



Full wwPDB EM Validation Report ⓘ

Jun 29, 2025 – 03:03 am BST

PDB ID : 8ROR / pdb_00008ror
EMDB ID : EMD-19402
Title : Single-particle cryo-EM of Mycoplasma pneumoniae adhesin P1 complexed with the anti-adhesive Fab fragment.
Authors : Vizarraga, D.; Kawamoto, A.; Marcos-Silva, M.; Fita, I.; Miyata, M.; Pinyol, J.; Namba, K.; Kenri, T.
Deposited on : 2024-01-12
Resolution : 2.39 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

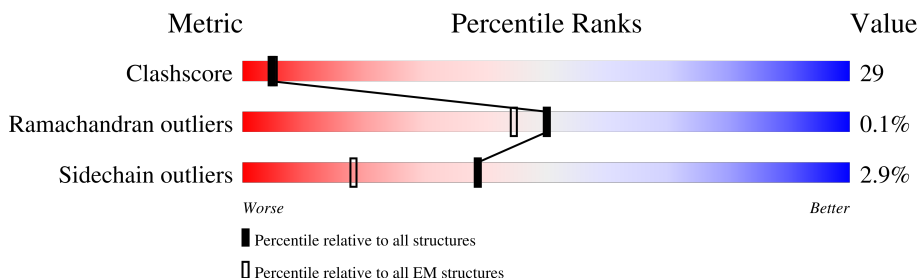
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.39 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	1457	<div> <div>71%</div> <div>43% 49% 7%</div> </div>
2	L	218	<div> <div>69%</div> <div>61% 38%</div> </div>
3	H	222	<div> <div>84%</div> <div>61% 37%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14205 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 Adhesin P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	1349	Total	C	N	O	S	9	0
			10563	6659	1841	2053	10		

- Molecule 2 is a protein called Light Chain Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	218	Total	C	N	O	S	0	0
			1698	1066	288	337	7		

- Molecule 3 is a protein called Heavy Chain Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	222	Total	C	N	O	S	0	0
			1675	1057	271	337	10		

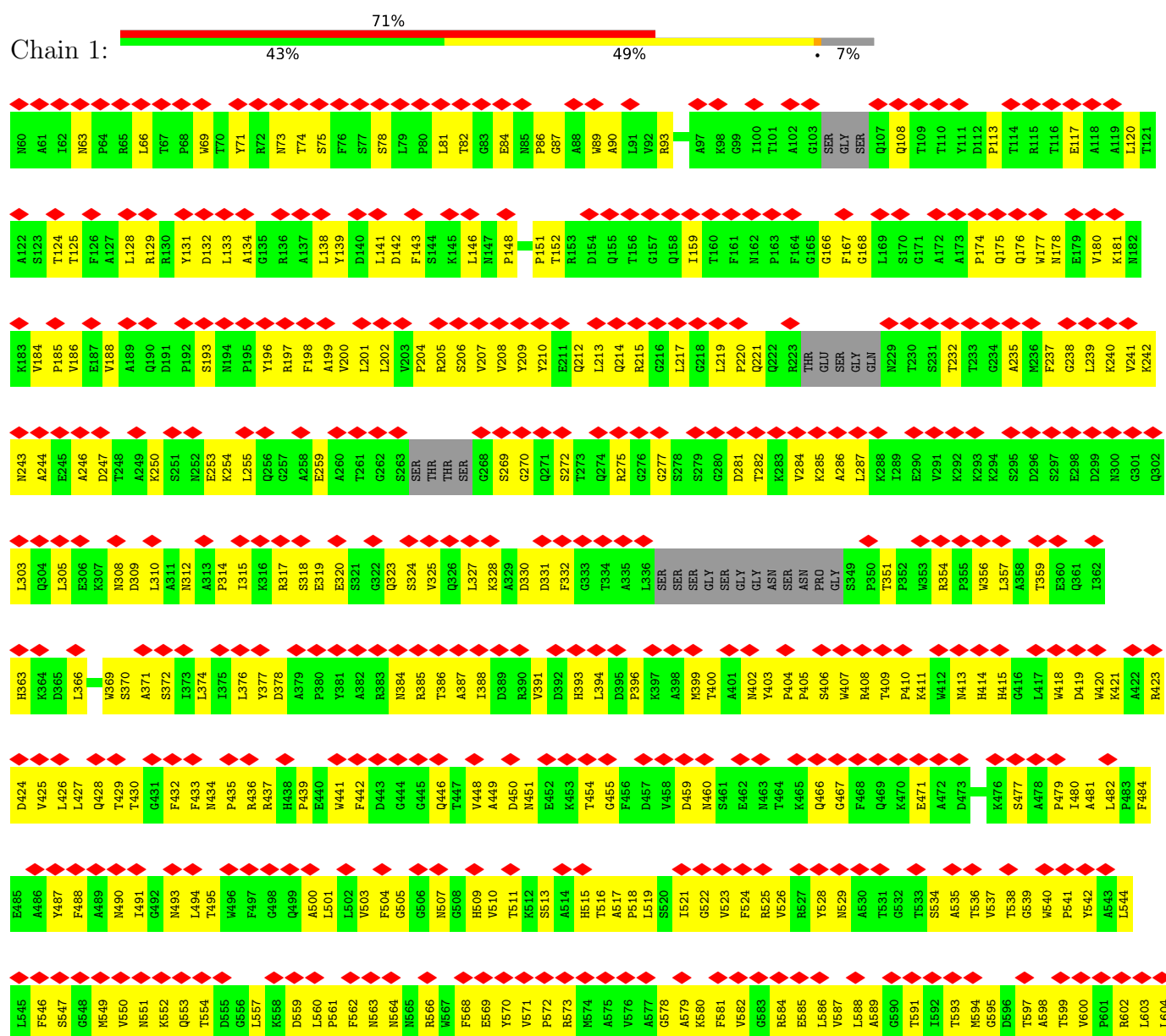
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	1	267	Total	O	0
			267	267	
4	H	2	Total	O	0
			2	2	

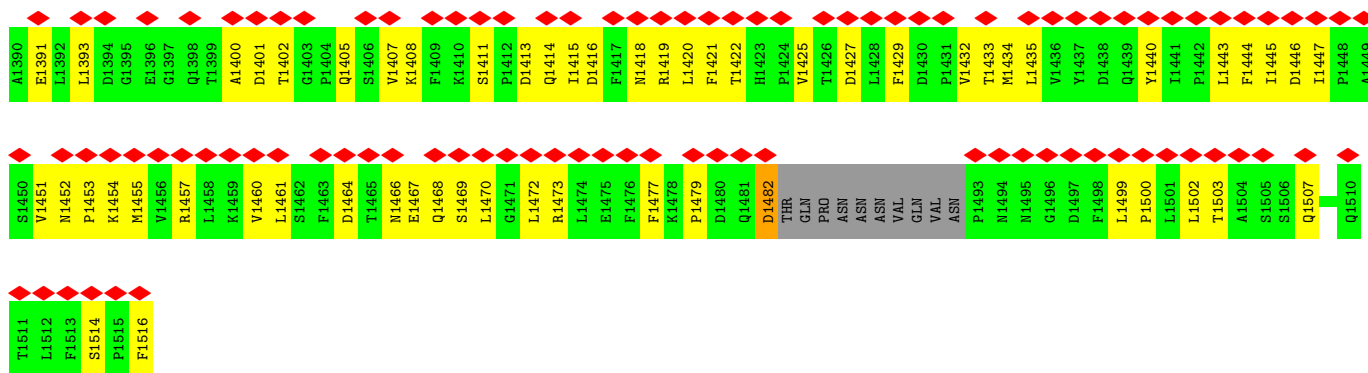
3 Residue-property plots

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

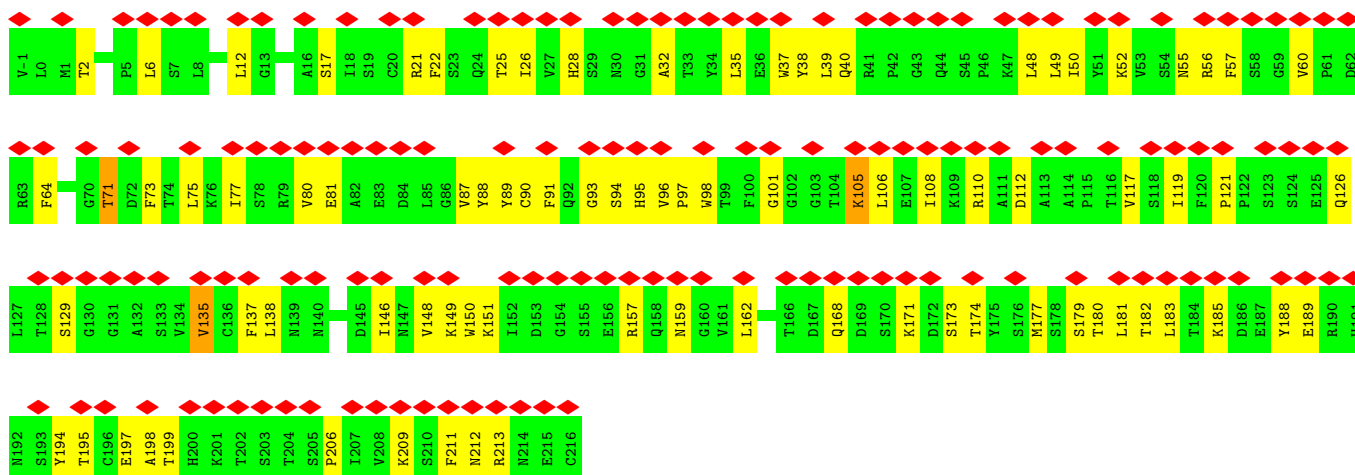
• Molecule 1: Adhesin P1



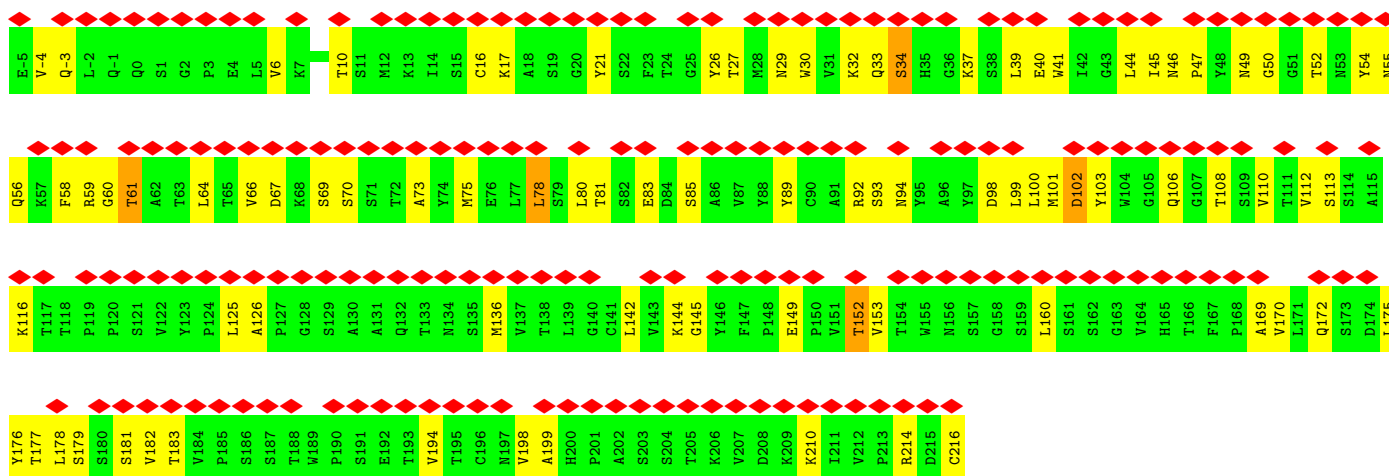
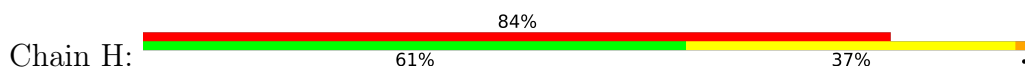
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T1269	K1270	L1271	R1272	Q1273	S1274	F1275	G1276	T1277	D1278	H1279	S1280	T1281	Q1282	P1283	Q1284	P1285	Q1286	S1287	L1288	K1289	T1290	T1291	T1292	P1293	V1294	F1295	G1296	T1297	S1298	S1299	G1300	N1301	L1302	S1303	S1304	K1305	L1306	S1307	GLY	GLY	GLY	ALA	GLY	GLY	GLY	SER	SER	GLY	GLY	GLN	SER	GLY	VAL	D1324	L1325	S1326	P1327	V1328		
K1088	A1089	T1090	L1091	I1092	T1093	P1094	L1096	A1097	W1098	T1099	P1100	Q1101	D1102	V1103	G1104	N1105	L1106	V1107	N1108	S1109	G1110	T1111	T1112	V1113	S1114	F1115	Q1116	L1117	W1120	L1121	V1122	T1123	F1124	T1125	D1126	F1127	V1128	K1129	P1130	R1131	A1132	G1133	Y1134	L1135	G1136	L1137	Q1138	L1139	T1140	G1141	K1079	T1080	P1081	E1082	Q1083	N1084	N1085	A1147	T1148	
Q1149	R1150	A1151	L1152	T1153	W1154	A1155	P1156	R1157	P1158	W1159	A1160	A1161	F1162	G1163	G1164	S1165	W1166	V1167	N1168	R1169	S1169	G1170	G1171	R1172	V1173	E1174	S1175	W1176	W1177	D1178	K1180	G1181	W1182	W1183	A1184	D1185	Q1186	A1187	Q1188	T1189	S1189	Q1190	S1191	Q1192	GLY	SER	THR	THR	THR	ALA	ARG	ASN	A1202	L1203	P1204	E1205	N1206	P1207	N1208	
A1209	L1210	A1211	F1212	Q1213	V1214	S1215	V1216	E1217	E1218	A1219	S1220	A1221	Y1222	G1223	P1224	N1225	T1226	SER	SER	GLY	GLN	THR	GLN	S1233	T1234	N1235	S1236	S1237	P1238	Y1239	L1240	H1241	L1242	V1243	K1244	P1245	K1246	K1247	V1248	T1249	Q1250	S1251	D1252	K1253	L1254	T1255	D1256	Q1257	L1258	K1259	N1260	L1261	L1262	D1263	P1264	N1265	Q1266	V1267	R1268	
E1269	K1270	L1271	R1272	Q1273	S1274	F1275	G1276	T1277	D1278	H1279	S1280	T1281	Q1282	P1283	Q1284	P1285	Q1286	S1287	L1288	K1289	T1290	T1291	T1292	P1293	V1294	F1295	G1296	T1297	S1298	S1299	G1300	N1301	L1302	S1303	S1304	K1305	L1306	S1307	GLY	GLY	GLY	ALA	GLY	GLY	GLY	SER	SER	GLY	GLY	GLN	SER	GLY	VAL	D1324	L1325	S1326	P1327	V1328		
Y605	D606	E607	L608	E609	S610	N611	N612	N613	L614	V615	A616	Q617	G618	Q619	G620	L621	L622	R623	E624	D625	L626	Q627	L628	F629	T630	P631	Y632	G633	W634	A635	N636	R637	P638	D639	L640	P641	I642	G643	A644	W645	S646	S647	S648	S649	S650	S651	S652	H653	N654	A655	P656	Y657	Y658	F659	H660	N661	N662	P663	D664	
W665	Q666	D667	R668	P669	I670	Q671	N672	N673	V674	D675	A676	F677	I678	Q679	K679	G680	W681	E682	D683	K684	N685	L686	G687	D688	D689	T689	K691	Y692	I693	Y694	P695	Y696	R697	Y698	Y699	G699	W700	G701	W702	A703	W704	Q705	W706	Y707	N708	W709	S710	N711	K712	L713	T714	D715	Q716	L718	N719	A720	D721	V722	N724	
E725	N726	A727	Y728	Q729	N730	N731	S732	L733	F734	A735	A736	I737	L738	N739	W740	E741	L742	L743	A744	A745	L746	P747	D748	K749	I811	V750	K751	Y752	G753	K754	E755	F758	A759	A760	N761	E762	Y763	E764	R765	F766	N767	Q768	K769	L770	T771	V772	A773	P774	T775	Q776	T777	T778	N779	W780	S781	H782	F783	S784	P785	
T786	L787	S788	R789	F790	S791	T792	T793	F794	N795	L796	V797	G798	S799	W800	L801	D802	Q803	W804	L805	D806	Y807	W808	P809	W810	I811	G812	N813	G814	Y815	R816	Y817	G818	N819	N820	R822	G823	W824	D825	D826	I827	T828	A829	P830	Q831	THR	SER	ALA	GLY	SER	SER	GLY	ILE	SER	THR	ASN	THR	SER			
GLY	S847	R848	S849	F850	L851	P852	T853	F854	S855	N856	I857	G858	V859	G860	L861	K862	A863	N864	V865	Q866	A867	T868	L869	G870	G871	SER	GLN	THR	MET	ILE	THR	GLY	SER	PRO	ARG	ARG	THR	LEU	ASP	GLN	A888	N889	L890	Q891	L892	W893	T894	G895	A896	G897	W898	R899	N900	D901	K902	Q903	Q904	S905		
G906	Q907	S908	D909	E910	N911	H912	T913	K914	L1035	T915	T916	S917	A918	T919	G920	N921	D922	Q923	Q924	GLY	GLN	SER	G928	T929	S930	A931	G932	N933	P934	S935	S936	L937	R938	Q939	D940	N941	I942	S943	K944	S945	G946	D947	S948	L949	T950	T951	Q952	D953	G954	N955	A956	T957	D958	Q959	Q960	E961	A962	T963	N964	Y965
T966	N967	L968	P969	P970	N971	L972	T973	P974	T975	A976	D977	W978	P979	N980	A981	L982	S983	F984	T985	N986	K987	N988	N989	A990	Q991	R992	A993	Q994	L995	F996	L997	R998	Q999	L1000	L1001	G1002	S1003	I1004	P1005	V1006	L1007	V1008	N1009	R1010	S1011	G1012	N1016	K1017	F1018	Q1019	A1020	T1021	D1022	Q1023	K1024	W1025	S1026	Y1027		
T1028	D1029	L1030	H1031	S1032	D1033	Q1034	T1035	K1036	L1037	N1038	L1039	P1040	A1041	Y1042	G1043	E1044	V1045	M1046	G1047	L1048	L1049	N1050	P1051	A1052	L1053	V1054	E1055	T1056	Y1057	F1058	G1059	N1060	T1061	R1062	A1063	G1064	G1065	S1066	G1067	SER	ASN	THR	T1071	S1072	P1073	P1074	G1075	I1076	F1077	F1078	K1079	T1080	P1081	E1082	Q1083	N1084	N1085	D1086	S1087	
K1088	A1089	T1090	L1091	I1092	T1093	P1094	L1096	A1097	W1098	T1099	P1100	Q1101	D1102	V1103	G1104	N1105	L1106	V1107	N1108	S1109	G1110	T1111	T1112	V1113	S1114	F1115	Q1116	L1117	W1120	L1121	V1122	T1123	F1124	T1125	D1126	F1127	V1128	K1129	P1130	R1131	A1132	G1133	Y1134	L1135	G1136	L1137	Q1138	L1139	T1140	G1141	K1079	T1080	P1081	E1082	Q1083	N1084	N1085	A1147	T1148	
Q1149	R1150	A1151	L1152	T1153	W1154	A1155	P1156	R1157	P1158	W1159	A1160	A1161	F1162	G1163	G1164	S1165	W1166	V1167	N1168	R1169	S1169	G1170	G1171	R1172	V1173	E1174	S1175	W1176	W1177	D1178	K1180	G1181	W1182	W1183	A1184	D1185	Q1186	A1187	Q1188	T1189	S1189	Q1190	S1191	Q1192	GLY	SER	THR	THR	THR	ALA	ARG	ASN	A1202	L1203	P1204	E1205	N1206	P1207	N1208	
A1209	L1210	A1211	F1212	Q1213	V1214	S1215	V1216	E1217	E1218	A1219	S1220	A1221	Y1222	G1223	P1224	N1225	T1226	SER	SER	GLY	GLN	THR	GLN	S1233	T1234	N1235	S1236	S1237	P1238	Y1239	L1240	H1241	L1242	V1243	K1244	P1245	K1246	K1247	V1248	T1249	Q1250	S1251	D1252	K1253	L1254	T1255	D1256	Q1257	L1258	K1259	N1260	L1261	L1262	D1263	P1264	N1265	Q1266	V1267	R1268	
E1269	K1270	L1271	R1272	Q1273	S1274	F1275	G1276	T1277	D1278	H1279	S1280	T1281	Q1282	P1283	Q1284	P1285	Q1286	S1287	L1288	K1289	T1290	T1291	T1292	P1293	V1294	F1295	G1296	T1297	S1298	S1299	G1300	N1301	L1302	S1303	S1304	K1305	L1306	S1307	GLY	GLY	GLY	ALA	GLY	GLY	GLY	SER	SER	GLY	GLY	GLN	SER	GLY	VAL	D1324	L1325	S1326	P1327	V1328		



