



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 09:05 PM UTC

PDB ID : 7RZA / pdb_00007rza
EMDB ID : EMD-24756
Title : Structure of the complex of AMPA receptor GluA2 with auxiliary subunit GSG1L bound to agonist quisqualate
Authors : Gangwar, S.P.; Klykov, O.V.; Yelshanskaya, M.V.; Sobolevsky, A.I.
Deposited on : 2021-08-27
Resolution : 4.26 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:

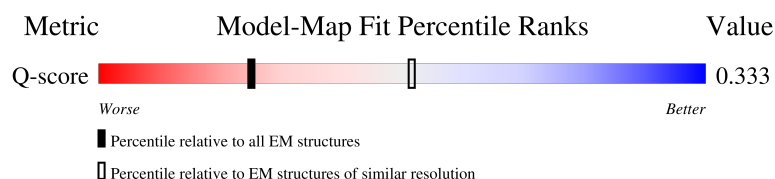
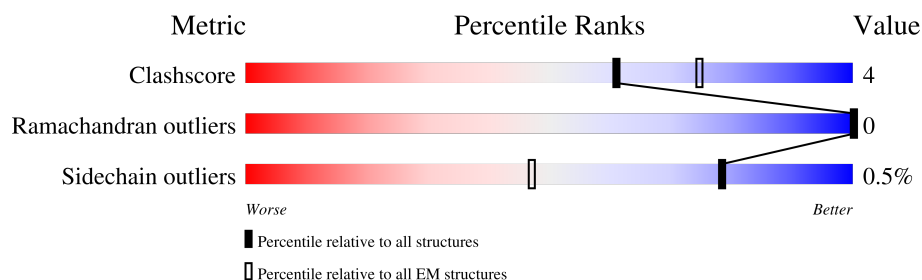
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 4.26 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	4601 (3.76 - 4.76)

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	1154	7% 73% 12% 15%
1	B	1154	5% 60% 8% 32%
1	C	1154	7% 72% 12% 15%
1	D	1154	6% 60% 8% 32%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27850 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	981	Total	C	N	O	S	0	0
			7713	4964	1276	1431	42		
1	B	785	Total	C	N	O	S	0	0
			6186	3973	1027	1156	30		
1	C	981	Total	C	N	O	S	0	0
			7713	4964	1276	1431	42		
1	D	785	Total	C	N	O	S	0	0
			6186	3973	1027	1156	30		

