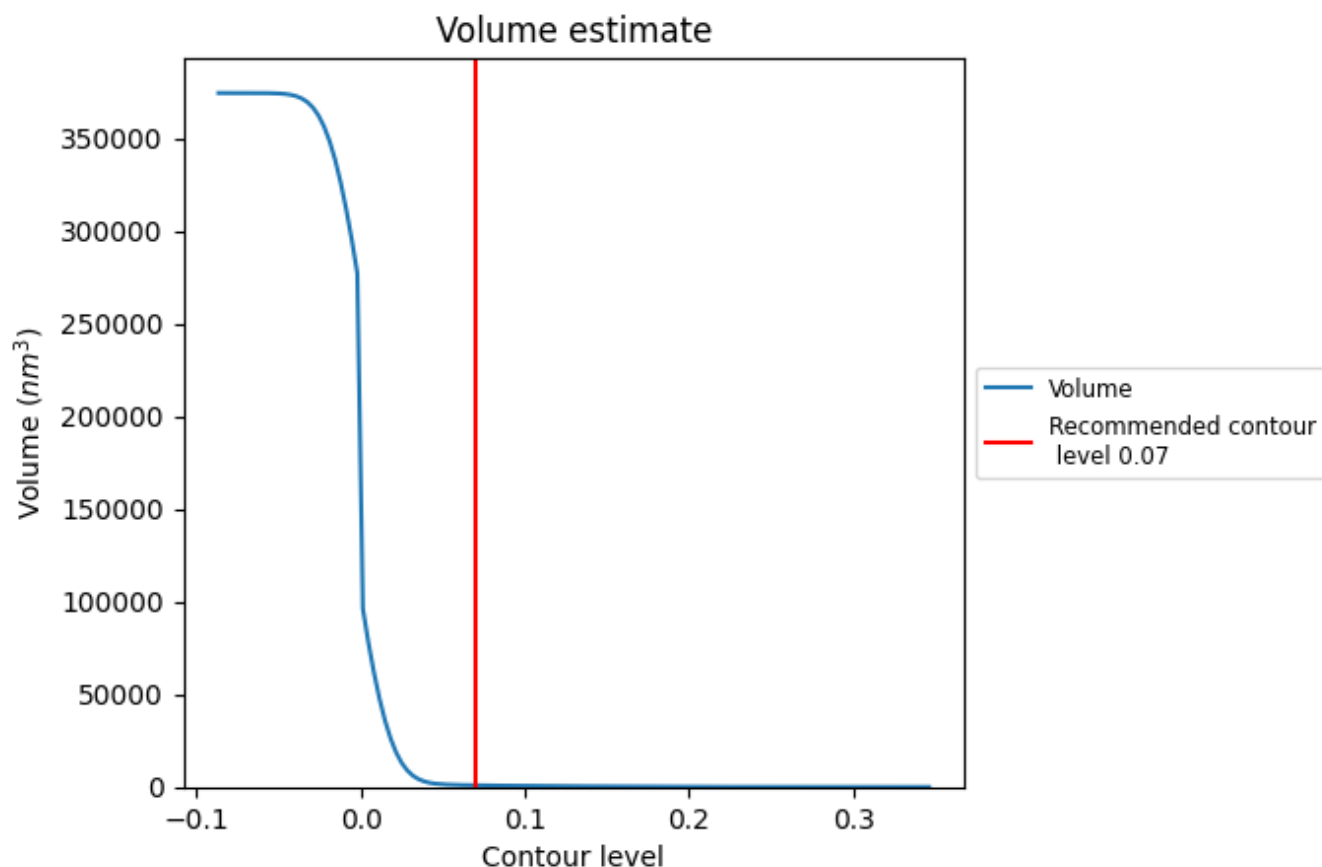
This section contains the results of statistical analysis of the map.

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.