• Molecule 2: Light Chain Fab



• Molecule 3: Heavy Chain Fab



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4312408	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.027	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	188.0, 188.0, 188.0	wwPDB
Map dimensions	376, 376, 376	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5, 0.5, 0.5	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1	0.22	0/10826	0.38	2/14749 (0.0%)
2	L	0.13	0/1739	0.32	0/2361
3	H	0.15	0/1718	0.36	0/2349
All	All	0.20	0/14283	0.37	2/19459 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	448	VAL	N-CA-C	-5.60	107.28	112.43
1	1	958	ASP	CB-CA-C	-5.38	110.35	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	10563	0	10175	682	0
2	L	1698	0	1638	73	0
3	H	1675	0	1630	77	0
4	1	267	0	0	14	0
4	H	2	0	0	0	0
All	All	14205	0	13443	804	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 29.

All (804) 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)
3:H:214:ARG:H	3:H:214:ARG:HD3	1.39	0.86
1:1:374:LEU:HD13	1:1:388:ILE:HG12	1.61	0.82
1:1:1088:LYS:NZ	1:1:1253:LYS:O	2.12	0.82
1:1:733:LEU:HD21	1:1:1122:VAL:HG11	1.63	0.81
1:1:515:HIS:HE1	1:1:1209:ALA:HB3	1.48	0.79
1:1:217:LEU:HD11	1:1:439:PRO:HG2	1.65	0.78
1:1:202:LEU:O	1:1:371:ALA:HA	1.83	0.77
1:1:139:TYR:OH	1:1:378:ASP:OD1	2.01	0.77
1:1:399:MET:HG2	1:1:482:LEU:HD22	1.69	0.74
1:1:809:PRO:HA	1:1:816:ARG:HA	1.70	0.74
1:1:806:ASP:OD2	1:1:852:PRO:HB2	1.87	0.74
3:H:93:SER:HB3	3:H:101:MET:H	1.52	0.73
1:1:711:ASN:HB3	1:1:723:VAL:HG22	1.70	0.73
1:1:749:LYS:HA	1:1:749:LYS:HE2	1.71	0.73
1:1:851:LEU:HD12	1:1:1037:LEU:HD13	1.70	0.72
1:1:582:VAL:HG21	1:1:1128:VAL:HG21	1.70	0.72
1:1:704:TRP:HB2	1:1:983:SER:HA	1.68	0.72
1:1:640:LEU:HD12	1:1:693:ILE:HD13	1.71	0.72
3:H:102:ASP:OD1	3:H:103:TYR:N	2.21	0.72
1:1:525:ARG:NH2	1:1:748:ASP:OD1	2.22	0.72
1:1:617:GLN:O	1:1:728:TYR:OH	2.06	0.72
1:1:517:ALA:HA	1:1:1101:GLN:HE22	1.55	0.71
1:1:733:LEU:HD13	1:1:1117:LEU:HD22	1.73	0.71
1:1:1216:VAL:HG21	1:1:1252:ASP:HB3	1.72	0.71
1:1:1427:ASP:O	3:H:49:ASN:ND2	2.23	0.70
1:1:801:LEU:HD23	1:1:992:ARG:HB3	1.72	0.70
3:H:149:GLU:HG2	3:H:176:TYR:HE2	1.56	0.70
1:1:629:PHE:O	1:1:1043:GLY:N	2.21	0.69
3:H:136:MET:HE2	3:H:136:MET:HA	1.74	0.69
1:1:787:LEU:HD21	1:1:790:PHE:HB3	1.73	0.69
1:1:132:ASP:HB2	1:1:1502:LEU:HD13	1.73	0.69
1:1:617:GLN:NE2	1:1:624:GLU:O	2.25	0.69
2:L:189:GLU:OE2	2:L:213:ARG:NH2	2.26	0.69
1:1:1206:HIS:HB3	1:1:1209:ALA:HB2	1.74	0.69
1:1:460:ASN:H	1:1:466:GLN:HE21	1.41	0.68
2:L:21:ARG:HG3	2:L:21:ARG:HH11	1.57	0.68
2:L:81:GLU:OE2	2:L:81:GLU:N	2.26	0.68
1:1:81:LEU:O	1:1:86:PRO:HA	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:998:ARG:HD2	1:1:1001:LEU:HD12	1.74	0.68
1:1:561:PRO:HG2	1:1:594:MET:HB2	1.76	0.68
2:L:37:TRP:HB2	2:L:50:ILE:HB	1.73	0.68
1:1:1038:ASN:HA	1:1:1080:ILE:HG12	1.75	0.68
1:1:73:ASN:ND2	1:1:491:ILE:O	2.27	0.68
1:1:415:HIS:HB2	1:1:419:ASP:HB2	1.77	0.67
1:1:602:ARG:H	1:1:638:PRO:HB3	1.59	0.67
1:1:426:LEU:HD22	1:1:608:LEU:HD21	1.76	0.67
1:1:975:THR:HA	1:1:987:LYS:HE3	1.77	0.67
1:1:146:LEU:HD21	1:1:386:THR:HG21	1.76	0.67
2:L:49:LEU:HA	2:L:60:VAL:HG21	1.76	0.67
1:1:701:MET:N	1:1:983:SER:O	2.25	0.67
2:L:56:ARG:NH1	2:L:64:PHE:O	2.28	0.67
1:1:1434:MET:O	1:1:1460:VAL:N	2.24	0.66
1:1:584:ARG:NH2	2:L:71:THR:OG1	2.26	0.66
1:1:730:PRO:HB2	1:1:1100:PRO:HB2	1.76	0.66
1:1:1356:ASN:ND2	1:1:1369:LEU:O	2.28	0.66
1:1:1164:GLY:O	1:1:1175:SER:HA	1.95	0.66
1:1:180:VAL:HG21	1:1:391:VAL:HG11	1.78	0.66
1:1:674:VAL:HG22	1:1:678:ILE:HD12	1.77	0.66
1:1:604:LEU:HD11	1:1:660:HIS:HA	1.78	0.65
1:1:1172[A]:ARG:NH2	1:1:1373:ASN:OD1	2.30	0.65
1:1:235:ALA:HB1	1:1:239:LEU:HB3	1.78	0.65
1:1:1284:GLN:O	1:1:1286:GLN:NE2	2.30	0.65
1:1:1106:LEU:HD11	1:1:1113:VAL:HB	1.79	0.65
1:1:467:GLY:HA3	1:1:762:GLU:HG2	1.78	0.65
3:H:47:PRO:HA	3:H:66:VAL:HG21	1.79	0.65
1:1:394:LEU:HD11	1:1:503:VAL:HG21	1.79	0.64
1:1:573:ARG:NH2	1:1:727:ALA:O	2.24	0.64
1:1:585:GLU:HB3	1:1:737:ILE:HG23	1.80	0.64
1:1:662:ASN:ND2	1:1:932:GLY:O	2.31	0.64
1:1:509:HIS:NE2	1:1:1102:ASP:OD1	2.30	0.64
1:1:1009:ASN:ND2	1:1:1079:LYS:O	2.20	0.64
3:H:152:THR:HB	3:H:199:ALA:HB3	1.80	0.64
1:1:1369:LEU:HD12	1:1:1373:ASN:HB3	1.79	0.63
1:1:1447:ILE:HG21	1:1:1453:PRO:HG3	1.80	0.63
1:1:418:TRP:HB2	1:1:641:PRO:HB3	1.79	0.63
1:1:1332:SER:O	1:1:1336:VAL:HG23	1.98	0.63
1:1:611:ASN:HD22	1:1:630:THR:HB	1.64	0.63
1:1:310:LEU:HD13	1:1:418:TRP:HD1	1.64	0.63
1:1:725:GLU:OE1	1:1:726:ASN:N	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:197:ARG:NH1	4:1:1644:HOH:O	2.31	0.62
1:1:594:MET:N	1:1:731:ASN:OD1	2.28	0.62
3:H:94:ASN:HB2	3:H:99:LEU:HB2	1.81	0.62
1:1:629:PHE:CG	1:1:974:PRO:HG3	2.35	0.62
1:1:796:LEU:HD13	1:1:800:VAL:HG12	1.81	0.62
1:1:244:ALA:HB3	1:1:605:TYR:HB2	1.81	0.62
1:1:394:LEU:HA	1:1:537:VAL:HG11	1.81	0.62
1:1:519:LEU:O	4:1:1601:HOH:O	2.16	0.62
1:1:536:THR:OG1	1:1:748:ASP:OD2	2.15	0.62
1:1:921:MET:HE2	1:1:939:GLN:HG3	1.82	0.62
2:L:119:ILE:HG21	2:L:211:PHE:HB3	1.80	0.62
1:1:901:ASP:OD1	1:1:914:LYS:N	2.30	0.61
1:1:1354:ALA:O	1:1:1368:ARG:NH2	2.23	0.61
1:1:1179:LEU:HD11	1:1:1288:LEU:HB2	1.82	0.61
1:1:1126:ASP:HB2	1:1:1131:ARG:H	1.63	0.61
1:1:515:HIS:CE1	1:1:1209:ALA:HB3	2.33	0.61
1:1:602:ARG:NH2	4:1:1656:HOH:O	2.34	0.61
1:1:285:LYS:O	1:1:657:TYR:OH	2.12	0.61
1:1:436:ARG:HA	1:1:449:ALA:HB1	1.82	0.61
1:1:372:SER:HA	1:1:393:HIS:HA	1.83	0.60
1:1:811:ILE:HB	1:1:1120:TRP:HE1	1.66	0.60
1:1:1381:VAL:HG22	1:1:1393:LEU:HB3	1.82	0.60
1:1:625:ASP:OD1	1:1:728:TYR:N	2.34	0.60
1:1:731:ASN:ND2	4:1:1662:HOH:O	2.34	0.60
2:L:22:PHE:HB2	2:L:71:THR:HB	1.82	0.60
1:1:1039:LEU:HD13	1:1:1049:LEU:HD12	1.82	0.60
1:1:504:PHE:HD2	1:1:588:LEU:HD13	1.66	0.60
1:1:1005:PRO:HB2	1:1:1091:LEU:HD22	1.83	0.60
1:1:1078:PHE:HE1	1:1:1080:ILE:HD13	1.66	0.60
3:H:172:GLN:HE22	3:H:177:THR:HB	1.66	0.60
1:1:404:PRO:HD3	1:1:541:PRO:HG3	1.83	0.60
1:1:582:VAL:HB	1:1:1128:VAL:HG11	1.83	0.60
1:1:423:ARG:HB2	1:1:430:THR:HG22	1.84	0.60
1:1:809:PRO:HD2	1:1:1120:TRP:HH2	1.67	0.60
3:H:17:LYS:NZ	3:H:70:SER:O	2.32	0.60
1:1:413:ASN:ND2	1:1:419:ASP:OD2	2.26	0.60
1:1:956:ALA:O	1:1:957:ILE:HG13	2.02	0.60
1:1:1338:GLN:HG2	1:1:1364:VAL:HG23	1.84	0.60
1:1:851:LEU:HB2	1:1:1025[A]:TRP:HE3	1.66	0.60
3:H:160:LEU:HD21	3:H:182:VAL:HG21	1.84	0.59
1:1:275:ARG:NH1	1:1:667:ASP:OD2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:493:ASN:ND2	1:1:505:GLY:O	2.29	0.59
1:1:1113:VAL:HG23	1:1:1124:PHE:HB2	1.84	0.59
1:1:987:LYS:HG2	1:1:1047:GLY:HA2	1.84	0.59
2:L:194:TYR:HB2	2:L:211:PHE:CE1	2.36	0.59
1:1:200:VAL:HB	1:1:374:LEU:HG	1.85	0.59
1:1:426:LEU:HA	1:1:608:LEU:HD11	1.83	0.59
1:1:523:VAL:HG23	1:1:542:TYR:CE1	2.38	0.59
1:1:420:TRP:NE1	1:1:451:ASN:O	2.33	0.59
1:1:482:LEU:HG	1:1:487:TYR:HA	1.85	0.59
1:1:547:SER:HB3	1:1:568:PHE:HE1	1.67	0.59
1:1:566:ARG:HD2	1:1:755:GLU:HB2	1.83	0.59
3:H:194:VAL:H	3:H:210:LYS:HZ3	1.51	0.59
1:1:603:LEU:HD11	1:1:614:LEU:HB3	1.84	0.59
1:1:184:VAL:HG12	1:1:186:VAL:HG13	1.85	0.59
1:1:862:LYS:HD2	1:1:891:GLN:HG2	1.84	0.59
1:1:1009:ASN:HB3	1:1:1089:ALA:HB2	1.84	0.59
1:1:563:ASN:HB3	1:1:720:ALA:HB2	1.85	0.58
1:1:1098:TRP:HE1	1:1:1153:ILE:HG23	1.67	0.58
2:L:91:PHE:HE1	2:L:98:TRP:HB3	1.67	0.58
2:L:110:ARG:NH1	2:L:173:SER:O	2.36	0.58
1:1:328:LYS:O	1:1:436:ARG:NH1	2.35	0.58
2:L:97:PRO:HB3	3:H:55:ASN:HB2	1.83	0.58
1:1:423:ARG:HD3	1:1:430:THR:HA	1.84	0.58
1:1:1000:LEU:HD12	1:1:1117:LEU:HD23	1.86	0.58
1:1:1025[B]:TRP:HE1	1:1:1061:THR:HG21	1.68	0.58
3:H:116:LYS:HE2	3:H:116:LYS:H	1.67	0.58
1:1:796:LEU:HD11	1:1:1135:LEU:HD22	1.86	0.58
1:1:1357:THR:HB	1:1:1359:THR:HG22	1.85	0.58
1:1:1415:ILE:HD13	1:1:1420:LEU:HD22	1.85	0.58
2:L:40:GLN:OE1	3:H:33:GLN:NE2	2.27	0.58
1:1:242:LYS:HB3	1:1:325:VAL:HG11	1.85	0.58
1:1:410:PRO:HG2	1:1:442:PHE:CE2	2.39	0.58
1:1:1007:LEU:O	1:1:1078:PHE:HB2	2.04	0.58
1:1:142:ASP:O	1:1:146:LEU:N	2.37	0.58
1:1:319:GLU:HA	1:1:324:SER:HA	1.85	0.58
1:1:540:TRP:HB3	1:1:544:LEU:HD23	1.86	0.58
1:1:584:ARG:HH22	2:L:71:THR:HG1	1.51	0.58
1:1:602:ARG:NH1	4:1:1650:HOH:O	2.37	0.58
1:1:973:THR:O	1:1:986:ASN:ND2	2.37	0.58
1:1:1432:VAL:O	2:L:28:HIS:NE2	2.37	0.58
1:1:219:LEU:HD13	1:1:237:PHE:HB3	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:146:ILE:HD11	2:L:198:ALA:HB1	1.86	0.57
1:1:894:THR:O	1:1:971:ASN:ND2	2.37	0.57
1:1:247:ASP:N	1:1:314:PRO:O	2.31	0.57
1:1:1124:PHE:HA	1:1:1137:LEU:HD12	1.86	0.57
1:1:623:ARG:NH1	4:1:1683:HOH:O	2.37	0.57
1:1:956:ALA:HB2	1:1:962:ALA:HB2	1.87	0.57
1:1:957:ILE:HD12	1:1:958:ASP:HB2	1.86	0.57
1:1:394:LEU:HD22	1:1:524:PHE:HB3	1.86	0.57
1:1:1025[A]:TRP:HE1	1:1:1061:THR:HG21	1.70	0.57
1:1:661:ASN:ND2	1:1:700:GLY:O	2.30	0.57
1:1:419:ASP:OD1	1:1:602:ARG:NH2	2.37	0.57
1:1:896:ALA:O	1:1:975:THR:OG1	2.20	0.57
1:1:427:LEU:O	1:1:619:GLN:HB3	2.05	0.56
1:1:308:ASN:HD21	1:1:762:GLU:HG3	1.70	0.56
1:1:544:LEU:HD21	1:1:750:VAL:HG11	1.87	0.56
1:1:1183:TRP:NE1	1:1:1285:PRO:O	2.30	0.56
2:L:38:TYR:OH	3:H:100:LEU:O	2.23	0.56
1:1:1415:ILE:HB	1:1:1420:LEU:HD13	1.87	0.56
1:1:1120:TRP:CE3	1:1:1139:LEU:HB3	2.41	0.56
1:1:714:THR:HG1	1:1:719:SER:HG	1.50	0.56
1:1:305:LEU:HD23	1:1:308:ASN:HB2	1.88	0.56
1:1:1162:PHE:HE1	1:1:1175:SER:HB3	1.70	0.56
1:1:1470:LEU:HG	1:1:1472:LEU:HD21	1.87	0.56
2:L:108:ILE:N	2:L:168:GLN:OE1	2.38	0.56
1:1:198:PHE:CE2	1:1:378:ASP:HB3	2.41	0.56
1:1:859:VAL:HB	1:1:895:GLY:HA2	1.88	0.56