There are 1428 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	744	THR	ASN	conflict	UNP P19491
A	745	PRO	ALA	conflict	UNP P19491
A	754	SER	ASN	conflict	UNP P19491
A	758	VAL	LEU	conflict	UNP P19491
A	775	ALA	SER	conflict	UNP P19491
A	776	LYS	GLY	conflict	UNP P19491
A	777	ASP	GLY	conflict	UNP P19491
A	778	SER	GLY	conflict	UNP P19491
A	779	GLY	ASP	conflict	UNP P19491
A	999	GLY	-	expression tag	UNP P19491
A	1000	THR	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1001	GLY	-	expression tag	UNP P19491
A	1002	LYS	-	expression tag	UNP P19491
A	1003	THR	-	expression tag	UNP P19491
A	1004	SER	-	expression tag	UNP P19491
A	1005	ARG	-	expression tag	UNP P19491
A	1006	ARG	-	expression tag	UNP P19491
A	1007	GLY	-	expression tag	UNP P19491
A	1008	ARG	-	expression tag	UNP P19491
A	1009	ALA	-	expression tag	UNP P19491
A	1010	LEU	-	expression tag	UNP P19491
A	1011	LEU	-	expression tag	UNP P19491
A	1012	ALA	-	expression tag	UNP P19491
A	1013	VAL	-	expression tag	UNP P19491
A	1014	ALA	-	expression tag	UNP P19491
A	1015	LEU	-	expression tag	UNP P19491
A	1016	ASN	-	expression tag	UNP P19491
A	1017	LEU	-	expression tag	UNP P19491
A	1018	LEU	-	expression tag	UNP P19491
A	1019	ALA	-	expression tag	UNP P19491
A	1020	LEU	-	expression tag	UNP P19491
A	1021	LEU	-	expression tag	UNP P19491
A	1022	PHE	-	expression tag	UNP P19491
A	1023	ALA	-	expression tag	UNP P19491
A	1024	THR	-	expression tag	UNP P19491
A	1025	THR	-	expression tag	UNP P19491
A	1026	ALA	-	expression tag	UNP P19491
A	1027	PHE	-	expression tag	UNP P19491
A	1028	LEU	-	expression tag	UNP P19491
A	1029	THR	-	expression tag	UNP P19491
A	1030	THR	-	expression tag	UNP P19491
A	1031	TYR	-	expression tag	UNP P19491
A	1032	TRP	-	expression tag	UNP P19491
A	1033	CYS	-	expression tag	UNP P19491
A	1034	GLN	-	expression tag	UNP P19491
A	1035	GLY	-	expression tag	UNP P19491
A	1036	THR	-	expression tag	UNP P19491
A	1037	GLN	-	expression tag	UNP P19491
A	1038	ARG	-	expression tag	UNP P19491
A	1039	VAL	-	expression tag	UNP P19491
A	1040	PRO	-	expression tag	UNP P19491
A	1041	LYS	-	expression tag	UNP P19491
A	1042	PRO	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1043	GLY	-	expression tag	UNP P19491
A	1044	CYS	-	expression tag	UNP P19491
A	1045	GLY	-	expression tag	UNP P19491
A	1046	GLN	-	expression tag	UNP P19491
A	1047	GLY	-	expression tag	UNP P19491
A	1048	GLY	-	expression tag	UNP P19491
A	1049	GLY	-	expression tag	UNP P19491
A	1050	ALA	-	expression tag	UNP P19491
A	1051	ASN	-	expression tag	UNP P19491
A	1052	CYS	-	expression tag	UNP P19491
A	1053	PRO	-	expression tag	UNP P19491
A	1054	ASN	-	expression tag	UNP P19491
A	1055	SER	-	expression tag	UNP P19491
A	1056	GLY	-	expression tag	UNP P19491
A	1057	ALA	-	expression tag	UNP P19491
A	1058	ASN	-	expression tag	UNP P19491
A	1059	ALA	-	expression tag	UNP P19491
A	1060	THR	-	expression tag	UNP P19491
A	1061	ALA	-	expression tag	UNP P19491
A	1062	ASN	-	expression tag	UNP P19491
A	1063	SER	-	expression tag	UNP P19491
A	1064	THR	-	expression tag	UNP P19491
A	1065	ALA	-	expression tag	UNP P19491
A	1066	ALA	-	expression tag	UNP P19491
A	1067	PRO	-	expression tag	UNP P19491
A	1068	VAL	-	expression tag	UNP P19491
A	1069	ALA	-	expression tag	UNP P19491
A	1070	ALA	-	expression tag	UNP P19491
A	1071	SER	-	expression tag	UNP P19491
A	1072	PRO	-	expression tag	UNP P19491
A	1073	ALA	-	expression tag	UNP P19491
A	1074	GLY	-	expression tag	UNP P19491
A	1075	ALA	-	expression tag	UNP P19491
A	1076	PRO	-	expression tag	UNP P19491
A	1077	TYR	-	expression tag	UNP P19491
A	1078	SER	-	expression tag	UNP P19491
A	1079	TRP	-	expression tag	UNP P19491
A	1080	GLU	-	expression tag	UNP P19491
A	1081	ALA	-	expression tag	UNP P19491
A	1082	GLY	-	expression tag	UNP P19491
A	1083	ASP	-	expression tag	UNP P19491
A	1084	GLU	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1085	ARG	-	expression tag	UNP P19491
A	1086	PHE	-	expression tag	UNP P19491
A	1087	GLN	-	expression tag	UNP P19491
A	1088	LEU	-	expression tag	UNP P19491
A	1089	ARG	-	expression tag	UNP P19491
A	1090	ARG	-	expression tag	UNP P19491
A	1091	PHE	-	expression tag	UNP P19491
A	1092	HIS	-	expression tag	UNP P19491
A	1093	THR	-	expression tag	UNP P19491
A	1094	GLY	-	expression tag	UNP P19491
A	1095	ILE	-	expression tag	UNP P19491
A	1096	TRP	-	expression tag	UNP P19491
A	1097	TYR	-	expression tag	UNP P19491
A	1098	SER	-	expression tag	UNP P19491
A	1099	CYS	-	expression tag	UNP P19491
A	1100	GLU	-	expression tag	UNP P19491
A	1101	GLU	-	expression tag	UNP P19491
A	1102	GLU	-	expression tag	UNP P19491
A	1103	LEU	-	expression tag	UNP P19491
A	1104	GLY	-	expression tag	UNP P19491
A	1105	GLY	-	expression tag	UNP P19491
A	1106	PRO	-	expression tag	UNP P19491
A	1107	GLY	-	expression tag	UNP P19491
A	1108	GLU	-	expression tag	UNP P19491
A	1109	LYS	-	expression tag	UNP P19491
A	1110	CYS	-	expression tag	UNP P19491
A	1111	ARG	-	expression tag	UNP P19491
A	1112	SER	-	expression tag	UNP P19491
A	1113	PHE	-	expression tag	UNP P19491
A	1114	ILE	-	expression tag	UNP P19491
A	1115	ASP	-	expression tag	UNP P19491
A	1116	LEU	-	expression tag	UNP P19491
A	1117	ALA	-	expression tag	UNP P19491
A	1118	PRO	-	expression tag	UNP P19491
A	1119	ALA	-	expression tag	UNP P19491
A	1120	SER	-	expression tag	UNP P19491
A	1121	GLU	-	expression tag	UNP P19491
A	1122	LYS	-	expression tag	UNP P19491
A	1123	GLY	-	expression tag	UNP P19491
A	1124	VAL	-	expression tag	UNP P19491
A	1125	LEU	-	expression tag	UNP P19491
A	1126	TRP	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1127	LEU	-	expression tag	UNP P19491
A	1128	SER	-	expression tag	UNP P19491
A	1129	VAL	-	expression tag	UNP P19491
A	1130	VAL	-	expression tag	UNP P19491
A	1131	SER	-	expression tag	UNP P19491
A	1132	GLU	-	expression tag	UNP P19491
A	1133	VAL	-	expression tag	UNP P19491
A	1134	LEU	-	expression tag	UNP P19491
A	1135	TYR	-	expression tag	UNP P19491
A	1136	ILE	-	expression tag	UNP P19491
A	1137	LEU	-	expression tag	UNP P19491
A	1138	LEU	-	expression tag	UNP P19491
A	1139	LEU	-	expression tag	UNP P19491
A	1140	VAL	-	expression tag	UNP P19491
A	1141	VAL	-	expression tag	UNP P19491
A	1142	GLY	-	expression tag	UNP P19491
A	1143	PHE	-	expression tag	UNP P19491
A	1144	SER	-	expression tag	UNP P19491
A	1145	LEU	-	expression tag	UNP P19491
A	1146	MET	-	expression tag	UNP P19491
A	1147	CYS	-	expression tag	UNP P19491
A	1148	LEU	-	expression tag	UNP P19491
A	1149	GLU	-	expression tag	UNP P19491
A	1150	LEU	-	expression tag	UNP P19491
A	1151	LEU	-	expression tag	UNP P19491
A	1152	HIS	-	expression tag	UNP P19491
A	1153	SER	-	expression tag	UNP P19491
A	1154	SER	-	expression tag	UNP P19491
A	1155	SER	-	expression tag	UNP P19491
A	1156	VAL	-	expression tag	UNP P19491
A	1157	ILE	-	expression tag	UNP P19491
A	1158	ASP	-	expression tag	UNP P19491
A	1159	GLY	-	expression tag	UNP P19491
A	1160	LEU	-	expression tag	UNP P19491
A	1161	LYS	-	expression tag	UNP P19491
A	1162	LEU	-	expression tag	UNP P19491
A	1163	ASN	-	expression tag	UNP P19491
A	1164	ALA	-	expression tag	UNP P19491
A	1165	PHE	-	expression tag	UNP P19491
A	1166	ALA	-	expression tag	UNP P19491
A	1167	ALA	-	expression tag	UNP P19491
A	1168	VAL	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1169	PHE	-	expression tag	UNP P19491
A	1170	THR	-	expression tag	UNP P19491
A	1171	VAL	-	expression tag	UNP P19491
A	1172	LEU	-	expression tag	UNP P19491
A	1173	SER	-	expression tag	UNP P19491
A	1174	GLY	-	expression tag	UNP P19491
A	1175	LEU	-	expression tag	UNP P19491
A	1176	LEU	-	expression tag	UNP P19491
A	1177	GLY	-	expression tag	UNP P19491
A	1178	MET	-	expression tag	UNP P19491
A	1179	VAL	-	expression tag	UNP P19491
A	1180	ALA	-	expression tag	UNP P19491
A	1181	HIS	-	expression tag	UNP P19491
A	1182	MET	-	expression tag	UNP P19491
A	1183	MET	-	expression tag	UNP P19491
A	1184	TYR	-	expression tag	UNP P19491
A	1185	THR	-	expression tag	UNP P19491
A	1186	GLN	-	expression tag	UNP P19491
A	1187	VAL	-	expression tag	UNP P19491
A	1188	PHE	-	expression tag	UNP P19491
A	1189	GLN	-	expression tag	UNP P19491
A	1190	VAL	-	expression tag	UNP P19491
A	1191	THR	-	expression tag	UNP P19491
A	1192	VAL	-	expression tag	UNP P19491
A	1193	SER	-	expression tag	UNP P19491
A	1194	LEU	-	expression tag	UNP P19491
A	1195	GLY	-	expression tag	UNP P19491
A	1196	PRO	-	expression tag	UNP P19491
A	1197	GLU	-	expression tag	UNP P19491
A	1198	ASP	-	expression tag	UNP P19491
A	1199	TRP	-	expression tag	UNP P19491
A	1200	ARG	-	expression tag	UNP P19491
A	1201	PRO	-	expression tag	UNP P19491
A	1202	HIS	-	expression tag	UNP P19491
A	1203	SER	-	expression tag	UNP P19491
A	1204	TRP	-	expression tag	UNP P19491
A	1205	ASP	-	expression tag	UNP P19491
A	1206	TYR	-	expression tag	UNP P19491
A	1207	GLY	-	expression tag	UNP P19491
A	1208	TRP	-	expression tag	UNP P19491
A	1209	SER	-	expression tag	UNP P19491
A	1210	PHE	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1211	CYS	-	expression tag	UNP P19491
A	1212	LEU	-	expression tag	UNP P19491
A	1213	ALA	-	expression tag	UNP P19491
A	1214	TRP	-	expression tag	UNP P19491
A	1215	GLY	-	expression tag	UNP P19491
A	1216	SER	-	expression tag	UNP P19491
A	1217	PHE	-	expression tag	UNP P19491
A	1218	THR	-	expression tag	UNP P19491
A	1219	CYS	-	expression tag	UNP P19491
A	1220	CYS	-	expression tag	UNP P19491
A	1221	MET	-	expression tag	UNP P19491
A	1222	ALA	-	expression tag	UNP P19491
A	1223	ALA	-	expression tag	UNP P19491
A	1224	SER	-	expression tag	UNP P19491
A	1225	VAL	-	expression tag	UNP P19491
A	1226	THR	-	expression tag	UNP P19491
A	1227	THR	-	expression tag	UNP P19491
A	1228	LEU	-	expression tag	UNP P19491
A	1229	ASN	-	expression tag	UNP P19491
A	1230	SER	-	expression tag	UNP P19491
A	1231	TYR	-	expression tag	UNP P19491
A	1232	THR	-	expression tag	UNP P19491
A	1233	LYS	-	expression tag	UNP P19491
A	1234	THR	-	expression tag	UNP P19491
A	1235	VAL	-	expression tag	UNP P19491
A	1236	ILE	-	expression tag	UNP P19491
A	1237	GLU	-	expression tag	UNP P19491
A	1238	PHE	-	expression tag	UNP P19491
A	1239	ARG	-	expression tag	UNP P19491
A	1240	HIS	-	expression tag	UNP P19491
A	1241	LYS	-	expression tag	UNP P19491
A	1242	ARG	-	expression tag	UNP P19491
A	1243	LYS	-	expression tag	UNP P19491
A	1244	VAL	-	expression tag	UNP P19491
A	1245	PHE	-	expression tag	UNP P19491
A	1246	GLU	-	expression tag	UNP P19491
A	1247	GLN	-	expression tag	UNP P19491
A	1248	GLY	-	expression tag	UNP P19491
A	1249	TYR	-	expression tag	UNP P19491
A	1250	ARG	-	expression tag	UNP P19491
A	1251	GLU	-	expression tag	UNP P19491
A	1252	GLU	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1253	PRO	-	expression tag	UNP P19491
A	1254	THR	-	expression tag	UNP P19491
A	1255	PHE	-	expression tag	UNP P19491
A	1256	ILE	-	expression tag	UNP P19491
A	1257	ASP	-	expression tag	UNP P19491
A	1258	PRO	-	expression tag	UNP P19491
A	1259	GLU	-	expression tag	UNP P19491
A	1260	ALA	-	expression tag	UNP P19491
A	1261	ILE	-	expression tag	UNP P19491
A	1262	LYS	-	expression tag	UNP P19491
A	1263	TYR	-	expression tag	UNP P19491
A	1264	PHE	-	expression tag	UNP P19491
A	1265	ARG	-	expression tag	UNP P19491
A	1266	GLU	-	expression tag	UNP P19491
A	1267	ARG	-	expression tag	UNP P19491
A	1268	ILE	-	expression tag	UNP P19491
A	1269	GLU	-	expression tag	UNP P19491
A	1270	LYS	-	expression tag	UNP P19491
A	1271	GLY	-	expression tag	UNP P19491
A	1272	ASP	-	expression tag	UNP P19491
A	1273	VAL	-	expression tag	UNP P19491
A	1274	SER	-	expression tag	UNP P19491
A	1275	GLU	-	expression tag	UNP P19491
A	1276	GLU	-	expression tag	UNP P19491
A	1277	GLU	-	expression tag	UNP P19491
A	1278	ASP	-	expression tag	UNP P19491
A	1279	PHE	-	expression tag	UNP P19491
A	1280	ARG	-	expression tag	UNP P19491
A	1281	LEU	-	expression tag	UNP P19491
A	1282	ALA	-	expression tag	UNP P19491
A	1283	CYS	-	expression tag	UNP P19491
A	1284	ARG	-	expression tag	UNP P19491
A	1285	HIS	-	expression tag	UNP P19491
A	1286	GLU	-	expression tag	UNP P19491
A	1287	ARG	-	expression tag	UNP P19491
A	1288	TYR	-	expression tag	UNP P19491
A	1289	PRO	-	expression tag	UNP P19491
A	1290	THR	-	expression tag	UNP P19491
A	1291	ARG	-	expression tag	UNP P19491
A	1292	HIS	-	expression tag	UNP P19491
A	1293	GLN	-	expression tag	UNP P19491
A	1294	PRO	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1295	HIS	-	expression tag	UNP P19491
A	1296	MET	-	expression tag	UNP P19491
A	1297	GLY	-	expression tag	UNP P19491
A	1298	ASP	-	expression tag	UNP P19491
A	1299	SER	-	expression tag	UNP P19491
A	1300	TRP	-	expression tag	UNP P19491
A	1301	PRO	-	expression tag	UNP P19491
A	1302	ARG	-	expression tag	UNP P19491
A	1303	SER	-	expression tag	UNP P19491
A	1304	SER	-	expression tag	UNP P19491
A	1305	ALA	-	expression tag	UNP P19491
A	1306	HIS	-	expression tag	UNP P19491
A	1307	GLU	-	expression tag	UNP P19491
A	1308	ALA	-	expression tag	UNP P19491
A	1309	ALA	-	expression tag	UNP P19491
A	1310	GLU	-	expression tag	UNP P19491
A	1311	LEU	-	expression tag	UNP P19491
A	1312	ASN	-	expression tag	UNP P19491
A	1313	ARG	-	expression tag	UNP P19491
A	1314	GLN	-	expression tag	UNP P19491
A	1315	CYS	-	expression tag	UNP P19491
A	1316	TRP	-	expression tag	UNP P19491
A	1317	VAL	-	expression tag	UNP P19491
A	1318	LEU	-	expression tag	UNP P19491
A	1319	GLY	-	expression tag	UNP P19491
A	1320	HIS	-	expression tag	UNP P19491
A	1321	TRP	-	expression tag	UNP P19491
A	1322	VAL	-	expression tag	UNP P19491
A	1323	GLY	-	expression tag	UNP P19491
A	1324	THR	-	expression tag	UNP P19491
A	1325	GLY	-	expression tag	UNP P19491
A	1326	GLY	-	expression tag	UNP P19491
A	1327	LEU	-	expression tag	UNP P19491
A	1328	VAL	-	expression tag	UNP P19491
A	1329	PRO	-	expression tag	UNP P19491
A	1330	ARG	-	expression tag	UNP P19491
A	1331	GLY	-	expression tag	UNP P19491
A	1332	SER	-	expression tag	UNP P19491
A	1333	ALA	-	expression tag	UNP P19491
A	1334	ALA	-	expression tag	UNP P19491
A	1335	ALA	-	expression tag	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	744	THR	ASN	conflict	UNP P19491
B	745	PRO	ALA	conflict	UNP P19491
B	754	SER	ASN	conflict	UNP P19491
B	758	VAL	LEU	conflict	UNP P19491
B	775	ALA	SER	conflict	UNP P19491
B	776	LYS	GLY	conflict	UNP P19491
B	777	ASP	GLY	conflict	UNP P19491
B	778	SER	GLY	conflict	UNP P19491
B	779	GLY	ASP	conflict	UNP P19491
B	827	GLY	-	expression tag	UNP P19491
B	828	THR	-	expression tag	UNP P19491
B	829	GLY	-	expression tag	UNP P19491
B	830	LYS	-	expression tag	UNP P19491
B	831	THR	-	expression tag	UNP P19491
B	832	SER	-	expression tag	UNP P19491
B	833	ARG	-	expression tag	UNP P19491
B	834	ARG	-	expression tag	UNP P19491
B	835	GLY	-	expression tag	UNP P19491
B	836	ARG	-	expression tag	UNP P19491
B	837	ALA	-	expression tag	UNP P19491
B	838	LEU	-	expression tag	UNP P19491
B	839	LEU	-	expression tag	UNP P19491
B	840	ALA	-	expression tag	UNP P19491
B	841	VAL	-	expression tag	UNP P19491
B	842	ALA	-	expression tag	UNP P19491
B	843	LEU	-	expression tag	UNP P19491
B	844	ASN	-	expression tag	UNP P19491
B	845	LEU	-	expression tag	UNP P19491
B	846	LEU	-	expression tag	UNP P19491
B	847	ALA	-	expression tag	UNP P19491
B	848	LEU	-	expression tag	UNP P19491
B	849	LEU	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	850	PHE	-	expression tag	UNP P19491
B	851	ALA	-	expression tag	UNP P19491
B	852	THR	-	expression tag	UNP P19491
B	853	THR	-	expression tag	UNP P19491
B	854	ALA	-	expression tag	UNP P19491
B	855	PHE	-	expression tag	UNP P19491
B	856	LEU	-	expression tag	UNP P19491
B	857	THR	-	expression tag	UNP P19491
B	858	THR	-	expression tag	UNP P19491
B	859	TYR	-	expression tag	UNP P19491
B	860	TRP	-	expression tag	UNP P19491
B	861	CYS	-	expression tag	UNP P19491
B	862	GLN	-	expression tag	UNP P19491
B	863	GLY	-	expression tag	UNP P19491
B	864	THR	-	expression tag	UNP P19491
B	865	GLN	-	expression tag	UNP P19491
B	866	ARG	-	expression tag	UNP P19491
B	867	VAL	-	expression tag	UNP P19491
B	868	PRO	-	expression tag	UNP P19491
B	869	LYS	-	expression tag	UNP P19491
B	870	PRO	-	expression tag	UNP P19491
B	871	GLY	-	expression tag	UNP P19491
B	872	CYS	-	expression tag	UNP P19491
B	873	GLY	-	expression tag	UNP P19491
B	874	GLN	-	expression tag	UNP P19491
B	875	GLY	-	expression tag	UNP P19491
B	876	GLY	-	expression tag	UNP P19491
B	877	GLY	-	expression tag	UNP P19491
B	878	ALA	-	expression tag	UNP P19491
B	879	ASN	-	expression tag	UNP P19491
B	880	CYS	-	expression tag	UNP P19491
B	881	PRO	-	expression tag	UNP P19491
B	882	ASN	-	expression tag	UNP P19491
B	883	SER	-	expression tag	UNP P19491
B	884	GLY	-	expression tag	UNP P19491
B	885	ALA	-	expression tag	UNP P19491
B	886	ASN	-	expression tag	UNP P19491
B	887	ALA	-	expression tag	UNP P19491
B	888	THR	-	expression tag	UNP P19491
B	889	ALA	-	expression tag	UNP P19491
B	890	ASN	-	expression tag	UNP P19491
B	891	SER	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	892	THR	-	expression tag	UNP P19491
B	893	ALA	-	expression tag	UNP P19491
B	894	ALA	-	expression tag	UNP P19491
B	895	PRO	-	expression tag	UNP P19491
B	896	VAL	-	expression tag	UNP P19491
B	897	ALA	-	expression tag	UNP P19491
B	898	ALA	-	expression tag	UNP P19491
B	899	SER	-	expression tag	UNP P19491
B	900	PRO	-	expression tag	UNP P19491
B	901	ALA	-	expression tag	UNP P19491
B	902	GLY	-	expression tag	UNP P19491
B	903	ALA	-	expression tag	UNP P19491
B	904	PRO	-	expression tag	UNP P19491
B	905	TYR	-	expression tag	UNP P19491
B	906	SER	-	expression tag	UNP P19491
B	907	TRP	-	expression tag	UNP P19491
B	908	GLU	-	expression tag	UNP P19491
B	909	ALA	-	expression tag	UNP P19491
B	910	GLY	-	expression tag	UNP P19491
B	911	ASP	-	expression tag	UNP P19491
B	912	GLU	-	expression tag	UNP P19491
B	913	ARG	-	expression tag	UNP P19491
B	914	PHE	-	expression tag	UNP P19491
B	915	GLN	-	expression tag	UNP P19491
B	916	LEU	-	expression tag	UNP P19491
B	917	ARG	-	expression tag	UNP P19491
B	918	ARG	-	expression tag	UNP P19491
B	919	PHE	-	expression tag	UNP P19491
B	920	HIS	-	expression tag	UNP P19491
B	921	THR	-	expression tag	UNP P19491
B	922	GLY	-	expression tag	UNP P19491
B	923	ILE	-	expression tag	UNP P19491
B	924	TRP	-	expression tag	UNP P19491
B	925	TYR	-	expression tag	UNP P19491
B	926	SER	-	expression tag	UNP P19491
B	927	CYS	-	expression tag	UNP P19491
B	928	GLU	-	expression tag	UNP P19491
B	929	GLU	-	expression tag	UNP P19491
B	930	GLU	-	expression tag	UNP P19491
B	931	LEU	-	expression tag	UNP P19491
B	932	GLY	-	expression tag	UNP P19491
B	933	GLY	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	934	PRO	-	expression tag	UNP P19491
B	935	GLY	-	expression tag	UNP P19491
B	936	GLU	-	expression tag	UNP P19491
B	937	LYS	-	expression tag	UNP P19491
B	938	CYS	-	expression tag	UNP P19491
B	939	ARG	-	expression tag	UNP P19491
B	940	SER	-	expression tag	UNP P19491
B	941	PHE	-	expression tag	UNP P19491
B	942	ILE	-	expression tag	UNP P19491
B	943	ASP	-	expression tag	UNP P19491
B	944	LEU	-	expression tag	UNP P19491
B	945	ALA	-	expression tag	UNP P19491
B	946	PRO	-	expression tag	UNP P19491
B	947	ALA	-	expression tag	UNP P19491
B	948	SER	-	expression tag	UNP P19491
B	949	GLU	-	expression tag	UNP P19491
B	950	LYS	-	expression tag	UNP P19491
B	951	GLY	-	expression tag	UNP P19491
B	952	VAL	-	expression tag	UNP P19491
B	953	LEU	-	expression tag	UNP P19491
B	954	TRP	-	expression tag	UNP P19491
B	955	LEU	-	expression tag	UNP P19491
B	956	SER	-	expression tag	UNP P19491
B	957	VAL	-	expression tag	UNP P19491
B	958	VAL	-	expression tag	UNP P19491
B	959	SER	-	expression tag	UNP P19491
B	960	GLU	-	expression tag	UNP P19491
B	961	VAL	-	expression tag	UNP P19491
B	962	LEU	-	expression tag	UNP P19491
B	963	TYR	-	expression tag	UNP P19491
B	964	ILE	-	expression tag	UNP P19491
B	965	LEU	-	expression tag	UNP P19491
B	966	LEU	-	expression tag	UNP P19491
B	967	LEU	-	expression tag	UNP P19491
B	968	VAL	-	expression tag	UNP P19491
B	969	VAL	-	expression tag	UNP P19491
B	970	GLY	-	expression tag	UNP P19491
B	971	PHE	-	expression tag	UNP P19491
B	972	SER	-	expression tag	UNP P19491
B	973	LEU	-	expression tag	UNP P19491
B	974	MET	-	expression tag	UNP P19491
B	975	CYS	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	976	LEU	-	expression tag	UNP P19491
B	977	GLU	-	expression tag	UNP P19491
B	978	LEU	-	expression tag	UNP P19491
B	979	LEU	-	expression tag	UNP P19491
B	980	HIS	-	expression tag	UNP P19491
B	981	SER	-	expression tag	UNP P19491
B	982	SER	-	expression tag	UNP P19491
B	983	SER	-	expression tag	UNP P19491
B	984	VAL	-	expression tag	UNP P19491
B	985	ILE	-	expression tag	UNP P19491
B	986	ASP	-	expression tag	UNP P19491
B	987	GLY	-	expression tag	UNP P19491
B	988	LEU	-	expression tag	UNP P19491
B	989	LYS	-	expression tag	UNP P19491
B	990	LEU	-	expression tag	UNP P19491
B	991	ASN	-	expression tag	UNP P19491
B	992	ALA	-	expression tag	UNP P19491
B	993	PHE	-	expression tag	UNP P19491
B	994	ALA	-	expression tag	UNP P19491
B	995	ALA	-	expression tag	UNP P19491
B	996	VAL	-	expression tag	UNP P19491
B	997	PHE	-	expression tag	UNP P19491
B	998	THR	-	expression tag	UNP P19491
B	999	VAL	-	expression tag	UNP P19491
B	1000	LEU	-	expression tag	UNP P19491
B	1001	SER	-	expression tag	UNP P19491
B	1002	GLY	-	expression tag	UNP P19491
B	1003	LEU	-	expression tag	UNP P19491
B	1004	LEU	-	expression tag	UNP P19491
B	1005	GLY	-	expression tag	UNP P19491
B	1006	MET	-	expression tag	UNP P19491
B	1007	VAL	-	expression tag	UNP P19491
B	1008	ALA	-	expression tag	UNP P19491
B	1009	HIS	-	expression tag	UNP P19491
B	1010	MET	-	expression tag	UNP P19491
B	1011	MET	-	expression tag	UNP P19491
B	1012	TYR	-	expression tag	UNP P19491
B	1013	THR	-	expression tag	UNP P19491
B	1014	GLN	-	expression tag	UNP P19491
B	1015	VAL	-	expression tag	UNP P19491
B	1016	PHE	-	expression tag	UNP P19491
B	1017	GLN	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1018	VAL	-	expression tag	UNP P19491
B	1019	THR	-	expression tag	UNP P19491
B	1020	VAL	-	expression tag	UNP P19491
B	1021	SER	-	expression tag	UNP P19491
B	1022	LEU	-	expression tag	UNP P19491
B	1023	GLY	-	expression tag	UNP P19491
B	1024	PRO	-	expression tag	UNP P19491
B	1025	GLU	-	expression tag	UNP P19491
B	1026	ASP	-	expression tag	UNP P19491
B	1027	TRP	-	expression tag	UNP P19491
B	1028	ARG	-	expression tag	UNP P19491
B	1029	PRO	-	expression tag	UNP P19491
B	1030	HIS	-	expression tag	UNP P19491
B	1031	SER	-	expression tag	UNP P19491
B	1032	TRP	-	expression tag	UNP P19491
B	1033	ASP	-	expression tag	UNP P19491
B	1034	TYR	-	expression tag	UNP P19491
B	1035	GLY	-	expression tag	UNP P19491
B	1036	TRP	-	expression tag	UNP P19491
B	1037	SER	-	expression tag	UNP P19491
B	1038	PHE	-	expression tag	UNP P19491
B	1039	CYS	-	expression tag	UNP P19491
B	1040	LEU	-	expression tag	UNP P19491
B	1041	ALA	-	expression tag	UNP P19491
B	1042	TRP	-	expression tag	UNP P19491
B	1043	GLY	-	expression tag	UNP P19491
B	1044	SER	-	expression tag	UNP P19491
B	1045	PHE	-	expression tag	UNP P19491
B	1046	THR	-	expression tag	UNP P19491
B	1047	CYS	-	expression tag	UNP P19491
B	1048	CYS	-	expression tag	UNP P19491
B	1049	MET	-	expression tag	UNP P19491
B	1050	ALA	-	expression tag	UNP P19491
B	1051	ALA	-	expression tag	UNP P19491
B	1052	SER	-	expression tag	UNP P19491
B	1053	VAL	-	expression tag	UNP P19491
B	1054	THR	-	expression tag	UNP P19491
B	1055	THR	-	expression tag	UNP P19491
B	1056	LEU	-	expression tag	UNP P19491
B	1057	ASN	-	expression tag	UNP P19491
B	1058	SER	-	expression tag	UNP P19491
B	1059	TYR	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1060	THR	-	expression tag	UNP P19491
B	1061	LYS	-	expression tag	UNP P19491
B	1062	THR	-	expression tag	UNP P19491
B	1063	VAL	-	expression tag	UNP P19491
B	1064	ILE	-	expression tag	UNP P19491
B	1065	GLU	-	expression tag	UNP P19491
B	1066	PHE	-	expression tag	UNP P19491
B	1067	ARG	-	expression tag	UNP P19491
B	1068	HIS	-	expression tag	UNP P19491
B	1069	LYS	-	expression tag	UNP P19491
B	1070	ARG	-	expression tag	UNP P19491
B	1071	LYS	-	expression tag	UNP P19491
B	1072	VAL	-	expression tag	UNP P19491
B	1073	PHE	-	expression tag	UNP P19491
B	1074	GLU	-	expression tag	UNP P19491
B	1075	GLN	-	expression tag	UNP P19491
B	1076	GLY	-	expression tag	UNP P19491
B	1077	TYR	-	expression tag	UNP P19491
B	1078	ARG	-	expression tag	UNP P19491
B	1079	GLU	-	expression tag	UNP P19491
B	1080	GLU	-	expression tag	UNP P19491
B	1081	PRO	-	expression tag	UNP P19491
B	1082	THR	-	expression tag	UNP P19491
B	1083	PHE	-	expression tag	UNP P19491
B	1084	ILE	-	expression tag	UNP P19491
B	1085	ASP	-	expression tag	UNP P19491
B	1086	PRO	-	expression tag	UNP P19491
B	1087	GLU	-	expression tag	UNP P19491
B	1088	ALA	-	expression tag	UNP P19491
B	1089	ILE	-	expression tag	UNP P19491
B	1090	LYS	-	expression tag	UNP P19491
B	1091	TYR	-	expression tag	UNP P19491
B	1092	PHE	-	expression tag	UNP P19491
B	1093	ARG	-	expression tag	UNP P19491
B	1094	GLU	-	expression tag	UNP P19491
B	1095	ARG	-	expression tag	UNP P19491
B	1096	ILE	-	expression tag	UNP P19491
B	1097	GLU	-	expression tag	UNP P19491
B	1098	LYS	-	expression tag	UNP P19491
B	1099	GLY	-	expression tag	UNP P19491
B	1100	ASP	-	expression tag	UNP P19491
B	1101	VAL	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1102	SER	-	expression tag	UNP P19491
B	1103	GLU	-	expression tag	UNP P19491
B	1104	GLU	-	expression tag	UNP P19491
B	1105	GLU	-	expression tag	UNP P19491
B	1106	ASP	-	expression tag	UNP P19491
B	1107	PHE	-	expression tag	UNP P19491
B	1108	ARG	-	expression tag	UNP P19491
B	1109	LEU	-	expression tag	UNP P19491
B	1110	ALA	-	expression tag	UNP P19491
B	1111	CYS	-	expression tag	UNP P19491
B	1112	ARG	-	expression tag	UNP P19491
B	1113	HIS	-	expression tag	UNP P19491
B	1114	GLU	-	expression tag	UNP P19491
B	1115	ARG	-	expression tag	UNP P19491
B	1116	TYR	-	expression tag	UNP P19491
B	1117	PRO	-	expression tag	UNP P19491
B	1118	THR	-	expression tag	UNP P19491
B	1119	ARG	-	expression tag	UNP P19491
B	1120	HIS	-	expression tag	UNP P19491
B	1121	GLN	-	expression tag	UNP P19491
B	1122	PRO	-	expression tag	UNP P19491
B	1123	HIS	-	expression tag	UNP P19491
B	1124	MET	-	expression tag	UNP P19491
B	1125	GLY	-	expression tag	UNP P19491
B	1126	ASP	-	expression tag	UNP P19491
B	1127	SER	-	expression tag	UNP P19491
B	1128	TRP	-	expression tag	UNP P19491
B	1129	PRO	-	expression tag	UNP P19491
B	1130	ARG	-	expression tag	UNP P19491
B	1131	SER	-	expression tag	UNP P19491
B	1132	SER	-	expression tag	UNP P19491
