



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 05:03 PM UTC

PDB ID : 6V85 / pdb_00006v85
EMDB ID : EMD-21095
Title : Parainfluenza virus 5 L-P complex
Authors : Abdella, R.; He, Y.
Deposited on : 2019-12-10
Resolution : 4.38 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:

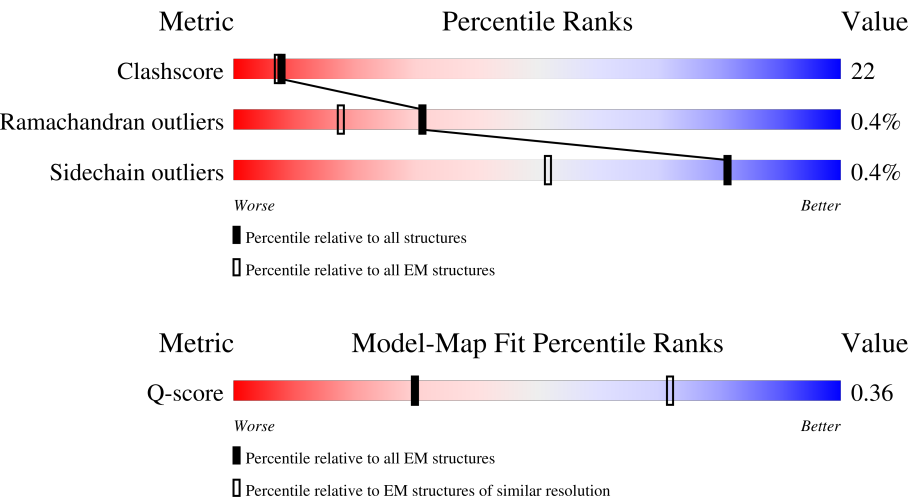
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.38 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	3702 (3.88 - 4.88)

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	2255	8% 47% 37% 16%
2	B	392	15% 14% 82%
2	C	392	15% 15% 81%
2	D	392	15% 16% 82%

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Mol	Chain	Length	Quality of chain
2	E	392	14%15%81%
2	F	392	8%88%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17878 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1901	Total	C	N	O	S	0	0
			15200	9769	2578	2770	83		

- Molecule 2 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	47	Total	C	N	O	S	0	0
			374	238	64	70	2		
2	B	72	Total	C	N	O	S	4	0
			569	350	101	115	3		
2	C	74	Total	C	N	O	S	4	0
			582	357	103	119	3		
2	D	72	Total	C	N	O	S	4	0
			569	350	101	115	3		
2	E	74	Total	C	N	O	S	4	0
			582	357	103	119	3		

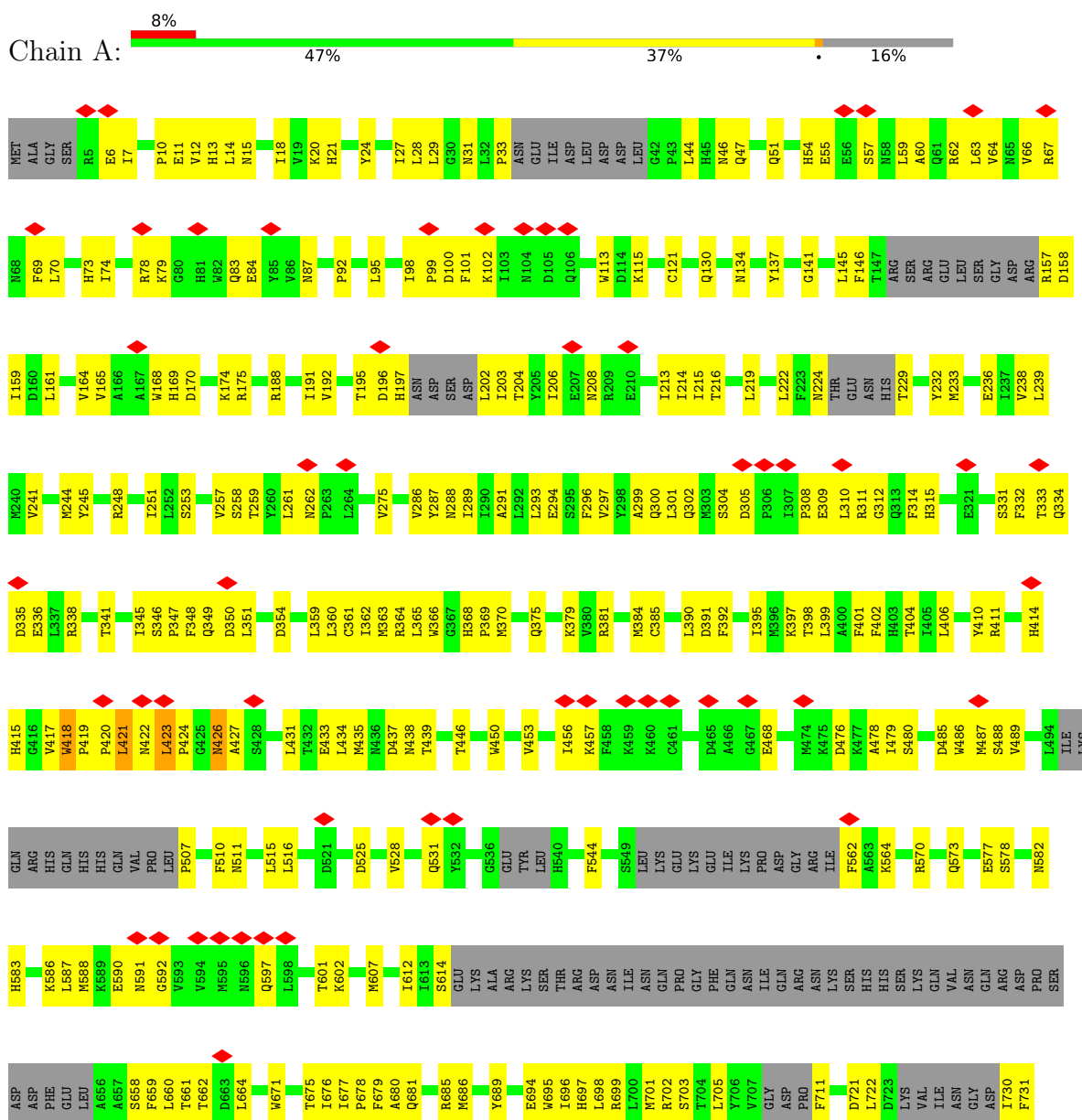
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Zn	0
			2	2	

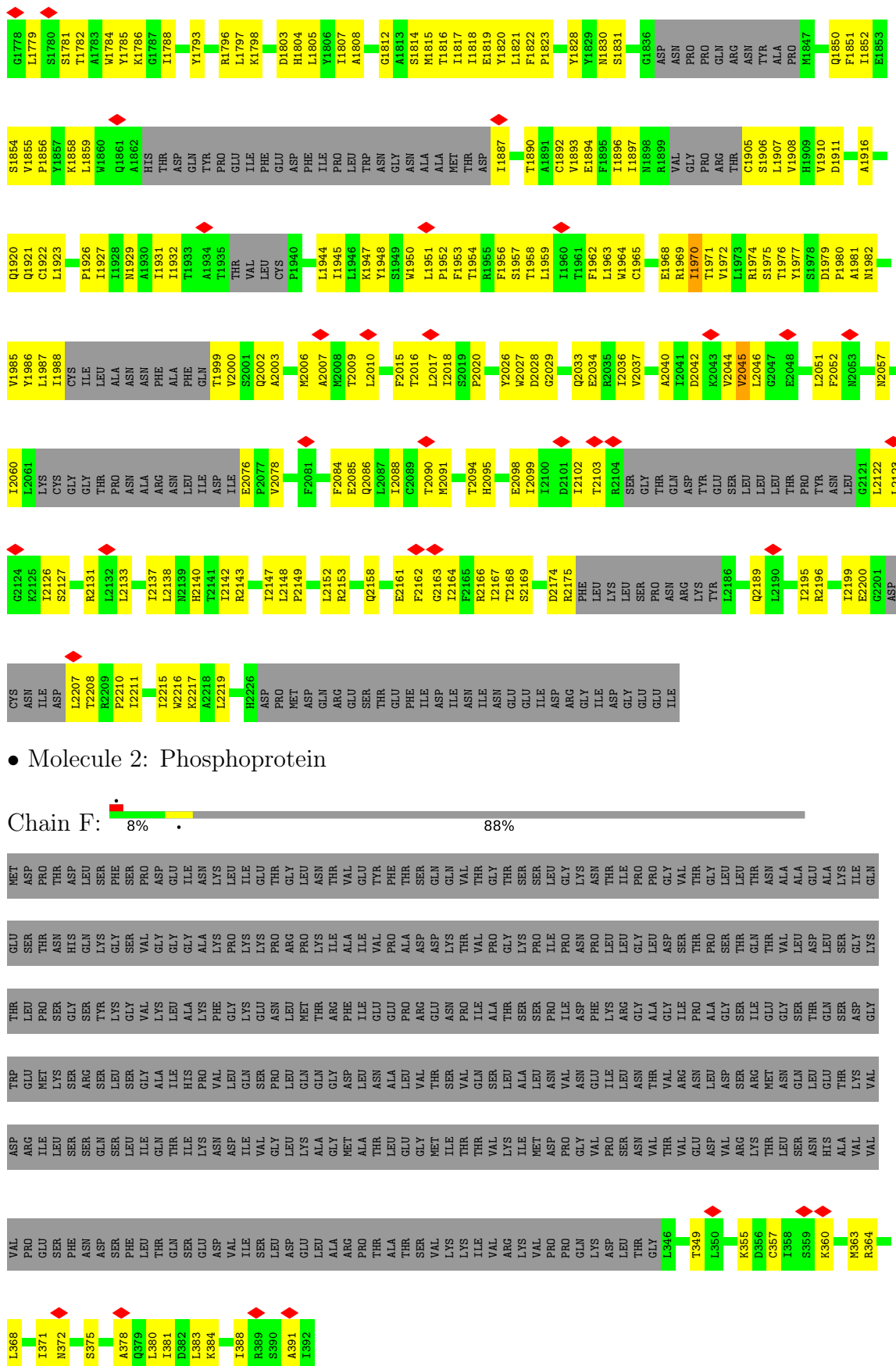
3 Residue-property plots

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: RNA-directed RNA polymerase L