1:1:977:ASP:HA	1:1:985:THR:HG23	1.87	0.56
1:1:1033:ASP:OD1	1:1:1035:THR:OG1	2.23	0.56
1:1:653:HIS:ND1	1:1:935:ASP:OD1	2.33	0.56
1:1:1178:ASP:OD2	1:1:1180:LYS:NZ	2.39	0.56
3:H:33:GLN:HB2	3:H:39:LEU:HD23	1.87	0.56
3:H:54:TYR:HE2	3:H:64:LEU:HD13	1.71	0.56
1:1:124:THR:O	1:1:205:ARG:NH1	2.39	0.55
1:1:405:PRO:HB3	1:1:408:ARG:HH22	1.71	0.55
3:H:27:THR:O	3:H:93:SER:OG	2.24	0.55
1:1:1126:ASP:HB3	1:1:1131:ARG:HE	1.70	0.55
1:1:410:PRO:HG2	1:1:442:PHE:HE2	1.72	0.55
1:1:517:ALA:HA	1:1:1101:GLN:NE2	2.21	0.55
1:1:856:ASN:ND2	1:1:975:THR:O	2.35	0.55
1:1:869:LEU:HD22	1:1:965:TYR:CG	2.41	0.55
1:1:897:GLY:HA3	1:1:973:THR:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1096:LEU:O	1:1:1208:ASN:ND2	2.38	0.55
1:1:781:SER:O	1:1:784:SER:OG	2.25	0.55
1:1:800:VAL:HG13	1:1:1331:VAL:HG11	1.89	0.55
1:1:1212:PHE:HB2	1:1:1262:LEU:HD21	1.88	0.55
2:L:138:LEU:HB2	2:L:177:MET:HB3	1.89	0.55
1:1:703:ALA:HA	1:1:988:ASN:HB3	1.88	0.55
2:L:90:CYS:O	2:L:101:GLY:N	2.38	0.55
1:1:557:LEU:HD11	1:1:801:LEU:HD22	1.89	0.54
2:L:194:TYR:HB2	2:L:211:PHE:HE1	1.72	0.54
1:1:237:PHE:CE2	1:1:1262:LEU:HD13	2.42	0.54
1:1:853:THR:HG22	1:1:1048:LEU:HB2	1.90	0.54
1:1:1002:GLY:HA3	1:1:1096:LEU:HD12	1.90	0.54
1:1:1464:ASP:O	1:1:1468:GLN:N	2.40	0.54
3:H:149:GLU:HG2	3:H:176:TYR:CE2	2.42	0.54
1:1:580:LYS:NZ	4:1:1701:HOH:O	2.40	0.54
1:1:627:GLN:CD	1:1:991:GLN:HB2	2.32	0.54
3:H:64:LEU:HD12	3:H:75:MET:HG3	1.88	0.54
1:1:73:ASN:HB2	1:1:510:VAL:HB	1.88	0.54
1:1:89:TRP:CZ3	1:1:128:LEU:HB3	2.42	0.54
1:1:359:THR:HG23	1:1:396:PRO:HB2	1.89	0.54
1:1:418:TRP:CH2	1:1:639:ASP:HA	2.42	0.54
1:1:429:THR:HG21	1:1:437:ARG:HG3	1.89	0.54
1:1:519:LEU:HD21	1:1:1101:GLN:HG2	1.89	0.54
1:1:519:LEU:HD11	1:1:730:PRO:HD3	1.90	0.54
1:1:589:ALA:HA	1:1:735:ALA:HA	1.88	0.54
1:1:219:LEU:HD21	1:1:1203:LEU:HD22	1.89	0.54
1:1:221:GLN:NE2	1:1:330:ASP:O	2.41	0.54
1:1:255:LEU:HD21	1:1:309:ASP:HB3	1.89	0.54
1:1:899:ARG:CZ	1:1:972:LEU:HG	2.37	0.54
1:1:269:SER:OG	1:1:270:GLY:N	2.38	0.54
1:1:133:LEU:HD21	1:1:1499:LEU:HB3	1.90	0.54
1:1:1044:GLU:HA	1:1:1091:LEU:HD21	1.89	0.54
1:1:152:THR:N	1:1:168:GLY:O	2.32	0.53
1:1:184:VAL:O	1:1:202:LEU:HA	2.08	0.53
1:1:819:ASN:HB3	1:1:850[A]:PHE:HD2	1.73	0.53
1:1:1009:ASN:HA	1:1:1258:LEU:HD21	1.89	0.53
1:1:945:SER:O	1:1:948:SER:OG	2.26	0.53
2:L:89:TYR:OH	3:H:33:GLN:NE2	2.41	0.53
3:H:16:CYS:HB3	3:H:73:ALA:HB3	1.91	0.53
1:1:74:THR:HG21	1:1:493:ASN:H	1.74	0.53
1:1:829:ALA:O	1:1:831:GLN:NE2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1288:LEU:HD11	1:1:1374:ALA:HB1	1.91	0.53
1:1:1454[A]:LYS:O	3:H:56:GLN:NE2	2.37	0.53
1:1:423:ARG:NH2	1:1:724:ASN:O	2.40	0.53
1:1:488:PHE:HA	1:1:491:ILE:HB	1.91	0.53
1:1:1405:GLN:N	1:1:1405:GLN:OE1	2.42	0.53
1:1:641:PRO:HD2	1:1:693:ILE:HD11	1.90	0.52
1:1:87:GLY:HA3	1:1:131:TYR:O	2.09	0.52
1:1:237:PHE:HE2	1:1:1262:LEU:HD13	1.74	0.52
1:1:557:LEU:HB2	1:1:560:LEU:HD11	1.90	0.52
1:1:1411:SER:OG	1:1:1413:ASP:OD1	2.26	0.52
3:H:34:SER:HB2	3:H:37:LYS:HD3	1.90	0.52
1:1:174:PRO:HG2	1:1:177:TRP:HB2	1.90	0.52
1:1:286:ALA:HB2	1:1:695:PRO:HD3	1.90	0.52
1:1:510:VAL:HG13	1:1:511:THR:HG23	1.92	0.52
1:1:562:PHE:HB2	1:1:713:LEU:HG	1.91	0.52
1:1:597:THR:HG22	1:1:710:SER:HB2	1.92	0.52
1:1:459:ASP:OD1	1:1:459:ASP:N	2.43	0.52
1:1:494:LEU:HG	1:1:501:LEU:HD21	1.92	0.52
1:1:721:ASP:HA	1:1:770:LEU:HD13	1.90	0.52
1:1:1005:PRO:HD2	1:1:1045:VAL:HG21	1.92	0.52
1:1:1042:TYR:HE1	1:1:1215:SER:HB3	1.75	0.52
1:1:239:LEU:HD22	1:1:1213:GLN:HG3	1.90	0.52
1:1:259:GLU:HG2	1:1:285:LYS:HG2	1.90	0.52
1:1:495:THR:HG21	1:1:586:LEU:HD11	1.92	0.52
1:1:998:ARG:NH2	1:1:1003:SER:O	2.43	0.52
1:1:1461:LEU:HD11	1:1:1473:ARG:HB2	1.91	0.52
1:1:591:THR:OG1	1:1:1100:PRO:O	2.25	0.52
1:1:808:VAL:HG22	1:1:1366:VAL:HG11	1.90	0.52
1:1:1018:PHE:CZ	1:1:1023:GLN:HB2	2.44	0.52
1:1:1203:LEU:HD12	1:1:1204:PRO:HD2	1.90	0.52
1:1:1421:PHE:HB3	1:1:1468:GLN:HG2	1.90	0.52
1:1:1042:TYR:CE1	1:1:1215:SER:HB3	2.44	0.52
3:H:41:TRP:HZ2	3:H:44:LEU:HD23	1.74	0.52
3:H:136:MET:SD	3:H:183:THR:HB	2.49	0.52
1:1:175:GLN:O	1:1:176:GLN:HG2	2.10	0.52
1:1:184:VAL:HG11	1:1:208:VAL:HG21	1.92	0.52
1:1:581:PHE:HE1	1:1:740:PRO:HG3	1.75	0.52
1:1:698:TYR:HB3	1:1:704:TRP:HH2	1.75	0.52
1:1:809:PRO:HD2	1:1:1120:TRP:CH2	2.43	0.52
1:1:519:LEU:HB2	1:1:573:ARG:HB3	1.92	0.51
1:1:254:LYS:HG2	1:1:646:SER:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:407:TRP:CH2	1:1:571:VAL:HG13	2.44	0.51
1:1:1000:LEU:HD21	1:1:1139:LEU:HD13	1.92	0.51
1:1:232:THR:HG22	1:1:1250:GLN:HE22	1.75	0.51
1:1:410:PRO:HB2	1:1:433:PHE:O	2.10	0.51
1:1:1001:LEU:HD21	1:1:1117:LEU:HD11	1.93	0.51
1:1:1012:GLY:N	1:1:1016:ASN:O	2.41	0.51
3:H:153:VAL:HG22	3:H:198:VAL:HG22	1.93	0.51
1:1:1097:ALA:HB1	1:1:1207:PRO:HG2	1.92	0.51
2:L:149:LYS:O	2:L:197:GLU:N	2.39	0.51
1:1:255:LEU:HD12	1:1:644:ALA:HB2	1.92	0.51
1:1:404:PRO:HD2	1:1:407:TRP:CD2	2.46	0.51
1:1:437:ARG:HG2	1:1:620:GLY:HA2	1.92	0.51
1:1:636:ASN:ND2	4:1:1693:HOH:O	2.43	0.51
1:1:1432:VAL:HG11	3:H:100:LEU:HD11	1.93	0.51
1:1:167:PHE:HZ	1:1:196:TYR:HB3	1.75	0.51
1:1:851:LEU:HB2	1:1:1025[A]:TRP:CE3	2.44	0.51
1:1:1440:TYR:HD1	1:1:1443:LEU:HD21	1.76	0.51
2:L:93:GLY:O	2:L:98:TRP:NE1	2.43	0.51
1:1:315:ILE:HD11	1:1:646:SER:HB2	1.92	0.51
1:1:941:ASN:HB3	1:1:956:ALA:HA	1.93	0.51
1:1:1125:THR:OG1	1:1:1126:ASP:OD1	2.28	0.51
1:1:1261:LEU:HD22	1:1:1267:VAL:HG22	1.91	0.51
1:1:1479:PRO:HB2	1:1:1482:ASP:HA	1.92	0.51
1:1:89:TRP:HB3	1:1:188:VAL:HG21	1.93	0.51
1:1:856:ASN:OD1	1:1:987:LYS:NZ	2.44	0.51
1:1:1429:PHE:CG	1:1:1460:VAL:HG21	2.45	0.51
3:H:32:LYS:HD2	3:H:58:PHE:CZ	2.46	0.51
2:L:37:TRP:CH2	2:L:90:CYS:HB3	2.46	0.51
1:1:217:LEU:HB3	1:1:515:HIS:HB2	1.92	0.50
1:1:912:HIS:HA	1:1:970:PRO:HD3	1.93	0.50
1:1:1063:ALA:HB3	1:1:1073:SER:HB3	1.93	0.50
1:1:1135:LEU:N	1:1:1300:GLY:O	2.41	0.50
1:1:627:GLN:OE1	1:1:1046:ASN:ND2	2.44	0.50
1:1:729:GLN:NE2	4:1:1643:HOH:O	2.31	0.50
2:L:173:SER:O	2:L:173:SER:OG	2.28	0.50
1:1:201:LEU:HD11	1:1:491:ILE:HG23	1.93	0.50
1:1:429:THR:OG1	1:1:437:ARG:NE	2.37	0.50
1:1:593:THR:HB	1:1:727:ALA:HB3	1.94	0.50
1:1:327:LEU:HD11	1:1:619:GLN:HB2	1.93	0.50
1:1:561:PRO:HD3	1:1:990:ALA:HB2	1.93	0.50
1:1:584:ARG:NH1	2:L:22:PHE:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:46:ASN:O	3:H:50:GLY:N	2.44	0.50
1:1:405:PRO:HB3	1:1:408:ARG:NH2	2.26	0.50
3:H:32:LYS:O	3:H:40:GLU:N	2.41	0.50
1:1:143:PHE:HE2	1:1:185:PRO:HB3	1.77	0.50
1:1:406:SER:HB2	1:1:758:PHE:CZ	2.47	0.50
1:1:108:GLN:NE2	1:1:214:GLN:O	2.45	0.50
1:1:370:SER:OG	1:1:393:HIS:HB3	2.11	0.50
1:1:620:GLY:HA2	1:1:728:TYR:HE2	1.76	0.50
1:1:664:ASP:CG	1:1:899:ARG:HH12	2.20	0.50
1:1:610:SER:HB3	1:1:1245:PRO:HG2	1.94	0.50
3:H:83:GLU:CD	3:H:83:GLU:H	2.19	0.50
1:1:199:ALA:HB1	1:1:501:LEU:HD22	1.94	0.50
3:H:61:THR:O	3:H:78:LEU:N	2.44	0.50
1:1:407:TRP:CG	1:1:480:ILE:HD12	2.47	0.49
2:L:117:VAL:HG22	2:L:138:LEU:HG	1.93	0.49
1:1:1160:ALA:O	1:1:1163:ARG:NH1	2.43	0.49
1:1:1362:ASP:OD1	1:1:1362:ASP:N	2.41	0.49
1:1:275:ARG:HA	1:1:656:PRO:HG3	1.94	0.49
1:1:759:ALA:HB1	1:1:764[A]:GLU:HB3	1.94	0.49
1:1:632:TYR:CD2	1:1:1245:PRO:HD2	2.47	0.49
1:1:1123:THR:O	1:1:1137:LEU:HA	2.13	0.49
1:1:402:ASN:ND2	1:1:538:THR:OG1	2.44	0.49
1:1:413:ASN:HA	1:1:758:PHE:CZ	2.48	0.49
1:1:1012:GLY:O	1:1:1017:LYS:NZ	2.41	0.49
1:1:1302:LEU:HD22	1:1:1331:VAL:HG22	1.93	0.49
1:1:66:LEU:HD21	1:1:125:THR:HB	1.95	0.49
1:1:132:ASP:HB3	1:1:138:LEU:HD11	1.95	0.49
1:1:415:HIS:HB3	1:1:418:TRP:CE2	2.47	0.49
1:1:611:ASN:HB3	1:1:630:THR:HB	1.95	0.49
1:1:673:VAL:HG22	1:1:942:ILE:HD12	1.94	0.49
1:1:677:PHE:CZ	1:1:942:ILE:HD11	2.48	0.49
1:1:1161:ALA:O	1:1:1178:ASP:N	2.24	0.49
1:1:1249:THR:H	1:1:1252:ASP:HB2	1.77	0.49
3:H:80:LEU:HB3	3:H:112:VAL:HG11	1.94	0.49
1:1:411:LYS:HD3	1:1:450:ASP:O	2.13	0.49
1:1:669:PRO:HD2	1:1:965:TYR:OH	2.12	0.49
1:1:675:ASP:HA	1:1:679:LYS:HB2	1.94	0.49
1:1:1334:TRP:CH2	1:1:1364:VAL:HA	2.48	0.49
1:1:557:LEU:HD21	1:1:801:LEU:HD22	1.94	0.49
1:1:408:ARG:HA	1:1:479:PRO:HB3	1.94	0.49
2:L:91:PHE:CE1	2:L:98:TRP:HB3	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:45:ILE:HD12	3:H:52:THR:HG22	1.95	0.49
1:1:204:PRO:HD2	1:1:488:PHE:CZ	2.47	0.48
1:1:584:ARG:HH11	1:1:584:ARG:HG2	1.78	0.48
1:1:691:LYS:H	1:1:766:PHE:HZ	1.60	0.48
1:1:817:TYR:O	1:1:853:THR:OG1	2.15	0.48
1:1:210:TYR:CD2	1:1:213:LEU:HD12	2.48	0.48
1:1:305:LEU:HD11	1:1:763:TYR:HB2	1.96	0.48
1:1:434:ASN:N	1:1:725:GLU:OE2	2.32	0.48
1:1:441:TRP:CH2	1:1:573:ARG:HD2	2.49	0.48
1:1:523:VAL:HG23	1:1:542:TYR:HE1	1.79	0.48
1:1:978:TRP:O	1:1:985:THR:OG1	2.32	0.48
1:1:1024:LYS:HB2	1:1:1036:LYS:HB3	1.95	0.48
1:1:1338:GLN:HG3	1:1:1360:GLY:HA2	1.95	0.48
1:1:612:LEU:HB3	1:1:1213:GLN:CB	2.43	0.48
1:1:667:ASP:HB3	1:1:673:VAL:HG11	1.95	0.48
1:1:1025[B]:TRP:NE1	1:1:1061:THR:HG21	2.28	0.48
1:1:1477:PHE:CG	3:H:56:GLN:HG2	2.49	0.48
2:L:135:VAL:HG12	2:L:180:THR:HG23	1.95	0.48
1:1:220:PRO:HB3	1:1:331:ASP:HB3	1.96	0.48
1:1:407:TRP:HB3	1:1:480:ILE:HB	1.94	0.48
1:1:487:TYR:O	1:1:491:ILE:HG12	2.14	0.48
1:1:821:HIS:CD2	1:1:852:PRO:HD3	2.48	0.48
1:1:133:LEU:CD2	1:1:1499:LEU:HB3	2.43	0.48
1:1:861:LEU:HD12	1:1:900:ASN:CG	2.39	0.48
1:1:897:GLY:HA2	1:1:1239:TYR:CD2	2.48	0.48
1:1:1008:VAL:HG23	1:1:1258:LEU:HD11	1.95	0.48
1:1:1010:ARG:HB2	1:1:1018:PHE:HB2	1.95	0.48
1:1:446:GLN:HA	1:1:449:ALA:HB2	1.95	0.48
1:1:359:THR:OG1	1:1:481:ALA:HB1	2.14	0.48
1:1:490:ASN:O	1:1:490:ASN:ND2	2.44	0.48
1:1:528:TYR:CD2	1:1:535:ALA:HB2	2.49	0.48