B	1133	ALA	-	expression tag	UNP P19491
B	1134	HIS	-	expression tag	UNP P19491
B	1135	GLU	-	expression tag	UNP P19491
B	1136	ALA	-	expression tag	UNP P19491
B	1137	ALA	-	expression tag	UNP P19491
B	1138	GLU	-	expression tag	UNP P19491
B	1139	LEU	-	expression tag	UNP P19491
B	1140	ASN	-	expression tag	UNP P19491
B	1141	ARG	-	expression tag	UNP P19491
B	1142	GLN	-	expression tag	UNP P19491
B	1143	CYS	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1144	TRP	-	expression tag	UNP P19491
B	1145	VAL	-	expression tag	UNP P19491
B	1146	LEU	-	expression tag	UNP P19491
B	1147	GLY	-	expression tag	UNP P19491
B	1148	HIS	-	expression tag	UNP P19491
B	1149	TRP	-	expression tag	UNP P19491
B	1150	VAL	-	expression tag	UNP P19491
B	1151	GLY	-	expression tag	UNP P19491
B	1152	THR	-	expression tag	UNP P19491
B	1153	GLY	-	expression tag	UNP P19491
B	1154	GLY	-	expression tag	UNP P19491
B	1155	LEU	-	expression tag	UNP P19491
B	1156	VAL	-	expression tag	UNP P19491
B	1157	PRO	-	expression tag	UNP P19491
B	1158	ARG	-	expression tag	UNP P19491
B	1159	GLY	-	expression tag	UNP P19491
B	1160	SER	-	expression tag	UNP P19491
B	1161	ALA	-	expression tag	UNP P19491
B	1162	ALA	-	expression tag	UNP P19491
B	1163	ALA	-	expression tag	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	744	THR	ASN	conflict	UNP P19491
C	745	PRO	ALA	conflict	UNP P19491
C	754	SER	ASN	conflict	UNP P19491
C	758	VAL	LEU	conflict	UNP P19491
C	775	ALA	SER	conflict	UNP P19491
C	776	LYS	GLY	conflict	UNP P19491
C	777	ASP	GLY	conflict	UNP P19491
C	778	SER	GLY	conflict	UNP P19491
C	779	GLY	ASP	conflict	UNP P19491
C	999	GLY	-	expression tag	UNP P19491
C	1000	THR	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1001	GLY	-	expression tag	UNP P19491
C	1002	LYS	-	expression tag	UNP P19491
C	1003	THR	-	expression tag	UNP P19491
C	1004	SER	-	expression tag	UNP P19491
C	1005	ARG	-	expression tag	UNP P19491
C	1006	ARG	-	expression tag	UNP P19491
C	1007	GLY	-	expression tag	UNP P19491
C	1008	ARG	-	expression tag	UNP P19491
C	1009	ALA	-	expression tag	UNP P19491
C	1010	LEU	-	expression tag	UNP P19491
C	1011	LEU	-	expression tag	UNP P19491
C	1012	ALA	-	expression tag	UNP P19491
C	1013	VAL	-	expression tag	UNP P19491
C	1014	ALA	-	expression tag	UNP P19491
C	1015	LEU	-	expression tag	UNP P19491
C	1016	ASN	-	expression tag	UNP P19491
C	1017	LEU	-	expression tag	UNP P19491
C	1018	LEU	-	expression tag	UNP P19491
C	1019	ALA	-	expression tag	UNP P19491
C	1020	LEU	-	expression tag	UNP P19491
C	1021	LEU	-	expression tag	UNP P19491
C	1022	PHE	-	expression tag	UNP P19491
C	1023	ALA	-	expression tag	UNP P19491
C	1024	THR	-	expression tag	UNP P19491
C	1025	THR	-	expression tag	UNP P19491
C	1026	ALA	-	expression tag	UNP P19491
C	1027	PHE	-	expression tag	UNP P19491
C	1028	LEU	-	expression tag	UNP P19491
C	1029	THR	-	expression tag	UNP P19491
C	1030	THR	-	expression tag	UNP P19491
C	1031	TYR	-	expression tag	UNP P19491
C	1032	TRP	-	expression tag	UNP P19491
C	1033	CYS	-	expression tag	UNP P19491
C	1034	GLN	-	expression tag	UNP P19491
C	1035	GLY	-	expression tag	UNP P19491
C	1036	THR	-	expression tag	UNP P19491
C	1037	GLN	-	expression tag	UNP P19491
C	1038	ARG	-	expression tag	UNP P19491
C	1039	VAL	-	expression tag	UNP P19491
C	1040	PRO	-	expression tag	UNP P19491
C	1041	LYS	-	expression tag	UNP P19491
C	1042	PRO	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1043	GLY	-	expression tag	UNP P19491
C	1044	CYS	-	expression tag	UNP P19491
C	1045	GLY	-	expression tag	UNP P19491
C	1046	GLN	-	expression tag	UNP P19491
C	1047	GLY	-	expression tag	UNP P19491
C	1048	GLY	-	expression tag	UNP P19491
C	1049	GLY	-	expression tag	UNP P19491
C	1050	ALA	-	expression tag	UNP P19491
C	1051	ASN	-	expression tag	UNP P19491
C	1052	CYS	-	expression tag	UNP P19491
C	1053	PRO	-	expression tag	UNP P19491
C	1054	ASN	-	expression tag	UNP P19491
C	1055	SER	-	expression tag	UNP P19491
C	1056	GLY	-	expression tag	UNP P19491
C	1057	ALA	-	expression tag	UNP P19491
C	1058	ASN	-	expression tag	UNP P19491
C	1059	ALA	-	expression tag	UNP P19491
C	1060	THR	-	expression tag	UNP P19491
C	1061	ALA	-	expression tag	UNP P19491
C	1062	ASN	-	expression tag	UNP P19491
C	1063	SER	-	expression tag	UNP P19491
C	1064	THR	-	expression tag	UNP P19491
C	1065	ALA	-	expression tag	UNP P19491
C	1066	ALA	-	expression tag	UNP P19491
C	1067	PRO	-	expression tag	UNP P19491
C	1068	VAL	-	expression tag	UNP P19491
C	1069	ALA	-	expression tag	UNP P19491
C	1070	ALA	-	expression tag	UNP P19491
C	1071	SER	-	expression tag	UNP P19491
C	1072	PRO	-	expression tag	UNP P19491
C	1073	ALA	-	expression tag	UNP P19491
C	1074	GLY	-	expression tag	UNP P19491
C	1075	ALA	-	expression tag	UNP P19491
C	1076	PRO	-	expression tag	UNP P19491
C	1077	TYR	-	expression tag	UNP P19491
C	1078	SER	-	expression tag	UNP P19491
C	1079	TRP	-	expression tag	UNP P19491
C	1080	GLU	-	expression tag	UNP P19491
C	1081	ALA	-	expression tag	UNP P19491
C	1082	GLY	-	expression tag	UNP P19491
C	1083	ASP	-	expression tag	UNP P19491
C	1084	GLU	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1085	ARG	-	expression tag	UNP P19491
C	1086	PHE	-	expression tag	UNP P19491
C	1087	GLN	-	expression tag	UNP P19491
C	1088	LEU	-	expression tag	UNP P19491
C	1089	ARG	-	expression tag	UNP P19491
C	1090	ARG	-	expression tag	UNP P19491
C	1091	PHE	-	expression tag	UNP P19491
C	1092	HIS	-	expression tag	UNP P19491
C	1093	THR	-	expression tag	UNP P19491
C	1094	GLY	-	expression tag	UNP P19491
C	1095	ILE	-	expression tag	UNP P19491
C	1096	TRP	-	expression tag	UNP P19491
C	1097	TYR	-	expression tag	UNP P19491
C	1098	SER	-	expression tag	UNP P19491
C	1099	CYS	-	expression tag	UNP P19491
C	1100	GLU	-	expression tag	UNP P19491
C	1101	GLU	-	expression tag	UNP P19491
C	1102	GLU	-	expression tag	UNP P19491
C	1103	LEU	-	expression tag	UNP P19491
C	1104	GLY	-	expression tag	UNP P19491
C	1105	GLY	-	expression tag	UNP P19491
C	1106	PRO	-	expression tag	UNP P19491
C	1107	GLY	-	expression tag	UNP P19491
C	1108	GLU	-	expression tag	UNP P19491
C	1109	LYS	-	expression tag	UNP P19491
C	1110	CYS	-	expression tag	UNP P19491
C	1111	ARG	-	expression tag	UNP P19491
C	1112	SER	-	expression tag	UNP P19491
C	1113	PHE	-	expression tag	UNP P19491
C	1114	ILE	-	expression tag	UNP P19491
C	1115	ASP	-	expression tag	UNP P19491
C	1116	LEU	-	expression tag	UNP P19491
C	1117	ALA	-	expression tag	UNP P19491
C	1118	PRO	-	expression tag	UNP P19491
C	1119	ALA	-	expression tag	UNP P19491
C	1120	SER	-	expression tag	UNP P19491
C	1121	GLU	-	expression tag	UNP P19491
C	1122	LYS	-	expression tag	UNP P19491
C	1123	GLY	-	expression tag	UNP P19491
C	1124	VAL	-	expression tag	UNP P19491
C	1125	LEU	-	expression tag	UNP P19491
C	1126	TRP	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1127	LEU	-	expression tag	UNP P19491
C	1128	SER	-	expression tag	UNP P19491
C	1129	VAL	-	expression tag	UNP P19491
C	1130	VAL	-	expression tag	UNP P19491
C	1131	SER	-	expression tag	UNP P19491
C	1132	GLU	-	expression tag	UNP P19491
C	1133	VAL	-	expression tag	UNP P19491
C	1134	LEU	-	expression tag	UNP P19491
C	1135	TYR	-	expression tag	UNP P19491
C	1136	ILE	-	expression tag	UNP P19491
C	1137	LEU	-	expression tag	UNP P19491
C	1138	LEU	-	expression tag	UNP P19491
C	1139	LEU	-	expression tag	UNP P19491
C	1140	VAL	-	expression tag	UNP P19491
C	1141	VAL	-	expression tag	UNP P19491
C	1142	GLY	-	expression tag	UNP P19491
C	1143	PHE	-	expression tag	UNP P19491
C	1144	SER	-	expression tag	UNP P19491
C	1145	LEU	-	expression tag	UNP P19491
C	1146	MET	-	expression tag	UNP P19491
C	1147	CYS	-	expression tag	UNP P19491
C	1148	LEU	-	expression tag	UNP P19491
C	1149	GLU	-	expression tag	UNP P19491
C	1150	LEU	-	expression tag	UNP P19491
C	1151	LEU	-	expression tag	UNP P19491
C	1152	HIS	-	expression tag	UNP P19491
C	1153	SER	-	expression tag	UNP P19491
C	1154	SER	-	expression tag	UNP P19491
C	1155	SER	-	expression tag	UNP P19491
C	1156	VAL	-	expression tag	UNP P19491
C	1157	ILE	-	expression tag	UNP P19491
C	1158	ASP	-	expression tag	UNP P19491
C	1159	GLY	-	expression tag	UNP P19491
C	1160	LEU	-	expression tag	UNP P19491
C	1161	LYS	-	expression tag	UNP P19491
C	1162	LEU	-	expression tag	UNP P19491
C	1163	ASN	-	expression tag	UNP P19491
C	1164	ALA	-	expression tag	UNP P19491
C	1165	PHE	-	expression tag	UNP P19491
C	1166	ALA	-	expression tag	UNP P19491
C	1167	ALA	-	expression tag	UNP P19491
C	1168	VAL	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1169	PHE	-	expression tag	UNP P19491
C	1170	THR	-	expression tag	UNP P19491
C	1171	VAL	-	expression tag	UNP P19491
C	1172	LEU	-	expression tag	UNP P19491
C	1173	SER	-	expression tag	UNP P19491
C	1174	GLY	-	expression tag	UNP P19491
C	1175	LEU	-	expression tag	UNP P19491
C	1176	LEU	-	expression tag	UNP P19491
C	1177	GLY	-	expression tag	UNP P19491
C	1178	MET	-	expression tag	UNP P19491
C	1179	VAL	-	expression tag	UNP P19491
C	1180	ALA	-	expression tag	UNP P19491
C	1181	HIS	-	expression tag	UNP P19491
C	1182	MET	-	expression tag	UNP P19491
C	1183	MET	-	expression tag	UNP P19491
C	1184	TYR	-	expression tag	UNP P19491
C	1185	THR	-	expression tag	UNP P19491
C	1186	GLN	-	expression tag	UNP P19491
C	1187	VAL	-	expression tag	UNP P19491
C	1188	PHE	-	expression tag	UNP P19491
C	1189	GLN	-	expression tag	UNP P19491
C	1190	VAL	-	expression tag	UNP P19491
C	1191	THR	-	expression tag	UNP P19491
C	1192	VAL	-	expression tag	UNP P19491
C	1193	SER	-	expression tag	UNP P19491
C	1194	LEU	-	expression tag	UNP P19491
C	1195	GLY	-	expression tag	UNP P19491
C	1196	PRO	-	expression tag	UNP P19491
C	1197	GLU	-	expression tag	UNP P19491
C	1198	ASP	-	expression tag	UNP P19491
C	1199	TRP	-	expression tag	UNP P19491
C	1200	ARG	-	expression tag	UNP P19491
C	1201	PRO	-	expression tag	UNP P19491
C	1202	HIS	-	expression tag	UNP P19491
C	1203	SER	-	expression tag	UNP P19491
C	1204	TRP	-	expression tag	UNP P19491
C	1205	ASP	-	expression tag	UNP P19491
C	1206	TYR	-	expression tag	UNP P19491
C	1207	GLY	-	expression tag	UNP P19491
C	1208	TRP	-	expression tag	UNP P19491
C	1209	SER	-	expression tag	UNP P19491
C	1210	PHE	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1211	CYS	-	expression tag	UNP P19491
C	1212	LEU	-	expression tag	UNP P19491
C	1213	ALA	-	expression tag	UNP P19491
C	1214	TRP	-	expression tag	UNP P19491
C	1215	GLY	-	expression tag	UNP P19491
C	1216	SER	-	expression tag	UNP P19491
C	1217	PHE	-	expression tag	UNP P19491
C	1218	THR	-	expression tag	UNP P19491
C	1219	CYS	-	expression tag	UNP P19491
C	1220	CYS	-	expression tag	UNP P19491
C	1221	MET	-	expression tag	UNP P19491
C	1222	ALA	-	expression tag	UNP P19491
C	1223	ALA	-	expression tag	UNP P19491
C	1224	SER	-	expression tag	UNP P19491
C	1225	VAL	-	expression tag	UNP P19491
C	1226	THR	-	expression tag	UNP P19491
C	1227	THR	-	expression tag	UNP P19491
C	1228	LEU	-	expression tag	UNP P19491
C	1229	ASN	-	expression tag	UNP P19491
C	1230	SER	-	expression tag	UNP P19491
C	1231	TYR	-	expression tag	UNP P19491
C	1232	THR	-	expression tag	UNP P19491
C	1233	LYS	-	expression tag	UNP P19491
C	1234	THR	-	expression tag	UNP P19491
C	1235	VAL	-	expression tag	UNP P19491
C	1236	ILE	-	expression tag	UNP P19491
C	1237	GLU	-	expression tag	UNP P19491
C	1238	PHE	-	expression tag	UNP P19491
C	1239	ARG	-	expression tag	UNP P19491
C	1240	HIS	-	expression tag	UNP P19491
C	1241	LYS	-	expression tag	UNP P19491
C	1242	ARG	-	expression tag	UNP P19491
C	1243	LYS	-	expression tag	UNP P19491
C	1244	VAL	-	expression tag	UNP P19491
C	1245	PHE	-	expression tag	UNP P19491
C	1246	GLU	-	expression tag	UNP P19491
C	1247	GLN	-	expression tag	UNP P19491
C	1248	GLY	-	expression tag	UNP P19491
C	1249	TYR	-	expression tag	UNP P19491
C	1250	ARG	-	expression tag	UNP P19491
C	1251	GLU	-	expression tag	UNP P19491
C	1252	GLU	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1253	PRO	-	expression tag	UNP P19491
C	1254	THR	-	expression tag	UNP P19491
C	1255	PHE	-	expression tag	UNP P19491
C	1256	ILE	-	expression tag	UNP P19491
C	1257	ASP	-	expression tag	UNP P19491
C	1258	PRO	-	expression tag	UNP P19491
C	1259	GLU	-	expression tag	UNP P19491
C	1260	ALA	-	expression tag	UNP P19491
C	1261	ILE	-	expression tag	UNP P19491
C	1262	LYS	-	expression tag	UNP P19491
C	1263	TYR	-	expression tag	UNP P19491
C	1264	PHE	-	expression tag	UNP P19491
C	1265	ARG	-	expression tag	UNP P19491
C	1266	GLU	-	expression tag	UNP P19491
C	1267	ARG	-	expression tag	UNP P19491
C	1268	ILE	-	expression tag	UNP P19491
C	1269	GLU	-	expression tag	UNP P19491
C	1270	LYS	-	expression tag	UNP P19491
C	1271	GLY	-	expression tag	UNP P19491
C	1272	ASP	-	expression tag	UNP P19491
C	1273	VAL	-	expression tag	UNP P19491
C	1274	SER	-	expression tag	UNP P19491
C	1275	GLU	-	expression tag	UNP P19491
C	1276	GLU	-	expression tag	UNP P19491
C	1277	GLU	-	expression tag	UNP P19491
C	1278	ASP	-	expression tag	UNP P19491
C	1279	PHE	-	expression tag	UNP P19491
C	1280	ARG	-	expression tag	UNP P19491
C	1281	LEU	-	expression tag	UNP P19491
C	1282	ALA	-	expression tag	UNP P19491
C	1283	CYS	-	expression tag	UNP P19491
C	1284	ARG	-	expression tag	UNP P19491
C	1285	HIS	-	expression tag	UNP P19491
C	1286	GLU	-	expression tag	UNP P19491
C	1287	ARG	-	expression tag	UNP P19491
C	1288	TYR	-	expression tag	UNP P19491
C	1289	PRO	-	expression tag	UNP P19491
C	1290	THR	-	expression tag	UNP P19491
C	1291	ARG	-	expression tag	UNP P19491
C	1292	HIS	-	expression tag	UNP P19491
C	1293	GLN	-	expression tag	UNP P19491
C	1294	PRO	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1295	HIS	-	expression tag	UNP P19491
C	1296	MET	-	expression tag	UNP P19491
C	1297	GLY	-	expression tag	UNP P19491
C	1298	ASP	-	expression tag	UNP P19491
C	1299	SER	-	expression tag	UNP P19491
C	1300	TRP	-	expression tag	UNP P19491
C	1301	PRO	-	expression tag	UNP P19491
C	1302	ARG	-	expression tag	UNP P19491
C	1303	SER	-	expression tag	UNP P19491
C	1304	SER	-	expression tag	UNP P19491
C	1305	ALA	-	expression tag	UNP P19491
C	1306	HIS	-	expression tag	UNP P19491
C	1307	GLU	-	expression tag	UNP P19491
C	1308	ALA	-	expression tag	UNP P19491
C	1309	ALA	-	expression tag	UNP P19491
C	1310	GLU	-	expression tag	UNP P19491
C	1311	LEU	-	expression tag	UNP P19491
C	1312	ASN	-	expression tag	UNP P19491
C	1313	ARG	-	expression tag	UNP P19491
C	1314	GLN	-	expression tag	UNP P19491
C	1315	CYS	-	expression tag	UNP P19491
C	1316	TRP	-	expression tag	UNP P19491
C	1317	VAL	-	expression tag	UNP P19491
C	1318	LEU	-	expression tag	UNP P19491
C	1319	GLY	-	expression tag	UNP P19491
C	1320	HIS	-	expression tag	UNP P19491
C	1321	TRP	-	expression tag	UNP P19491
C	1322	VAL	-	expression tag	UNP P19491
C	1323	GLY	-	expression tag	UNP P19491
C	1324	THR	-	expression tag	UNP P19491
C	1325	GLY	-	expression tag	UNP P19491
C	1326	GLY	-	expression tag	UNP P19491
C	1327	LEU	-	expression tag	UNP P19491
C	1328	VAL	-	expression tag	UNP P19491
C	1329	PRO	-	expression tag	UNP P19491
C	1330	ARG	-	expression tag	UNP P19491
C	1331	GLY	-	expression tag	UNP P19491
C	1332	SER	-	expression tag	UNP P19491
C	1333	ALA	-	expression tag	UNP P19491
C	1334	ALA	-	expression tag	UNP P19491
C	1335	ALA	-	expression tag	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	744	THR	ASN	conflict	UNP P19491
D	745	PRO	ALA	conflict	UNP P19491
D	754	SER	ASN	conflict	UNP P19491
D	758	VAL	LEU	conflict	UNP P19491
D	775	ALA	SER	conflict	UNP P19491
D	776	LYS	GLY	conflict	UNP P19491
D	777	ASP	GLY	conflict	UNP P19491
D	778	SER	GLY	conflict	UNP P19491
D	779	GLY	ASP	conflict	UNP P19491
D	827	GLY	-	expression tag	UNP P19491
D	828	THR	-	expression tag	UNP P19491
D	829	GLY	-	expression tag	UNP P19491
D	830	LYS	-	expression tag	UNP P19491
D	831	THR	-	expression tag	UNP P19491
D	832	SER	-	expression tag	UNP P19491
D	833	ARG	-	expression tag	UNP P19491
D	834	ARG	-	expression tag	UNP P19491
D	835	GLY	-	expression tag	UNP P19491
D	836	ARG	-	expression tag	UNP P19491
D	837	ALA	-	expression tag	UNP P19491
D	838	LEU	-	expression tag	UNP P19491
D	839	LEU	-	expression tag	UNP P19491
D	840	ALA	-	expression tag	UNP P19491
D	841	VAL	-	expression tag	UNP P19491
D	842	ALA	-	expression tag	UNP P19491
D	843	LEU	-	expression tag	UNP P19491
D	844	ASN	-	expression tag	UNP P19491
D	845	LEU	-	expression tag	UNP P19491
D	846	LEU	-	expression tag	UNP P19491
D	847	ALA	-	expression tag	UNP P19491
D	848	LEU	-	expression tag	UNP P19491
D	849	LEU	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	850	PHE	-	expression tag	UNP P19491
D	851	ALA	-	expression tag	UNP P19491
D	852	THR	-	expression tag	UNP P19491
D	853	THR	-	expression tag	UNP P19491
D	854	ALA	-	expression tag	UNP P19491
D	855	PHE	-	expression tag	UNP P19491
D	856	LEU	-	expression tag	UNP P19491
D	857	THR	-	expression tag	UNP P19491
D	858	THR	-	expression tag	UNP P19491
D	859	TYR	-	expression tag	UNP P19491
D	860	TRP	-	expression tag	UNP P19491
D	861	CYS	-	expression tag	UNP P19491
D	862	GLN	-	expression tag	UNP P19491
D	863	GLY	-	expression tag	UNP P19491
D	864	THR	-	expression tag	UNP P19491
D	865	GLN	-	expression tag	UNP P19491
D	866	ARG	-	expression tag	UNP P19491
D	867	VAL	-	expression tag	UNP P19491
D	868	PRO	-	expression tag	UNP P19491
D	869	LYS	-	expression tag	UNP P19491
D	870	PRO	-	expression tag	UNP P19491
D	871	GLY	-	expression tag	UNP P19491
D	872	CYS	-	expression tag	UNP P19491
D	873	GLY	-	expression tag	UNP P19491
D	874	GLN	-	expression tag	UNP P19491
D	875	GLY	-	expression tag	UNP P19491
D	876	GLY	-	expression tag	UNP P19491
D	877	GLY	-	expression tag	UNP P19491
D	878	ALA	-	expression tag	UNP P19491
D	879	ASN	-	expression tag	UNP P19491
D	880	CYS	-	expression tag	UNP P19491
D	881	PRO	-	expression tag	UNP P19491
D	882	ASN	-	expression tag	UNP P19491
D	883	SER	-	expression tag	UNP P19491
D	884	GLY	-	expression tag	UNP P19491
D	885	ALA	-	expression tag	UNP P19491
D	886	ASN	-	expression tag	UNP P19491
D	887	ALA	-	expression tag	UNP P19491
D	888	THR	-	expression tag	UNP P19491
D	889	ALA	-	expression tag	UNP P19491
D	890	ASN	-	expression tag	UNP P19491
D	891	SER	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	892	THR	-	expression tag	UNP P19491
D	893	ALA	-	expression tag	UNP P19491
D	894	ALA	-	expression tag	UNP P19491
D	895	PRO	-	expression tag	UNP P19491
D	896	VAL	-	expression tag	UNP P19491
D	897	ALA	-	expression tag	UNP P19491
D	898	ALA	-	expression tag	UNP P19491
D	899	SER	-	expression tag	UNP P19491
D	900	PRO	-	expression tag	UNP P19491
D	901	ALA	-	expression tag	UNP P19491
D	902	GLY	-	expression tag	UNP P19491
D	903	ALA	-	expression tag	UNP P19491
D	904	PRO	-	expression tag	UNP P19491
D	905	TYR	-	expression tag	UNP P19491
D	906	SER	-	expression tag	UNP P19491
D	907	TRP	-	expression tag	UNP P19491
D	908	GLU	-	expression tag	UNP P19491
D	909	ALA	-	expression tag	UNP P19491
D	910	GLY	-	expression tag	UNP P19491
D	911	ASP	-	expression tag	UNP P19491
D	912	GLU	-	expression tag	UNP P19491
D	913	ARG	-	expression tag	UNP P19491
D	914	PHE	-	expression tag	UNP P19491
D	915	GLN	-	expression tag	UNP P19491
D	916	LEU	-	expression tag	UNP P19491
D	917	ARG	-	expression tag	UNP P19491
D	918	ARG	-	expression tag	UNP P19491
D	919	PHE	-	expression tag	UNP P19491
D	920	HIS	-	expression tag	UNP P19491
D	921	THR	-	expression tag	UNP P19491
D	922	GLY	-	expression tag	UNP P19491
D	923	ILE	-	expression tag	UNP P19491
D	924	TRP	-	expression tag	UNP P19491
D	925	TYR	-	expression tag	UNP P19491
D	926	SER	-	expression tag	UNP P19491
D	927	CYS	-	expression tag	UNP P19491
D	928	GLU	-	expression tag	UNP P19491
D	929	GLU	-	expression tag	UNP P19491
D	930	GLU	-	expression tag	UNP P19491
D	931	LEU	-	expression tag	UNP P19491
D	932	GLY	-	expression tag	UNP P19491
D	933	GLY	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	934	PRO	-	expression tag	UNP P19491
D	935	GLY	-	expression tag	UNP P19491
D	936	GLU	-	expression tag	UNP P19491
D	937	LYS	-	expression tag	UNP P19491
D	938	CYS	-	expression tag	UNP P19491
D	939	ARG	-	expression tag	UNP P19491
D	940	SER	-	expression tag	UNP P19491
D	941	PHE	-	expression tag	UNP P19491
D	942	ILE	-	expression tag	UNP P19491
D	943	ASP	-	expression tag	UNP P19491
D	944	LEU	-	expression tag	UNP P19491
D	945	ALA	-	expression tag	UNP P19491
D	946	PRO	-	expression tag	UNP P19491
D	947	ALA	-	expression tag	UNP P19491
D	948	SER	-	expression tag	UNP P19491
D	949	GLU	-	expression tag	UNP P19491
D	950	LYS	-	expression tag	UNP P19491
D	951	GLY	-	expression tag	UNP P19491
D	952	VAL	-	expression tag	UNP P19491
D	953	LEU	-	expression tag	UNP P19491
D	954	TRP	-	expression tag	UNP P19491
D	955	LEU	-	expression tag	UNP P19491
D	956	SER	-	expression tag	UNP P19491
D	957	VAL	-	expression tag	UNP P19491
D	958	VAL	-	expression tag	UNP P19491
D	959	SER	-	expression tag	UNP P19491
D	960	GLU	-	expression tag	UNP P19491
D	961	VAL	-	expression tag	UNP P19491
D	962	LEU	-	expression tag	UNP P19491
D	963	TYR	-	expression tag	UNP P19491
D	964	ILE	-	expression tag	UNP P19491
D	965	LEU	-	expression tag	UNP P19491
D	966	LEU	-	expression tag	UNP P19491
D	967	LEU	-	expression tag	UNP P19491
D	968	VAL	-	expression tag	UNP P19491
D	969	VAL	-	expression tag	UNP P19491
D	970	GLY	-	expression tag	UNP P19491
D	971	PHE	-	expression tag	UNP P19491
D	972	SER	-	expression tag	UNP P19491
D	973	LEU	-	expression tag	UNP P19491
D	974	MET	-	expression tag	UNP P19491
D	975	CYS	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	976	LEU	-	expression tag	UNP P19491
D	977	GLU	-	expression tag	UNP P19491
D	978	LEU	-	expression tag	UNP P19491
D	979	LEU	-	expression tag	UNP P19491
D	980	HIS	-	expression tag	UNP P19491
D	981	SER	-	expression tag	UNP P19491
D	982	SER	-	expression tag	UNP P19491
D	983	SER	-	expression tag	UNP P19491
D	984	VAL	-	expression tag	UNP P19491
D	985	ILE	-	expression tag	UNP P19491
D	986	ASP	-	expression tag	UNP P19491
D	987	GLY	-	expression tag	UNP P19491
D	988	LEU	-	expression tag	UNP P19491
D	989	LYS	-	expression tag	UNP P19491
D	990	LEU	-	expression tag	UNP P19491
D	991	ASN	-	expression tag	UNP P19491
D	992	ALA	-	expression tag	UNP P19491
D	993	PHE	-	expression tag	UNP P19491
D	994	ALA	-	expression tag	UNP P19491
D	995	ALA	-	expression tag	UNP P19491
D	996	VAL	-	expression tag	UNP P19491
D	997	PHE	-	expression tag	UNP P19491
D	998	THR	-	expression tag	UNP P19491
D	999	VAL	-	expression tag	UNP P19491
D	1000	LEU	-	expression tag	UNP P19491
D	1001	SER	-	expression tag	UNP P19491
D	1002	GLY	-	expression tag	UNP P19491
D	1003	LEU	-	expression tag	UNP P19491
D	1004	LEU	-	expression tag	UNP P19491
D	1005	GLY	-	expression tag	UNP P19491
D	1006	MET	-	expression tag	UNP P19491
D	1007	VAL	-	expression tag	UNP P19491
D	1008	ALA	-	expression tag	UNP P19491
D	1009	HIS	-	expression tag	UNP P19491
D	1010	MET	-	expression tag	UNP P19491
D	1011	MET	-	expression tag	UNP P19491
D	1012	TYR	-	expression tag	UNP P19491
D	1013	THR	-	expression tag	UNP P19491
D	1014	GLN	-	expression tag	UNP P19491
D	1015	VAL	-	expression tag	UNP P19491
D	1016	PHE	-	expression tag	UNP P19491
D	1017	GLN	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1018	VAL	-	expression tag	UNP P19491
D	1019	THR	-	expression tag	UNP P19491
D	1020	VAL	-	expression tag	UNP P19491
D	1021	SER	-	expression tag	UNP P19491
D	1022	LEU	-	expression tag	UNP P19491
D	1023	GLY	-	expression tag	UNP P19491
D	1024	PRO	-	expression tag	UNP P19491
D	1025	GLU	-	expression tag	UNP P19491
D	1026	ASP	-	expression tag	UNP P19491
D	1027	TRP	-	expression tag	UNP P19491
D	1028	ARG	-	expression tag	UNP P19491
D	1029	PRO	-	expression tag	UNP P19491
D	1030	HIS	-	expression tag	UNP P19491
D	1031	SER	-	expression tag	UNP P19491
D	1032	TRP	-	expression tag	UNP P19491
D	1033	ASP	-	expression tag	UNP P19491
D	1034	TYR	-	expression tag	UNP P19491
D	1035	GLY	-	expression tag	UNP P19491
D	1036	TRP	-	expression tag	UNP P19491
D	1037	SER	-	expression tag	UNP P19491
D	1038	PHE	-	expression tag	UNP P19491
D	1039	CYS	-	expression tag	UNP P19491
D	1040	LEU	-	expression tag	UNP P19491
D	1041	ALA	-	expression tag	UNP P19491
D	1042	TRP	-	expression tag	UNP P19491
D	1043	GLY	-	expression tag	UNP P19491
D	1044	SER	-	expression tag	UNP P19491
D	1045	PHE	-	expression tag	UNP P19491
D	1046	THR	-	expression tag	UNP P19491
D	1047	CYS	-	expression tag	UNP P19491
D	1048	CYS	-	expression tag	UNP P19491
D	1049	MET	-	expression tag	UNP P19491
D	1050	ALA	-	expression tag	UNP P19491
D	1051	ALA	-	expression tag	UNP P19491
D	1052	SER	-	expression tag	UNP P19491
D	1053	VAL	-	expression tag	UNP P19491
D	1054	THR	-	expression tag	UNP P19491
D	1055	THR	-	expression tag	UNP P19491
D	1056	LEU	-	expression tag	UNP P19491
D	1057	ASN	-	expression tag	UNP P19491
D	1058	SER	-	expression tag	UNP P19491
D	1059	TYR	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1060	THR	-	expression tag	UNP P19491
D	1061	LYS	-	expression tag	UNP P19491
D	1062	THR	-	expression tag	UNP P19491
D	1063	VAL	-	expression tag	UNP P19491
D	1064	ILE	-	expression tag	UNP P19491
D	1065	GLU	-	expression tag	UNP P19491
D	1066	PHE	-	expression tag	UNP P19491
D	1067	ARG	-	expression tag	UNP P19491
D	1068	HIS	-	expression tag	UNP P19491
D	1069	LYS	-	expression tag	UNP P19491
D	1070	ARG	-	expression tag	UNP P19491
D	1071	LYS	-	expression tag	UNP P19491
D	1072	VAL	-	expression tag	UNP P19491
D	1073	PHE	-	expression tag	UNP P19491
D	1074	GLU	-	expression tag	UNP P19491
D	1075	GLN	-	expression tag	UNP P19491
D	1076	GLY	-	expression tag	UNP P19491
D	1077	TYR	-	expression tag	UNP P19491
D	1078	ARG	-	expression tag	UNP P19491
D	1079	GLU	-	expression tag	UNP P19491
D	1080	GLU	-	expression tag	UNP P19491
D	1081	PRO	-	expression tag	UNP P19491
D	1082	THR	-	expression tag	UNP P19491
D	1083	PHE	-	expression tag	UNP P19491
D	1084	ILE	-	expression tag	UNP P19491
D	1085	ASP	-	expression tag	UNP P19491
D	1086	PRO	-	expression tag	UNP P19491
D	1087	GLU	-	expression tag	UNP P19491
D	1088	ALA	-	expression tag	UNP P19491
D	1089	ILE	-	expression tag	UNP P19491
D	1090	LYS	-	expression tag	UNP P19491
D	1091	TYR	-	expression tag	UNP P19491
D	1092	PHE	-	expression tag	UNP P19491
D	1093	ARG	-	expression tag	UNP P19491
D	1094	GLU	-	expression tag	UNP P19491
D	1095	ARG	-	expression tag	UNP P19491
D	1096	ILE	-	expression tag	UNP P19491
D	1097	GLU	-	expression tag	UNP P19491
D	1098	LYS	-	expression tag	UNP P19491
D	1099	GLY	-	expression tag	UNP P19491
D	1100	ASP	-	expression tag	UNP P19491
D	1101	VAL	-	expression tag	UNP P19491