SER	LEU	LYS	THR	PRO	HIS	VAL	PRO	GLY	THR	SER	CYS	ILE	GLU	ASP	ASP	SER	LEU	C1731	T1732	T1733	T1734	Y1735	W1738	I1739	I1740	VAL	E1741	ASN	PRO	ARG	LEU	A1673	A1674	F1675	Y1676	I1677	I1678	T1682	L1683	R1684	L1685	L1686	I1687	I1690	R1691	A1699	V1700	T1701	SER	TYR	TYR	GLU	SER	LEU	GLU	TYR	ILE	ASP
D1564	Y1565	I1566	K1578	I1581	N1582	V1583	S1585	G1588	D1589	L1590	E1591	L1592	V1593	V1594	SER	GLU	ASP	SER	LEU	ASN	VAL	GLU	ASN	R1605	S1606	M1607	N1608	L1609	I1610	A1611	R1612	K1613	L1614	T1615	L1616	L1617	S1618	L1619	I1620	H1621	L1625	E1626	L1627	P1628	K1629	I1630	K1631	G1632	F1633	S1634	P1635	D1636	E1637					
L1487	F1488	M1489	Y1490	W1493	E1494	L1497	S1500	Y1501	Q1502	M1503	Y1504	Y1505	L1506	R1507	V1508	T1509	G1510	W1511	S1512	N1513	I1514	V1515	D1516	M1520	R1523	R1524	M1606	M1607	N1608	L1609	I1610	A1611	R1612	K1613	L1614	T1615	L1616	L1617	S1618	L1619	I1620	H1621	L1625	E1626	L1627	P1628	K1629	I1630	K1631	G1632	F1633	S1634	P1635	D1636	E1637			
SER	PHE	GLN	ALA	GLN	GLY	ASN	ASP	VAL	ASP	THR	THR	T1438	Q1442	F1443	T1444	A1445	R1446	I1449	M1450	A1451	I1452	T1453	GLY	LEU	ASP	GLU	VAL	ILE	VAL	ALA	SER	THR	ASN	ASP	ALA	ILE	VAL	PHE	ASP	GLU	ASP	PRO	LEU	SER	GLU	TYR	VAL	ASN	TRP	I1476	S1477	E1478	C1479	M1480	Y1481	E1486		
G1344	L1345	I1356	N1357	R1358	T1359	F1360	S1363	H1366	L1367	H1368	T1369	C1373	C1374	L1375	R1376	D1379	L1383	E1384	I1385	A1386	V1389	K1390	P1391	H1392	I1393	L1394	V1395	Y1396	Y1397	SER	ASN	LYS	PHE	VAL	PHE	ASP	GLU	ASP	PRO	LEU	SER	GLU	TYR	GLU	THR	ALA	LYS	LEU	SER	LEU	SER	LEU						
I1250	W1251	A1252	F1253	E1258	R1270	W1271	N1272	L1275	E1276	Q1277	L1278	P1285	T1286	S1287	A1288	H1292	R1293	L1294	D1295	D1296	G1297	T1298	T1299	W1214	L1300	L1301	K1302	F1303	T1304	P1305	A1306	S1307	S1308	F1311	S1312	S1313	S1318	N1319	D1320	E1321	Q1322	Y1323	L1324	T1325	D1328	K1329	T1330	A1331	S1332	M1334								
E1162	D1165	E1168	G1172	V1176	Y1180	Q1183	C1184	ALA	ALA	GLY	ASP	ASN	ARG	F1191	T1192	W1193	F1194	S1198	G1203	P1206	M1209	R1213	W1214	P1215	Y1216	S1219	R1220	E1223	R1224	R1225	VAL	ALA	SER	MET	ALA	Y1231	I1232	R1233	G1234	A1235	S1236	L1239	L1243	R1244														
T1067	S1068	Q1076	K1088	S1089	L1090	I1092	K1093	P1094	L1095	S1096	K1099	E1102	I1103	L1104	D1105	Y1106	N1107	I1108	N1109	Y1110	L1111	N1114	L1118	K1119	N1120	A1121	I1122	E1123	P1124	Y1127	L1128	K1129	A1130	M1131	T1132	L1133	E1134	T1135	C1136	S1137	N1143	W1149	P1151	L1152	L1153	G1160	L1161											
N980	L981	K985	P986	Q987	W991	A992	F993	P998	Y999	S1000	I1001	N1002	Y1005	P1009	T1010	R1015	H1016	T1017	Q1018	M1022	P1028	M1029	L1030	R1031	G1032	I1033	F1034	S1035	D1036	N1043	H1044	L1045	F1048	L1049	L1050	D1051	R1052	E1053	V1054	P1055	F1056	P1057	R1058	V1059	I1062	I1063												
Y894	M895	K898	Q899	L900	S901	Y902	I905	Q908	I911	P912	Q913	D914	Q915	T917	L918	E919	Y920	I921	N922	L930	S935	Q936	L937	L940	N941	Y942	L943	S944	C945	R946	R947	L948	F949	N950	R951	N952	D955	P956	V957	V958	V961	L967	K985	D886	I887	C888	L891											
E820	Q821	E822	T823	I824	I825	S826	S827	H828	F829	F830	V831	R835	I836	F837	T844	Q845	A846	L847	K848	Y849	A850	L853	C854	L855	V859	L860	G861	E862	C863	T864	Q865	S866	S867	C868	S869	N870	L871	A872	V875	M876	R877	L878	T879	E880	V883	E884	K885	D886	I887	C888	L891							
I732	P735	ARG	GLY	G738	I739	S740	E741	L742	C743	Q744	K745	A746	L747	T748	S751	I752	A753	L754	I755	L756	L757	S758	M767	S768	M769	G772	D773	N774	Q775	T781	R782	V783	L790	E791	K792	R793	T794	I795	A796	F797	C800	L807	N810	N811	G815	H816	H817	L818	K819									



● Molecule 2: Phosphoprotein



LYS MET ARG GLU GLU TYR LEU LEU LYS ILE	PRO	GLU	D241	THR	GLU	TRP	THR	GLU	ASP	MET	THR	GLU	ASP	THR	ASN	GLY	THR	GLN	LYS	LEU	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY
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● Molecule 2: Phosphoprotein



LYS	MET	ARG	GLU	TYR	LEU	LEU	LEU	LYS	ILE	ASN	GLN	GLU	ALA	SER	ASP	VAL	ILE	GLU	SER	GLY	ALA	ASN	LYS	LEU	ILE	GLY	THR	GLY	LEU	THR	ASN	GLY	ALA	GLU	ALA	LYS	ILE	GLN																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
PRO	GLU	SER	PHE	ASN	ASP	SER	PHE	LEU	LYS	THR	GLN	GLU	ALA	SER	ASP	VAL	ILE	GLU	ASP	GLY	ALA	ASN	LYS	LEU	ILE	GLY	THR	GLY	LEU	THR	ASN	GLY	ALA	GLU	ALA	LYS	ILE	GLN																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
R242	I243	L244	S245	S246	Q247	S248	L249	T250	Q251	T252	I253	K254	N255	D256	I257	V258	L260	K261	A262	G263	M264	T266	L267	E268	G269	M270	I271	THR	THR	VAL	PRO	PRO	GLN	LYS	ASP	MET	ASP	PRO	GLY	VAL	PRO	GLN	LYS	ILE	ARG	VAL	PRO	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR	GLY	LEU	THR</

● Molecule 2: Phosphoprotein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	102493	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.091	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	403.2, 403.2, 403.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.31	0/15514	0.56	5/21035 (0.0%)
2	B	0.32	0/575	0.52	0/776
2	C	0.25	0/588	0.46	0/794
2	D	0.28	0/575	0.44	0/776
2	E	0.28	0/588	0.49	0/794
2	F	0.19	0/375	0.33	0/498
All	All	0.30	0/18215	0.55	5/24673 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1374	CYS	CA-C-N	7.14	129.97	122.97
1	A	1374	CYS	C-N-CA	7.14	129.97	122.97
1	A	1375	VAL	O-C-N	6.71	126.95	121.85
1	A	2045	VAL	N-CA-C	-5.32	106.33	112.98
1	A	1375	VAL	N-CA-C	-5.26	106.53	111.48

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	15200	0	15373	750	0
2	B	569	0	600	25	0
2	C	582	0	611	20	0
2	D	569	0	600	18	0
2	E	582	0	611	26	0
2	F	374	0	414	12	0
3	A	2	0	0	0	0
All	All	17878	0	18209	809	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 22.