1:1:629:PHE:CE2	1:1:631:PRO:HG3	2.49	0.48
1:1:828:THR:HA	1:1:1027:TYR:H	1.79	0.48
1:1:1432:VAL:HG11	3:H:100:LEU:HD21	1.95	0.48
1:1:560:LEU:O	1:1:713:LEU:N	2.46	0.48
2:L:93:GLY:HA3	3:H:100:LEU:CD1	2.44	0.48
1:1:87:GLY:HA2	1:1:133:LEU:HA	1.95	0.47
3:H:144:LYS:HD2	3:H:177:THR:HG21	1.95	0.47
1:1:277:GLY:HA2	1:1:281:ASP:HB3	1.96	0.47
1:1:432:PHE:O	1:1:726:ASN:ND2	2.47	0.47
1:1:433:PHE:HE2	1:1:441:TRP:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1038:ASN:C	1:1:1051:PRO:HG3	2.39	0.47
3:H:126:ALA:O	3:H:214:ARG:NH2	2.48	0.47
1:1:86:PRO:HG3	1:1:1500:PRO:HG3	1.95	0.47
1:1:419:ASP:OD2	1:1:423:ARG:HD2	2.14	0.47
1:1:243:ASN:HB3	1:1:606:ASP:HA	1.97	0.47
1:1:428:GLN:NE2	4:1:1650:HOH:O	2.40	0.47
1:1:631:PRO:HA	1:1:634:TRP:CD2	2.49	0.47
1:1:678:ILE:O	1:1:682:GLU:N	2.48	0.47
1:1:901:ASP:OD2	1:1:1235:ASN:HB2	2.14	0.47
1:1:494:LEU:HB3	1:1:501:LEU:HD11	1.95	0.47
1:1:549:MET:HG2	1:1:787:LEU:HD22	1.95	0.47
1:1:1419:ARG:HH22	1:1:1440:TYR:HE1	1.63	0.47
2:L:119:ILE:HD11	2:L:209:LYS:HB3	1.97	0.47
3:H:125:LEU:HD11	3:H:142:LEU:HB2	1.97	0.47
1:1:402:ASN:HB2	1:1:539:GLY:O	2.14	0.47
1:1:117:GLU:HB2	1:1:369:TRP:CH2	2.49	0.47
1:1:399:MET:HA	1:1:539:GLY:O	2.15	0.47
1:1:403:TYR:OH	1:1:521:ILE:HG21	2.14	0.47
1:1:513:SER:H	1:1:516:THR:HG1	1.63	0.47
1:1:566:ARG:HH22	1:1:768:GLN:HB2	1.79	0.47
1:1:599:THR:HA	1:1:614:LEU:HD11	1.97	0.47
1:1:896:ALA:HB3	1:1:1049:LEU:HD13	1.96	0.47
1:1:1408:LYS:NZ	1:1:1503:THR:O	2.43	0.47
1:1:1452:ASN:HD22	1:1:1453:PRO:HD2	1.79	0.47
1:1:159:ILE:HG13	1:1:377:TYR:CZ	2.50	0.47
1:1:490:ASN:ND2	1:1:522:GLY:O	2.38	0.47
1:1:587:VAL:HG11	1:1:1113:VAL:HG21	1.96	0.47
1:1:1149:GLN:HG2	1:1:1288:LEU:HD21	1.96	0.47
1:1:63:ASN:O	1:1:129:ARG:NH2	2.47	0.47
1:1:84:GLU:HG3	1:1:1473:ARG:HH22	1.79	0.47
1:1:310:LEU:HD13	1:1:418:TRP:CD1	2.48	0.47
1:1:642:ILE:HG13	4:1:1698:HOH:O	2.15	0.47
2:L:212:ASN:OD1	2:L:213:ARG:N	2.48	0.47
1:1:1407:VAL:HG13	1:1:1445:ILE:HD12	1.96	0.47
2:L:117:VAL:HB	2:L:209:LYS:HG3	1.96	0.47
1:1:74:THR:HG21	1:1:493:ASN:N	2.31	0.46
1:1:113:PRO:HA	1:1:356:TRP:CH2	2.50	0.46
1:1:405:PRO:HD3	1:1:752:TYR:CG	2.50	0.46
1:1:563:ASN:ND2	1:1:719:SER:OG	2.37	0.46
1:1:566:ARG:HH11	1:1:755:GLU:HA	1.80	0.46
1:1:742:LEU:O	1:1:746:LEU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1098:TRP:CZ2	1:1:1153:ILE:HA	2.50	0.46
1:1:71:TYR:CG	1:1:186:VAL:HB	2.50	0.46
1:1:631:PRO:HA	1:1:634:TRP:CE2	2.50	0.46
3:H:-4:VAL:HG11	3:H:92:ARG:HD3	1.97	0.46
1:1:167:PHE:CE2	1:1:377:TYR:HB3	2.51	0.46
1:1:240[B]:LYS:O	1:1:619:GLN:NE2	2.44	0.46
1:1:420:TRP:CD1	1:1:454:THR:HG21	2.50	0.46
1:1:1176:VAL:HG13	1:1:1377:MET:HE1	1.97	0.46
1:1:1454[B]:LYS:HE2	3:H:60:GLY:HA3	1.97	0.46
2:L:39:LEU:HB2	2:L:49:LEU:HD11	1.98	0.46
2:L:151:LYS:HB2	2:L:195:THR:HG22	1.96	0.46
1:1:78:SER:HA	1:1:90:ALA:HA	1.98	0.46
1:1:504:PHE:HA	1:1:523:VAL:HG22	1.96	0.46
1:1:544:LEU:HG	1:1:783:PHE:CG	2.50	0.46
1:1:546:PHE:HB3	1:1:549:MET:SD	2.55	0.46
1:1:503:VAL:HB	1:1:524:PHE:HB2	1.97	0.46
1:1:622:LEU:HD22	1:1:1212:PHE:HA	1.96	0.46
1:1:1039:LEU:HD12	1:1:1040:PRO:HD2	1.98	0.46
2:L:57:PHE:CZ	3:H:102:ASP:HB2	2.50	0.46
1:1:239:LEU:HD11	1:1:615:VAL:HG12	1.98	0.46
1:1:287:LEU:HB2	1:1:693:ILE:HB	1.96	0.46
1:1:396:PRO:O	1:1:400:THR:HG23	2.15	0.46
1:1:563:ASN:O	1:1:711:ASN:HB2	2.16	0.46
1:1:240[A]:LYS:O	1:1:619:GLN:NE2	2.44	0.46
1:1:743:LEU:HA	1:1:746:LEU:HD12	1.96	0.46
2:L:87:VAL:HA	2:L:105:LYS:HA	1.97	0.46
1:1:131:TYR:CZ	1:1:1385:VAL:HG21	2.51	0.46
1:1:807:TYR:OH	1:1:1360:GLY:HA3	2.16	0.46
1:1:1144:ALA:O	1:1:1150:ARG:HB2	2.15	0.46
1:1:525:ARG:CZ	1:1:540:TRP:HZ2	2.28	0.46
1:1:640:LEU:HB3	1:1:644:ALA:HB3	1.97	0.46
1:1:854:PHE:CD1	1:1:995:LEU:HD13	2.51	0.46
1:1:1176:VAL:HB	1:1:1384:ILE:HD11	1.98	0.46
1:1:1185:ASP:HA	1:1:1188:GLN:HG2	1.98	0.46
2:L:126:GLN:O	2:L:129:SER:OG	2.32	0.46
1:1:113:PRO:HA	1:1:356:TRP:CZ2	2.51	0.45
1:1:525:ARG:NH1	1:1:746:LEU:O	2.44	0.45
1:1:711:ASN:OD1	1:1:711:ASN:N	2.48	0.45
1:1:810:TRP:CZ3	1:1:1057:TYR:HA	2.51	0.45
1:1:1150:ARG:HD2	1:1:1275:PHE:CD2	2.51	0.45
1:1:1174:GLU:HG2	1:1:1291:THR:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:134:ALA:HB2	1:1:1402:THR:HG23	1.98	0.45
1:1:317:ARG:HG2	1:1:425:VAL:HA	1.98	0.45
1:1:400:THR:HA	1:1:403:TYR:CG	2.51	0.45
1:1:862:LYS:HE3	1:1:893:TRP:NE1	2.30	0.45
1:1:1055:GLU:OE2	1:1:1062:ARG:N	2.47	0.45
1:1:1464:ASP:O	1:1:1468:GLN:CA	2.64	0.45
3:H:54:TYR:CE2	3:H:64:LEU:HD13	2.51	0.45
1:1:554:THR:HA	1:1:790:PHE:O	2.16	0.45
1:1:573:ARG:HH21	1:1:726:ASN:HB3	1.82	0.45
1:1:620:GLY:HA2	1:1:728:TYR:CE2	2.51	0.45
1:1:629:PHE:HA	1:1:702:TRP:HE1	1.82	0.45
1:1:755:GLU:OE1	1:1:775:THR:OG1	2.34	0.45
2:L:26:ILE:HA	2:L:95:HIS:CE1	2.52	0.45
1:1:730:PRO:HD2	1:1:1100:PRO:HG2	1.99	0.45
1:1:1042:TYR:CD1	1:1:1042:TYR:C	2.95	0.45
1:1:1214:VAL:HG22	1:1:1216:VAL:HG22	1.98	0.45
1:1:244:ALA:N	1:1:605:TYR:O	2.50	0.45
1:1:507:ASN:HB2	1:1:1101:GLN:O	2.16	0.45
1:1:573:ARG:NH2	1:1:726:ASN:HB3	2.31	0.45
1:1:595:GLY:HA3	1:1:711:ASN:OD1	2.17	0.45
1:1:854:PHE:HE1	1:1:995:LEU:HD22	1.82	0.45
1:1:998:ARG:HA	1:1:1001:LEU:HD12	1.98	0.45
1:1:1416:ASP:HB2	1:1:1418:ASN:ND2	2.32	0.45
1:1:1427:ASP:OD1	1:1:1427:ASP:C	2.59	0.45
2:L:171:LYS:H	2:L:171:LYS:HG2	1.57	0.45
3:H:144:LYS:HB3	3:H:144:LYS:HE2	1.64	0.45
1:1:455:GLY:N	1:1:477:SER:HB3	2.31	0.45
1:1:1141:GLY:O	1:1:1369:LEU:N	2.40	0.45
2:L:185:LYS:O	2:L:189:GLU:HG2	2.16	0.45
3:H:-4:VAL:HG22	3:H:21:TYR:CD1	2.52	0.45
3:H:169:ALA:HB1	3:H:177:THR:H	1.81	0.45
1:1:71:TYR:CE1	1:1:510:VAL:HG21	2.51	0.45
1:1:207:VAL:O	1:1:510:VAL:HG22	2.16	0.45
1:1:707:TYR:HA	1:1:712:LYS:HD3	1.99	0.45
1:1:1097:ALA:HB3	1:1:1158:PRO:HD3	1.99	0.45
1:1:1211:ALA:O	1:1:1213:GLN:NE2	2.49	0.45
2:L:157:ARG:HH22	2:L:183:LEU:HD11	1.81	0.45
1:1:794:PHE:HB3	1:1:796:LEU:HG	1.99	0.45
1:1:1152:LEU:HD21	1:1:1177:TRP:CD2	2.51	0.45
1:1:202:LEU:O	1:1:371:ALA:CA	2.61	0.45
1:1:235:ALA:HB2	1:1:241:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:504:PHE:CD2	1:1:588:LEU:HD13	2.50	0.45
1:1:647:SER:HB3	1:1:654:ASN:HA	1.99	0.45
1:1:1262:LEU:HD23	1:1:1262:LEU:HA	1.68	0.45
1:1:1454[B]:LYS:O	3:H:56:GLN:NE2	2.38	0.45
1:1:594:MET:HG3	1:1:731:ASN:OD1	2.17	0.44
1:1:799:SER:O	1:1:803:GLN:HG2	2.17	0.44
1:1:978:TRP:H	1:1:985:THR:HG23	1.81	0.44
1:1:1058:PHE:HB3	1:1:1074:PRO:HD2	1.99	0.44
2:L:112:ASP:OD1	2:L:112:ASP:N	2.50	0.44
1:1:247:ASP:HB3	1:1:250:LYS:HB2	1.98	0.44
1:1:253:GLU:O	1:1:312:ASN:HB3	2.18	0.44
1:1:542:TYR:HB2	1:1:572:PRO:O	2.17	0.44
3:H:29:ASN:OD1	3:H:29:ASN:N	2.50	0.44
1:1:482:LEU:HD12	1:1:482:LEU:HA	1.72	0.44
1:1:1099:THR:H	1:1:1102:ASP:CG	2.25	0.44
1:1:1140:THR:HG21	1:1:1292:THR:HA	2.00	0.44
1:1:148:PRO:HB3	1:1:388:ILE:HD12	1.98	0.44
1:1:598:ALA:HA	1:1:627:GLN:HA	2.00	0.44
2:L:52:LYS:HB3	2:L:55:ASN:OD1	2.17	0.44
1:1:134:ALA:O	1:1:1400:ALA:N	2.51	0.44
1:1:437:ARG:HD2	1:1:725:GLU:CD	2.43	0.44
1:1:629:PHE:CZ	1:1:631:PRO:HG3	2.52	0.44
1:1:862:LYS:HD2	1:1:891:GLN:CG	2.46	0.44
1:1:997:LEU:HD21	1:1:1100:PRO:HB3	1.98	0.44
1:1:1126:ASP:O	1:1:1130:PRO:HA	2.17	0.44
1:1:1165:SER:HA	1:1:1175:SER:HA	1.99	0.44
1:1:1214:VAL:HB	1:1:1254:LEU:HG	2.00	0.44
1:1:1432:VAL:HG21	3:H:100:LEU:HD21	1.99	0.44
1:1:151:PRO:HG3	1:1:377:TYR:CD2	2.52	0.44
1:1:284:VAL:HG12	1:1:695:PRO:HG2	1.99	0.44
1:1:410:PRO:HG3	1:1:480:ILE:HG13	2.00	0.44
1:1:594:MET:SD	1:1:732:SER:HB2	2.57	0.44
1:1:631:PRO:HB2	1:1:701:MET:HE1	1.99	0.44
1:1:166:GLY:HA3	1:1:384:ASN:HB2	1.99	0.44
1:1:285:LYS:O	1:1:695:PRO:HG3	2.17	0.44
1:1:589:ALA:HB3	1:1:1106:LEU:HD13	1.99	0.44
1:1:656:PRO:HG2	1:1:695:PRO:HA	2.00	0.44
1:1:747:PRO:HG2	1:1:779:ASN:HB2	2.00	0.44
1:1:1418:ASN:O	1:1:1422:THR:N	2.51	0.44
2:L:32:ALA:HB1	2:L:52:LYS:HD2	2.00	0.44
1:1:206:SER:HB3	1:1:356:TRP:CZ3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:357:LEU:HD12	1:1:484:PHE:CD2	2.53	0.44
1:1:515:HIS:NE2	1:1:1204:PRO:O	2.50	0.44
1:1:517:ALA:HB2	1:1:623:ARG:HH21	1.82	0.44
1:1:560:LEU:HD13	1:1:562:PHE:HE2	1.82	0.44
1:1:1139:LEU:HB2	1:1:1366:VAL:HG13	1.99	0.44
1:1:69:TRP:CH2	1:1:186:VAL:HG12	2.53	0.44
1:1:796:LEU:HD21	1:1:1135:LEU:HA	1.98	0.44
1:1:974:PRO:HB3	1:1:1046:ASN:HA	2.00	0.44
1:1:1407:VAL:HA	1:1:1446:ASP:O	2.18	0.44
1:1:1418:ASN:O	1:1:1422:THR:HG23	2.17	0.44
3:H:214:ARG:HH12	3:H:216:CYS:HB3	1.82	0.44
1:1:254:LYS:HA	1:1:314:PRO:HG3	2.00	0.43
1:1:414:HIS:ND1	1:1:569:GLU:OE2	2.51	0.43
1:1:441:TRP:HE1	1:1:521:ILE:HB	1.83	0.43
1:1:604:LEU:HD12	1:1:607:GLU:HG3	2.00	0.43
1:1:811:ILE:HD11	1:1:1142:LEU:H	1.82	0.43
2:L:39:LEU:HD13	2:L:88:TYR:CE1	2.53	0.43
1:1:120:LEU:HD13	1:1:209:TYR:HD2	1.83	0.43
1:1:611:ASN:HA	1:1:1042:TYR:OH	2.18	0.43
1:1:801:LEU:O	1:1:805:LEU:HG	2.18	0.43
1:1:915:PHE:CE1	1:1:919:THR:HG21	2.53	0.43
1:1:1137:LEU:HD23	1:1:1139:LEU:HD21	2.00	0.43
1:1:1235:ASN:CG	1:1:1240:LEU:HD13	2.44	0.43
1:1:1254:LEU:HD23	1:1:1254:LEU:HA	1.79	0.43
2:L:40:GLN:NE2	3:H:89:TYR:OH	2.50	0.43
2:L:150:TRP:HB3	2:L:181:LEU:HD11	1.99	0.43
3:H:30:TRP:CD1	3:H:64:LEU:HG	2.53	0.43
1:1:1467:GLU:OE2	1:1:1469:SER:HB3	2.19	0.43
1:1:407:TRP:CD2	1:1:480:ILE:HD12	2.54	0.43
1:1:415:HIS:HB2	1:1:419:ASP:CB	2.45	0.43
1:1:604:LEU:HA	1:1:658:TYR:OH	2.18	0.43
1:1:613:ASN:ND2	1:1:1213:GLN:O	2.47	0.43
1:1:1023:GLN:HG2	1:1:1025[A]:TRP:CZ2	2.53	0.43
1:1:1102:ASP:HB3	1:1:1159:TRP:CE3	2.53	0.43
1:1:275:ARG:NH1	1:1:695:PRO:O	2.38	0.43
1:1:668:ARG:HG3	1:1:963:THR:O	2.19	0.43