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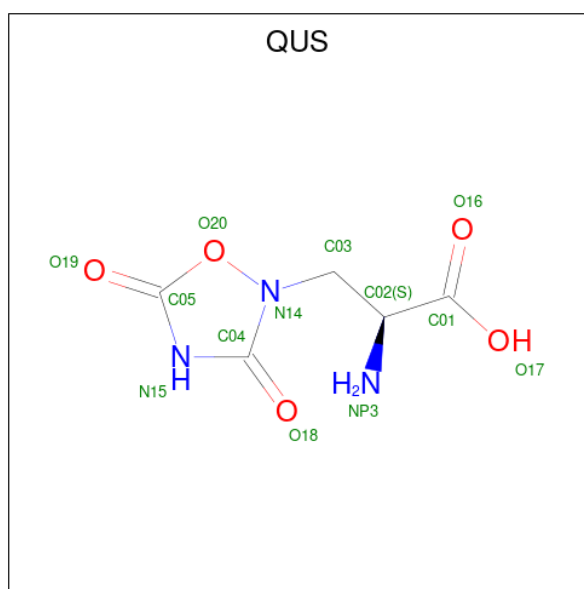
Chain	Residue	Modelled	Actual	Comment	Reference
D	1102	SER	-	expression tag	UNP P19491
D	1103	GLU	-	expression tag	UNP P19491
D	1104	GLU	-	expression tag	UNP P19491
D	1105	GLU	-	expression tag	UNP P19491
D	1106	ASP	-	expression tag	UNP P19491
D	1107	PHE	-	expression tag	UNP P19491
D	1108	ARG	-	expression tag	UNP P19491
D	1109	LEU	-	expression tag	UNP P19491
D	1110	ALA	-	expression tag	UNP P19491
D	1111	CYS	-	expression tag	UNP P19491
D	1112	ARG	-	expression tag	UNP P19491
D	1113	HIS	-	expression tag	UNP P19491
D	1114	GLU	-	expression tag	UNP P19491
D	1115	ARG	-	expression tag	UNP P19491
D	1116	TYR	-	expression tag	UNP P19491
D	1117	PRO	-	expression tag	UNP P19491
D	1118	THR	-	expression tag	UNP P19491
D	1119	ARG	-	expression tag	UNP P19491
D	1120	HIS	-	expression tag	UNP P19491
D	1121	GLN	-	expression tag	UNP P19491
D	1122	PRO	-	expression tag	UNP P19491
D	1123	HIS	-	expression tag	UNP P19491
D	1124	MET	-	expression tag	UNP P19491
D	1125	GLY	-	expression tag	UNP P19491
D	1126	ASP	-	expression tag	UNP P19491
D	1127	SER	-	expression tag	UNP P19491
D	1128	TRP	-	expression tag	UNP P19491
D	1129	PRO	-	expression tag	UNP P19491
D	1130	ARG	-	expression tag	UNP P19491
D	1131	SER	-	expression tag	UNP P19491
D	1132	SER	-	expression tag	UNP P19491
D	1133	ALA	-	expression tag	UNP P19491
D	1134	HIS	-	expression tag	UNP P19491
D	1135	GLU	-	expression tag	UNP P19491
D	1136	ALA	-	expression tag	UNP P19491
D	1137	ALA	-	expression tag	UNP P19491
D	1138	GLU	-	expression tag	UNP P19491
D	1139	LEU	-	expression tag	UNP P19491
D	1140	ASN	-	expression tag	UNP P19491
D	1141	ARG	-	expression tag	UNP P19491
D	1142	GLN	-	expression tag	UNP P19491
D	1143	CYS	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1144	TRP	-	expression tag	UNP P19491
D	1145	VAL	-	expression tag	UNP P19491
D	1146	LEU	-	expression tag	UNP P19491
D	1147	GLY	-	expression tag	UNP P19491
D	1148	HIS	-	expression tag	UNP P19491
D	1149	TRP	-	expression tag	UNP P19491
D	1150	VAL	-	expression tag	UNP P19491
D	1151	GLY	-	expression tag	UNP P19491
D	1152	THR	-	expression tag	UNP P19491
D	1153	GLY	-	expression tag	UNP P19491
D	1154	GLY	-	expression tag	UNP P19491
D	1155	LEU	-	expression tag	UNP P19491
D	1156	VAL	-	expression tag	UNP P19491
D	1157	PRO	-	expression tag	UNP P19491
D	1158	ARG	-	expression tag	UNP P19491
D	1159	GLY	-	expression tag	UNP P19491
D	1160	SER	-	expression tag	UNP P19491
D	1161	ALA	-	expression tag	UNP P19491
D	1162	ALA	-	expression tag	UNP P19491
D	1163	ALA	-	expression tag	UNP P19491