All (809) 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:A:410:TYR:CE1	1:A:414:HIS:HD2	1.32	1.48
1:A:1950:TRP:CE3	1:A:1956:PHE:CE1	2.16	1.33
1:A:1950:TRP:HE3	1:A:1956:PHE:CD1	1.47	1.31
1:A:410:TYR:CE1	1:A:414:HIS:CD2	2.17	1.29
1:A:1746:LEU:HB3	1:A:1748:LYS:NZ	1.50	1.25
2:E:266:THR:HG22	2:E:270:MET:HE2	1.15	1.15
1:A:1950:TRP:CZ3	1:A:1956:PHE:CE1	2.36	1.13
1:A:1793:TYR:OH	1:A:1971:THR:HG21	1.46	1.13
1:A:1476:ILE:N	1:A:1535:SER:HG	1.45	1.12
1:A:1184:CYS:HA	1:A:1368:HIS:HE1	1.17	1.09
1:A:410:TYR:CZ	1:A:414:HIS:CD2	2.40	1.08
1:A:418:TRP:HB2	1:A:419:PRO:HD2	1.31	1.07
1:A:1950:TRP:CE3	1:A:1956:PHE:CD1	2.37	1.05
2:B:264:MET:HE1	2:C:263:GLY:C	1.83	1.04
1:A:1950:TRP:HE3	1:A:1956:PHE:CE1	1.64	1.04
1:A:1746:LEU:HB3	1:A:1748:LYS:HZ2	1.01	1.03
2:D:264:MET:HE1	2:E:263:GLY:C	1.83	1.03
1:A:2208:THR:HG23	1:A:2211:ILE:HG12	1.43	1.01
1:A:2208:THR:CG2	1:A:2211:ILE:CG1	2.38	1.01
1:A:1191:PHE:HB2	1:A:1321:GLU:HB2	1.45	0.99
1:A:1954:THR:O	1:A:1958:THR:HG23	1.63	0.99
2:E:266:THR:CG2	2:E:270:MET:HE2	1.94	0.98
1:A:418:TRP:CB	1:A:419:PRO:HD2	1.94	0.96
1:A:2208:THR:HG23	1:A:2211:ILE:CG1	1.95	0.95
2:C:268:GLU:HG2	2:D:267:LEU:HD11	1.49	0.95
2:B:267:LEU:HD11	2:E:268:GLU:HG2	1.49	0.94
1:A:1184:CYS:HA	1:A:1368:HIS:CE1	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:TRP:CB	1:A:419:PRO:CD	2.46	0.93
2:B:264:MET:HE1	2:C:263:GLY:CA	1.99	0.93
2:D:264:MET:HE1	2:E:263:GLY:CA	1.99	0.93
1:A:410:TYR:OH	1:A:414:HIS:CD2	2.22	0.92
2:E:266:THR:HG22	2:E:270:MET:CE	2.00	0.91
1:A:2208:THR:CG2	1:A:2211:ILE:HG13	2.01	0.90
1:A:1191:PHE:HB2	1:A:1321:GLU:CB	2.02	0.89
1:A:422:ASN:HA	1:A:453:VAL:CG2	2.01	0.89
1:A:422:ASN:OD1	1:A:453:VAL:CG2	2.20	0.88
2:D:264:MET:HE1	2:E:263:GLY:HA3	1.55	0.88
1:A:422:ASN:C	1:A:453:VAL:HG23	1.99	0.86
1:A:2208:THR:CG2	1:A:2211:ILE:HG12	2.03	0.86
1:A:830:PHE:HB3	1:A:837:PHE:HB2	1.56	0.86
2:B:264:MET:HE1	2:C:263:GLY:HA3	1.55	0.86
1:A:422:ASN:OD1	1:A:453:VAL:HG21	1.75	0.85
1:A:1743:ASN:O	1:A:1743:ASN:ND2	2.08	0.85
1:A:1193:TRP:NE1	1:A:1318:SER:OG	2.09	0.85
1:A:410:TYR:HE1	1:A:414:HIS:CD2	1.74	0.85
1:A:422:ASN:HA	1:A:453:VAL:HG21	1.58	0.84
1:A:422:ASN:O	1:A:453:VAL:HG23	1.77	0.83
1:A:361:CYS:HB2	1:A:848:LYS:HB2	1.58	0.83
1:A:1808:ALA:H	1:A:1830:ASN:HB3	1.44	0.82
1:A:1746:LEU:CB	1:A:1748:LYS:HZ2	1.90	0.82
1:A:1793:TYR:HH	1:A:1971:THR:HG21	1.39	0.82
1:A:417:VAL:HG23	1:A:437:ASP:OD2	1.80	0.81
1:A:1765:LYS:NZ	1:A:1982:ASN:O	2.13	0.81
1:A:99:PRO:HB3	1:A:102:LYS:HB2	1.63	0.81
1:A:417:VAL:HA	1:A:437:ASP:OD2	1.80	0.81
1:A:1660:LEU:O	1:A:1663:PHE:HB2	1.82	0.80
1:A:1746:LEU:O	1:A:1748:LYS:HD2	1.81	0.80
1:A:418:TRP:HB2	1:A:419:PRO:CD	2.07	0.80
1:A:69:PHE:O	1:A:73:HIS:HB2	1.83	0.80
1:A:1193:TRP:NE1	1:A:1318:SER:HG	1.80	0.80
1:A:100:ASP:HB2	1:A:222:LEU:HD11	1.64	0.79
1:A:831:VAL:HG22	1:A:836:ILE:HG22	1.64	0.79
1:A:1746:LEU:CB	1:A:1748:LYS:NZ	2.41	0.79
1:A:1963:LEU:HD23	1:A:1987:LEU:HD21	1.65	0.79
1:A:1054:VAL:H	1:A:1383:LEU:HD13	1.47	0.79
1:A:457:LYS:H	1:A:685:ARG:HG2	1.48	0.78
1:A:1180:TYR:OH	1:A:1922:CYS:HB3	1.82	0.78
1:A:1476:ILE:N	1:A:1535:SER:OG	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:SER:HB2	1:A:564:LYS:HG3	1.64	0.78
1:A:961:VAL:HG23	1:A:1137:SER:HB3	1.65	0.78
1:A:476:ASP:HB2	1:A:515:LEU:HB2	1.66	0.78
1:A:1656:SER:OG	1:A:1659:ASN:ND2	2.17	0.78
1:A:1950:TRP:CZ3	1:A:1956:PHE:HE1	2.02	0.77
1:A:410:TYR:HH	1:A:414:HIS:CD2	2.01	0.77
1:A:1963:LEU:CD2	1:A:1987:LEU:CD2	2.63	0.77
1:A:2189:GLN:HA	1:A:2195:ILE:HD11	1.65	0.77
1:A:410:TYR:HE1	1:A:414:HIS:HD2	0.83	0.76
1:A:251:ILE:HG21	1:A:362:ILE:HG21	1.65	0.76
1:A:206:ILE:HB	1:A:213:ILE:HB	1.68	0.76
1:A:51:GLN:O	1:A:55:GLU:HB2	1.85	0.75
1:A:419:PRO:HG2	1:A:422:ASN:HB2	1.68	0.75
1:A:1793:TYR:OH	1:A:1971:THR:CG2	2.31	0.75
1:A:1816:THR:HG23	1:A:1817:ILE:HD12	1.66	0.75
1:A:302:GLN:NE2	1:A:310:LEU:O	2.20	0.75
1:A:1446:ARG:NH1	1:A:1593:VAL:O	2.20	0.75
1:A:525:ASP:HB3	1:A:528:VAL:HG12	1.69	0.74
1:A:1501:TYR:HB2	1:A:1614:LEU:HG	1.68	0.74
1:A:1950:TRP:HB3	1:A:1956:PHE:CG	2.23	0.74
1:A:1784:TRP:HB2	1:A:1817:ILE:HD13	1.70	0.74
1:A:1920:GLN:NE2	1:A:1922:CYS:SG	2.61	0.74
1:A:398:THR:HG23	1:A:679:PHE:HZ	1.53	0.73
1:A:1963:LEU:CD2	1:A:1987:LEU:HD21	2.18	0.73
1:A:1300:THR:HG22	1:A:1301:LEU:H	1.52	0.73
1:A:1746:LEU:HB3	1:A:1748:LYS:HZ3	1.53	0.73
1:A:421:LEU:N	1:A:421:LEU:HD12	2.02	0.73
1:A:602:LYS:NZ	1:A:1215:PRO:O	2.21	0.73
1:A:1534:ALA:HB2	1:A:1760:ASN:HB2	1.69	0.73
1:A:2208:THR:HG21	1:A:2211:ILE:HG13	1.69	0.73
1:A:1803:ASP:H	1:A:1906:SER:HB3	1.53	0.72
1:A:1950:TRP:CE3	1:A:1956:PHE:CZ	2.75	0.72
1:A:1926:PRO:HG2	1:A:1962:PHE:HE1	1.55	0.72
1:A:2158:GLN:O	1:A:2161:GLU:C	2.33	0.72
1:A:2166:ARG:HH22	1:A:2200:GLU:HA	1.55	0.71
1:A:426:ASN:ND2	2:B:259:GLY:HA2	2.04	0.71
1:A:346:SER:O	1:A:349:GLN:NE2	2.23	0.71
1:A:422:ASN:OD1	1:A:453:VAL:HB	1.90	0.71
1:A:1446:ARG:HH12	1:A:1594:VAL:HA	1.55	0.71
1:A:418:TRP:HB3	1:A:419:PRO:CD	2.19	0.71
1:A:1659:ASN:O	1:A:1663:PHE:N	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2208:THR:HG21	1:A:2211:ILE:CG1	2.21	0.70
1:A:411:ARG:HH12	1:A:415:HIS:HA	1.56	0.70
1:A:422:ASN:OD1	1:A:453:VAL:CB	2.40	0.70
1:A:1616:LEU:HD13	1:A:1642:LEU:HG	1.71	0.70
1:A:332:PHE:HB3	1:A:336:GLU:HB3	1.74	0.69
1:A:1950:TRP:HZ3	1:A:1956:PHE:CE1	2.03	0.69
1:A:1856:PRO:HA	1:A:1859:LEU:HB3	1.72	0.69
1:A:130:GLN:NE2	1:A:134:ASN:OD1	2.25	0.69
1:A:2207:LEU:HD12	1:A:2207:LEU:N	2.07	0.69
1:A:2164:ILE:HB	1:A:2207:LEU:HG	1.73	0.69
1:A:998:PRO:HB3	1:A:1057:PRO:HB2	1.74	0.69
2:B:267:LEU:CD1	2:E:268:GLU:HG2	2.22	0.69
1:A:410:TYR:OH	1:A:414:HIS:NE2	2.25	0.68
1:A:1950:TRP:HZ3	1:A:1956:PHE:HE1	1.38	0.68
1:A:78:ARG:NH2	1:A:79:LYS:O	2.26	0.68
1:A:994:LEU:HD22	1:A:1050:LEU:HD21	1.76	0.68
1:A:1948:TYR:CE2	1:A:1959:LEU:HD22	2.29	0.68
1:A:401:PHE:HA	1:A:404:THR:HG22	1.76	0.68
1:A:1592:LEU:HD22	1:A:1615:THR:HG21	1.73	0.68
1:A:1775:ARG:HD3	1:A:1782:THR:HB	1.76	0.68
1:A:2006:MET:O	1:A:2009:THR:OG1	2.12	0.68
1:A:206:ILE:HG22	1:A:208:ASN:HD22	1.59	0.67
1:A:1963:LEU:HD22	1:A:1987:LEU:CD2	2.23	0.67
2:C:268:GLU:HG2	2:D:267:LEU:CD1	2.22	0.67
1:A:1613:LYS:NZ	1:A:1634:SER:O	2.28	0.67
1:A:1963:LEU:HD22	1:A:1987:LEU:HD23	1.77	0.67