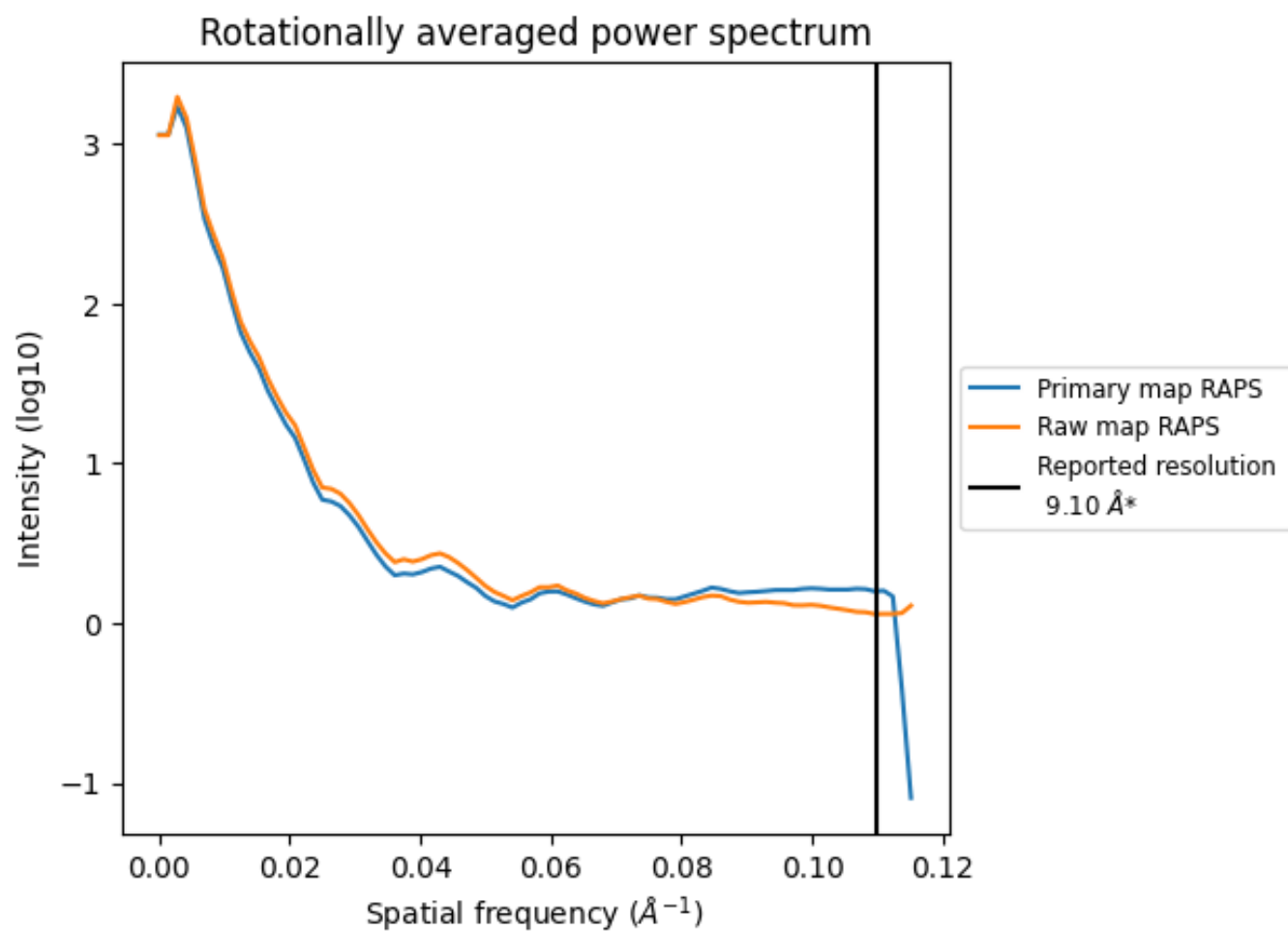
7.2 Volume estimate [i](#)



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](#)