- Molecule 2 is (S)-2-AMINO-3-(3,5-DIOXO-[1,2,4]OXADIAZOLIDIN-2-YL)-PROPIONIC ACID (CCD ID: QUS) (formula: C₅H₇N₃O₅) (labeled as "Ligand of Interest" by depositor).

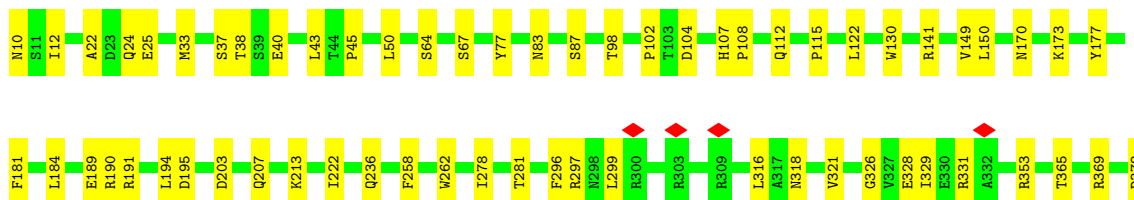


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			13	5	3	5	

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Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total 13	C 5	N 3	O 5	0
2	C	1	Total 13	C 5	N 3	O 5	0
2	D	1	Total 13	C 5	N 3	O 5	0





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	118416	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.076	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0077	Depositor
Map size ($\text{\AA}$)	298.8, 298.8, 298.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QUS

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	0.28	0/7883	0.59	4/10664 (0.0%)
1	B	0.28	0/6317	0.59	3/8533 (0.0%)
1	C	0.28	0/7883	0.59	4/10664 (0.0%)
1	D	0.28	0/6317	0.59	3/8533 (0.0%)
All	All	0.28	0/28400	0.59	14/38394 (0.0%)

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	3
1	C	0	3
1	D	0	3
All	All	0	12

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1153	SER	CA-C-N	5.75	128.78	120.79
1	C	1153	SER	C-N-CA	5.75	128.78	120.79
1	A	1153	SER	CA-C-N	5.71	128.73	120.79
1	A	1153	SER	C-N-CA	5.71	128.73	120.79
1	B	233	LEU	N-CA-C	-5.51	106.56	113.72
1	D	233	LEU	N-CA-C	-5.50	106.57	113.72
1	D	774	GLY	CA-C-N	5.50	128.41	120.38
1	D	774	GLY	C-N-CA	5.50	128.41	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	774	GLY	CA-C-N	5.47	128.37	120.38
1	B	774	GLY	C-N-CA	5.47	128.37	120.38
1	A	1197	GLU	CA-C-N	5.30	134.25	124.82
1	A	1197	GLU	C-N-CA	5.30	134.25	124.82
1	C	1197	GLU	CA-C-N	5.28	134.22	124.82
1	C	1197	GLU	C-N-CA	5.28	134.22	124.82

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1118	PRO	Peptide
1	A	318	ASN	Peptide
1	A	378	ASP	Peptide
1	B	318	ASN	Peptide
1	B	678	GLU	Peptide
1	B	679	PRO	Peptide
1	C	1118	PRO	Peptide
1	C	318	ASN	Peptide
1	C	378	ASP	Peptide
1	D	318	ASN	Peptide
1	D	678	GLU	Peptide
1	D	679	PRO	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7713	0	7694	80	0
1	B	6186	0	6181	54	0
1	C	7713	0	7694	84	0
1	D	6186	0	6181	53	0
2	A	13	0	6	1	0
2	B	13	0	6	0	0
2	C	13	0	6	1	0
2	D	13	0	6	2	0
All	All	27850	0	27774	246	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 (246) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:VAL:HG22	1:C:803:LEU:HD11	1.75	0.69
1:A:451:GLY:O	1:A:485:ARG:NH2	2.28	0.67
1:C:451:GLY:O	1:C:485:ARG:NH2	2.28	0.67
1:B:235:ILE:HD12	1:B:242:VAL:HG21	1.80	0.64
1:D:235:ILE:HD12	1:D:242:VAL:HG21	1.80	0.63
1:C:115:PRO:HG3	1:C:353:ARG:HD3	1.80	0.63
1:A:756:GLN:CG	1:A:758:VAL:HG23	2.30	0.62
1:C:756:GLN:CG	1:C:758:VAL:HG23	2.30	0.62
1:A:115:PRO:HG3	1:A:353:ARG:HD3	1.80	0.62
1:D:364:LYS:HD2	1:D:369:ARG:HD3	1.82	0.61
1:C:296:PHE:HA	1:C:299:LEU:HD23	1.83	0.61
1:B:364:LYS:HD2	1:B:369:ARG:HD3	1.82	0.60
1:A:296:PHE:HA	1:A:299:LEU:HD23	1.83	0.60
1:B:650:LEU:HD23	1:B:652:SER:H	1.67	0.59
1:A:803:LEU:HD11	1:D:536:VAL:HG22	1.84	0.59
1:A:756:GLN:HG2	1:A:758:VAL:HG23	1.85	0.59
1:A:786:ALA:HA	1:D:619:ASN:HD21	1.68	0.58
1:C:756:GLN:HG2	1:C:758:VAL:HG23	1.85	0.58
1:B:301:LYS:O	1:B:303:ARG:NH1	2.37	0.58
1:D:650:LEU:HD23	1:D:652:SER:H	1.67	0.58
1:B:711:TYR:OH	1:B:770:LYS:NZ	2.37	0.58
1:D:301:LYS:O	1:D:303:ARG:NH1	2.37	0.58
1:C:369:ARG:HH22	1:C:387:THR:HA	1.68	0.58
1:D:711:TYR:OH	1:D:770:LYS:NZ	2.37	0.58
1:A:574:PHE:HE1	1:D:596:LEU:HD13	1.68	0.57
1:C:570:GLU:O	1:C:575:ASN:ND2	2.38	0.57
1:C:1031:TYR:HD1	1:C:1034:GLN:HE22	1.52	0.57
1:A:1031:TYR:HD1	1:A:1034:GLN:HE22	1.51	0.57
1:A:570:GLU:O	1:A:575:ASN:ND2	2.38	0.56
1:A:369:ARG:HH22	1:A:387:THR:HA	1.68	0.56
1:C:190:ARG:HE	1:C:469:TYR:HB3	1.71	0.56
1:D:337:GLN:HE21	1:D:344:ASN:HD21	1.53	0.56
1:B:337:GLN:HE21	1:B:344:ASN:HD21	1.53	0.55
1:C:10:ASN:N	1:C:40:GLU:O	2.40	0.55
1:A:544:SER:HB3	1:A:569:ASN:HD21	1.72	0.55
1:C:610:LEU:HD21	1:D:613:ILE:HD12	1.87	0.55
1:C:1102:GLU:H	1:C:1107:GLY:HA3	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:PRO:O	1:B:619:ASN:ND2	2.39	0.55
1:C:141:ARG:NH2	1:C:195:ASP:OD2	2.39	0.55
1:A:190:ARG:HE	1:A:469:TYR:HB3	1.71	0.55
1:D:405:TYR:OH	1:D:496:MET:SD	2.65	0.55
1:C:536:VAL:HG22	1:D:803:LEU:HD21	1.88	0.55
1:A:1013:VAL:HG22	1:A:1146:MET:HB3	1.89	0.55
1:A:10:ASN:N	1:A:40:GLU:O	2.40	0.54
1:A:756:GLN:CD	1:A:758:VAL:CG2	2.80	0.54
1:A:756:GLN:CD	1:A:758:VAL:HG21	2.33	0.54
1:D:520:PRO:O	1:D:619:ASN:ND2	2.39	0.54
1:A:1102:GLU:H	1:A:1107:GLY:HA3	1.72	0.54
1:C:177:TYR:HD2	1:C:207:GLN:HG3	1.73	0.54
1:C:756:GLN:CD	1:C:758:VAL:HG21	2.33	0.54
1:A:405:TYR:OH	1:A:496:MET:SD	2.62	0.54
1:C:544:SER:HB3	1:C:569:ASN:HD21	1.71	0.54
1:C:1013:VAL:HG22	1:C:1146:MET:HB3	1.89	0.54
1:B:503:MET:HE1	1:B:690:VAL:HG22	1.89	0.54
1:B:756:GLN:HB2	1:B:758:VAL:HG23	1.90	0.54
1:B:521:LEU:HD13	1:B:616:TYR:HD1	1.73	0.54
1:C:756:GLN:CD	1:C:758:VAL:CG2	2.80	0.53
1:D:503:MET:HE1	1:D:690:VAL:HG22	1.89	0.53
1:D:570:GLU:O	1:D:575:ASN:ND2	2.39	0.53
1:A:639:LEU:HD22	1:A:647:TYR:HE1	1.74	0.53
1:B:232:LEU:HD23	1:B:363:LEU:HD22	1.91	0.53
1:B:405:TYR:OH	1:B:496:MET:SD	2.65	0.53
1:B:596:LEU:HD13	1:C:574:PHE:HE1	1.73	0.53
1:C:655:THR:OG1	2:C:1401:QUS:O18	2.26	0.53
1:A:33:MET:O	1:A:37:SER:OG	2.27	0.53
1:C:639:LEU:HD22	1:C:647:TYR:HE1	1.74	0.53
1:D:521:LEU:HD13	1:D:616:TYR:HD1	1.73	0.53
1:A:141:ARG:NH2	1:A:195:ASP:OD2	2.39	0.53
1:B:570:GLU:O	1:B:575:ASN:ND2	2.39	0.53
1:D:756:GLN:HB2	1:D:758:VAL:HG23	1.90	0.53
1:C:22:ALA:HB1	1:C:25:GLU:HB2	1.91	0.53
1:A:177:TYR:HD2	1:A:207:GLN:HG3	1.72	0.53
1:C:644:GLU:OE2	1:C:699:LYS:NZ	2.42	0.52
1:A:22:ALA:HB1	1:A:25:GLU:HB2	1.91	0.52
1:C:1040:PRO:O	1:C:1086:PHE:N	2.42	0.52
1:C:33:MET:O	1:C:37:SER:OG	2.27	0.52
1:A:644:GLU:OE2	1:A:699:LYS:NZ	2.42	0.52
1:D:544:SER:O	1:D:569:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:SER:O	1:B:569:ASN:ND2	2.42	0.52
1:B:611:ILE:HG21	1:C:795:VAL:HG21	1.91	0.52
1:A:1040:PRO:O	1:A:1086:PHE:N	2.42	0.52
1:D:328:GLU:OE1	1:D:331:ARG:NH2	2.39	0.52
1:A:328:GLU:HG2	1:A:331:ARG:HH21	1.76	0.51
1:B:24:GLN:HE21	1:B:278:ILE:HD12	1.75	0.51
1:D:232:LEU:HD23	1:D:363:LEU:HD22	1.91	0.51
1:A:538:VAL:HG21	1:A:1221:MET:HB3	1.91	0.51
1:D:24:GLN:HE21	1:D:278:ILE:HD12	1.75	0.51
1:C:538:VAL:HG21	1:C:1221:MET:HB3	1.92	0.51
1:B:619:ASN:HD21	1:C:786:ALA:HA	1.75	0.51
1:C:328:GLU:HG2	1:C:331:ARG:HH21	1.76	0.51
1:A:487:GLU:HG3	1:A:488:VAL:HG13	1.93	0.51
1:A:681:VAL:O	1:A:700:TYR:OH	2.25	0.51
1:B:79:LYS:HD3	1:B:142:GLY:HA2	1.94	0.50
1:A:181:PHE:HB3	1:A:213:LYS:HE3	1.93	0.50
1:D:79:LYS:HD3	1:D:142:GLY:HA2	1.94	0.50
1:A:619:ASN:HD22	1:A:622:ALA:HB3	1.77	0.50
1:A:33:MET:HE2	1:A:45:PRO:HD3	1.94	0.49
1:A:536:VAL:HG22	1:B:803:LEU:HD21	1.93	0.49
1:A:630:VAL:HG23	1:A:632:PRO:HD3	1.94	0.49
1:A:655:THR:OG1	2:A:1401:QUS:O18	2.26	0.49
1:C:405:TYR:OH	1:C:496:MET:SD	2.62	0.49
1:C:630:VAL:HG23	1:C:632:PRO:HD3	1.94	0.49
1:A:173:LYS:NZ	1:A:203:ASP:OD2	2.33	0.49
1:B:399:THR:HB	1:B:406:VAL:HG21	1.95	0.49
1:C:33:MET:HE2	1:C:45:PRO:HD3	1.94	0.49
1:C:181:PHE:HB3	1:C:213:LYS:HE3	1.93	0.49
1:C:619:ASN:HD22	1:C:622:ALA:HB3	1.76	0.49
1:C:487:GLU:HG3	1:C:488:VAL:HG13	1.93	0.49
1:A:567:SER:OG	1:A:568:THR:N	2.46	0.49
1:B:77:TYR:HE2	1:B:98:THR:HG21	1.77	0.49
1:C:25:GLU:OE2	1:C:281:THR:OG1	2.27	0.49
1:C:681:VAL:O	1:C:700:TYR:OH	2.25	0.49
1:D:522:ALA:H	1:D:525:ILE:HD12	1.78	0.49
1:C:711:TYR:HB2	1:C:767:TRP:HE1	1.78	0.48
1:D:475:ALA:HB3	1:D:735:ALA:HB3	1.95	0.48
1:D:77:TYR:HE2	1:D:98:THR:HG21	1.77	0.48
1:D:399:THR:HB	1:D:406:VAL:HG21	1.95	0.48
1:A:711:TYR:HB2	1:A:767:TRP:HE1	1.78	0.47
1:B:30:ARG:HB2	1:B:270:TYR:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:SER:H	1:B:325:GLN:HG2	1.78	0.47
1:C:516:SER:OG	1:C:791:ASN:O	2.32	0.47
1:A:516:SER:OG	1:A:791:ASN:O	2.32	0.47
1:B:522:ALA:H	1:B:525:ILE:HD12	1.78	0.47
1:C:1182:MET:HE1	1:D:789:LEU:HD11	1.95	0.47
1:A:587:GLN:HG3	1:D:606:TRP:CD1	2.50	0.47
1:B:475:ALA:HB3	1:B:735:ALA:HB3	1.95	0.47
1:C:316:LEU:HD13	1:C:321:VAL:HB	1.97	0.47
1:D:30:ARG:HB2	1:D:270:TYR:HE1	1.79	0.47
1:D:307:SER:H	1:D:325:GLN:HG2	1.78	0.47
1:A:64:SER:O	1:A:67:SER:OG	2.30	0.47
1:A:130:TRP:CD2	1:A:191:ARG:HD3	2.50	0.47
1:A:1182:MET:HE1	1:B:789:LEU:HD11	1.96	0.47
1:C:529:ILE:O	1:C:533:TYR:N	2.46	0.47
1:A:661:ARG:NH2	1:D:754:SER:O	2.48	0.47
1:C:130:TRP:CD2	1:C:191:ARG:HD3	2.50	0.47
1:D:579:PHE:HB2	1:D:591:ILE:HD11	1.97	0.47
1:C:1153:SER:OG	1:C:1154:SER:N	2.48	0.47
1:C:606:TRP:CD1	1:D:587:GLN:HE21	2.33	0.47
1:A:102:PRO:HA	1:A:112:GLN:HG2	1.97	0.46
1:B:502:ILE:HG12	1:B:703:LEU:HG	1.96	0.46
1:B:754:SER:O	1:C:661:ARG:NH2	2.48	0.46
1:D:489:ILE:HD12	1:D:735:ALA:HB1	1.97	0.46
1:B:328:GLU:OE1	1:B:331:ARG:NH2	2.39	0.46
1:C:64:SER:O	1:C:67:SER:OG	2.30	0.46
1:C:567:SER:OG	1:C:568:THR:N	2.46	0.46
1:C:716:LYS:HG3	1:C:772:GLU:HG2	1.97	0.46
1:C:102:PRO:HA	1:C:112:GLN:HG2	1.97	0.46
1:A:316:LEU:HD13	1:A:321:VAL:HB	1.97	0.46
1:B:489:ILE:HD12	1:B:735:ALA:HB1	1.97	0.46
1:C:170:ASN:HA	1:C:173:LYS:HD3	1.96	0.46
1:C:1190:VAL:O	1:C:1194:LEU:N	2.42	0.46
1:A:729:SER:HB3	1:D:497:SER:HB3	1.98	0.46
1:C:38:THR:OG1	1:C:297:ARG:NH2	2.49	0.46
1:C:236:GLN:NE2	1:C:365:THR:O	2.44	0.46
1:D:502:ILE:HG12	1:D:703:LEU:HG	1.96	0.46
1:A:24:GLN:HE21	1:A:278:ILE:HD12	1.80	0.46
1:D:394:THR:HA	1:D:439:LYS:HB2	1.98	0.46
1:A:170:ASN:HA	1:A:173:LYS:HD3	1.97	0.46
1:A:716:LYS:HG3	1:A:772:GLU:HG2	1.97	0.46
1:C:705:GLU:OE1	1:C:732:TYR:OH	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:GLU:OE2	1:A:281:THR:OG1	2.27	0.46
1:A:83:ASN:ND2	1:B:80:LYS:O	2.48	0.46
1:A:793:ALA:HA	1:A:796:PHE:HD2	1.81	0.46
1:C:793:ALA:HA	1:C:796:PHE:HD2	1.81	0.45
1:A:639:LEU:O	1:A:647:TYR:OH	2.27	0.45
1:A:1098:SER:N	1:A:1111:ARG:O	2.48	0.45
1:D:30:ARG:NH2	1:D:269:GLU:O	2.48	0.45
1:A:326:GLY:HA2	1:A:329:ILE:HD12	1.99	0.45
1:B:579:PHE:HB2	1:B:591:ILE:HD11	1.97	0.45
1:A:38:THR:OG1	1:A:297:ARG:NH2	2.49	0.45
1:C:24:GLN:HE21	1:C:278:ILE:HD12	1.80	0.45
1:A:529:ILE:O	1:A:533:TYR:N	2.46	0.45
1:C:1123:GLY:HA2	1:C:1126:TRP:HD1	1.81	0.45
1:B:394:THR:HA	1:B:439:LYS:HB2	1.98	0.45
1:C:690:VAL:HG21	1:C:712:ILE:HD13	1.98	0.44
1:A:795:VAL:HG21	1:D:611:ILE:HG21	1.99	0.44
1:C:87:SER:OG	1:D:56:PHE:N	2.47	0.44
1:A:690:VAL:HG21	1:A:712:ILE:HD13	1.98	0.44
1:A:1153:SER:OG	1:A:1154:SER:N	2.48	0.44
1:B:30:ARG:NH2	1:B:269:GLU:O	2.48	0.44
1:B:504:ILE:HG21	1:B:633:ILE:HD11	2.00	0.44
1:B:318:ASN:HD22	1:B:318:ASN:HA	1.64	0.44
1:B:742:LEU:HA	1:B:745:PRO:HD2	2.00	0.44
1:A:258:PHE:O	1:A:262:TRP:N	2.51	0.44
1:D:742:LEU:HA	1:D:745:PRO:HD2	2.00	0.44
1:A:236:GLN:NE2	1:A:365:THR:O	2.44	0.43
1:A:1099:CYS:HA	1:A:1110:CYS:HA	2.00	0.43
1:B:529:ILE:O	1:B:533:TYR:N	2.50	0.43
1:B:710:GLU:O	1:B:714:GLN:NE2	2.51	0.43
1:C:173:LYS:NZ	1:C:203:ASP:OD2	2.33	0.43
1:C:194:LEU:HD11	1:C:222:ILE:HG12	2.00	0.43
1:A:1123:GLY:HA2	1:A:1126:TRP:HD1	1.81	0.43
1:C:1099:CYS:HA	1:C:1110:CYS:HA	2.00	0.43
1:D:504:ILE:HG21	1:D:633:ILE:HD11	2.00	0.43
1:A:194:LEU:HD11	1:A:222:ILE:HG12	2.00	0.43
1:C:607:PHE:HD1	1:D:585:MET:HE1	1.84	0.43
1:A:604:VAL:HG12	1:B:799:LEU:HD12	2.01	0.43
1:C:326:GLY:HA2	1:C:329:ILE:HD12	1.99	0.43
1:C:258:PHE:O	1:C:262:TRP:N	2.51	0.43
1:B:86:THR:HG22	1:B:110:VAL:HG21	2.00	0.42
1:C:83:ASN:ND2	1:D:80:LYS:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ILE:HG23	1:D:130:TRP:HB2	2.01	0.42
1:D:710:GLU:O	1:D:714:GLN:NE2	2.51	0.42
1:B:692:ARG:O	1:B:696:SER:OG	2.31	0.42
1:B:592:SER:HA	1:B:593:PRO:HD3	1.93	0.42
1:A:1190:VAL:O	1:A:1194:LEU:N	2.42	0.42
1:B:572:GLY:O	1:B:576:SER:N	2.53	0.42
1:C:1098:SER:N	1:C:1111:ARG:O	2.48	0.42
1:D:86:THR:HG22	1:D:110:VAL:HG21	2.00	0.42
1:B:489:ILE:HG22	1:B:737:PRO:HA	2.02	0.42
1:B:606:TRP:CD1	1:C:587:GLN:HG3	2.55	0.42
1:D:127:TYR:HB2	1:D:380:MET:HG3	2.01	0.42
1:A:88:PHE:HE1	1:B:56:PHE:HA	1.85	0.42
1:A:729:SER:OG	1:D:729:SER:OG	2.27	0.42
1:C:184:LEU:HB3	1:C:189:GLU:HB2	2.02	0.42
1:A:489:ILE:HG22	1:A:737:PRO:HA	2.01	0.41
1:C:107:HIS:HA	1:C:108:PRO:HD3	1.93	0.41
1:D:489:ILE:HG22	1:D:737:PRO:HA	2.02	0.41
1:D:686:THR:OG1	2:D:1301:QUS:O19	2.33	0.41
1:A:77:TYR:HE1	1:A:98:THR:HG21	1.85	0.41
1:C:122:LEU:HD23	1:C:122:LEU:HA	1.91	0.41
2:D:1301:QUS:O20	2:D:1301:QUS:NP3	2.53	0.41
1:A:642:GLN:NE2	1:A:644:GLU:OE1	2.54	0.41
1:A:702:TYR:HE2	1:A:704:LEU:HD13	1.86	0.41
1:C:104:ASP:OD1	1:C:104:ASP:N	2.54	0.41
1:A:184:LEU:HB3	1:A:189:GLU:HB2	2.02	0.41
1:B:127:TYR:HB2	1:B:380:MET:HG3	2.01	0.41
1:C:573:ILE:HD12	1:C:573:ILE:HA	1.95	0.41
1:B:800:VAL:HA	1:B:803:LEU:HD12	2.03	0.41
1:C:150:LEU:HD23	1:C:150:LEU:HA	1.92	0.41
1:D:529:ILE:O	1:D:533:TYR:N	2.50	0.41
1:B:125:ILE:HG23	1:B:130:TRP:HB2	2.01	0.41
1:B:270:TYR:HB2	1:B:273:ALA:HB2	2.03	0.41
1:C:122:LEU:HD21	1:C:149:VAL:HG12	2.03	0.41
1:C:642:GLN:NE2	1:C:644:GLU:OE1	2.54	0.41
1:A:150:LEU:HD23	1:A:150:LEU:HA	1.92	0.41
1:A:246:GLN:HE21	1:A:248:VAL:H	1.69	0.41
1:C:77:TYR:HE1	1:C:98:THR:HG21	1.85	0.41
1:B:174:ASP:HB3	1:B:178:ARG:HH22	1.86	0.40
1:C:489:ILE:HG22	1:C:737:PRO:HA	2.01	0.40
1:C:466:GLU:HG2	1:C:471:LYS:HE2	2.03	0.40
1:D:800:VAL:HA	1:D:803:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:639:LEU:O	1:C:647:TYR:OH	2.27	0.40
1:A:122:LEU:HD21	1:A:149:VAL:HG12	2.02	0.40
1:A:18:PHE:HA	1:A:19:PRO:HD3	1.98	0.40
1:C:12:ILE:HD11	1:C:43:LEU:HG	2.03	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	973/1154 (84%)	926 (95%)	47 (5%)	0	100	100
1	B	779/1154 (68%)	750 (96%)	29 (4%)	0	100	100
1	C	973/1154 (84%)	926 (95%)	47 (5%)	0	100	100
1	D	779/1154 (68%)	750 (96%)	29 (4%)	0	100	100
All	All	3504/4616 (76%)	3352 (96%)	152 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	834/969 (86%)	829 (99%)	5 (1%)	78	80
1	B	669/969 (69%)	666 (100%)	3 (0%)	84	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	834/969 (86%)	829 (99%)	5 (1%)	78	80
1	D	669/969 (69%)	666 (100%)	3 (0%)	84	82
All	All	3006/3876 (78%)	2990 (100%)	16 (0%)	78	81