1:A:1972:VAL:HG22	1:A:1985:VAL:HG22	1.76	0.67
1:A:827:SER:OG	1:A:828:HIS:ND1	2.28	0.67
1:A:294:GLU:HA	1:A:363:MET:HE1	1.75	0.66
1:A:1379:ASP:HB3	1:A:2127:SER:HB3	1.77	0.66
1:A:2166:ARG:NH2	1:A:2200:GLU:OE1	2.28	0.66
1:A:426:ASN:HB3	2:B:258:VAL:HG12	1.78	0.66
1:A:1120:ASN:ND2	1:A:1121:ALA:O	2.28	0.66
1:A:1564:ASP:OD1	1:A:1565:TYR:N	2.29	0.66
1:A:29:LEU:HD23	1:A:63:LEU:HD12	1.78	0.66
1:A:1581:ILE:HD13	1:A:1584:LEU:HD12	1.76	0.66
1:A:1784:TRP:HE1	1:A:2057:ASN:ND2	1.94	0.66
1:A:12:VAL:O	1:A:13:HIS:ND1	2.29	0.66
1:A:1533:LEU:HD22	1:A:1566:ILE:HA	1.77	0.66
1:A:251:ILE:HG13	1:A:362:ILE:HD12	1.77	0.65
1:A:1963:LEU:CD2	1:A:1987:LEU:HD23	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:MET:HB3	1:A:507:PRO:HA	1.78	0.65
1:A:1784:TRP:HE1	1:A:2057:ASN:HD21	1.43	0.65
1:A:961:VAL:CG2	1:A:1137:SER:HB3	2.26	0.65
1:A:1746:LEU:O	1:A:1748:LYS:CD	2.43	0.65
1:A:1319:ASN:HB3	1:A:1762:HIS:HB3	1.77	0.65
1:A:2164:ILE:HD12	1:A:2164:ILE:H	1.62	0.65
1:A:13:HIS:HA	1:A:239:LEU:HD21	1.79	0.64
1:A:418:TRP:CZ2	1:A:438:ASN:O	2.50	0.64
1:A:169:HIS:O	1:A:174:LYS:NZ	2.28	0.64
1:A:1805:LEU:O	1:A:1908:VAL:HA	1.97	0.64
2:B:264:MET:CE	2:C:263:GLY:C	2.68	0.64
1:A:807:LEU:O	1:A:811:ASN:ND2	2.24	0.64
1:A:696:ILE:HG13	1:A:697:HIS:H	1.63	0.64
1:A:914:ASP:OD1	1:A:915:GLN:N	2.31	0.64
1:A:1184:CYS:CA	1:A:1368:HIS:HE1	2.04	0.64
1:A:1633:PHE:HB3	1:A:1635:PRO:HD2	1.80	0.64
1:A:423:LEU:HG	1:A:431:LEU:HA	1.80	0.63
1:A:936:GLN:HG2	1:A:956:PRO:HB2	1.80	0.63
1:A:2046:LEU:HD13	1:A:2153:ARG:HH22	1.63	0.63
1:A:305:ASP:OD1	1:A:311:ARG:NH2	2.22	0.63
1:A:1818:ILE:O	1:A:1822:PHE:N	2.31	0.63
1:A:597:GLN:NE2	1:A:1303:PHE:O	2.28	0.63
1:A:422:ASN:CA	1:A:453:VAL:CG2	2.74	0.63
1:A:1972:VAL:HB	1:A:1987:LEU:HD12	1.81	0.63
1:A:137:TYR:HD1	1:A:141:GLY:HA2	1.63	0.63
1:A:866:SER:O	1:A:869:SER:HB3	1.99	0.63
1:A:361:CYS:SG	1:A:848:LYS:N	2.71	0.63
1:A:916:ILE:HD11	1:A:1108:ILE:HG23	1.80	0.62
1:A:11:GLU:O	1:A:188:ARG:NH1	2.32	0.62
1:A:297:VAL:HB	1:A:360:LEU:HD12	1.80	0.62
1:A:420:PRO:HB2	1:A:421:LEU:HD12	1.80	0.62
1:A:1605:ARG:HG3	1:A:1608:ASN:HD21	1.63	0.62
1:A:204:THR:HG22	1:A:215:ILE:HB	1.81	0.62
1:A:299:ALA:HB2	1:A:314:PHE:HD2	1.65	0.62
1:A:431:LEU:HG	1:A:435:MET:HE3	1.81	0.62
1:A:875:VAL:O	1:A:879:THR:HG23	2.00	0.62
1:A:1198:SER:OG	1:A:1358:ARG:NH2	2.33	0.62
1:A:861:GLY:HA3	1:A:1010:THR:HB	1.82	0.62
1:A:1134:GLU:H	1:A:1134:GLU:CD	2.08	0.62
1:A:976:TRP:O	1:A:980:ASN:ND2	2.33	0.61
1:A:1999:THR:HG22	1:A:2000:VAL:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1613:LYS:HE3	1:A:1639:CYS:N	2.14	0.61
1:A:1948:TYR:CD2	1:A:1959:LEU:CD2	2.83	0.61
1:A:1830:ASN:OD1	1:A:1831:SER:N	2.33	0.61
1:A:411:ARG:HG2	1:A:439:THR:HA	1.82	0.61
1:A:1771:HIS:CE1	1:A:1775:ARG:HH12	2.18	0.61
1:A:301:LEU:HG	1:A:829:PHE:HE1	1.66	0.61
1:A:516:LEU:HD11	1:A:1088:LYS:HG2	1.83	0.61
1:A:658:SER:HA	1:A:827:SER:HA	1.82	0.61
1:A:468:GLU:OE2	1:A:582:ASN:ND2	2.33	0.61
1:A:835:ARG:NH2	1:A:1304:THR:O	2.33	0.61
1:A:2076:GLU:HG3	1:A:2078:VAL:HG23	1.82	0.61
1:A:422:ASN:CA	1:A:453:VAL:HG23	2.30	0.61
1:A:98:ILE:HG13	1:A:99:PRO:HD2	1.82	0.60
1:A:1446:ARG:O	1:A:1450:ASN:HB2	2.01	0.60
2:B:270:MET:O	2:B:270:MET:HG2	2.01	0.60
1:A:1805:LEU:HG	1:A:1908:VAL:HG13	1.83	0.60
1:A:410:TYR:O	1:A:414:HIS:HB2	2.02	0.60
1:A:362:ILE:HD11	1:A:847:LEU:HB3	1.84	0.60
1:A:411:ARG:NH1	1:A:415:HIS:HA	2.16	0.60
1:A:1172:GLY:HA2	1:A:1367:LEU:HA	1.84	0.60
1:A:1481:TYR:OH	1:A:2161:GLU:O	2.15	0.60
1:A:864:THR:O	1:A:867:SER:OG	2.15	0.60
1:A:2095:HIS:CG	1:A:2133:LEU:HD13	2.37	0.60
1:A:1028:PRO:O	1:A:1030:LEU:N	2.35	0.59
1:A:1746:LEU:HD13	1:A:1748:LYS:HZ1	1.67	0.59
1:A:66:VAL:HG13	1:A:214:ILE:HG21	1.83	0.59
1:A:1779:LEU:O	1:A:2217:LYS:NZ	2.28	0.59
1:A:1950:TRP:O	1:A:1982:ASN:ND2	2.32	0.59
1:A:165:VAL:HG23	1:A:894:TYR:HE2	1.68	0.59
1:A:486:TRP:HA	1:A:489:VAL:HG12	1.85	0.59
1:A:943:LEU:HB3	1:A:947:ARG:HB2	1.84	0.59
1:A:1974:ARG:HA	1:A:1985:VAL:HG23	1.83	0.59
1:A:1544:ARG:NH1	1:A:2034:GLU:OE2	2.36	0.59
1:A:1975:SER:O	1:A:2033:GLN:NE2	2.23	0.59
1:A:421:LEU:HD12	1:A:421:LEU:H	1.67	0.59
1:A:1000:SER:O	1:A:1149:TRP:NE1	2.35	0.59
1:A:1750:PRO:HG3	1:A:2015:PHE:HA	1.85	0.58
1:A:2138:LEU:HD21	1:A:2215:ILE:HG21	1.84	0.58
1:A:1127:TYR:HA	1:A:1130:ALA:HB3	1.85	0.58
1:A:1331:ALA:HA	1:A:1334:ASN:HB2	1.84	0.58
1:A:1538:SER:HB2	1:A:1763:ASN:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:PHE:CE2	1:A:359:LEU:HD22	2.39	0.58
1:A:113:TRP:CZ2	1:A:902:TYR:HB2	2.39	0.58
1:A:399:LEU:HD22	1:A:678:PRO:HB3	1.85	0.58
2:B:253:ILE:HG23	2:E:257:ILE:CD1	2.33	0.58
2:C:257:ILE:CD1	2:D:253:ILE:HG23	2.33	0.58
1:A:671:TRP:HB3	1:A:676:ILE:HD11	1.85	0.58
1:A:1561:ALA:HB3	1:A:1751:ILE:HG12	1.85	0.58
1:A:397:LYS:HG2	1:A:450:TRP:HZ3	1.69	0.58
1:A:418:TRP:HZ2	1:A:438:ASN:O	1.85	0.58
1:A:297:VAL:HG21	1:A:360:LEU:HB2	1.86	0.58
1:A:950:ASN:OD1	1:A:952:ASN:ND2	2.30	0.58
1:A:2028:ASP:OD1	1:A:2029:GLY:N	2.37	0.57
1:A:2158:GLN:O	1:A:2161:GLU:O	2.22	0.57
2:D:264:MET:CE	2:E:263:GLY:C	2.68	0.57
1:A:590:GLU:O	1:A:768:SER:OG	2.17	0.57
1:A:1615:THR:O	1:A:1618:SER:OG	2.19	0.57
1:A:411:ARG:HD3	1:A:418:TRP:CD1	2.40	0.57
1:A:485:ASP:O	1:A:488:SER:OG	2.20	0.57
1:A:528:VAL:HG23	1:A:531:GLN:HE21	1.70	0.57
1:A:10:PRO:HB2	1:A:188:ARG:HH12	1.69	0.57
1:A:1911:ASP:OD1	1:A:1911:ASP:N	2.35	0.57
1:A:294:GLU:OE2	1:A:364:ARG:HB2	2.05	0.56
1:A:18:ILE:HG23	1:A:370:MET:HA	1.88	0.56
1:A:392:PHE:CE2	2:B:270:MET:HB2	2.40	0.56
1:A:478:ALA:O	1:A:570:ARG:NH1	2.38	0.56
1:A:1034:PHE:HD1	1:A:1076:GLN:HE22	1.52	0.56
1:A:1209:ASN:OD1	1:A:1213:ARG:NH2	2.36	0.56
1:A:1582:ASN:O	1:A:1585:SER:HB3	2.05	0.56
1:A:1971:THR:O	1:A:1988:ILE:HG23	2.05	0.56
1:A:261:LEU:HG	1:A:262:ASN:H	1.70	0.56
1:A:310:LEU:HD13	1:A:826:SER:HA	1.87	0.56
1:A:578:SER:O	1:A:582:ASN:HB2	2.05	0.56
1:A:662:THR:OG1	1:A:775:GLN:NE2	2.38	0.56
1:A:1687:LEU:O	1:A:1690:ILE:HG22	2.05	0.56
1:A:1739:ILE:HG22	1:A:1740:ILE:HG23	1.86	0.56
1:A:1820:TYR:HB2	1:A:2060:ILE:HD12	1.87	0.56
1:A:2051:LEU:HG	1:A:2052:PHE:H	1.71	0.56
1:A:31:ASN:HB2	1:A:67:ARG:HD3	1.88	0.56
2:F:378:ALA:HA	2:F:381:ILE:HD12	1.88	0.56
1:A:758:SER:OG	1:A:810:ASN:ND2	2.36	0.56
1:A:1892:CYS:O	1:A:1896:ILE:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1927:ILE:O	1:A:1931:ILE:HG12	2.05	0.56