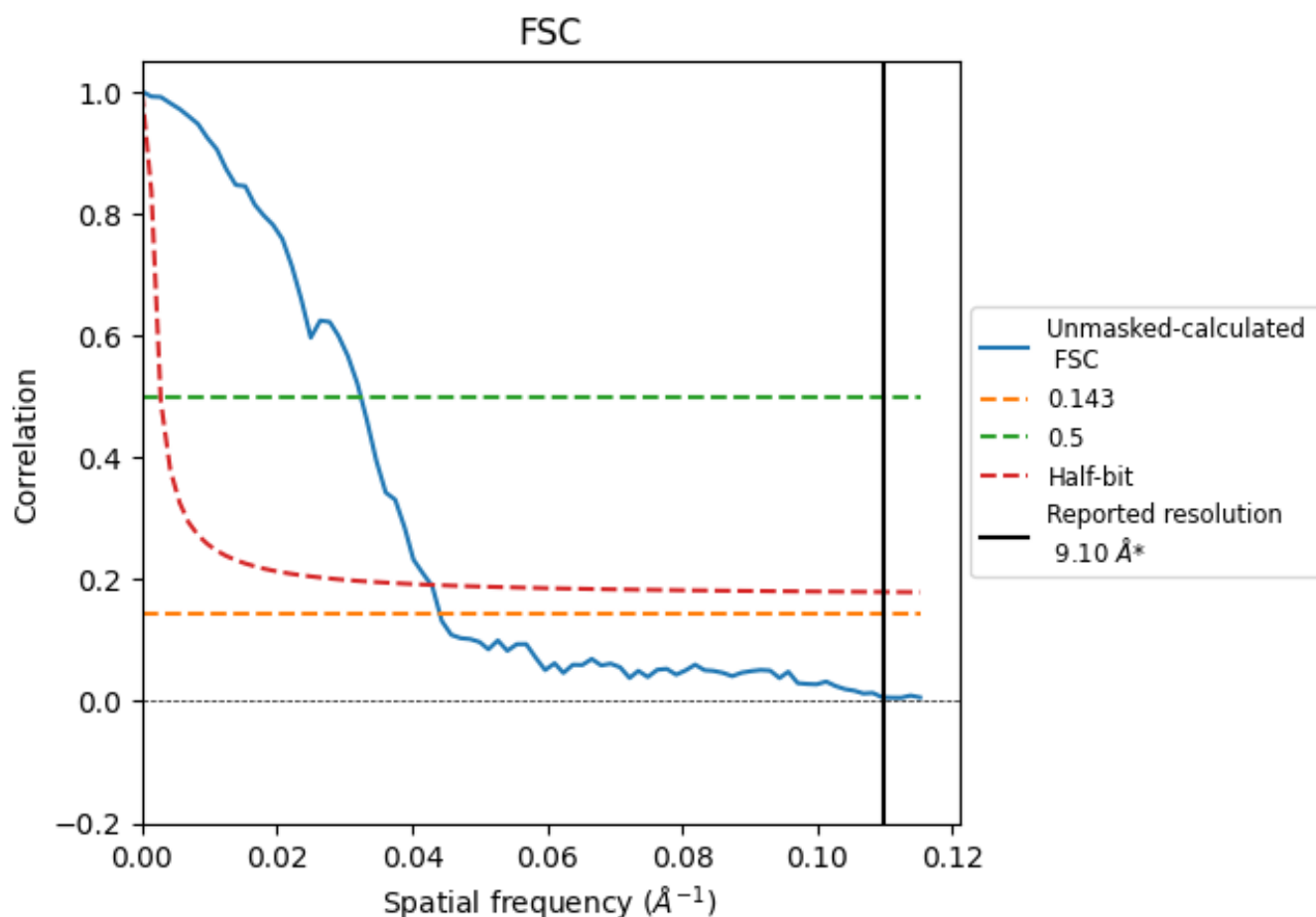


*Reported resolution corresponds to spatial frequency of $0.110 \text{ \AA}^{-1}$

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 $0.110 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

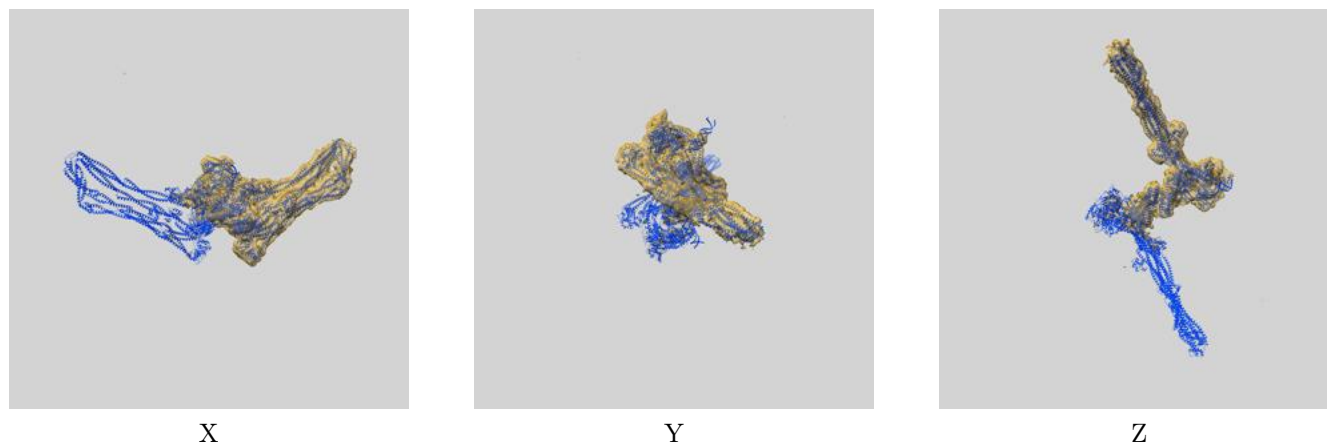
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	22.68	30.86	23.36