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	489	ILE
1	A	498	LEU
1	A	787	LEU
1	A	1134	LEU
1	B	215	VAL
1	B	318	ASN
1	B	596	LEU
1	C	50	LEU
1	C	489	ILE
1	C	498	LEU
1	C	787	LEU
1	C	1134	LEU
1	D	215	VAL
1	D	318	ASN
1	D	596	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	13	GLN
1	A	60	ASN
1	A	170	ASN
1	A	214	HIS
1	A	246	GLN
1	A	311	ASN
1	A	435	HIS
1	A	508	GLN
1	A	569	ASN
1	A	619	ASN
1	A	1189	GLN
1	A	1202	HIS

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Mol	Chain	Res	Type
1	B	10	ASN
1	B	24	GLN
1	B	49	ASN
1	B	60	ASN
1	B	214	HIS
1	B	311	ASN
1	B	318	ASN
1	B	344	ASN
1	B	569	ASN
1	B	587	GLN
1	B	619	ASN
1	B	642	GLN
1	B	714	GLN
1	C	10	ASN
1	C	13	GLN
1	C	83	ASN
1	C	170	ASN
1	C	214	HIS
1	C	246	GLN
1	C	311	ASN
1	C	508	GLN
1	C	569	ASN
1	C	619	ASN
1	C	1016	ASN
1	C	1189	GLN
1	C	1202	HIS
1	D	10	ASN
1	D	24	GLN
1	D	49	ASN
1	D	60	ASN
1	D	107	HIS
1	D	214	HIS
1	D	311	ASN
1	D	318	ASN
1	D	344	ASN
1	D	569	ASN
1	D	642	GLN
1	D	714	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	QUS	B	1301	-	9,13,13	5.76	3 (33%)	10,18,18	2.89	5 (50%)
2	QUS	C	1401	-	9,13,13	5.71	3 (33%)	10,18,18	2.85	4 (40%)
2	QUS	D	1301	-	9,13,13	5.76	3 (33%)	10,18,18	2.89	5 (50%)
2	QUS	A	1401	-	9,13,13	5.74	3 (33%)	10,18,18	2.84	4 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	QUS	B	1301	-	-	4/6/8/8	0/1/1/1
2	QUS	C	1401	-	-	3/6/8/8	0/1/1/1
2	QUS	D	1301	-	-	4/6/8/8	0/1/1/1
2	QUS	A	1401	-	-	4/6/8/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301	QUS	O19-C05	12.97	1.45	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1301	QUS	O19-C05	12.94	1.45	1.21
2	A	1401	QUS	O19-C05	12.91	1.45	1.21
2	C	1401	QUS	O19-C05	12.85	1.45	1.21
2	D	1301	QUS	O18-C04	10.48	1.41	1.23
2	B	1301	QUS	O18-C04	10.43	1.41	1.23
2	A	1401	QUS	O18-C04	10.16	1.41	1.23
2	C	1401	QUS	O18-C04	10.11	1.41	1.23
2	C	1401	QUS	C04-N14	-3.68	1.32	1.39
2	A	1401	QUS	C04-N14	-3.67	1.32	1.39
2	B	1301	QUS	C04-N14	-2.97	1.34	1.39
2	D	1301	QUS	C04-N14	-2.97	1.34	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1401	QUS	O20-N14-C03	6.10	125.95	113.83
2	A	1401	QUS	O20-N14-C03	6.07	125.90	113.83
2	B	1301	QUS	O20-N14-C03	5.99	125.72	113.83
2	D	1301	QUS	O20-N14-C03	5.95	125.66	113.83
2	A	1401	QUS	C04-N15-C05	-4.07	105.73	112.62
2	C	1401	QUS	C04-N15-C05	-4.06	105.74	112.62
2	A	1401	QUS	O20-C05-N15	3.82	109.58	106.14
2	C	1401	QUS	O20-C05-N15	3.79	109.56	106.14
2	D	1301	QUS	C04-N15-C05	-3.77	106.23	112.62
2	B	1301	QUS	C04-N15-C05	-3.76	106.24	112.62
2	B	1301	QUS	O20-C05-N15	3.57	109.36	106.14
2	D	1301	QUS	O20-C05-N15	3.54	109.33	106.14
2	D	1301	QUS	O20-C05-O19	2.83	125.41	122.95
2	B	1301	QUS	O20-C05-O19	2.76	125.36	122.95
2	D	1301	QUS	O19-C05-N15	-2.70	125.26	129.68
2	B	1301	QUS	O19-C05-N15	-2.69	125.29	129.68
2	C	1401	QUS	O19-C05-N15	-2.11	126.23	129.68
2	A	1401	QUS	O19-C05-N15	-2.09	126.26	129.68

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1401	QUS	O16-C01-C02-C03
2	B	1301	QUS	O16-C01-C02-C03
2	B	1301	QUS	O16-C01-C02-NP3
2	B	1301	QUS	O17-C01-C02-C03

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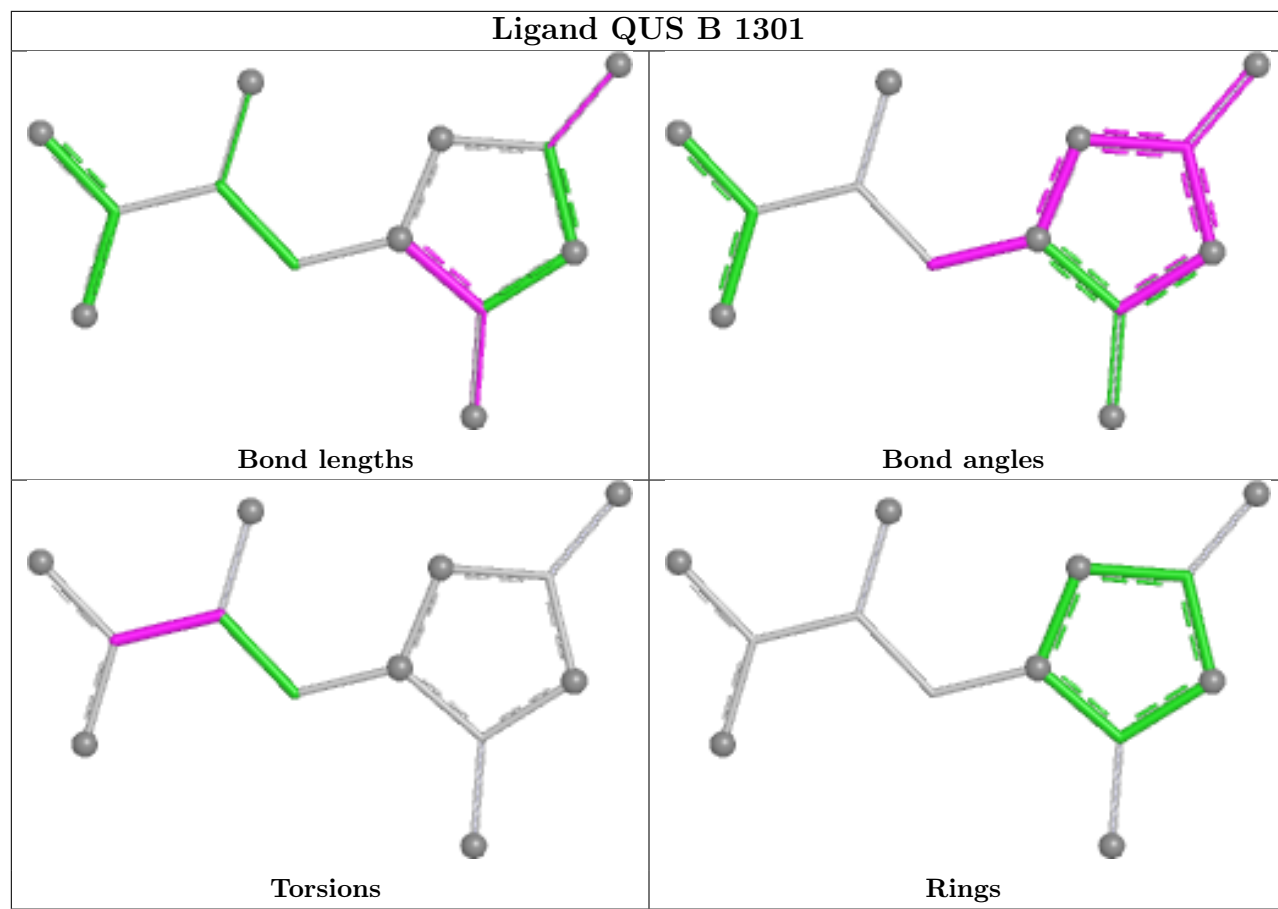
Mol	Chain	Res	Type	Atoms
2	C	1401	QUS	O16-C01-C02-C03
2	D	1301	QUS	O16-C01-C02-C03
2	D	1301	QUS	O16-C01-C02-NP3
2	D	1301	QUS	O17-C01-C02-C03
2	B	1301	QUS	O17-C01-C02-NP3
2	D	1301	QUS	O17-C01-C02-NP3
2	A	1401	QUS	O17-C01-C02-C03
2	C	1401	QUS	O17-C01-C02-C03
2	A	1401	QUS	O17-C01-C02-NP3
2	C	1401	QUS	O17-C01-C02-NP3
2	A	1401	QUS	O16-C01-C02-NP3

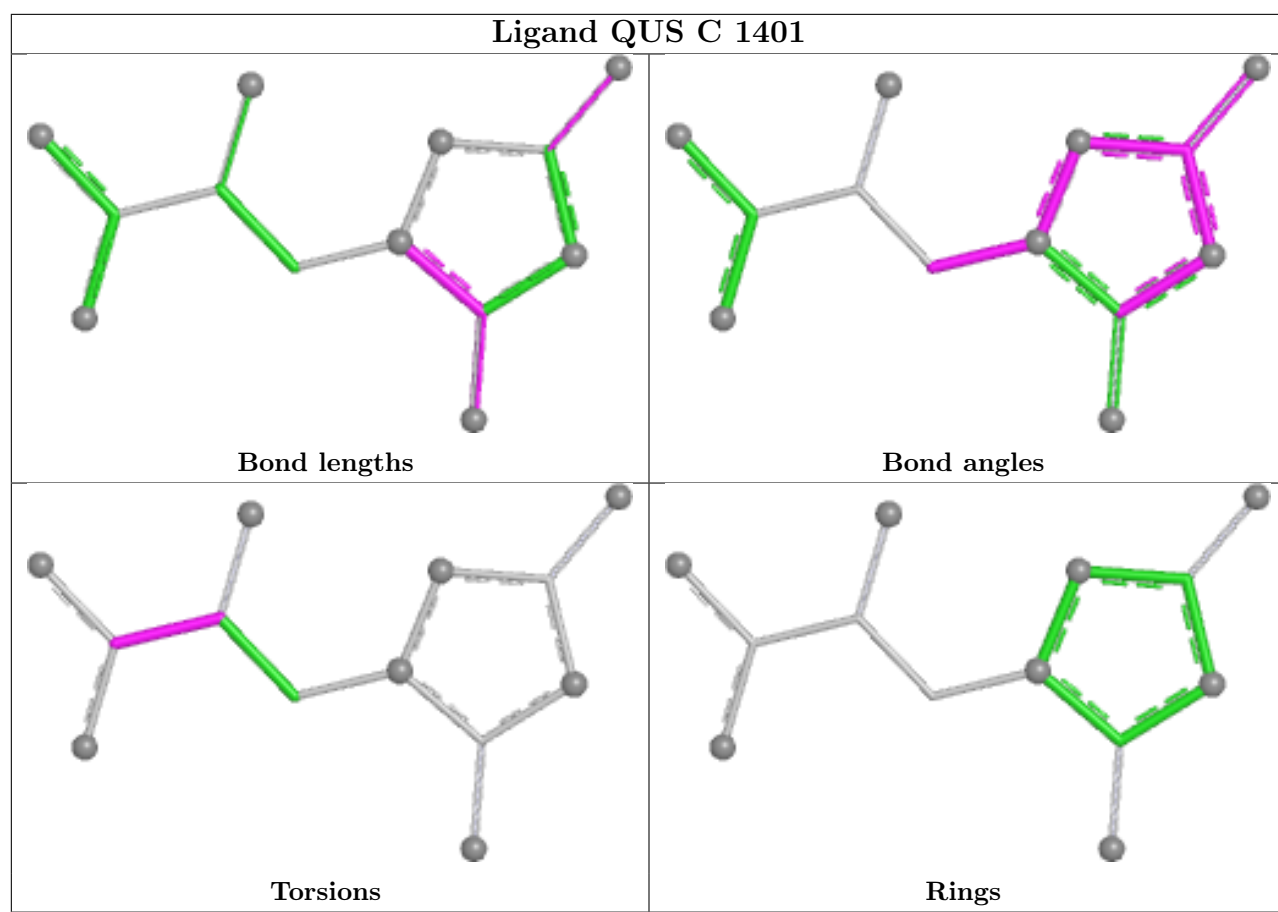
There are no ring outliers.