1:A:1950:TRP:HB3	1:A:1956:PHE:CB	2.35	0.56
1:A:418:TRP:HB3	1:A:419:PRO:HD3	1.86	0.56
1:A:1741:GLU:HA	1:A:1969:ARG:H	1.71	0.56
1:A:739:ILE:HG21	1:A:742:LEU:HB2	1.86	0.56
1:A:1180:TYR:OH	1:A:1922:CYS:CB	2.52	0.56
1:A:1180:TYR:HH	1:A:1922:CYS:HB3	1.70	0.56
1:A:1250:ILE:HG23	1:A:1252:ALA:H	1.71	0.56
1:A:1781:SER:OG	1:A:1812:GLY:O	2.24	0.56
2:F:355:LYS:HA	2:F:364:ARG:HH12	1.70	0.56
2:D:253:ILE:O	2:D:257:ILE:HG13	2.06	0.56
1:A:54:HIS:O	1:A:54:HIS:ND1	2.36	0.56
1:A:591:ASN:ND2	1:A:768:SER:OG	2.39	0.56
1:A:864:THR:H	1:A:1107:ASN:HD21	1.53	0.56
1:A:1206:PRO:HA	1:A:1213:ARG:HH21	1.71	0.56
1:A:1595:THR:HA	1:A:1676:ALA:HB3	1.88	0.56
1:A:169:HIS:ND1	1:A:170:ASP:OD1	2.36	0.55
1:A:544:PHE:HD2	1:A:699:ARG:HH11	1.53	0.55
1:A:1050:LEU:O	1:A:1055:ILE:HG21	2.06	0.55
1:A:991:TRP:CD2	1:A:1152:LEU:HD21	2.42	0.55
1:A:1442:GLN:HG2	1:A:1490:TYR:CE2	2.41	0.55
1:A:2095:HIS:ND1	1:A:2133:LEU:HB2	2.21	0.55
1:A:1134:GLU:OE1	1:A:1134:GLU:N	2.22	0.55
1:A:1852:ILE:HA	1:A:1856:PRO:HG2	1.88	0.55
1:A:1855:VAL:HA	1:A:1858:LYS:HE2	1.88	0.55
1:A:1890:THR:HA	1:A:1893:VAL:HG12	1.88	0.55
1:A:1815:MET:HA	1:A:1818:ILE:HD13	1.88	0.55
1:A:1971:THR:H	1:A:1988:ILE:HG12	1.70	0.55
1:A:2086:GLN:O	1:A:2090:THR:HG23	2.06	0.55
1:A:456:ILE:HB	1:A:685:ARG:NH1	2.22	0.55
1:A:216:THR:OG1	1:A:219:LEU:N	2.40	0.55
1:A:662:THR:HG22	1:A:823:THR:HG22	1.88	0.55
1:A:1153:LEU:HD23	1:A:1153:LEU:H	1.70	0.55
1:A:62:ARG:O	1:A:66:VAL:HG23	2.07	0.55
1:A:864:THR:H	1:A:1107:ASN:ND2	2.05	0.55
1:A:695:TRP:HD1	1:A:698:LEU:HD12	1.72	0.54
1:A:781:THR:OG1	1:A:782:ARG:N	2.40	0.54
2:B:253:ILE:O	2:B:257:ILE:HG13	2.06	0.54
1:A:1052:ARG:HG3	1:A:1385:GLU:HG2	1.89	0.54
1:A:1735:TYR:HB2	1:A:1974:ARG:HH12	1.71	0.54
1:A:671:TRP:CH2	1:A:747:TRP:HA	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1191:PHE:HB2	1:A:1321:GLU:HB3	1.89	0.54
1:A:1765:LYS:HG3	1:A:1981:ALA:HB1	1.90	0.54
1:A:1803:ASP:OD1	1:A:1804:HIS:N	2.40	0.54
1:A:1830:ASN:HD22	1:A:1896:ILE:HD11	1.72	0.54
1:A:2196:ARG:O	1:A:2200:GLU:HG2	2.08	0.54
1:A:985:LYS:HD3	1:A:986:PRO:HD2	1.88	0.54
1:A:1180:TYR:CB	1:A:1887:ILE:HG23	2.37	0.54
1:A:1750:PRO:HA	1:A:2017:LEU:HD13	1.89	0.54
1:A:1357:ASN:HB3	1:A:1359:THR:HG23	1.89	0.54
2:C:257:ILE:HD13	2:D:253:ILE:HG23	1.90	0.54
1:A:27:ILE:HG13	1:A:28:LEU:HD12	1.89	0.54
1:A:341:THR:O	1:A:345:ILE:HG12	2.08	0.54
1:A:886:ASP:OD1	1:A:887:ILE:N	2.41	0.54
1:A:1807:ILE:HB	1:A:1910:VAL:HG12	1.89	0.54
1:A:426:ASN:OD1	1:A:426:ASN:N	2.26	0.54
1:A:696:ILE:HG13	1:A:697:HIS:N	2.23	0.54
1:A:826:SER:OG	1:A:827:SER:N	2.39	0.54
1:A:1500:SER:O	1:A:1503:MET:HB2	2.07	0.54
1:A:1971:THR:HG22	1:A:1988:ILE:HD13	1.90	0.54
1:A:300:GLN:HG2	1:A:348:PHE:HB3	1.90	0.53
1:A:811:ASN:O	1:A:815:GLY:N	2.41	0.53
1:A:1639:CYS:O	1:A:1643:THR:HG23	2.08	0.53
1:A:1740:ILE:CD1	1:A:1740:ILE:N	2.72	0.53
1:A:1968:GLU:N	1:A:1968:GLU:OE1	2.41	0.53
1:A:1613:LYS:HE3	1:A:1639:CYS:H	1.73	0.53
1:A:1743:ASN:HD22	1:A:1743:ASN:C	2.07	0.53
1:A:158:ASP:OD1	1:A:159:ILE:N	2.42	0.53
1:A:817:HIS:HB3	1:A:819:LYS:HE2	1.91	0.53
1:A:219:LEU:HD11	1:A:232:TYR:HB3	1.91	0.53
1:A:137:TYR:HA	1:A:141:GLY:HA2	1.90	0.53
1:A:1088:LYS:HA	1:A:1091:GLU:HG3	1.89	0.53
1:A:1271:VAL:O	1:A:1277:GLN:NE2	2.40	0.53
1:A:976:TRP:CD1	1:A:1120:ASN:HB3	2.44	0.53
1:A:1311:PHE:CE2	1:A:1356:ILE:HD11	2.44	0.53
1:A:1906:SER:OG	1:A:1907:LEU:N	2.41	0.53
1:A:1975:SER:OG	1:A:1976:THR:N	2.42	0.53
1:A:384:MET:SD	1:A:385:CYS:N	2.73	0.52
1:A:597:GLN:O	1:A:601:THR:HG23	2.10	0.52
1:A:661:THR:OG1	1:A:775:GLN:O	2.16	0.52
1:A:920:TYR:CE2	1:A:1111:LEU:HB3	2.43	0.52
1:A:1855:VAL:O	1:A:1858:LYS:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2006:MET:O	1:A:2010:LEU:HG	2.08	0.52
2:B:253:ILE:HG23	2:E:257:ILE:HD13	1.90	0.52
1:A:206:ILE:HG22	1:A:208:ASN:ND2	2.24	0.52
1:A:435:MET:HB2	1:A:1633:PHE:HE1	1.74	0.52
1:A:1763:ASN:HA	1:A:1766:LEU:HD13	1.90	0.52
1:A:1948:TYR:CD2	1:A:1959:LEU:HD23	2.44	0.52
1:A:1950:TRP:HZ2	1:A:2026:TYR:CG	2.27	0.52
1:A:1369:THR:HG22	1:A:1369:THR:O	2.10	0.52
1:A:1739:ILE:HG22	1:A:1740:ILE:HD12	1.90	0.52
1:A:1819:GLU:HG3	1:A:1823:PRO:HA	1.90	0.52
1:A:21:HIS:HD1	1:A:711:PHE:HA	1.75	0.52
1:A:301:LEU:HG	1:A:829:PHE:CE1	2.44	0.52
1:A:1191:PHE:CB	1:A:1321:GLU:HB2	2.29	0.52
1:A:937:LEU:HD21	1:A:981:LEU:HD13	1.91	0.52
1:A:1633:PHE:N	1:A:1637:GLU:OE1	2.39	0.52
1:A:1748:LYS:HG2	1:A:2020:PRO:HG3	1.91	0.52
1:A:1452:ILE:HG13	1:A:1528:ALA:HB3	1.92	0.52
1:A:614:SER:O	1:A:614:SER:OG	2.22	0.52
1:A:1757:ASP:N	1:A:1757:ASP:OD1	2.42	0.52
1:A:1793:TYR:O	1:A:1796:ARG:HB3	2.10	0.52
1:A:573:GLN:O	1:A:577:GLU:HG2	2.09	0.51
1:A:659:PHE:HE2	1:A:828:HIS:HA	1.75	0.51
1:A:950:ASN:OD1	1:A:951:ARG:N	2.43	0.51
1:A:164:VAL:O	1:A:168:TRP:HB2	2.10	0.51
1:A:287:TYR:CE2	1:A:369:PRO:HB3	2.45	0.51
1:A:364:ARG:O	1:A:364:ARG:HD3	2.09	0.51
1:A:941:ASN:ND2	1:A:944:SER:OG	2.37	0.51
1:A:1613:LYS:HE2	1:A:1638:LYS:HB2	1.92	0.51
2:C:266:THR:O	2:C:270:MET:HG3	2.10	0.51
1:A:1611:ALA:O	1:A:1615:THR:HG23	2.09	0.51
1:A:2076:GLU:O	1:A:2143:ARG:NE	2.43	0.51
1:A:835:ARG:HD2	1:A:845:GLN:HE22	1.75	0.51
1:A:1633:PHE:O	1:A:1638:LYS:NZ	2.42	0.51
1:A:1772:HIS:HA	1:A:1775:ARG:NH1	2.25	0.51
1:A:312:GLY:HA3	2:F:384:LYS:HE3	1.92	0.51
1:A:694:GLU:OE1	1:A:694:GLU:N	2.43	0.51
2:E:264:MET:O	2:E:268:GLU:HG3	2.11	0.51
1:A:354:ASP:OD1	1:A:844:THR:N	2.26	0.51
1:A:1030:LEU:HA	1:A:1033:ILE:HG13	1.93	0.51
1:A:1854:SER:O	1:A:1858:LYS:NZ	2.42	0.51
1:A:83:GLN:NE2	1:A:84:GLU:OE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LYS:HE2	1:A:175:ARG:HD3	1.92	0.50
1:A:671:TRP:HE1	1:A:816:HIS:CE1	2.29	0.50
1:A:955:ASP:HB3	1:A:958:VAL:HG22	1.94	0.50
1:A:986:PRO:HB2	1:A:1151:PRO:HG2	1.93	0.50
1:A:1980:PRO:HG3	1:A:2034:GLU:HG3	1.92	0.50
2:C:264:MET:O	2:C:268:GLU:HG3	2.11	0.50
1:A:57:SER:C	1:A:59:LEU:H	2.20	0.50
1:A:399:LEU:HA	1:A:679:PHE:CE1	2.46	0.50
1:A:935:SER:OG	1:A:941:ASN:N	2.45	0.50
1:A:457:LYS:N	1:A:685:ARG:HG2	2.23	0.50
1:A:901:SER:O	1:A:905:ILE:HG12	2.11	0.50
1:A:1239:LEU:O	1:A:1243:LEU:HD23	2.11	0.50
1:A:44:LEU:HD23	1:A:44:LEU:H	1.76	0.50
1:A:368:HIS:CD2	1:A:369:PRO:HD2	2.45	0.50
1:A:1067:THR:C	1:A:1270:ARG:HD3	2.35	0.50
1:A:1161:LEU:HB2	1:A:1162:GLU:CD	2.35	0.50