*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](#)

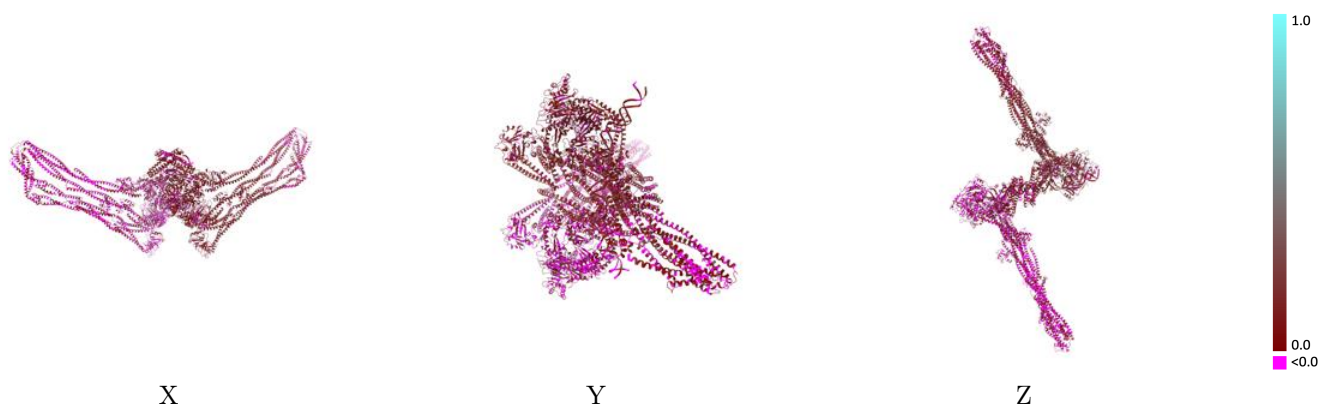
This section contains information regarding the fit between EMDB map EMD-51446 and PDB model 9GMA. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



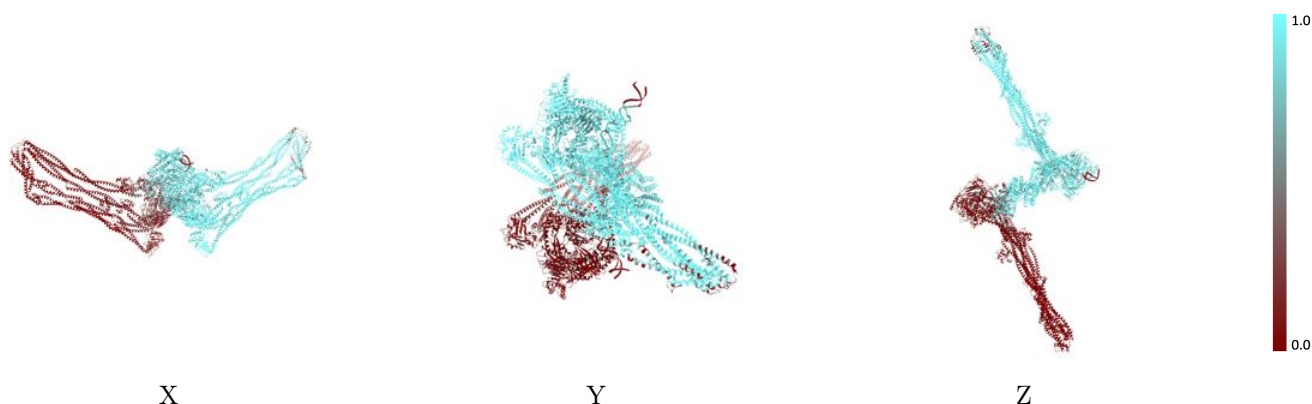
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