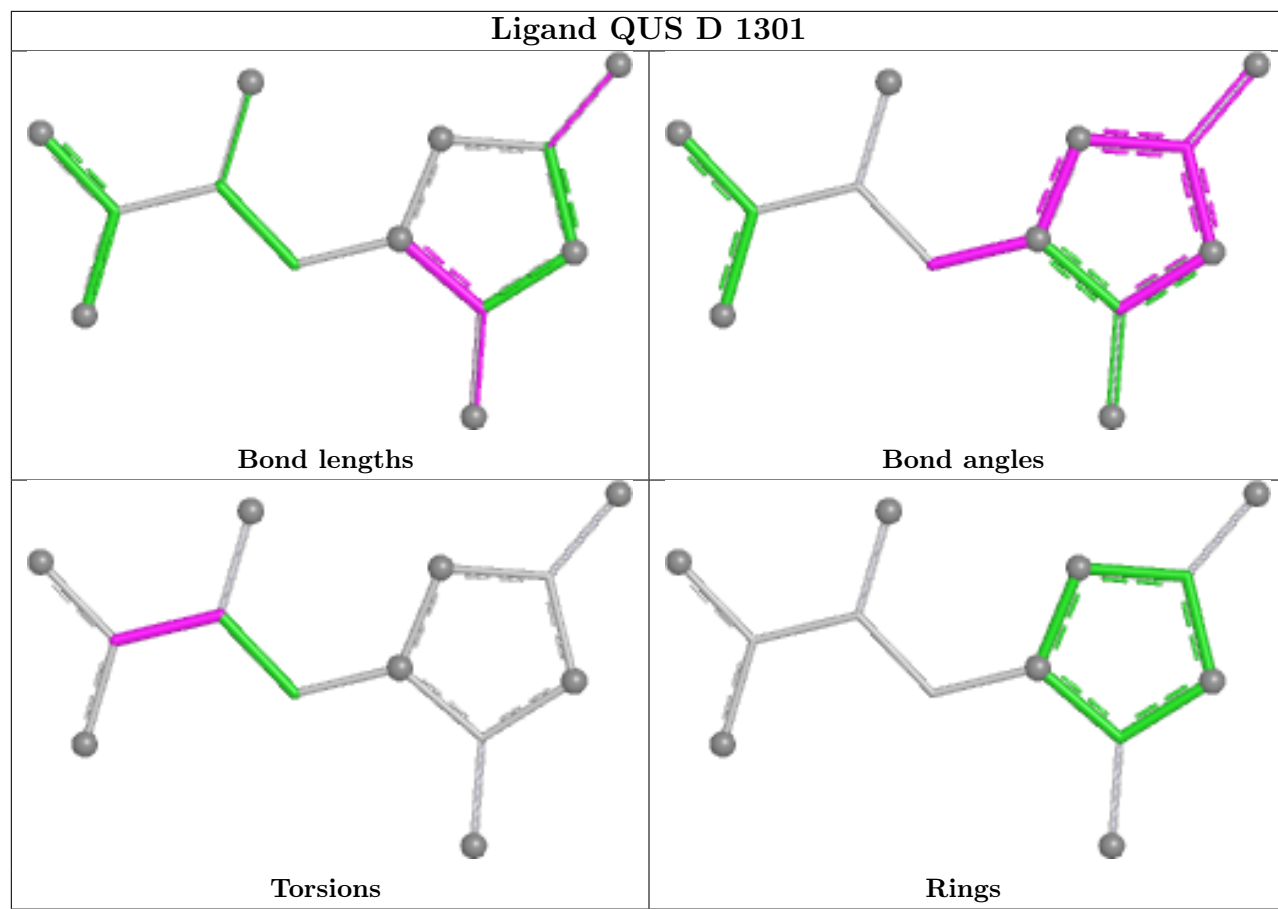
3 monomers are involved in 4 short contacts:

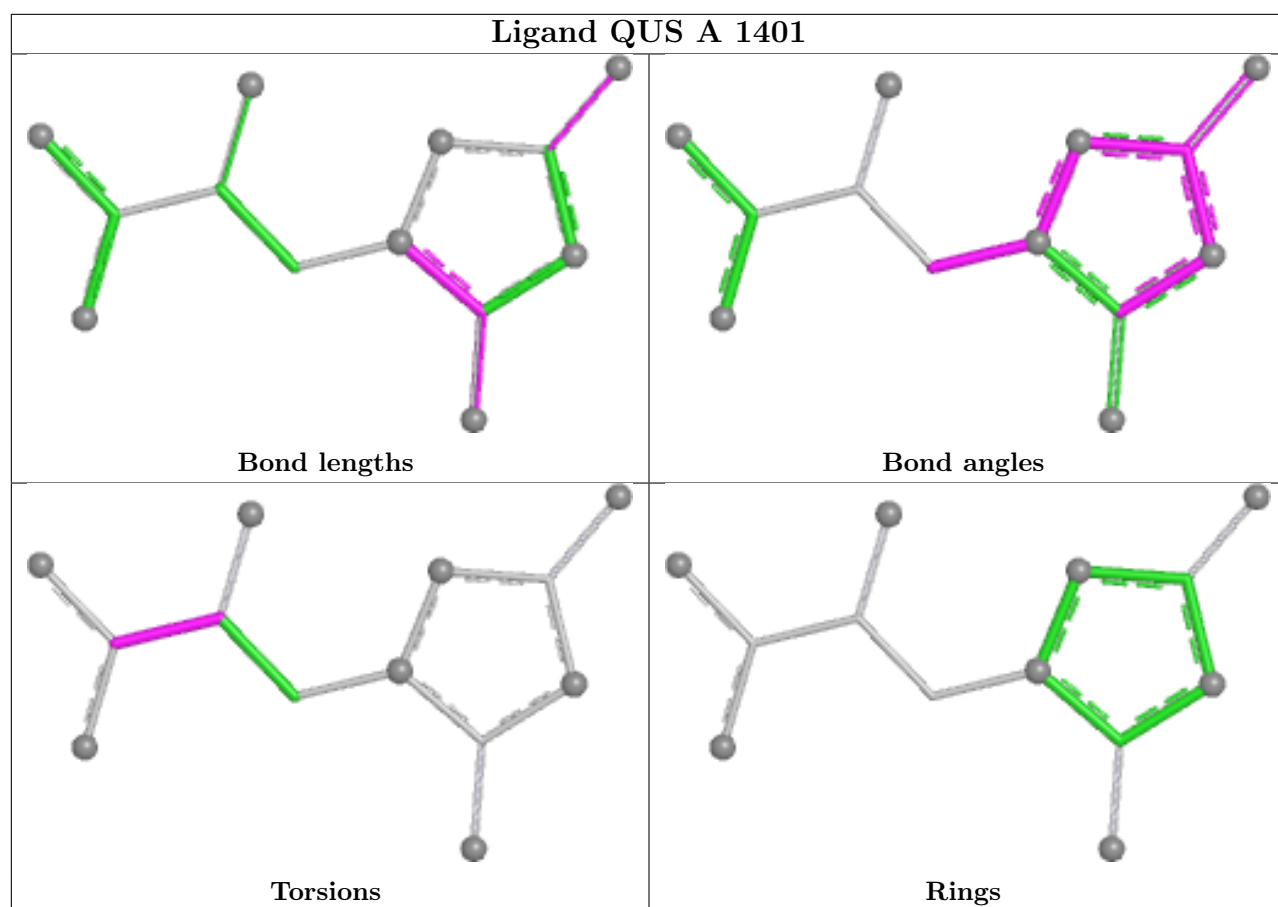
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1401	QUS	1	0
2	D	1301	QUS	2	0
2	A	1401	QUS	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

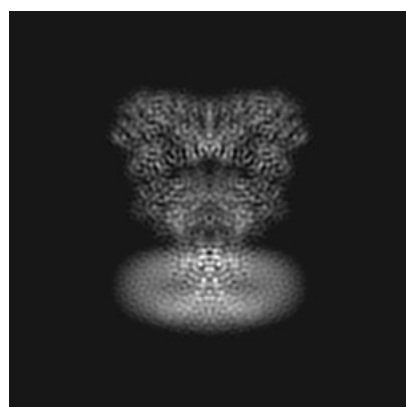
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24756. These allow visual inspection of the internal detail of the map and identification of artifacts.

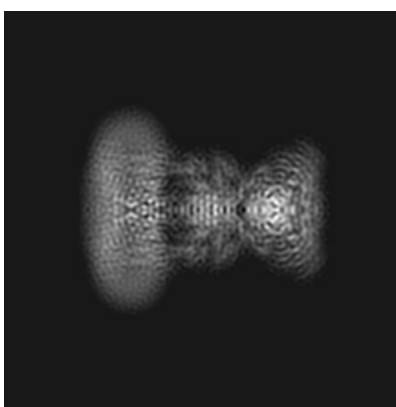
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

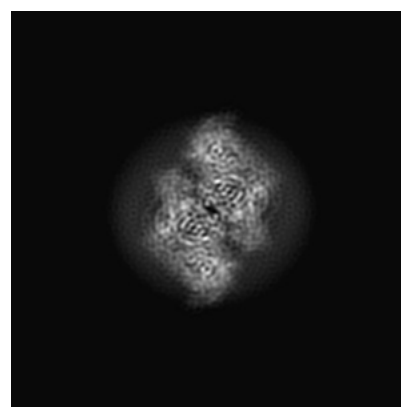
6.1.1 Primary map



X



Y

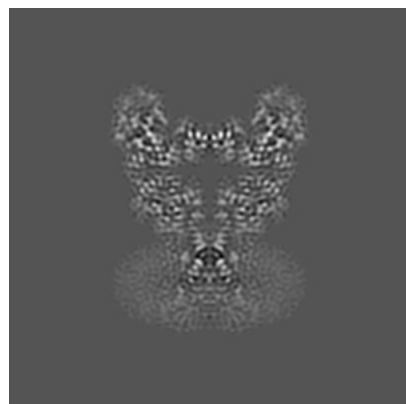


Z

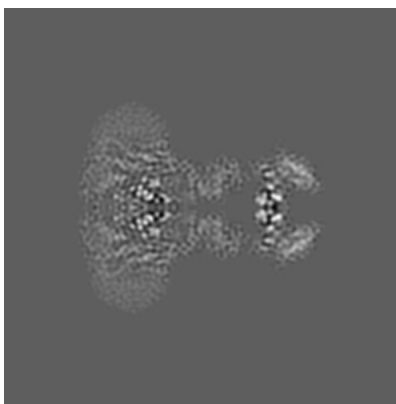
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

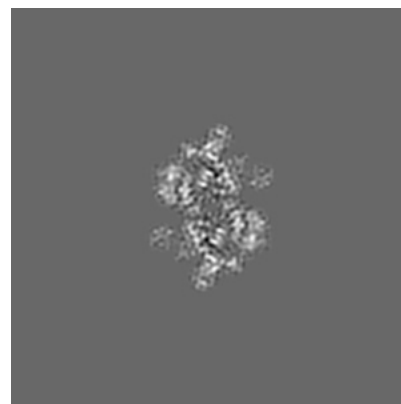
6.2.1 Primary map



X Index: 180



Y Index: 180



Z Index: 180

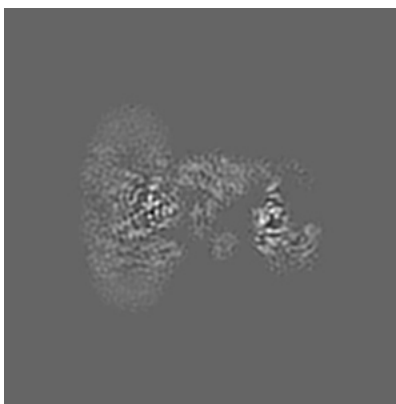
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

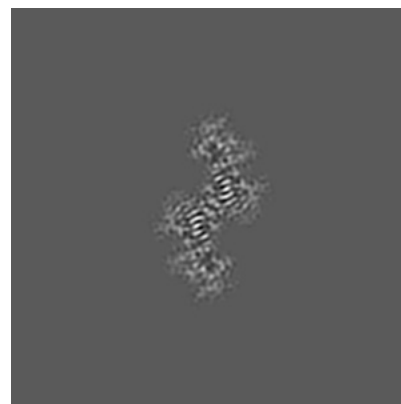
6.3.1 Primary map



X Index: 180



Y Index: 172

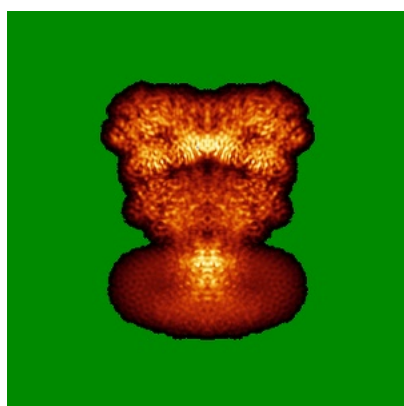


Z Index: 236

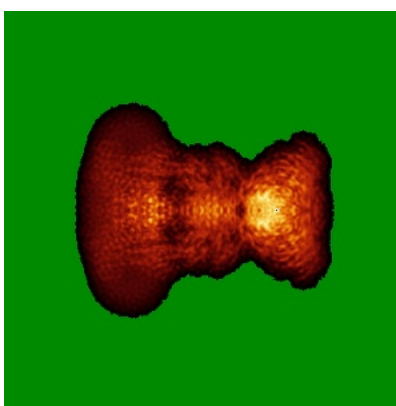
The images above show the largest variance slices of the map in three orthogonal directions.

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

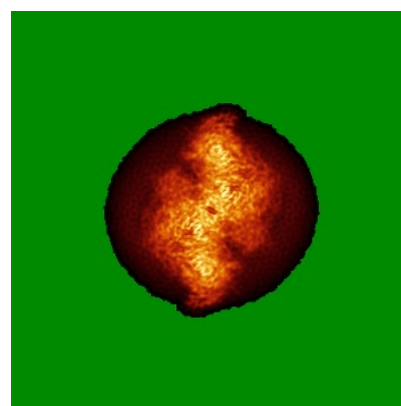
6.4.1 Primary map



X



Y

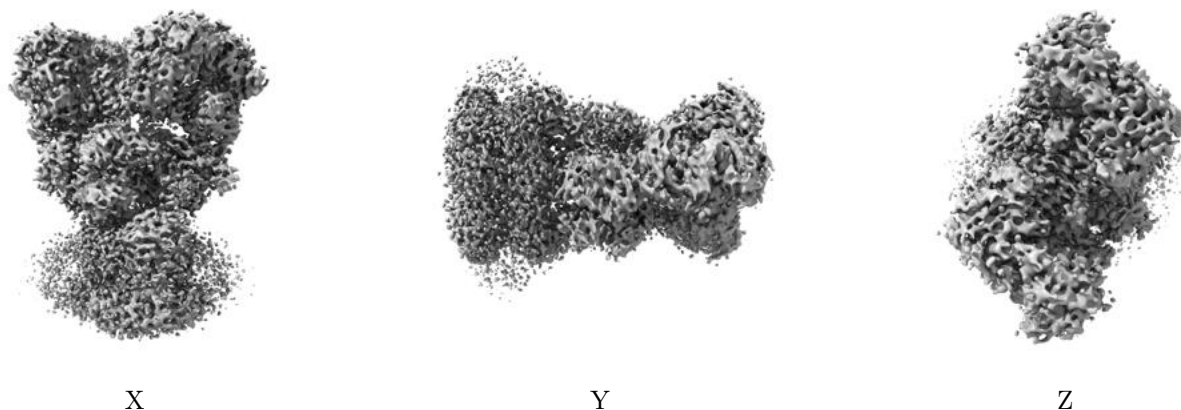


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0077. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

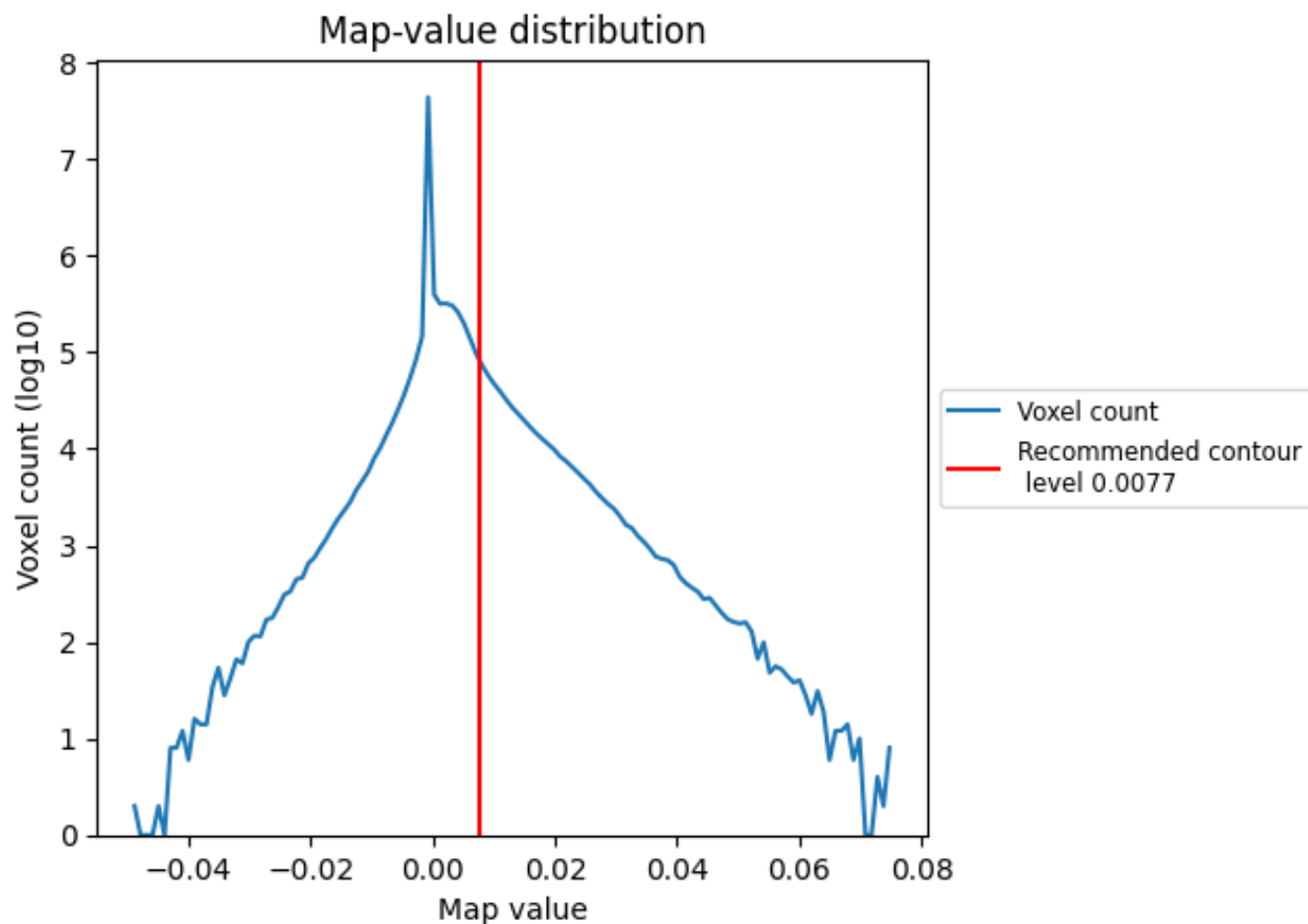
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