1:A:257:VAL:HG12	1:A:259:THR:HG23	1.93	0.50
1:A:790:LEU:O	1:A:794:THR:OG1	2.23	0.50
1:A:987:GLY:C	1:A:1002:ASN:HD21	2.18	0.50
1:A:1118:LEU:HG	1:A:1119:LYS:H	1.76	0.50
1:A:1905:CYS:N	1:A:1932:ILE:O	2.45	0.50
2:D:247:GLN:OE1	2:E:246:SER:HB3	2.12	0.50
1:A:900:LEU:HD22	1:A:940:LEU:HD12	1.93	0.50
1:A:2207:LEU:N	1:A:2207:LEU:CD1	2.73	0.50
1:A:196:ASP:O	1:A:197:HIS:ND1	2.44	0.50
1:A:880:GLU:OE2	1:A:1307:SER:OG	2.14	0.50
1:A:1180:TYR:HB2	1:A:1887:ILE:HG23	1.93	0.50
2:E:247:GLN:O	2:E:250:ILE:HB	2.12	0.50
1:A:1180:TYR:O	1:A:1887:ILE:HG21	2.11	0.50
1:A:1742:SER:HB2	1:A:1968:GLU:HG3	1.94	0.50
1:A:1948:TYR:CD2	1:A:1959:LEU:HD22	2.47	0.50
1:A:847:LEU:O	1:A:850:ALA:HB3	2.12	0.49
1:A:898:LYS:O	1:A:901:SER:OG	2.26	0.49
1:A:1615:THR:O	1:A:1619:LEU:HG	2.12	0.49
1:A:930:LEU:HD11	1:A:1114:ASN:ND2	2.26	0.49
1:A:976:TRP:HD1	1:A:1120:ASN:HB3	1.76	0.49
1:A:1740:ILE:O	1:A:1969:ARG:HA	2.13	0.49
1:A:1746:LEU:HD13	1:A:1748:LYS:NZ	2.27	0.49
1:A:46:ASN:N	1:A:47:GLN:OE1	2.45	0.49
1:A:797:PHE:HA	1:A:800:CYS:SG	2.52	0.49
1:A:2102:ILE:HD11	1:A:2126:ILE:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:GLN:OE1	2:C:246:SER:HB3	2.12	0.49
1:A:991:TRP:HB2	1:A:1043:ASN:OD1	2.12	0.49
1:A:677:ILE:HA	1:A:680:ALA:HB3	1.93	0.49
1:A:992:ALA:N	1:A:1043:ASN:OD1	2.45	0.49
1:A:1017:THR:HG22	1:A:1089:SER:OG	2.12	0.49
1:A:1511:TRP:O	1:A:1515:VAL:HG23	2.11	0.49
1:A:1511:TRP:O	1:A:1514:ILE:HG22	2.13	0.49
1:A:2127:SER:HB2	1:A:2131:ARG:HH21	1.76	0.49
2:C:247:GLN:O	2:C:250:ILE:HB	2.12	0.49
1:A:544:PHE:CE2	1:A:699:ARG:HB3	2.47	0.49
1:A:1005:TYR:HD2	1:A:1110:TYR:HA	1.78	0.49
1:A:660:LEU:HB3	1:A:825:ILE:HG13	1.95	0.49
1:A:695:TRP:CD1	1:A:698:LEU:HD12	2.48	0.49
1:A:1191:PHE:O	1:A:1321:GLU:CG	2.61	0.49
1:A:236:GLU:OE1	1:A:236:GLU:N	2.42	0.49
1:A:1786:LYS:HE3	1:A:1986:TYR:CG	2.47	0.49
1:A:1539:HIS:CE1	1:A:1766:LEU:H	2.31	0.48
1:A:562:PHE:N	1:A:740:GLU:OE1	2.46	0.48
1:A:391:ASP:HA	2:E:271:ILE:CD1	2.44	0.48
1:A:1357:ASN:CG	1:A:1358:ARG:H	2.20	0.48
1:A:2149:PRO:HB2	1:A:2152:LEU:HG	1.95	0.48
1:A:238:VAL:HA	1:A:241:VAL:HG22	1.95	0.48
1:A:392:PHE:HA	1:A:395:ILE:HG22	1.94	0.48
1:A:1750:PRO:HB2	1:A:1752:PRO:HD3	1.95	0.48
1:A:2016:THR:O	1:A:2017:LEU:HD12	2.12	0.48
1:A:1589:ASP:O	1:A:1590:LEU:HB2	2.13	0.48
1:A:1609:LEU:O	1:A:1613:LYS:HG2	2.13	0.48
1:A:332:PHE:HE2	1:A:335:ASP:H	1.61	0.48
1:A:479:ILE:C	1:A:564:LYS:HD2	2.39	0.48
1:A:417:VAL:CG2	1:A:437:ASP:OD2	2.57	0.48
1:A:2208:THR:HG23	1:A:2211:ILE:CB	2.43	0.48
1:A:891:LEU:O	1:A:895:MET:HG2	2.13	0.48
1:A:1769:PRO:HG2	1:A:2216:TRP:HE1	1.79	0.48
1:A:24:TYR:HA	1:A:27:ILE:HG12	1.94	0.48
1:A:1225:ARG:HB3	1:A:1684:ARG:HH22	1.79	0.48
1:A:1921:GLN:N	1:A:1921:GLN:OE1	2.47	0.48
1:A:423:LEU:C	1:A:423:LEU:HD13	2.39	0.47
1:A:607:MET:HG2	1:A:767:MET:HG2	1.94	0.47
1:A:1165:ASP:OD2	1:A:1168:GLU:N	2.33	0.47
1:A:1224:ARG:HG3	1:A:1293:ARG:HH21	1.77	0.47
2:F:380:LEU:HA	2:F:383:LEU:HD12	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:VAL:O	1:A:289:ILE:HG12	2.14	0.47
1:A:868:CYS:O	1:A:871:LEU:HB2	2.14	0.47
1:A:1206:PRO:HA	1:A:1213:ARG:NH2	2.29	0.47
1:A:1733:ASN:HD21	1:A:2036:ILE:HG21	1.79	0.47
1:A:101:PHE:CG	1:A:101:PHE:O	2.67	0.47
1:A:816:HIS:O	1:A:818:LEU:N	2.46	0.47
2:B:223:LEU:HD13	2:C:222:ILE:HG13	1.97	0.47
1:A:375:GLN:O	1:A:379:LYS:HG3	2.14	0.47
1:A:951:ARG:NH2	1:A:1306:ALA:O	2.48	0.47
1:A:92:PRO:HB2	1:A:95:LEU:HB2	1.97	0.47
1:A:853:LEU:HD13	1:A:895:MET:HE3	1.96	0.47
1:A:1739:ILE:CG2	1:A:1740:ILE:HD12	2.45	0.47
1:A:1740:ILE:HG21	1:A:2018:ILE:HG12	1.96	0.47
1:A:1786:LYS:HE3	1:A:1986:TYR:CD2	2.50	0.47
1:A:289:ILE:O	1:A:293:LEU:N	2.44	0.47
1:A:510:PHE:CG	1:A:511:ASN:N	2.82	0.47
1:A:1056:PHE:HB2	1:A:1059:VAL:HG22	1.96	0.47
1:A:244:MET:HE2	1:A:244:MET:HB3	1.75	0.47
2:F:375:SER:O	2:F:375:SER:OG	2.29	0.47
2:D:250:ILE:HG22	2:E:249:LEU:HD23	1.97	0.47
1:A:338:ARG:HH12	2:F:372:ASN:HD21	1.63	0.47
1:A:1048:PHE:HD2	1:A:1389:VAL:HG12	1.79	0.47
1:A:1803:ASP:CG	1:A:1906:SER:H	2.22	0.47
1:A:296:PHE:CZ	1:A:345:ILE:HD12	2.50	0.46
1:A:863:CYS:SG	1:A:1009:PRO:HD2	2.56	0.46
1:A:1768:ALA:HB3	1:A:1979:ASP:CG	2.40	0.46
1:A:664:LEU:HD12	1:A:664:LEU:HA	1.79	0.46
1:A:1131:MET:HE1	1:A:1143:ASN:ND2	2.30	0.46
1:A:1272:ASN:HD22	1:A:1395:VAL:H	1.63	0.46
1:A:2148:LEU:HD13	1:A:2153:ARG:HH11	1.79	0.46
1:A:361:CYS:CB	1:A:848:LYS:HB2	2.38	0.46
1:A:835:ARG:NH2	1:A:1306:ALA:H	2.13	0.46
1:A:835:ARG:HG2	1:A:845:GLN:OE1	2.15	0.46
1:A:872:ALA:O	1:A:876:MET:N	2.45	0.46
1:A:1052:ARG:NH2	1:A:1386:ALA:O	2.47	0.46
1:A:1160:GLY:O	1:A:1161:LEU:HD23	2.15	0.46
1:A:2167:ILE:HG13	1:A:2199:ILE:HG23	1.98	0.46
1:A:248:ARG:HA	1:A:365:LEU:HD21	1.96	0.46
1:A:1059:VAL:O	1:A:1063:ILE:HG12	2.15	0.46
1:A:1193:TRP:HZ3	1:A:1916:ALA:HB3	1.81	0.46
1:A:1449:ILE:HG21	1:A:1494:GLU:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1503:MET:HE2	1:A:1621:HIS:HE1	1.80	0.46
1:A:1605:ARG:HG3	1:A:1608:ASN:ND2	2.27	0.46
1:A:2174:ASP:OD1	1:A:2175:ARG:N	2.49	0.46
2:D:223:LEU:HD13	2:E:222:ILE:HG13	1.97	0.46
1:A:145:LEU:HD11	1:A:1360:PHE:HZ	1.80	0.46
1:A:287:TYR:CD2	1:A:369:PRO:HB3	2.50	0.46
1:A:885:LYS:HB3	1:A:948:LEU:HD11	1.98	0.46
1:A:1192:THR:O	1:A:1366:HIS:HD2	1.99	0.46
1:A:2163:GLY:H	1:A:2164:ILE:HD12	1.81	0.46
2:B:250:ILE:HG22	2:C:249:LEU:HD23	1.97	0.46
1:A:1045:LEU:HD13	1:A:1391:PRO:HD3	1.97	0.46
1:A:1633:PHE:HB2	1:A:1637:GLU:HB2	1.97	0.46
2:D:223:LEU:HG	2:D:227:ARG:CZ	2.46	0.46
1:A:57:SER:OG	1:A:59:LEU:HB2	2.16	0.46
1:A:402:PHE:CD2	1:A:679:PHE:HD1	2.34	0.46
1:A:417:VAL:CA	1:A:437:ASP:OD2	2.59	0.46
1:A:871:LEU:O	1:A:875:VAL:HG23	2.16	0.46
1:A:918:LEU:O	1:A:922:ASN:ND2	2.37	0.46
1:A:401:PHE:CE2	1:A:757:LEU:HA	2.50	0.46
1:A:418:TRP:CH2	1:A:433:GLU:O	2.69	0.46
1:A:1646:LEU:HA	1:A:1649:VAL:HG22	1.97	0.46
1:A:1950:TRP:CZ3	1:A:1956:PHE:CZ	2.95	0.46
2:C:233:MET:CE	2:D:233:MET:HE2	2.46	0.46
1:A:191:ILE:O	1:A:195:THR:HG23	2.15	0.46
1:A:333:THR:HG22	1:A:334:GLN:HG3	1.98	0.46
1:A:418:TRP:CD1	1:A:418:TRP:N	2.82	0.46
1:A:744:GLN:HA	1:A:747:TRP:CE3	2.51	0.46
1:A:2168:THR:OG1	1:A:2169:SER:N	2.49	0.46
1:A:859:VAL:HA	1:A:862:GLU:HB2	1.98	0.46
1:A:1660:LEU:HA	1:A:1663:PHE:CD2	2.51	0.46
1:A:1894:GLU:O	1:A:1897:ILE:HG22	2.16	0.46