1:1:750:VAL:HG22	1:1:783:PHE:CZ	2.54	0.43
1:1:1008:VAL:HG11	1:1:1076:ILE:HG22	2.00	0.43
1:1:1285:PRO:HG3	1:1:1376:LYS:HB3	2.01	0.43
2:L:40:GLN:NE2	3:H:33:GLN:OE1	2.37	0.43
3:H:145:GLY:HA2	3:H:175:LEU:HG	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:86:PRO:HB2	1:1:133:LEU:HB2	1.99	0.43
1:1:125:THR:HA	1:1:205:ARG:HH12	1.84	0.43
1:1:141:LEU:HD23	1:1:141:LEU:HA	1.76	0.43
1:1:402:ASN:HD21	1:1:538:THR:HG1	1.67	0.43
1:1:403:TYR:CE2	1:1:480:ILE:HG22	2.54	0.43
1:1:554:THR:HB	1:1:790:PHE:CE1	2.53	0.43
1:1:560:LEU:HD13	1:1:792:THR:HG21	1.99	0.43
1:1:827:ILE:HD11	1:1:1025[B]:TRP:CZ3	2.54	0.43
1:1:894:THR:HA	1:1:978:TRP:CH2	2.53	0.43
1:1:1514:SER:O	1:1:1516:PHE:N	2.51	0.43
2:L:137:PHE:CZ	3:H:179:SER:HB2	2.53	0.43
2:L:189:GLU:HA	2:L:213:ARG:NH1	2.34	0.43
1:1:128:LEU:HD23	1:1:128:LEU:HA	1.78	0.43
1:1:423:ARG:HH22	1:1:724:ASN:C	2.25	0.43
3:H:26:TYR:HB2	3:H:92:ARG:HG3	2.00	0.43
1:1:429:THR:HG22	1:1:436:ARG:HB3	2.01	0.43
1:1:493:ASN:HB3	1:1:578:GLY:HA2	2.00	0.43
1:1:603:LEU:O	4:1:1602:HOH:O	2.22	0.43
1:1:941:ASN:HA	1:1:962:ALA:HA	2.00	0.43
1:1:1112:THR:HB	1:1:1125:THR:HA	2.01	0.43
1:1:1259:LYS:HB2	1:1:1259:LYS:HE2	1.88	0.43
1:1:1464:ASP:O	1:1:1468:GLN:HA	2.19	0.43
2:L:52:LYS:HD3	3:H:98:ASP:HB2	1.99	0.43
3:H:29:ASN:HA	3:H:44:LEU:HA	2.01	0.43
3:H:32:LYS:HD2	3:H:58:PHE:CE2	2.54	0.43
1:1:108:GLN:HE22	1:1:214:GLN:HB2	1.84	0.43
1:1:193:SER:HA	2:L:25:THR:HG21	2.00	0.43
1:1:587:VAL:HG11	1:1:1113:VAL:HG11	2.01	0.43
1:1:629:PHE:HZ	1:1:972:LEU:O	2.02	0.43
1:1:634:TRP:HZ2	1:1:702:TRP:CE2	2.37	0.43
1:1:1150:ARG:HA	1:1:1153:ILE:HD12	1.99	0.43
2:L:37:TRP:HB3	2:L:75:LEU:HD22	2.00	0.43
1:1:1018:PHE:HZ	1:1:1023:GLN:HB2	1.83	0.43
1:1:377:TYR:HB2	1:1:387:ALA:HB3	2.00	0.42
1:1:402:ASN:O	1:1:752:TYR:OH	2.32	0.42
1:1:759:ALA:HB1	1:1:764[B]:GLU:HB3	2.01	0.42
1:1:939:GLN:O	1:1:954:GLY:N	2.52	0.42
1:1:990:ALA:O	1:1:994:GLN:HG3	2.18	0.42
2:L:48:LEU:HB2	3:H:102:ASP:HA	2.01	0.42
3:H:106:GLN:OE1	3:H:106:GLN:N	2.47	0.42
1:1:627:GLN:NE2	1:1:988:ASN:OD1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:811:ILE:HB	1:1:1120:TRP:NE1	2.32	0.42
1:1:1109:SER:OG	1:1:1171:GLY:O	2.29	0.42
1:1:1360:GLY:O	1:1:1364:VAL:N	2.49	0.42
1:1:1455:MET:HE2	3:H:56:GLN:HE21	1.84	0.42
2:L:121:PRO:HB3	2:L:211:PHE:CE2	2.55	0.42
2:L:162:LEU:HD23	2:L:162:LEU:HA	1.85	0.42
1:1:317:ARG:HE	1:1:424:ASP:CG	2.27	0.42
1:1:713:LEU:HD23	1:1:713:LEU:HA	1.73	0.42
2:L:39:LEU:HB3	2:L:49:LEU:HD21	2.00	0.42
3:H:-3:GLN:HA	3:H:-3:GLN:NE2	2.34	0.42
1:1:550:VAL:HG21	1:1:552:LYS:HE3	2.02	0.42
1:1:810:TRP:CZ2	1:1:812:GLY:HA3	2.54	0.42
1:1:968:LEU:HB3	1:1:984:PHE:CE2	2.54	0.42
2:L:148:VAL:HA	2:L:198:ALA:HA	2.01	0.42
1:1:414:HIS:N	1:1:569:GLU:OE2	2.22	0.42
1:1:579:ALA:HB1	1:1:586:LEU:HD11	2.00	0.42
1:1:997:LEU:O	1:1:1001:LEU:HG	2.20	0.42
1:1:1042:TYR:CZ	1:1:1245:PRO:HB3	2.54	0.42
1:1:1106:LEU:HD12	1:1:1114:SER:O	2.20	0.42
1:1:320:GLU:N	1:1:323:GLN:O	2.53	0.42
1:1:413:ASN:HD21	1:1:419:ASP:CG	2.22	0.42
1:1:421:LYS:C	1:1:642:ILE:HD11	2.45	0.42
1:1:516:THR:C	1:1:518:PRO:HD3	2.45	0.42
1:1:564:ASN:CG	1:1:570:TYR:HB3	2.44	0.42
1:1:627:GLN:O	1:1:991:GLN:NE2	2.52	0.42
1:1:1206:HIS:CD2	1:1:1264:PRO:HB2	2.54	0.42
2:L:35:LEU:HG	2:L:73:PHE:CG	2.55	0.42
3:H:41:TRP:CZ2	3:H:44:LEU:HD23	2.55	0.42
3:H:214:ARG:NH1	3:H:216:CYS:HB3	2.34	0.42
1:1:75:SER:HB2	1:1:1105:ASN:H	1.85	0.42
1:1:415:HIS:HB3	1:1:418:TRP:NE1	2.34	0.42
1:1:429:THR:HB	1:1:434:ASN:CB	2.50	0.42
1:1:491:ILE:HD13	1:1:491:ILE:HA	1.80	0.42
1:1:1386:ARG:HH11	1:1:1391:GLU:CD	2.27	0.42
2:L:12:LEU:HD13	2:L:80:VAL:O	2.18	0.42
1:1:210:TYR:HH	1:1:215:ARG:HH11	1.67	0.42
1:1:332:PHE:HZ	1:1:436:ARG:HG3	1.83	0.42
1:1:647:SER:HG	1:1:651:SER:HG	1.68	0.42
1:1:1009:ASN:HD22	1:1:1087:SER:HB2	1.84	0.42
2:L:199:THR:HG23	2:L:206:PRO:HG3	2.00	0.42
1:1:303:LEU:HD22	1:1:761:ASN:CG	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:538:THR:OG1	1:1:748:ASP:O	2.33	0.42
1:1:551:ASN:ND2	1:1:713:LEU:O	2.53	0.42
1:1:584:ARG:NH1	1:1:584:ARG:HG2	2.34	0.42
1:1:811:ILE:HG12	1:1:1153:ILE:HG12	2.01	0.42
1:1:1025[B]:TRP:CD1	1:1:1025[B]:TRP:N	2.87	0.42
1:1:1178:ASP:HB2	1:1:1381:VAL:O	2.19	0.42
1:1:1226:THR:O	1:1:1226:THR:OG1	2.37	0.42
2:L:77:ILE:HD12	2:L:106:LEU:HD11	2.00	0.42
2:L:149:LYS:HE3	2:L:149:LYS:HB3	1.91	0.42
1:1:246:ALA:HA	1:1:315:ILE:HD13	2.02	0.42
1:1:853:THR:O	1:1:1049:LEU:N	2.50	0.42
1:1:1074:PRO:HB3	1:1:1270:LYS:HB3	2.02	0.42
1:1:1407:VAL:HG21	1:1:1451:VAL:HG11	2.02	0.42
3:H:54:TYR:CD1	3:H:59:ARG:HD2	2.55	0.42
1:1:407:TRP:HA	1:1:432:PHE:HZ	1.86	0.41
1:1:804:VAL:O	1:1:808:VAL:HG23	2.20	0.41
1:1:810:TRP:HH2	1:1:1271:LEU:HD13	1.84	0.41
1:1:1420:LEU:HD23	1:1:1421:PHE:CE2	2.55	0.41
2:L:195:THR:OG1	2:L:209:LYS:O	2.35	0.41
1:1:436:ARG:HG2	1:1:619:GLN:O	2.20	0.41
1:1:742:LEU:O	1:1:746:LEU:HG	2.19	0.41
1:1:69:TRP:CD1	1:1:93:ARG:HB3	2.56	0.41
1:1:318:SER:O	1:1:325:VAL:HG12	2.19	0.41
1:1:597:THR:HA	1:1:600:VAL:HG23	2.02	0.41
1:1:998:ARG:NH1	4:1:1737:HOH:O	2.52	0.41
1:1:1444:PHE:CZ	1:1:1470:LEU:HD23	2.55	0.41
1:1:220:PRO:O	1:1:238:GLY:HA3	2.21	0.41
1:1:407:TRP:CZ2	1:1:571:VAL:HG22	2.55	0.41
1:1:423:ARG:HB3	1:1:428:GLN:HG2	2.03	0.41
1:1:636:ASN:OD1	1:1:658:TYR:HA	2.20	0.41
1:1:767:ASN:O	1:1:769:LYS:NZ	2.53	0.41
1:1:1039:LEU:HA	1:1:1051:PRO:HD3	2.01	0.41
1:1:1098:TRP:HZ2	1:1:1153:ILE:HA	1.84	0.41
1:1:1411:SER:OG	1:1:1414:GLN:HG2	2.21	0.41
3:H:6:VAL:HG11	3:H:80:LEU:HD13	2.01	0.41
1:1:415:HIS:C	1:1:765:ARG:HD2	2.46	0.41
1:1:549:MET:HA	1:1:553:GLN:OE1	2.20	0.41
1:1:665:TRP:HE1	1:1:933:ASN:HB3	1.85	0.41
1:1:811:ILE:O	1:1:1153:ILE:HD13	2.20	0.41
1:1:1210:LEU:HB2	1:1:1212:PHE:CE2	2.56	0.41
2:L:189:GLU:HA	2:L:213:ARG:HH12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:81:THR:O	3:H:112:VAL:HG21	2.20	0.41
1:1:624:GLU:CD	1:1:998:ARG:HH12	2.28	0.41
1:1:1113:VAL:CG2	1:1:1124:PHE:HB2	2.48	0.41
1:1:1457:ARG:NH1	2:L:96:VAL:HB	2.36	0.41
3:H:67:ASP:OD1	3:H:69:SER:OG	2.30	0.41
1:1:141:LEU:HD12	1:1:376:LEU:HD21	2.03	0.41
1:1:210:TYR:HE2	1:1:356:TRP:HB2	1.85	0.41
1:1:327:LEU:HD21	1:1:619:GLN:HB2	2.03	0.41
1:1:591:THR:HG21	1:1:1117:LEU:HD13	2.01	0.41
1:1:915:PHE:HA	1:1:968:LEU:HD11	2.02	0.41
1:1:1255:ASP:HB2	1:1:1258:LEU:HB2	2.01	0.41
2:L:137:PHE:CE1	3:H:179:SER:HB2	2.55	0.41
1:1:363:HIS:O	1:1:366:LEU:HG	2.21	0.41
1:1:385:ARG:HE	1:1:385:ARG:HB2	1.60	0.41
1:1:409:THR:HB	1:1:454:THR:O	2.20	0.41
1:1:731:ASN:HB2	1:1:994:GLN:OE1	2.20	0.41
3:H:108:THR:HG22	3:H:110:VAL:HG23	2.03	0.41
1:1:178:ASN:HA	1:1:181:LYS:NZ	2.36	0.41
1:1:198:PHE:HE2	1:1:378:ASP:HB3	1.83	0.41
1:1:310:LEU:HD22	1:1:418:TRP:HB3	2.02	0.41
1:1:471:GLU:OE2	1:1:471:GLU:HA	2.21	0.41
1:1:631:PRO:CB	1:1:701:MET:HE1	2.51	0.41
1:1:638:PRO:HD2	1:1:709:TRP:CE3	2.56	0.41
1:1:675:ASP:HA	1:1:679:LYS:CB	2.51	0.41
1:1:677:PHE:O	1:1:694:TYR:HB3	2.20	0.41
1:1:798:GLY:O	1:1:992:ARG:HD3	2.21	0.41
1:1:803:GLN:OE1	1:1:1332:SER:HB2	2.21	0.41
1:1:851:LEU:HD22	1:1:859:VAL:HG13	2.02	0.41
1:1:561:PRO:HG2	1:1:594:MET:CB	2.47	0.41
1:1:617:GLN:HE21	1:1:624:GLU:HB3	1.86	0.41
1:1:673:VAL:HG21	1:1:963:THR:HA	2.02	0.41
1:1:1006:VAL:HG23	1:1:1053:LEU:HB3	2.02	0.41
1:1:411:LYS:HG2	1:1:435:PRO:HD2	2.02	0.40
1:1:598:ALA:HB2	1:1:625:ASP:O	2.20	0.40
1:1:1090:THR:HB	1:1:1254:LEU:HD21	2.02	0.40
2:L:188:TYR:O	2:L:213:ARG:NH1	2.45	0.40
1:1:178:ASN:HA	1:1:181:LYS:HZ2	1.85	0.40
1:1:354:ARG:HB3	1:1:354:ARG:HH11	1.85	0.40
1:1:1168:ASN:OD1	1:1:1172[B]:ARG:N	2.50	0.40
2:L:21:ARG:HG3	2:L:21:ARG:NH1	2.29	0.40
3:H:175:LEU:HD12	3:H:175:LEU:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:159:ILE:HG13	1:1:377:TYR:CE1	2.56	0.40
1:1:369:TRP:HA	1:1:369:TRP:CE3	2.56	0.40
1:1:504:PHE:O	1:1:542:TYR:OH	2.31	0.40
1:1:587:VAL:HG22	1:1:737:ILE:CD1	2.50	0.40
1:1:612:LEU:HB3	1:1:1213:GLN:HB3	2.04	0.40
1:1:708:ASN:HB2	1:1:709:TRP:CE3	2.57	0.40
1:1:869:LEU:HD22	1:1:965:TYR:CD2	2.56	0.40
1:1:1003:SER:HB3	4:1:1669:HOH:O	2.21	0.40
1:1:1210:LEU:HB2	1:1:1212:PHE:CZ	2.56	0.40
1:1:272:SER:HB2	1:1:951:THR:O	2.21	0.40
1:1:406:SER:HB2	1:1:758:PHE:CE2	2.57	0.40
1:1:415:HIS:CB	1:1:419:ASP:HB2	2.48	0.40
1:1:504:PHE:CE2	1:1:588:LEU:HB2	2.56	0.40
1:1:529:ASN:OD1	1:1:529:ASN:N	2.54	0.40
1:1:603:LEU:HD23	1:1:634:TRP:HD1	1.87	0.40
1:1:1087:SER:O	1:1:1216:VAL:HA	2.22	0.40
1:1:1502:LEU:H	1:1:1502:LEU:HG	1.60	0.40
2:L:98:TRP:HB2	3:H:41:TRP:CD2	2.57	0.40
1:1:134:ALA:HB1	1:1:1400:ALA:O	2.21	0.40
1:1:212:GLN:O	1:1:214:GLN:NE2	2.54	0.40
1:1:500:ALA:HB1	1:1:525:ARG:HD2	2.03	0.40
1:1:547:SER:HB3	1:1:568:PHE:CE1	2.53	0.40
1:1:624:GLU:OE2	1:1:998:ARG:NH1	2.55	0.40
1:1:1082:GLU:HB2	1:1:1083:GLN:NE2	2.37	0.40
1:1:1098:TRP:CH2	1:1:1158:PRO:HB2	2.56	0.40
1:1:1166:TRP:CH2	1:1:1168:ASN:HA	2.57	0.40
1:1:1258:LEU:HD12	1:1:1258:LEU:HA	1.90	0.40
1:1:1433:THR:HB	1:1:1435:LEU:HG	2.04	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	1	1330/1457 (91%)	1252 (94%)	77 (6%)	1 (0%)	48	65
2	L	216/218 (99%)	205 (95%)	11 (5%)	0	100	100
3	H	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	25	38
All	All	1766/1897 (93%)	1665 (94%)	99 (6%)	2 (0%)	50	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	957	ILE
3	H	102	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	1141/1215 (94%)	1117 (98%)	24 (2%)	48	69
2	L	194/194 (100%)	183 (94%)	11 (6%)	17	29
3	H	193/193 (100%)	183 (95%)	10 (5%)	19	34
All	All	1528/1602 (95%)	1483 (97%)	45 (3%)	39	58