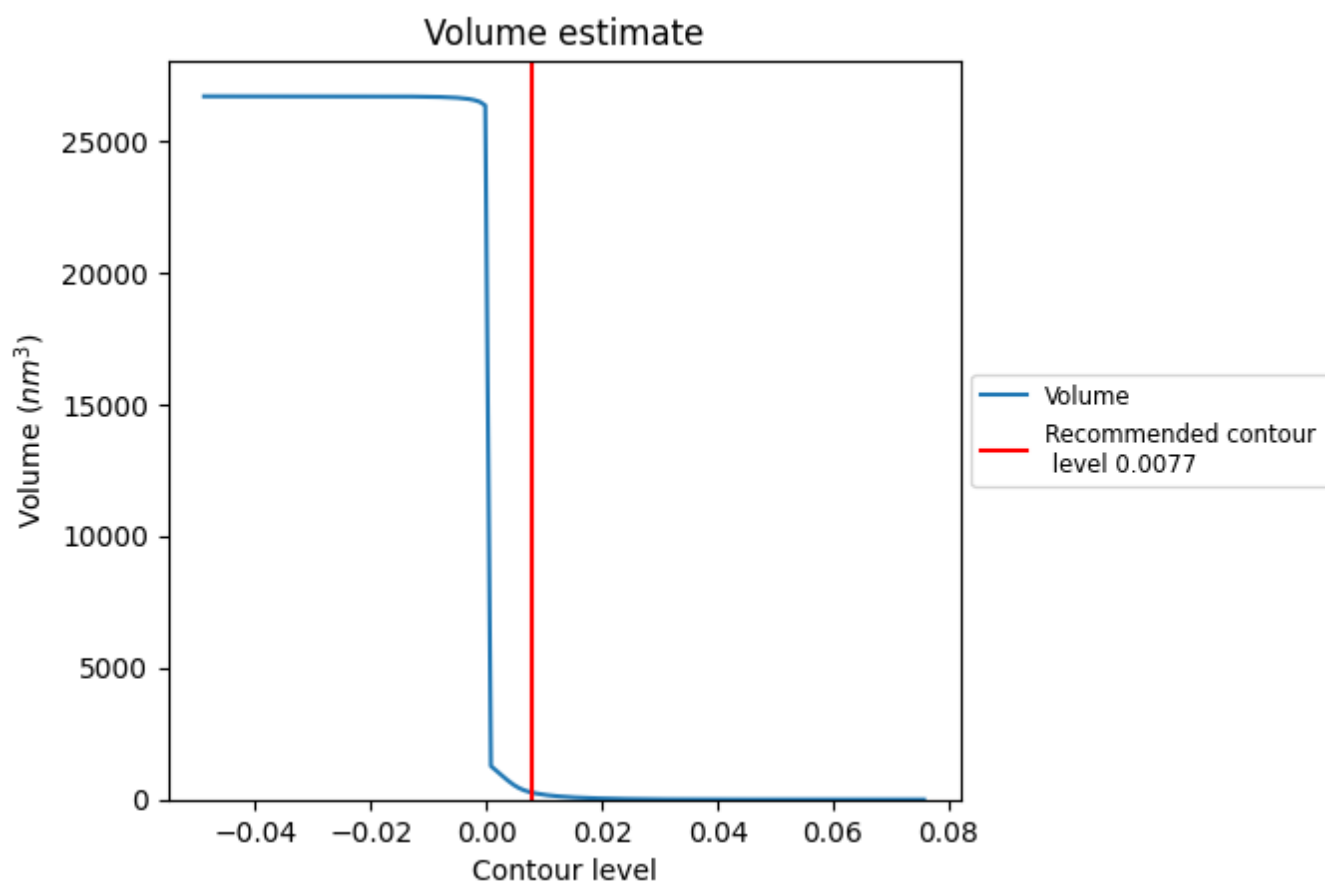
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

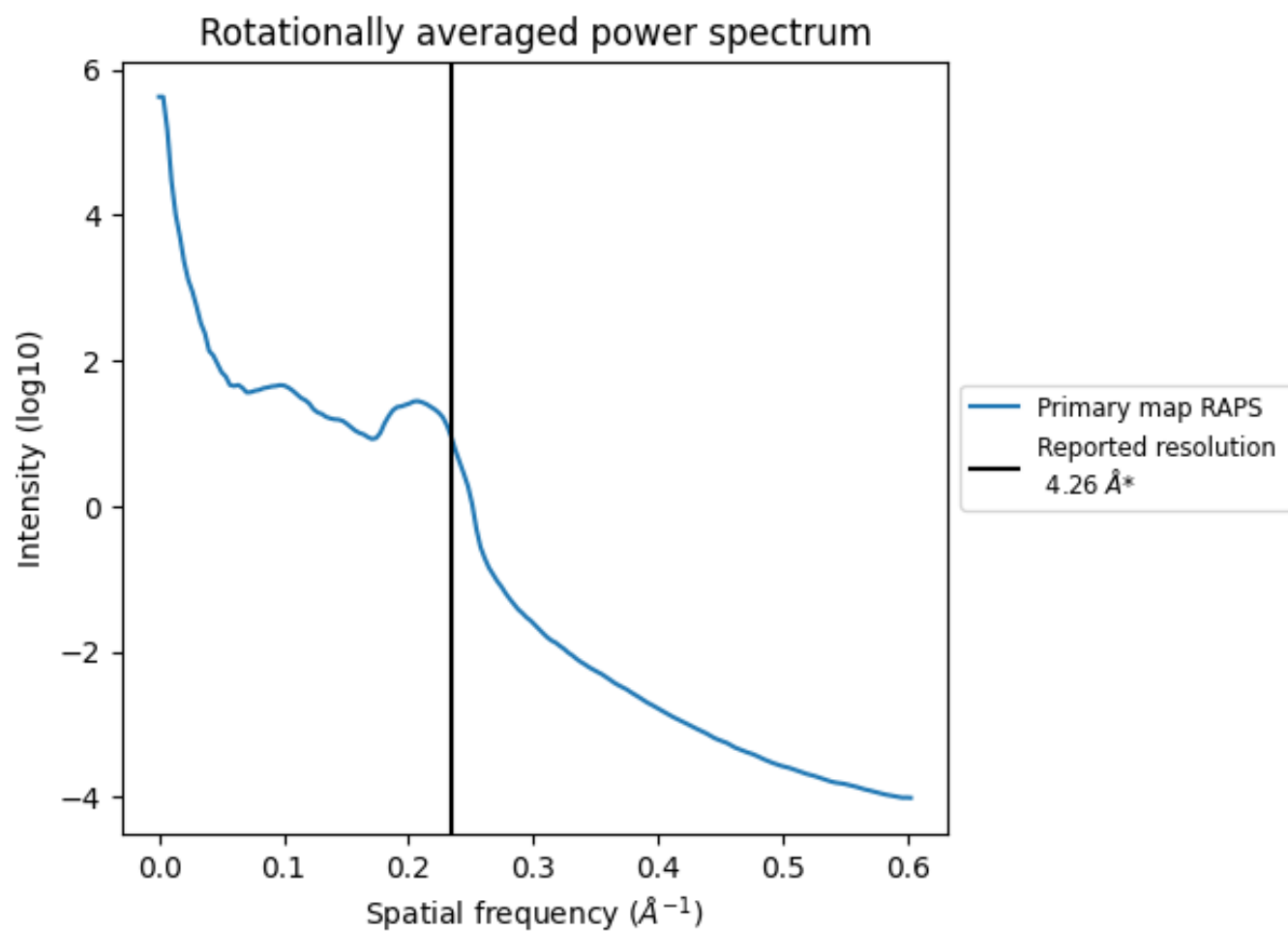
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 276 nm³; this corresponds to an approximate mass of 249 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

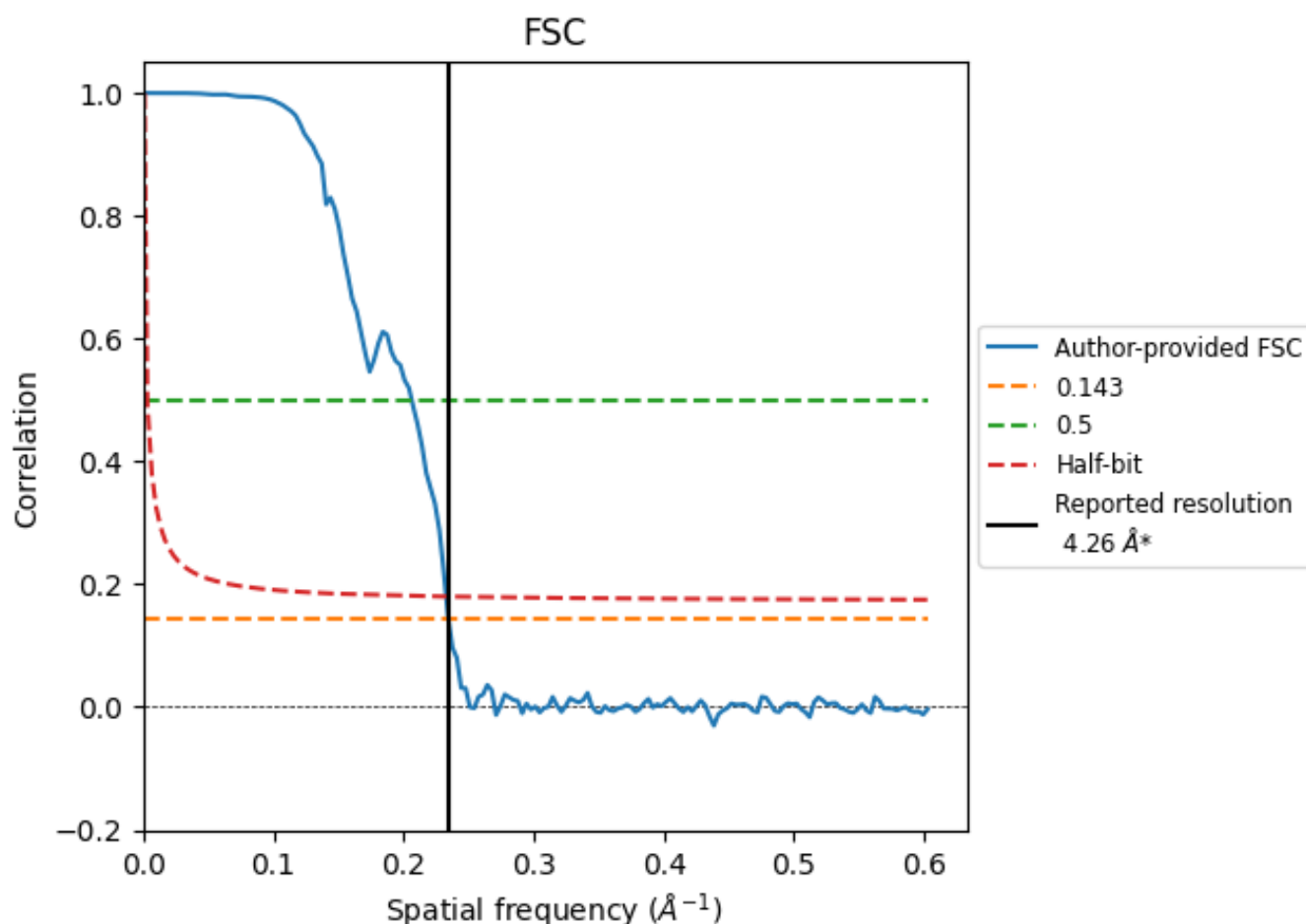


*Reported resolution corresponds to spatial frequency of 0.235 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.235 Å⁻¹

8.2 Resolution estimates [i](#)

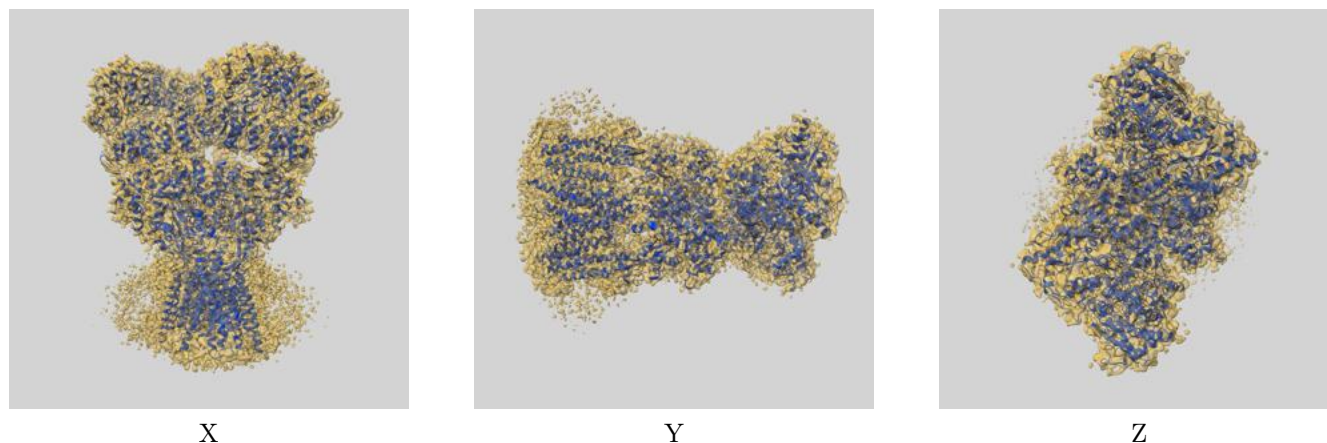
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.26	-	-
Author-provided FSC curve	4.27	4.85	4.30
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

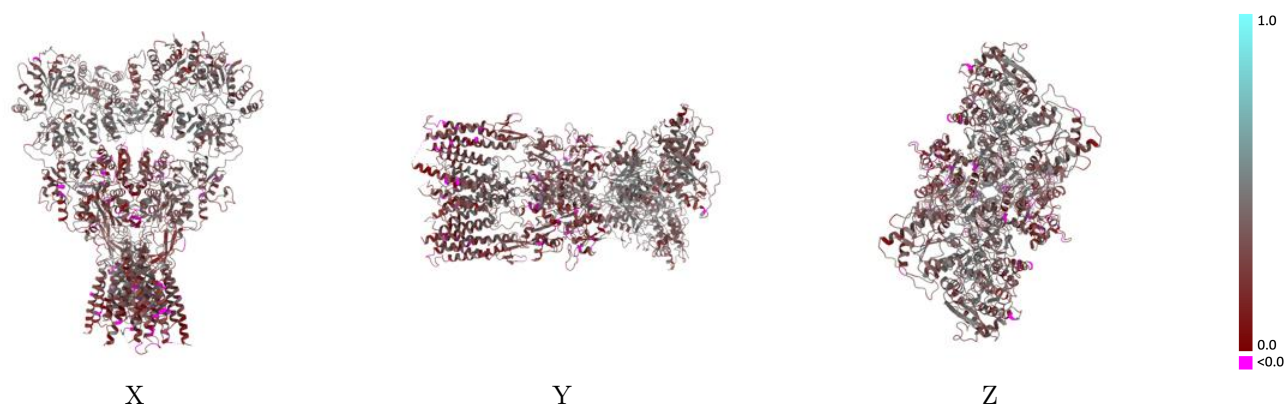
This section contains information regarding the fit between EMDB map EMD-24756 and PDB model 7RZA. Per-residue inclusion information can be found in section [3](#) on page [39](#).

9.1 Map-model overlay [i](#)



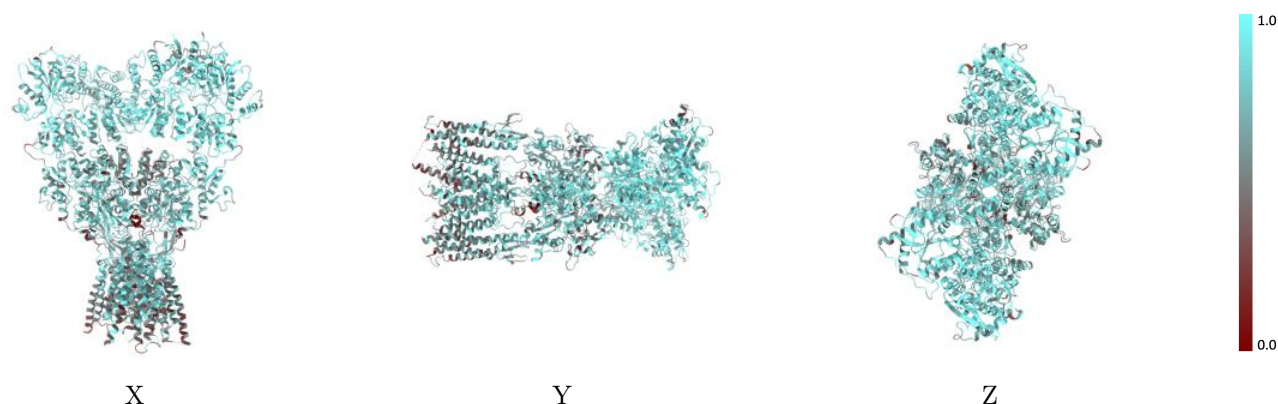
The images above show the 3D surface view of the map at the recommended contour level 0.0077 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



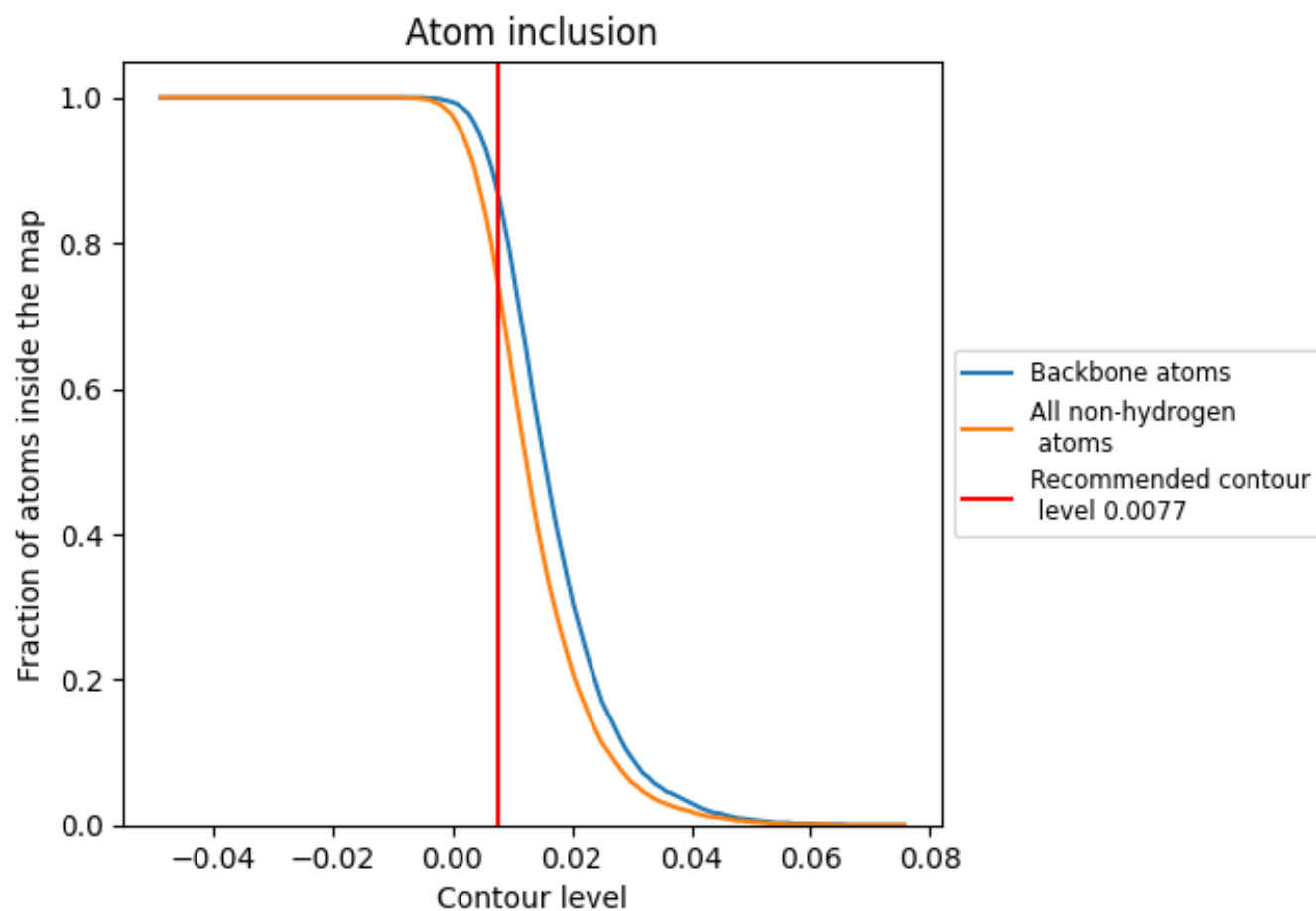
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0077).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 74% 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 (0.0077) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7440	0.3330
A	0.7400	0.3370
B	0.7450	0.3250
C	0.7460	0.3410
D	0.7460	0.3270