1:A:1948:TYR:CZ	1:A:1959:LEU:HD22	2.51	0.46
1:A:390:LEU:O	2:E:271:ILE:HD12	2.16	0.45
1:A:1497:LEU:O	1:A:1614:LEU:HD21	2.16	0.45
1:A:1646:LEU:HD23	1:A:1647:ARG:HD3	1.98	0.45
1:A:744:GLN:O	1:A:748:THR:HG23	2.15	0.45
1:A:1390:LYS:O	1:A:1392:HIS:NE2	2.49	0.45
1:A:1542:LEU:HD23	1:A:1542:LEU:HA	1.78	0.45
1:A:1593:VAL:HG23	1:A:1674:ALA:HB3	1.99	0.45
1:A:10:PRO:O	1:A:188:ARG:NH2	2.50	0.45
1:A:878:LEU:HG	1:A:883:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1018:GLN:O	1:A:1022:MET:HG2	2.16	0.45
1:A:1523:ARG:O	1:A:1524:ARG:HG3	2.17	0.45
1:A:1193:TRP:CZ3	1:A:1916:ALA:HB3	2.52	0.45
1:A:915:GLN:HA	1:A:918:LEU:HG	1.99	0.45
1:A:1444:THR:HG21	1:A:1480:MET:HG3	1.99	0.45
1:A:1911:ASP:HB3	1:A:1947:LYS:HB3	1.97	0.45
1:A:1929:ASN:HA	1:A:1932:ILE:HG22	1.98	0.45
1:A:1950:TRP:HB2	1:A:1953:PHE:HA	1.97	0.45
1:A:1099:LYS:HA	1:A:1102:GLU:HB2	1.97	0.45
1:A:1194:PHE:CZ	1:A:1344:GLY:HA3	2.52	0.45
1:A:1503:MET:HG3	1:A:1621:HIS:CE1	2.52	0.45
1:A:1539:HIS:N	1:A:1540:PRO:HD2	2.31	0.45
1:A:1608:ASN:OD1	1:A:1609:LEU:N	2.49	0.45
1:A:1740:ILE:HD11	1:A:1970:ILE:HG23	1.99	0.45
1:A:1786:LYS:HG3	1:A:1986:TYR:CE1	2.51	0.45
1:A:1820:TYR:HD1	1:A:1821:LEU:HD22	1.82	0.45
2:B:223:LEU:HG	2:B:227:ARG:CZ	2.46	0.45
1:A:70:LEU:O	1:A:74:ILE:HG12	2.16	0.45
1:A:1009:PRO:HB3	1:A:1103:ILE:HD12	1.98	0.45
1:A:1612:ARG:O	1:A:1616:LEU:HG	2.17	0.45
1:A:1740:ILE:HD13	1:A:1740:ILE:H	1.82	0.45
2:B:233:MET:HE2	2:E:233:MET:CE	2.46	0.45
1:A:60:ALA:O	1:A:64:VAL:HG23	2.17	0.45
1:A:202:LEU:HB3	1:A:203:ILE:H	1.56	0.45
1:A:418:TRP:HE3	1:A:422:ASN:HD22	1.65	0.45
1:A:1124:PRO:HB2	1:A:1127:TYR:CD2	2.52	0.45
1:A:1183:GLN:OE1	1:A:1183:GLN:HA	2.16	0.45
1:A:1244:ARG:NH2	1:A:1295:ASP:H	2.14	0.45
1:A:362:ILE:HG13	1:A:847:LEU:HD23	1.99	0.44
1:A:2122:LEU:C	1:A:2123:LEU:HD22	2.42	0.44
1:A:1051:ASP:O	1:A:1052:ARG:HD2	2.16	0.44
1:A:258:SER:HA	1:A:261:LEU:HD13	2.00	0.44
1:A:721:ASP:OD1	1:A:722:LEU:N	2.50	0.44
1:A:1093:LYS:O	1:A:1095:LEU:N	2.49	0.44
1:A:1216:TYR:HD2	1:A:1345:LEU:HD11	1.81	0.44
1:A:1224:ARG:HH11	1:A:1293:ARG:HE	1.66	0.44
1:A:1923:LEU:O	1:A:1927:ILE:HG13	2.18	0.44
1:A:2042:ASP:HA	1:A:2045:VAL:HG12	1.99	0.44
2:F:368:LEU:HD23	2:F:368:LEU:HA	1.81	0.44
1:A:115:LYS:HB2	1:A:115:LYS:HE2	1.75	0.44
1:A:347:PRO:HG2	1:A:348:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:LYS:HG2	1:A:1333:SER:HB3	2.00	0.44
1:A:2099:ILE:O	1:A:2103:THR:HG23	2.17	0.44
1:A:95:LEU:O	1:A:98:ILE:HG22	2.17	0.44
1:A:362:ILE:CG1	1:A:847:LEU:HB3	2.48	0.44
1:A:1294:LEU:HD12	1:A:1294:LEU:O	2.17	0.44
1:A:1735:TYR:HB2	1:A:1974:ARG:NH1	2.33	0.44
1:A:420:PRO:HB2	1:A:421:LEU:CD1	2.45	0.44
1:A:612:ILE:HG21	1:A:1213:ARG:NH1	2.33	0.44
1:A:1690:ILE:HG23	1:A:1691:ARG:NH2	2.33	0.44
1:A:2033:GLN:O	1:A:2037:VAL:HG22	2.18	0.44
1:A:2088:ILE:HG23	1:A:2137:ILE:HD12	1.99	0.44
1:A:2147:ILE:HD13	1:A:2147:ILE:HA	1.90	0.44
1:A:275:VAL:HB	1:A:366:TRP:CZ2	2.53	0.44
1:A:308:PRO:HB2	1:A:309:GLU:OE1	2.17	0.44
1:A:311:ARG:NH1	2:F:388:ILE:HG12	2.33	0.44
1:A:401:PHE:HE2	1:A:757:LEU:HA	1.82	0.44
1:A:855:LEU:HD12	1:A:855:LEU:HA	1.86	0.44
1:A:1216:TYR:CD2	1:A:1345:LEU:HD11	2.52	0.44
1:A:1630:ILE:HD12	1:A:1630:ILE:HA	1.89	0.44
2:B:264:MET:CE	2:C:263:GLY:HA3	2.38	0.44
1:A:350:ASP:O	1:A:351:LEU:HD23	2.17	0.44
1:A:1068:SER:OG	1:A:1393:ILE:HG21	2.18	0.44
1:A:1311:PHE:C	1:A:1313:SER:H	2.25	0.44
2:E:266:THR:CG2	2:E:270:MET:CE	2.77	0.44
1:A:204:THR:CG2	1:A:215:ILE:HB	2.47	0.43
1:A:659:PHE:CE2	1:A:828:HIS:HA	2.53	0.43
1:A:1028:PRO:C	1:A:1030:LEU:H	2.26	0.43
1:A:1540:PRO:HB3	1:A:2162:PHE:CE2	2.53	0.43
1:A:1616:LEU:O	1:A:1620:ILE:HG22	2.18	0.43
1:A:293:LEU:HD12	1:A:293:LEU:HA	1.79	0.43
1:A:381:ARG:HG3	1:A:732:ILE:HD13	1.99	0.43
1:A:582:ASN:HB3	1:A:583:HIS:HD2	1.82	0.43
1:A:1052:ARG:HG3	1:A:1385:GLU:HB3	1.99	0.43
2:F:368:LEU:HA	2:F:371:ILE:HD12	2.00	0.43
1:A:426:ASN:OD1	2:B:262:ALA:CB	2.66	0.43
1:A:586:LYS:O	1:A:588:MET:HG3	2.19	0.43
1:A:1443:PHE:HE2	1:A:1682:LEU:HB3	1.83	0.43
1:A:1578:LYS:O	1:A:1581:ILE:HB	2.19	0.43
1:A:59:LEU:HD13	1:A:62:ARG:HH11	1.84	0.43
1:A:245:TYR:HD1	1:A:245:TYR:HA	1.75	0.43
1:A:592:GLY:H	1:A:769:MET:HE1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:GLN:N	1:A:908:GLN:OE1	2.51	0.43
2:C:254:LYS:O	2:C:258:VAL:HG23	2.18	0.43
2:E:254:LYS:O	2:E:258:VAL:HG23	2.18	0.43
1:A:308:PRO:HB2	1:A:309:GLU:CD	2.44	0.43
1:A:744:GLN:O	1:A:747:TRP:HB2	2.19	0.43
1:A:390:LEU:HD13	1:A:675:THR:HB	2.01	0.43
1:A:1322:GLN:HE22	1:A:1325:THR:HG22	1.84	0.43
1:A:1785:TYR:O	1:A:1788:ILE:HG12	2.18	0.43
1:A:401:PHE:CE1	1:A:446:THR:HG23	2.54	0.43
1:A:423:LEU:HB2	1:A:434:LEU:HD22	2.01	0.43
1:A:1786:LYS:HB2	1:A:1977:TYR:CE2	2.53	0.43
1:A:1634:SER:HA	1:A:1638:LYS:NZ	2.34	0.43
1:A:1747:GLU:O	1:A:1747:GLU:HG3	2.19	0.43
1:A:99:PRO:HA	1:A:102:LYS:HG2	2.01	0.43
1:A:304:SER:O	1:A:304:SER:OG	2.37	0.43
1:A:783:VAL:HG21	1:A:792:LYS:HG2	2.01	0.43
1:A:1216:TYR:OH	1:A:1219:SER:OG	2.24	0.43
1:A:1606:SER:O	1:A:1610:ILE:HG23	2.18	0.43
1:A:2018:ILE:O	1:A:2018:ILE:HG13	2.19	0.43
1:A:315:HIS:HD2	2:F:349:THR:HG23	1.84	0.43
1:A:1646:LEU:HD22	1:A:1647:ARG:NH1	2.34	0.43
1:A:2007:ALA:HA	1:A:2010:LEU:HG	2.00	0.43
1:A:2026:TYR:HD2	1:A:2027:TRP:CD1	2.37	0.43
2:B:251:GLN:O	2:B:254:LYS:HB3	2.19	0.43
2:D:251:GLN:O	2:D:254:LYS:HB3	2.19	0.43
1:A:1741:GLU:C	1:A:1968:GLU:HB2	2.44	0.42
1:A:1775:ARG:HD3	1:A:1782:THR:CB	2.45	0.42
1:A:1797:LEU:HD12	1:A:1798:LYS:H	1.84	0.42
1:A:2016:THR:C	1:A:2017:LEU:HD12	2.44	0.42
1:A:192:VAL:O	1:A:195:THR:OG1	2.32	0.42
1:A:1897:ILE:HG13	1:A:1931:ILE:HD12	2.01	0.42
1:A:10:PRO:C	1:A:188:ARG:HH12	2.27	0.42
1:A:681:GLN:OE1	1:A:685:ARG:NH1	2.53	0.42
1:A:1009:PRO:HD3	1:A:1106:TYR:CD2	2.54	0.42
1:A:1067:THR:OG1	1:A:1068:SER:N	2.51	0.42
1:A:1486:GLU:HA	1:A:1489:MET:HB3	2.02	0.42
1:A:1964:TRP:CG	1:A:1964:TRP:O	2.72	0.42
1:A:2084:PHE:CE1	1:A:2085:GLU:HG3	2.54	0.42
1:A:791:GLU:O	1:A:795:ILE:HG12	2.19	0.42
1:A:956:PRO:HD2	1:A:999:TYR:CD2	2.55	0.42
1:A:1093:LYS:N	1:A:1094:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:PRO:N	1:A:188:ARG:HH22	2.18	0.42
1:A:479:ILE:O	1:A:564:LYS:HD2	2.20	0.42
1:A:1233:ARG:HA	1:A:1233:ARG:NE	2.34	0.42
1:A:1740:ILE:CD1	1:A:1740:ILE:H	2.32	0.42