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	82	THR
1	1	282	THR
1	1	351	THR
1	1	526	VAL
1	1	534	SER
1	1	559	ASP
1	1	664	ASP
1	1	688	ASP
1	1	718	LEU
1	1	725	GLU
1	1	784	SER

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Mol	Chain	Res	Type
1	1	789[A]	ARG
1	1	789[B]	ARG
1	1	826	ASP
1	1	943	SER
1	1	1087	SER
1	1	1126	ASP
1	1	1297	THR
1	1	1369	LEU
1	1	1401	ASP
1	1	1425	VAL
1	1	1466	ASN
1	1	1482	ASP
1	1	1507	GLN
2	L	2	THR
2	L	6	LEU
2	L	17	SER
2	L	71	THR
2	L	94	SER
2	L	105	LYS
2	L	135	VAL
2	L	159	ASN
2	L	174	THR
2	L	179	SER
2	L	182	THR
3	H	10	THR
3	H	34	SER
3	H	61	THR
3	H	78	LEU
3	H	85	SER
3	H	113	SER
3	H	152	THR
3	H	170	VAL
3	H	178	LEU
3	H	181	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	108	GLN
1	1	182	ASN
1	1	221	GLN
1	1	256	GLN

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Mol	Chain	Res	Type
1	1	300	ASN
1	1	415	HIS
1	1	611	ASN
1	1	613	ASN
1	1	782	HIS
1	1	889	ASN
1	1	952	GLN
1	1	960	GLN
1	1	980	ASN
1	1	1101	GLN
1	1	1266	GLN
1	1	1358	ASN
1	1	1378	ASN
1	1	1418	ASN
1	1	1494	ASN
2	L	40	GLN
2	L	163	ASN
2	L	214	ASN
3	H	33	GLN
3	H	172	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.

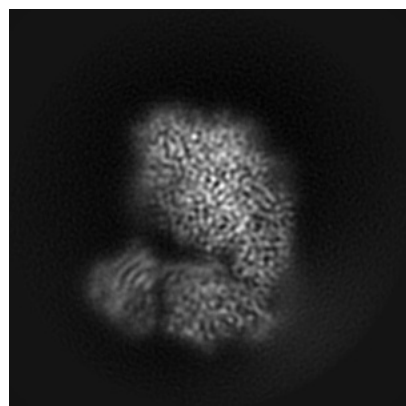
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19402. These allow visual inspection of the internal detail of the map and identification of artifacts.

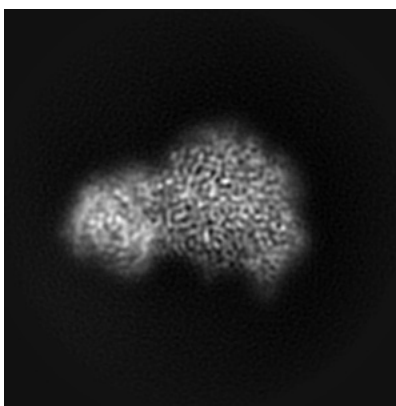
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

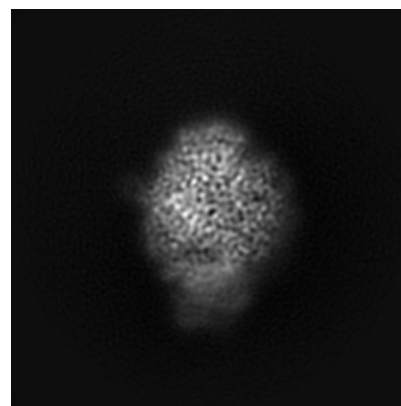
6.1.1 Primary map



X

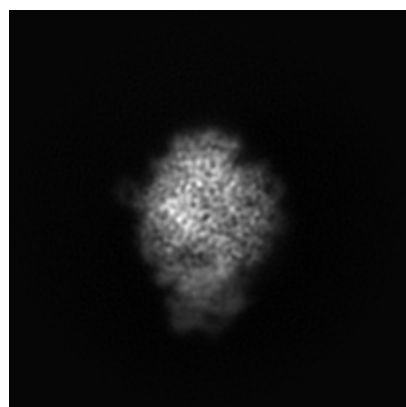


Y

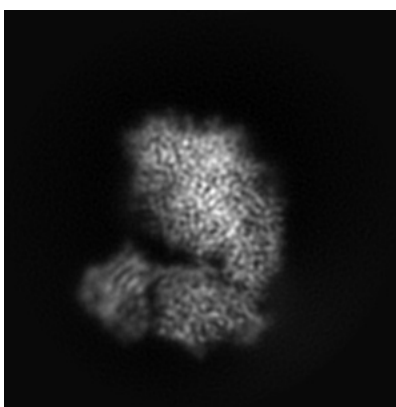


Z

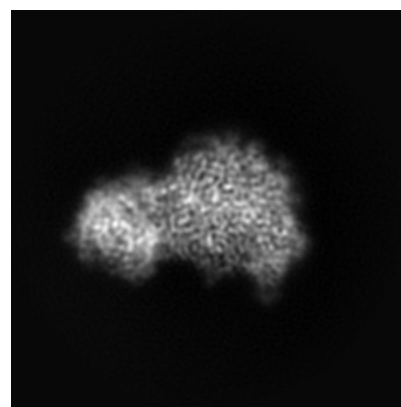
6.1.2 Raw map



X



Y

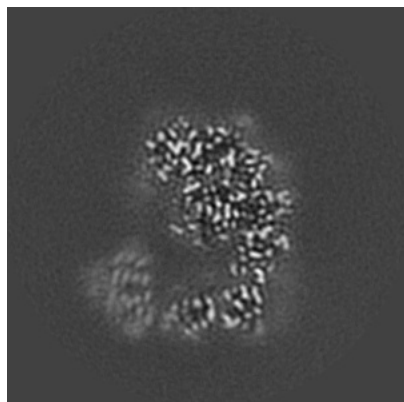


Z

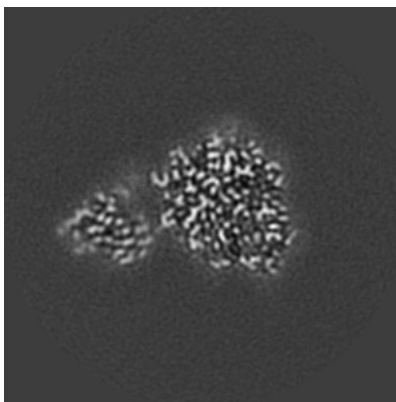
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

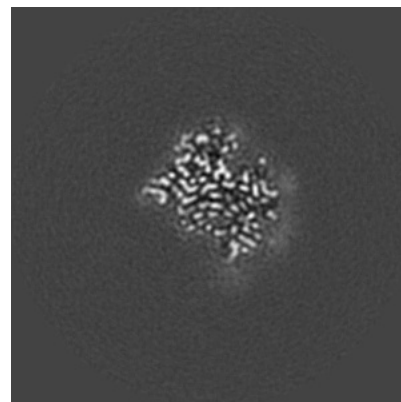
6.2.1 Primary map



X Index: 188

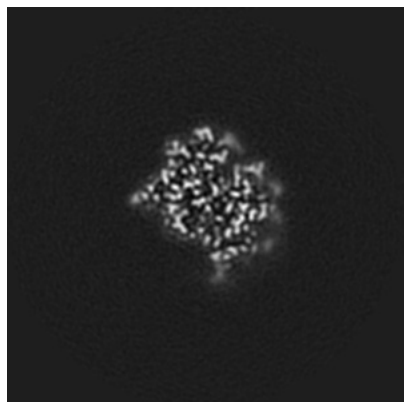


Y Index: 188

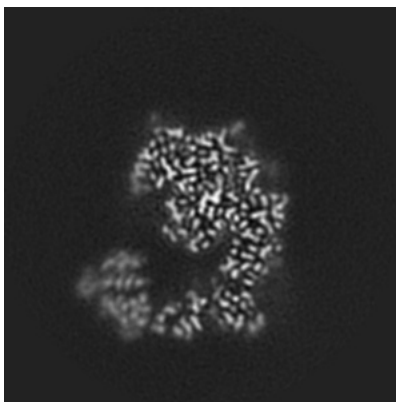


Z Index: 188

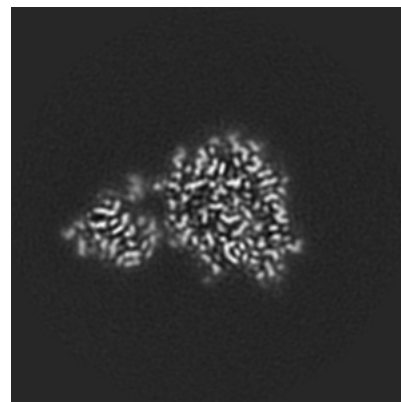
6.2.2 Raw map



X Index: 188



Y Index: 188

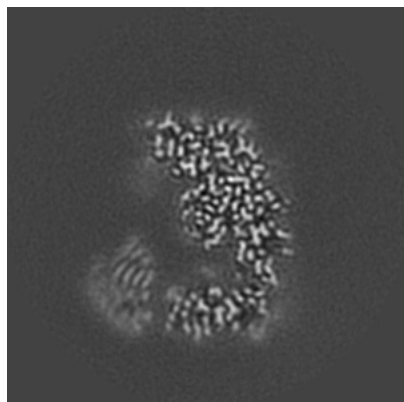


Z Index: 188

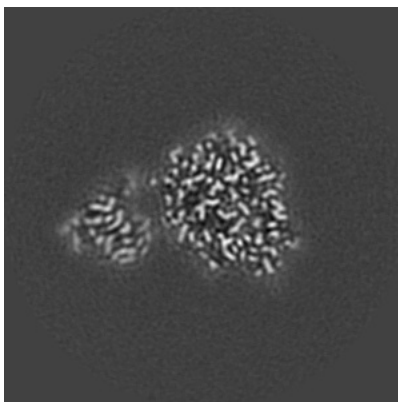
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