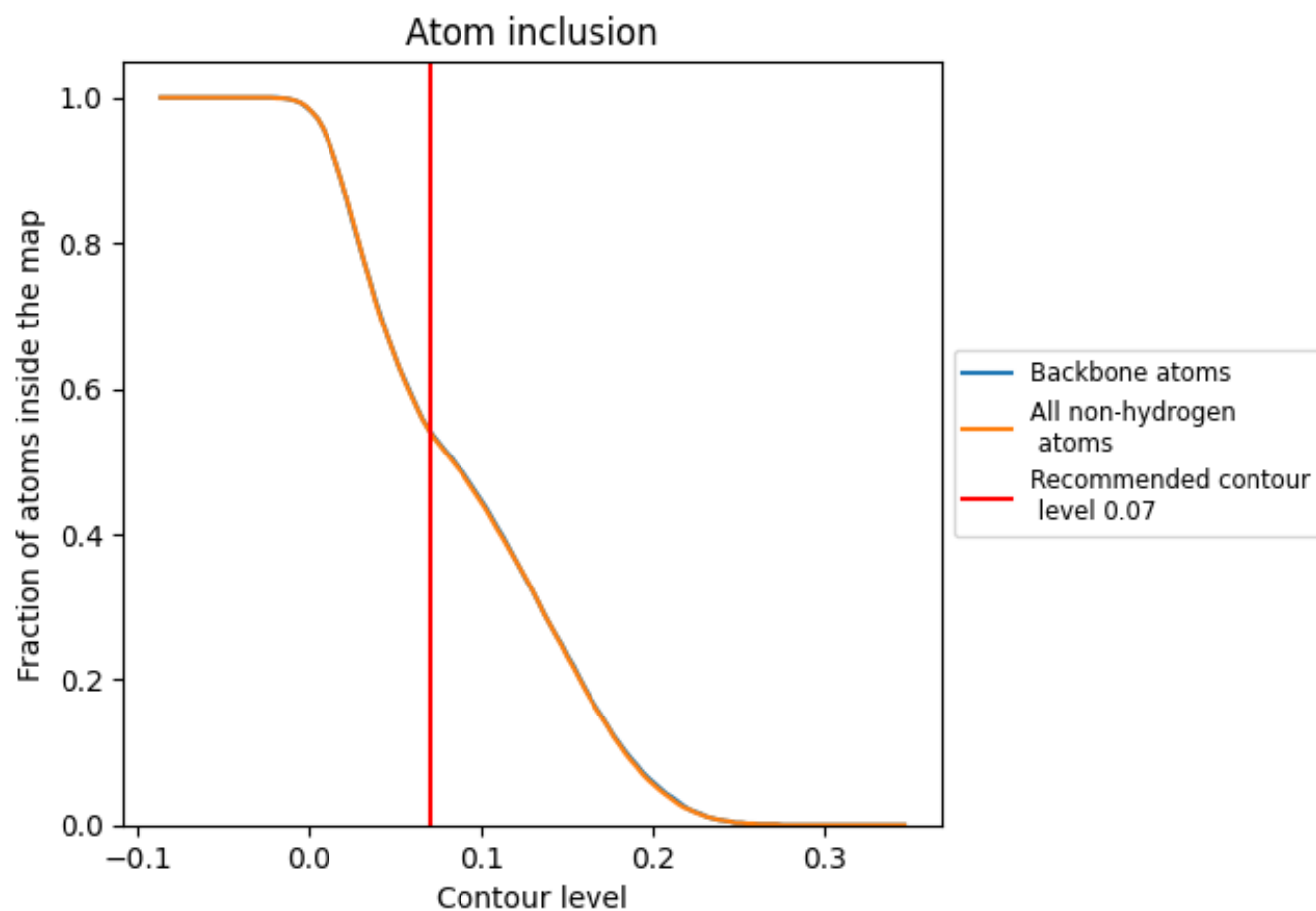
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

1.0

0.0

<0.0