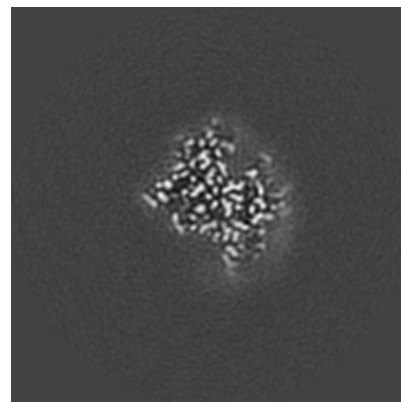
6.3.1 Primary map



X Index: 180

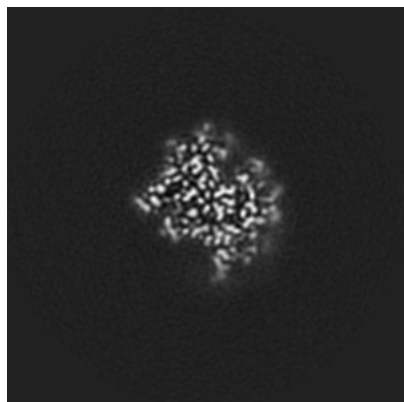


Y Index: 191

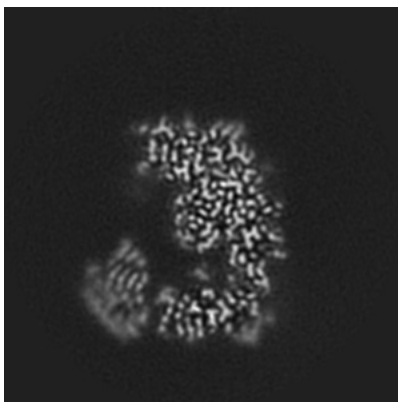


Z Index: 196

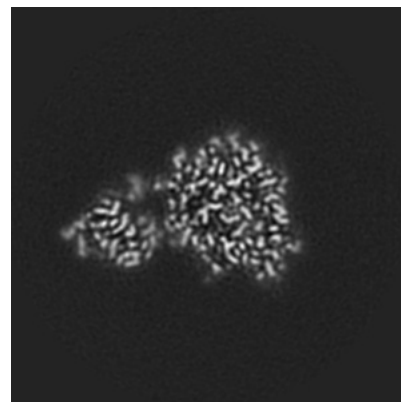
6.3.2 Raw map



X Index: 192



Y Index: 177

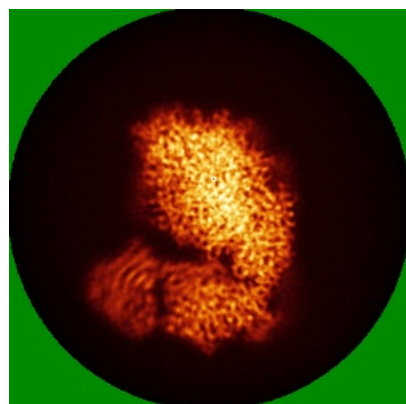


Z Index: 187

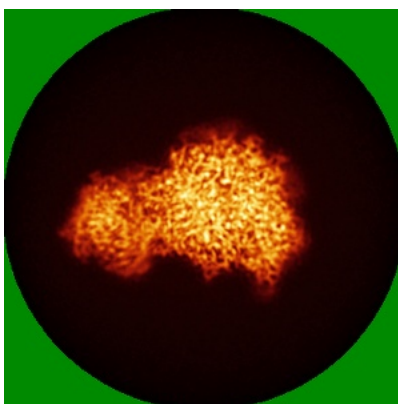
The images above show the largest variance slices of the map in three orthogonal directions.

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

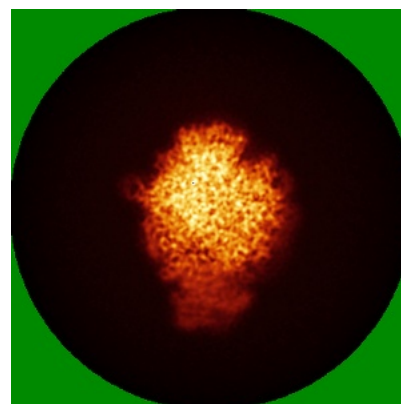
6.4.1 Primary map



X

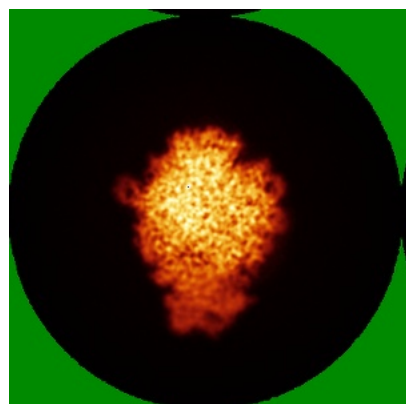


Y

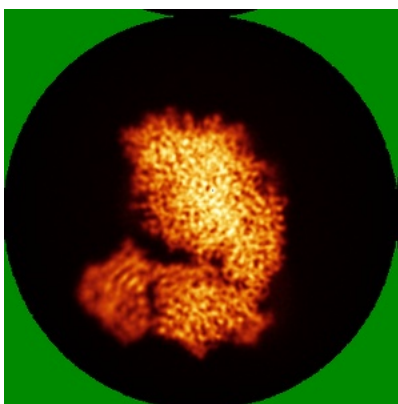


Z

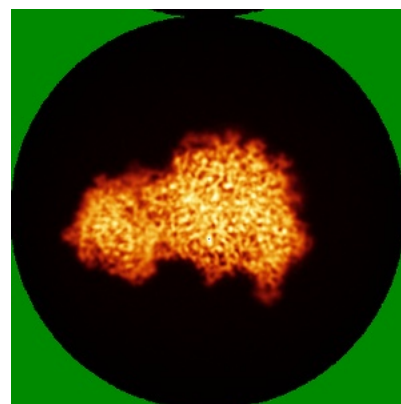
6.4.2 Raw map



X



Y

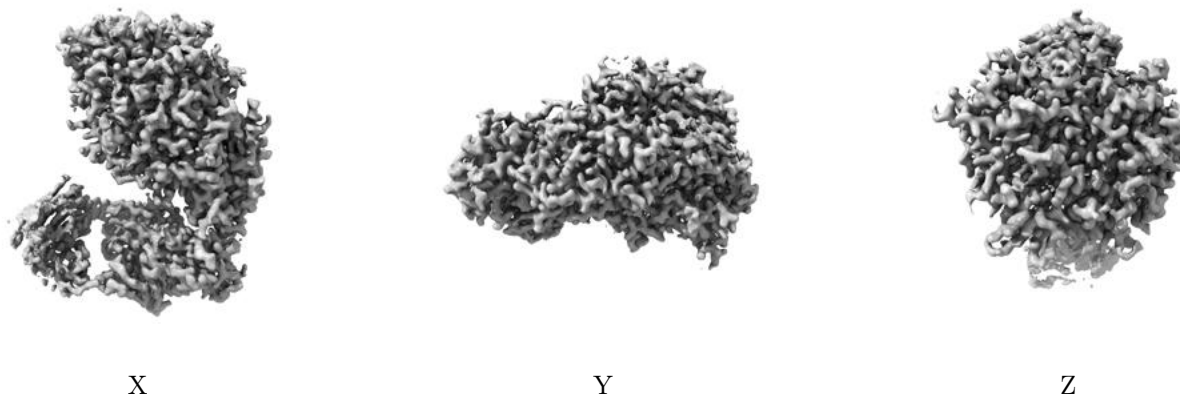


Z

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

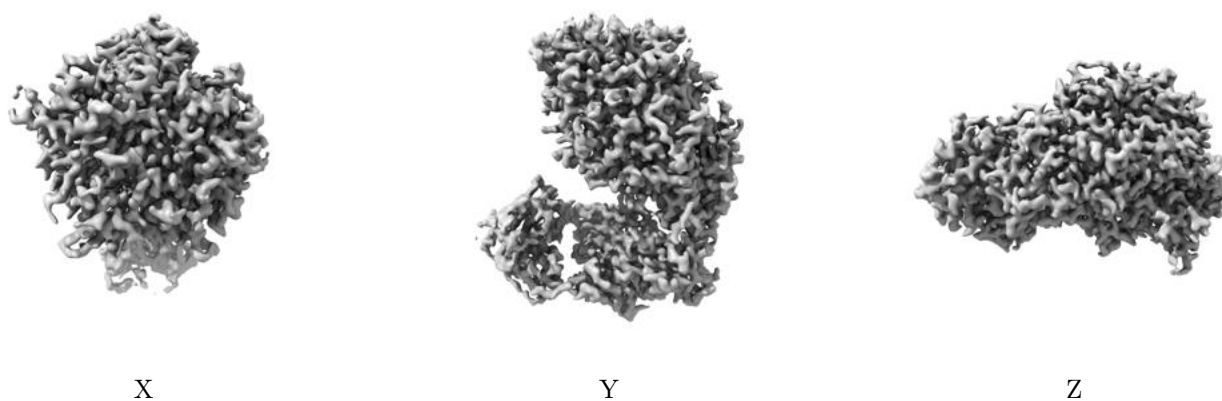
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

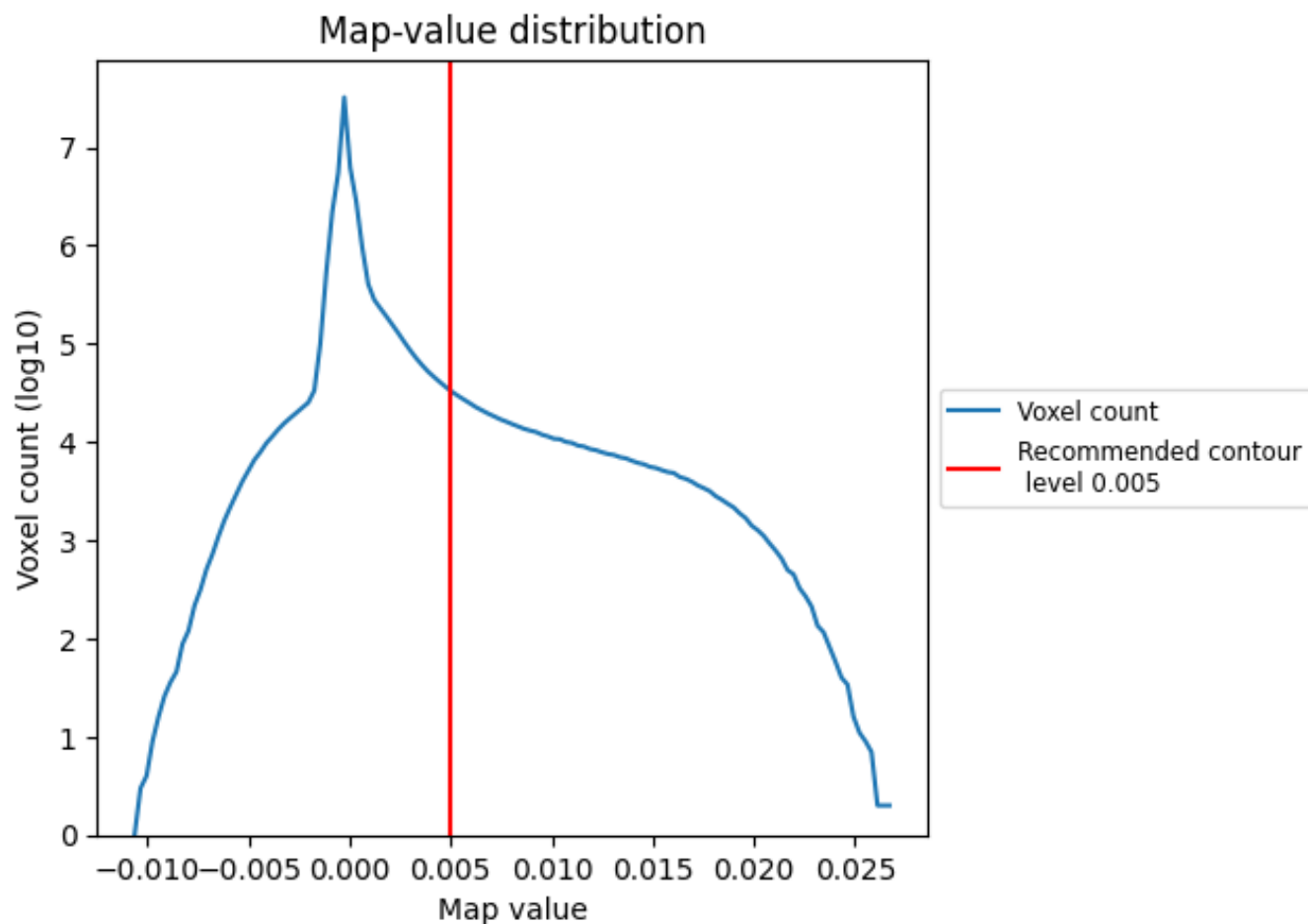
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

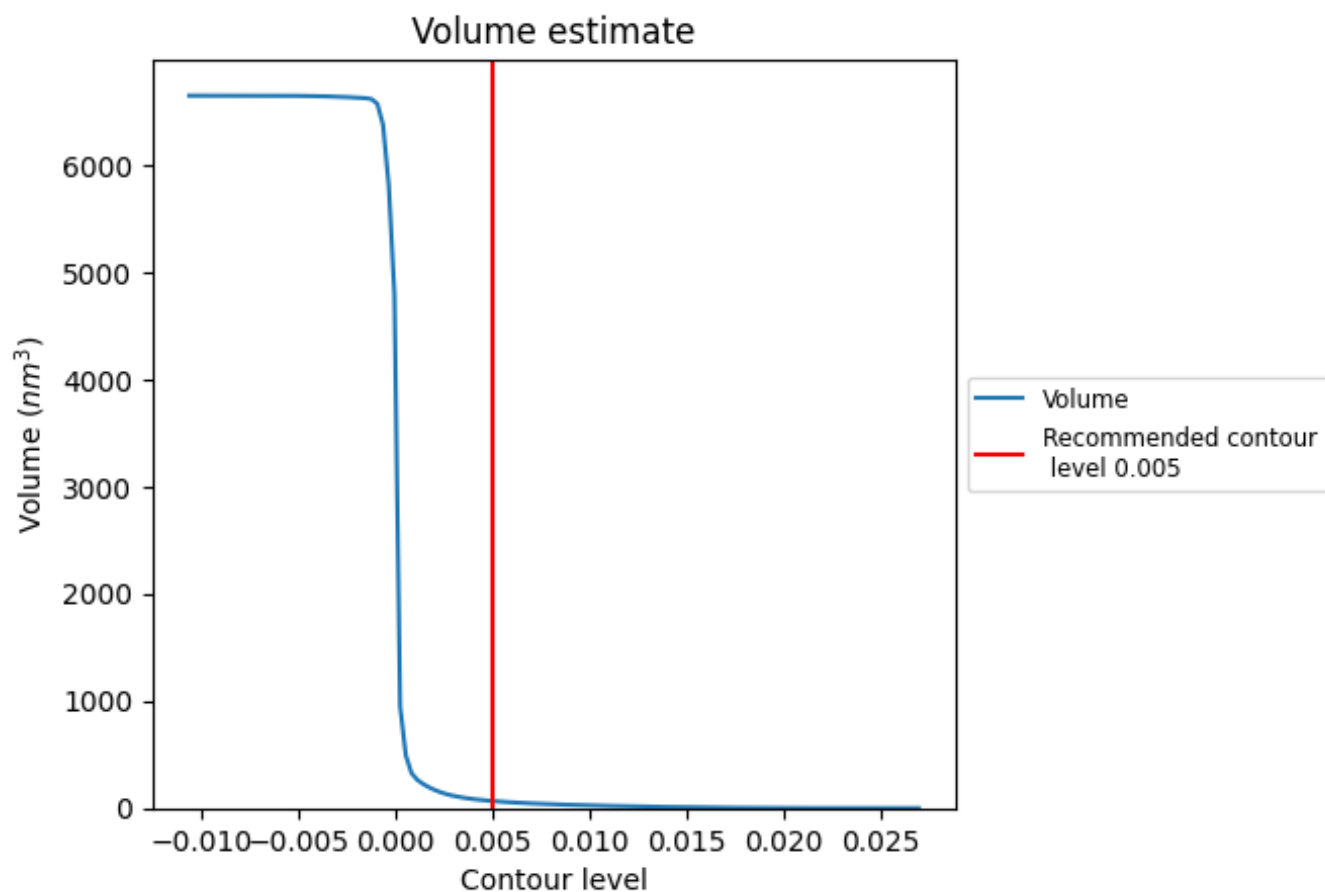
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

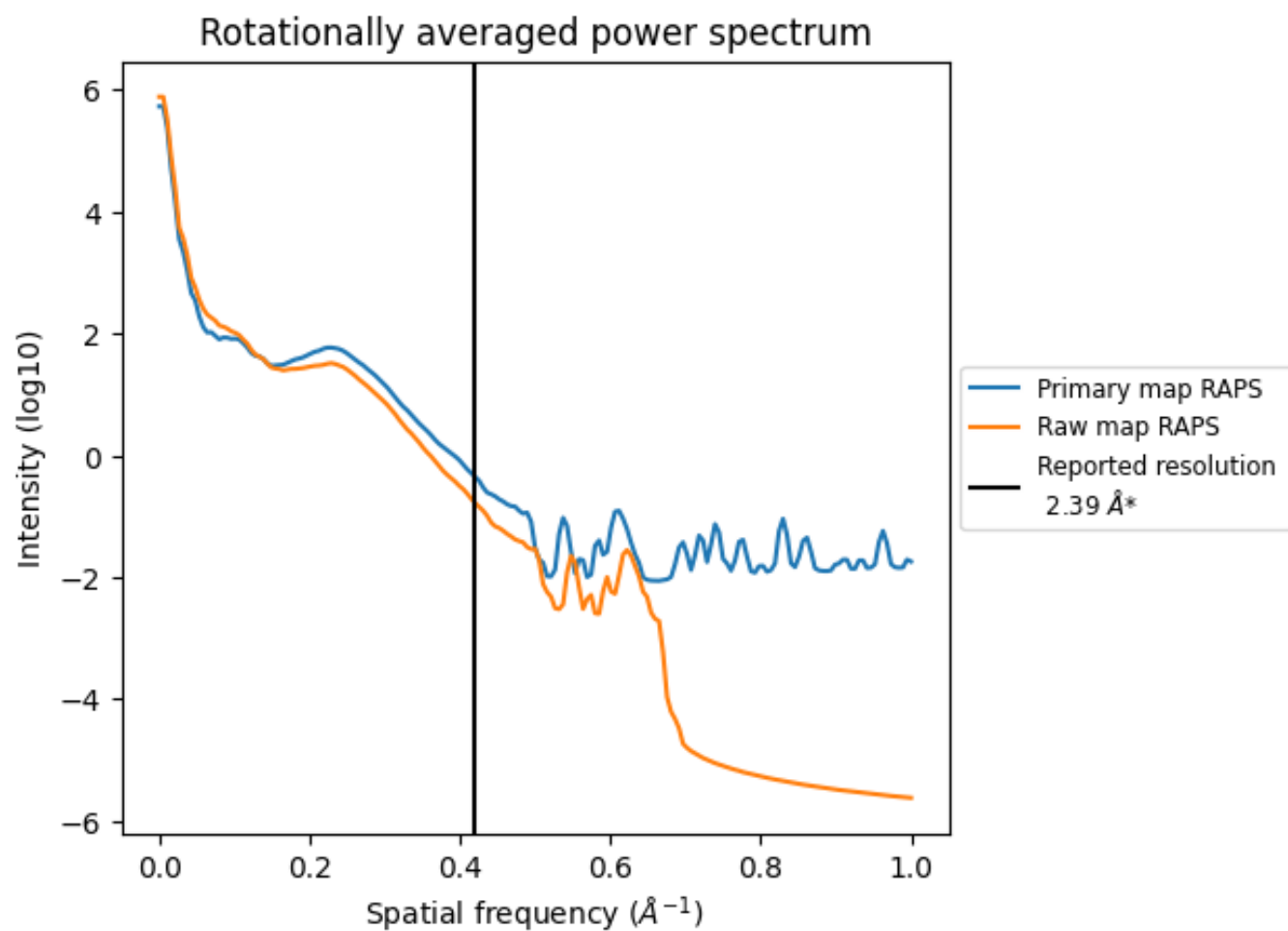
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 66 nm^3 ; this corresponds to an approximate mass of 60 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 ⓘ

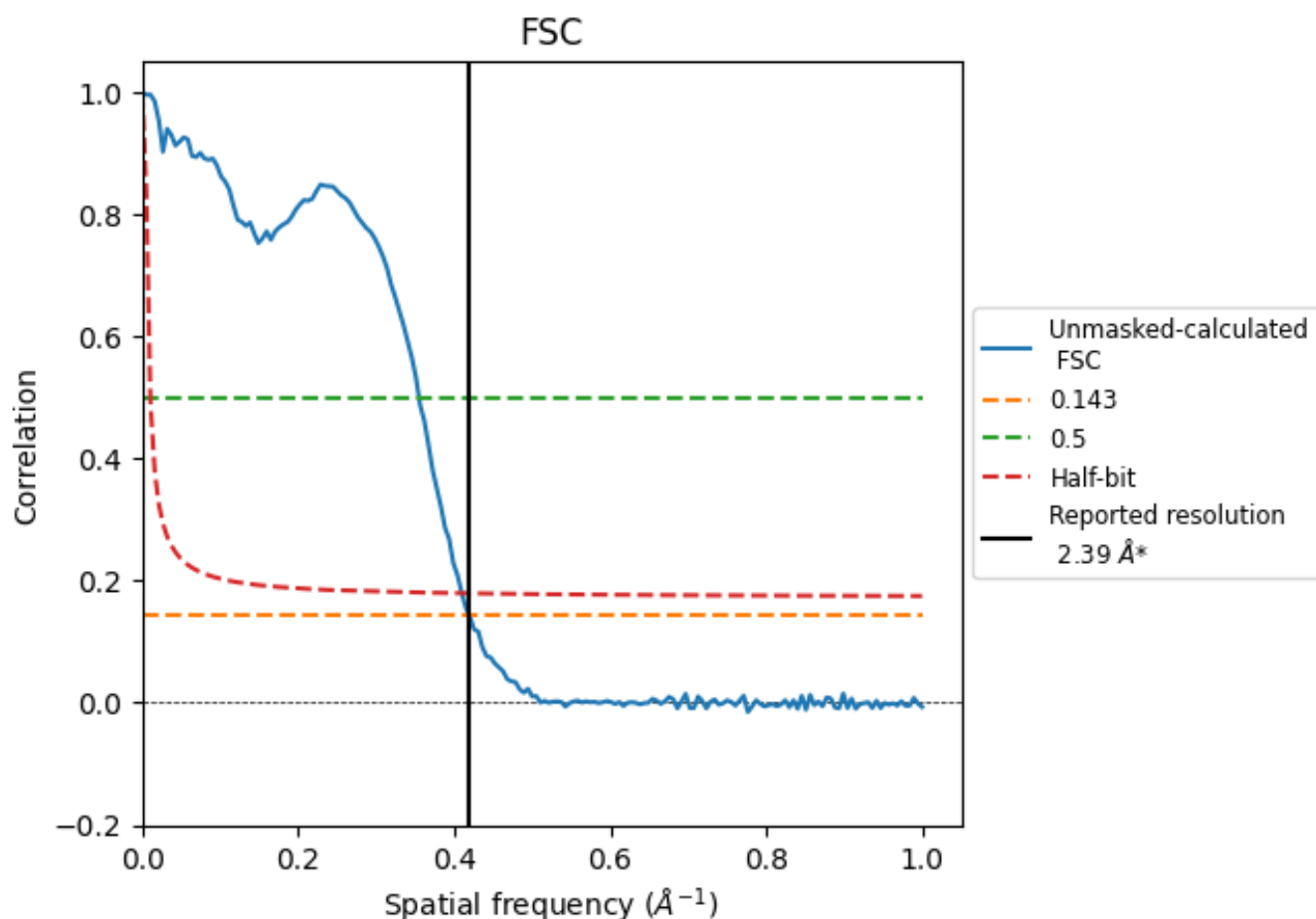


*Reported resolution corresponds to spatial frequency of 0.418 Å⁻¹

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 0.418 Å⁻¹

8.2 Resolution estimates [i](#)

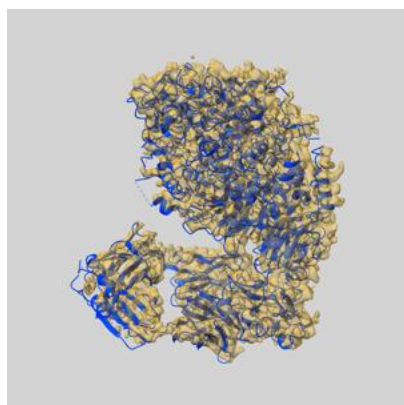
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.39	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.38	2.82	2.44

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

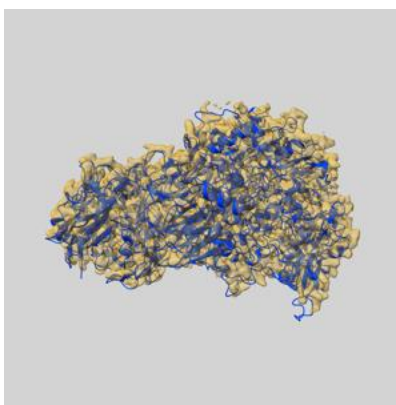
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19402 and PDB model 8ROR. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

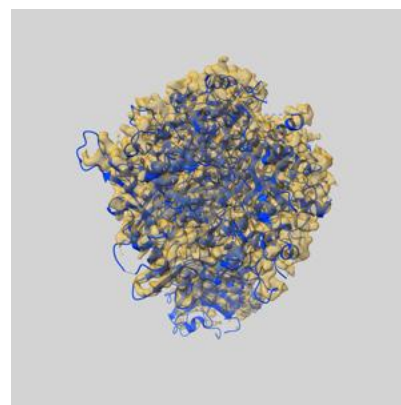
9.1 Map-model overlay [i](#)



X



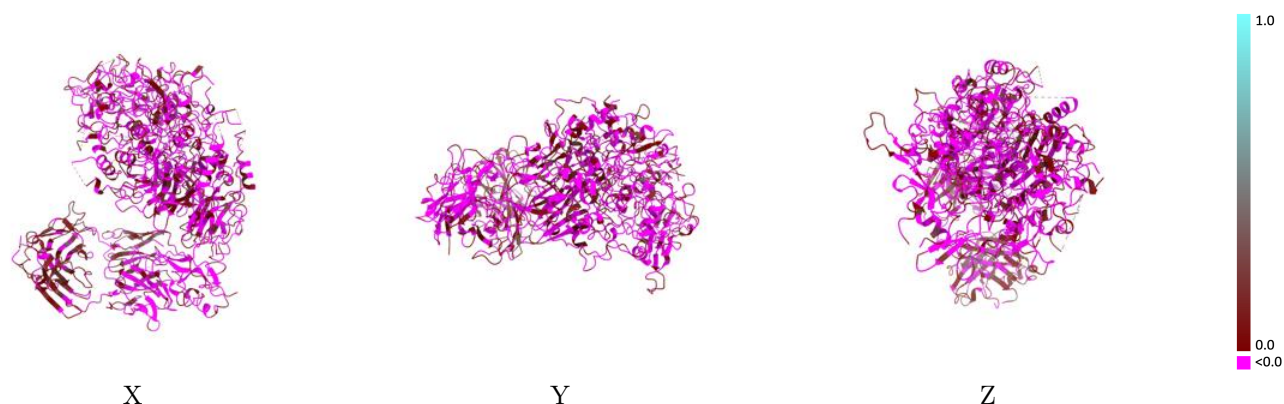
Y



Z

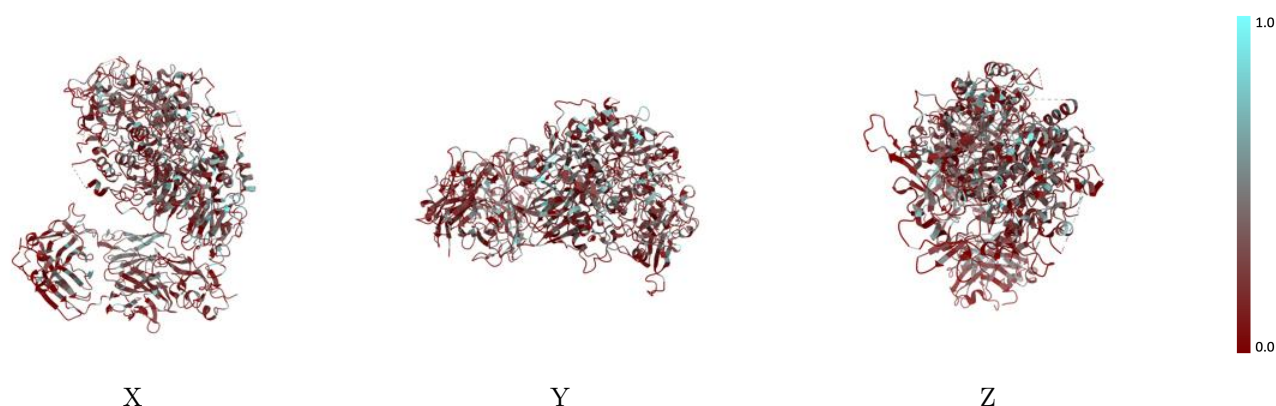
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



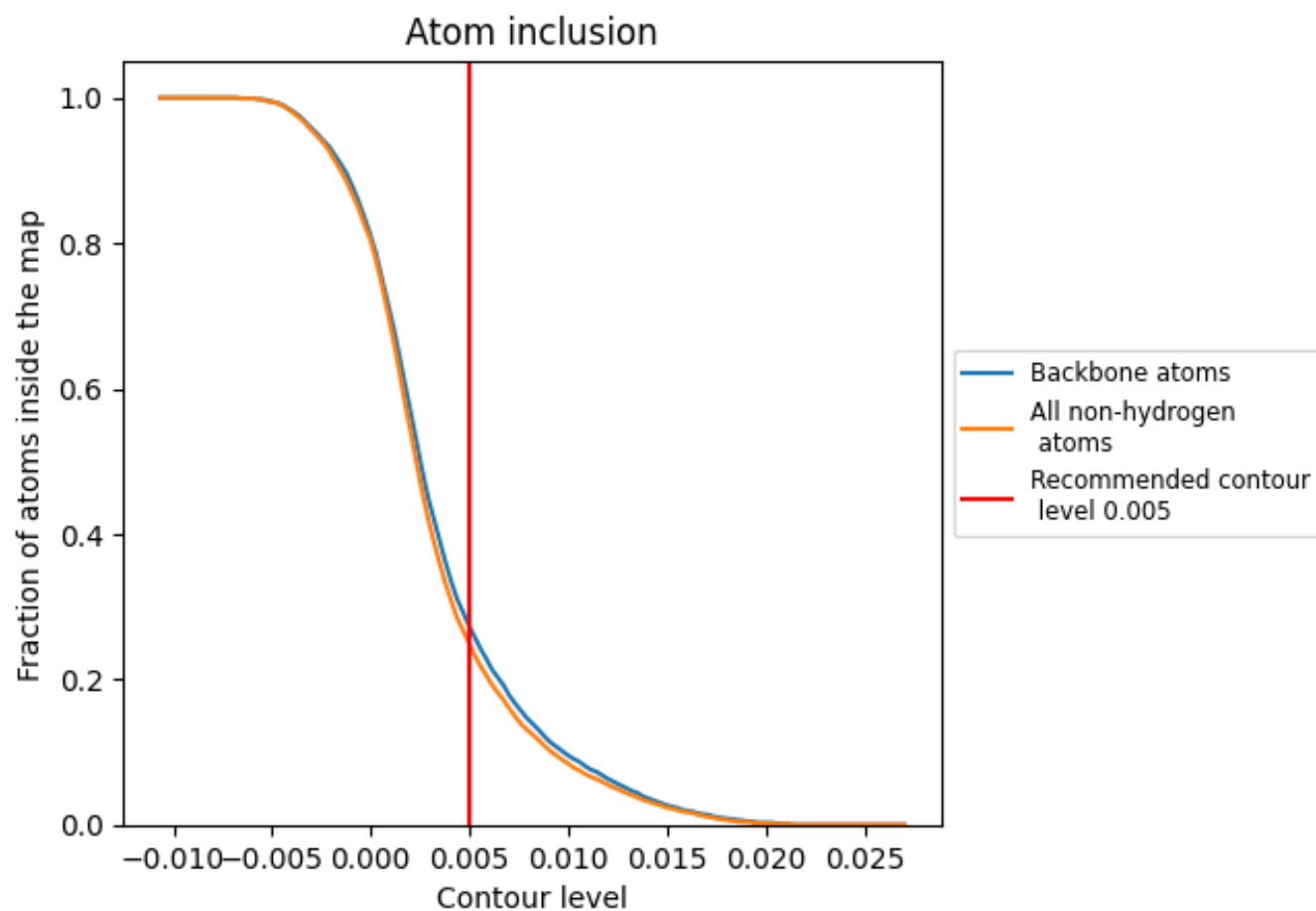
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 27% of all backbone atoms, 25% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.2480	<div></div> -0.0430
1	<div></div> 0.2520	<div></div> -0.0620
H	<div></div> 0.1980	<div></div> -0.0180
L	<div></div> 0.2780	<div></div> 0.0550