1:A:1750:PRO:HD3	1:A:2015:PHE:HD1	1.85	0.42
1:A:145:LEU:HD11	1:A:1360:PHE:CZ	2.54	0.42
1:A:224:ASN:OD1	1:A:229:THR:HB	2.19	0.42
1:A:879:THR:HG22	1:A:888:CYS:HB3	2.01	0.42
1:A:945:CYS:O	1:A:948:LEU:HB3	2.20	0.42
1:A:1108:ILE:HD13	1:A:1108:ILE:HA	1.86	0.42
1:A:920:TYR:CZ	1:A:1111:LEU:HD22	2.54	0.42
1:A:1005:TYR:CD2	1:A:1110:TYR:HA	2.53	0.42
1:A:1058:ARG:O	1:A:1062:ILE:HG12	2.20	0.42
1:A:1478:GLU:C	1:A:1480:MET:H	2.28	0.42
1:A:146:PHE:HB3	1:A:157:ARG:HH21	1.84	0.42
1:A:1951:LEU:HB3	1:A:1952:PRO:HD3	2.00	0.42
1:A:2091:MET:SD	1:A:2140:HIS:ND1	2.92	0.42
1:A:1295:ASP:OD1	1:A:1295:ASP:N	2.52	0.42
1:A:1690:ILE:HG23	1:A:1691:ARG:HH21	1.85	0.42
1:A:1851:PHE:O	1:A:1856:PRO:HD3	2.20	0.42
1:A:20:LYS:HE3	1:A:20:LYS:HB3	1.87	0.42
1:A:305:ASP:HA	1:A:311:ARG:NH1	2.34	0.42
1:A:1009:PRO:HD3	1:A:1106:TYR:CE2	2.54	0.42
1:A:1233:ARG:HE	1:A:1234:GLY:H	1.66	0.42
1:A:1493:TRP:O	1:A:1497:LEU:HG	2.20	0.42
1:A:1501:TYR:HA	1:A:1617:LEU:HD23	2.01	0.42
1:A:1740:ILE:HB	1:A:1741:GLU:H	1.78	0.42
1:A:1971:THR:HG22	1:A:1988:ILE:CD1	2.50	0.42
2:B:233:MET:HE2	2:E:233:MET:HE1	2.02	0.42
1:A:331:SER:HG	1:A:336:GLU:CD	2.28	0.41
1:A:362:ILE:HD11	1:A:847:LEU:C	2.45	0.41
1:A:379:LYS:HE3	1:A:379:LYS:HB2	1.75	0.41
1:A:745:LYS:O	1:A:748:THR:OG1	2.35	0.41
1:A:1123:GLU:N	1:A:1123:GLU:OE1	2.53	0.41
1:A:1438:THR:O	1:A:1442:GLN:HG3	2.19	0.41
1:A:1805:LEU:HD13	1:A:1828:TYR:HB3	2.01	0.41
1:A:2002:GLN:H	1:A:2002:GLN:CD	2.24	0.41
2:F:360:LYS:HG2	2:F:363:MET:HG2	2.02	0.41
2:D:264:MET:CE	2:E:263:GLY:HA3	2.38	0.41
1:A:698:LEU:O	1:A:701:MET:HB2	2.20	0.41
1:A:864:THR:N	1:A:1107:ASN:HD21	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1538:SER:C	1:A:1540:PRO:HD2	2.44	0.41
1:A:1963:LEU:C	1:A:1965:CYS:H	2.26	0.41
1:A:1136:CYS:SG	1:A:1168:GLU:OE2	2.78	0.41
1:A:1477:SER:HB3	1:A:1536:THR:HA	2.02	0.41
1:A:1540:PRO:HB3	1:A:2162:PHE:CD2	2.55	0.41
1:A:1629:LYS:HG2	1:A:1630:ILE:H	1.85	0.41
1:A:401:PHE:HE1	1:A:446:THR:HG23	1.85	0.41
1:A:751:SER:HA	1:A:754:VAL:HG22	2.01	0.41
1:A:876:MET:HE1	1:A:947:ARG:HD3	2.01	0.41
1:A:1449:ILE:O	1:A:1452:ILE:HG22	2.20	0.41
1:A:15:ASN:OD1	1:A:15:ASN:N	2.52	0.41
1:A:1231:TYR:CZ	1:A:1234:GLY:HA3	2.54	0.41
1:A:1509:VAL:HG12	1:A:1513:ASN:OD1	2.20	0.41
1:A:2002:GLN:HG2	1:A:2003:ALA:N	2.34	0.41
1:A:423:LEU:HG	1:A:431:LEU:CA	2.48	0.41
1:A:702:ARG:O	1:A:703:SER:OG	2.32	0.41
1:A:880:GLU:OE1	1:A:1308:SER:N	2.54	0.41
1:A:288:ASN:O	1:A:291:ALA:HB3	2.21	0.41
1:A:299:ALA:HB2	1:A:314:PHE:CD2	2.50	0.41
1:A:1015:ARG:O	1:A:1018:GLN:HG3	2.20	0.41
1:A:1243:LEU:HD13	1:A:1285:PRO:HG3	2.03	0.41
1:A:1304:THR:O	1:A:1306:ALA:N	2.54	0.41
1:A:1516:ASP:O	1:A:1520:MET:HG2	2.20	0.41
1:A:1814:SER:OG	1:A:1815:MET:N	2.54	0.41
1:A:2040:ALA:O	1:A:2044:VAL:HG23	2.20	0.41
1:A:2142:ILE:HG23	1:A:2219:LEU:HD13	2.03	0.41
2:F:357:CYS:SG	2:F:391:ALA:HB2	2.61	0.41
1:A:168:TRP:CG	1:A:253:SER:HG	2.39	0.41
1:A:485:ASP:O	1:A:488:SER:N	2.47	0.41
1:A:752:ILE:O	1:A:755:ILE:HG22	2.19	0.41
1:A:885:LYS:HB3	1:A:948:LEU:HD21	2.02	0.41
1:A:1646:LEU:HD11	1:A:1660:LEU:O	2.21	0.41
1:A:6:GLU:OE2	1:A:7:ILE:HG22	2.21	0.41
1:A:219:LEU:HD12	1:A:233:MET:O	2.21	0.41
1:A:332:PHE:CG	1:A:333:THR:N	2.89	0.41
1:A:363:MET:HE2	1:A:363:MET:HB3	1.88	0.41
1:A:1028:PRO:C	1:A:1030:LEU:N	2.78	0.41
1:A:1136:CYS:SG	1:A:1374:CYS:SG	3.19	0.41
1:A:1948:TYR:CG	1:A:1959:LEU:CD2	3.04	0.41
1:A:2098:GLU:O	1:A:2102:ILE:HG23	2.21	0.41
1:A:2208:THR:OG1	1:A:2210:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2211:ILE:O	1:A:2215:ILE:HG23	2.20	0.41
2:B:242:ARG:HB3	2:E:244:LEU:HD21	2.03	0.41
1:A:121:CYS:SG	1:A:161:LEU:HG	2.61	0.41
1:A:487:MET:CB	1:A:507:PRO:HA	2.49	0.41
1:A:1530:LEU:HD21	1:A:1760:ASN:HA	2.03	0.41
1:A:730:ILE:HG23	1:A:731:PHE:HD2	1.85	0.40
1:A:957:VAL:HG22	1:A:1001:ILE:HD11	2.03	0.40
1:A:1057:PRO:HG2	1:A:1161:LEU:HD11	2.03	0.40
1:A:1095:LEU:HG	1:A:1096:SER:H	1.86	0.40
1:A:1631:LYS:HD2	1:A:1632:GLY:N	2.36	0.40
1:A:1767:ASN:OD1	1:A:1767:ASN:N	2.50	0.40
1:A:1944:LEU:HD12	1:A:1945:ILE:H	1.87	0.40
1:A:33:PRO:O	1:A:87:ASN:ND2	2.55	0.40
1:A:168:TRP:CH2	1:A:895:MET:HE1	2.56	0.40
1:A:406:LEU:HD12	1:A:587:LEU:HD22	2.03	0.40
1:A:1002:ASN:HB2	1:A:1149:TRP:CZ3	2.54	0.40
1:A:1685:LYS:HE3	1:A:1685:LYS:HB3	1.86	0.40
2:C:250:ILE:HD13	2:D:250:ILE:HD11	2.03	0.40
1:A:287:TYR:CZ	1:A:369:PRO:HB3	2.55	0.40
1:A:422:ASN:CA	1:A:453:VAL:HG21	2.39	0.40
1:A:937:LEU:HG	1:A:937:LEU:O	2.20	0.40
1:A:967:LEU:HD22	1:A:972:CYS:SG	2.61	0.40
1:A:985:LYS:HD3	1:A:986:PRO:CD	2.52	0.40
1:A:994:LEU:HD12	1:A:1149:TRP:CD2	2.56	0.40
1:A:1626:GLU:OE2	1:A:1648:LYS:HB3	2.21	0.40
1:A:1629:LYS:HE2	1:A:1629:LYS:HB3	1.79	0.40
1:A:1772:HIS:HA	1:A:1775:ARG:HH11	1.85	0.40
2:B:250:ILE:HD11	2:E:250:ILE:HD13	2.03	0.40
2:C:233:MET:HE1	2:D:233:MET:HE2	2.02	0.40
1:A:299:ALA:HB1	1:A:315:HIS:HA	2.04	0.40
1:A:362:ILE:CD1	1:A:847:LEU:HB3	2.50	0.40
1:A:1176:VAL:HG12	1:A:1363:SER:OG	2.22	0.40
1:A:1777:LEU:HD23	1:A:1777:LEU:HA	1.87	0.40
1:A:7:ILE:HD12	1:A:7:ILE:HA	1.95	0.40
1:A:14:LEU:HD23	1:A:239:LEU:HD22	2.02	0.40
1:A:406:LEU:HD21	1:A:686:MET:SD	2.62	0.40
1:A:705:LEU:HB2	1:A:732:ILE:HB	2.04	0.40
1:A:1607:MET:HE3	1:A:1607:MET:HB2	1.85	0.40
1:A:1812:GLY:O	1:A:1850:GLN:NE2	2.54	0.40
1:A:1957:SER:OG	1:A:2017:LEU:HG	2.21	0.40
1:A:2094:THR:HG22	1:A:2098:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2148:LEU:HD13	1:A:2153:ARG:NH1	2.36	0.40
2:B:252:THR:HG21	2:E:254:LYS:HZ3	1.86	0.40
2:C:243:ILE:O	2:C:247:GLN:HG2	2.21	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	1843/2255 (82%)	1542 (84%)	292 (16%)	9 (0%)	24	62
2	B	74/392 (19%)	74 (100%)	0	0	100	100
2	C	76/392 (19%)	76 (100%)	0	0	100	100
2	D	74/392 (19%)	74 (100%)	0	0	100	100
2	E	76/392 (19%)	76 (100%)	0	0	100	100
2	F	45/392 (12%)	43 (96%)	2 (4%)	0	100	100
All	All	2188/4215 (52%)	1885 (86%)	294 (13%)	9 (0%)	31	66

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	418	TRP
1	A	1134	GLU
1	A	1738	TRP
1	A	1029	MET
1	A	1739	ILE
1	A	1746	LEU
1	A	424	PRO
1	A	427	ALA
1	A	1028	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1701/2019 (84%)	1692 (100%)	9 (0%)	81	81
2	B	68/342 (20%)	68 (100%)	0	100	100
2	C	70/342 (20%)	70 (100%)	0	100	100
2	D	68/342 (20%)	68 (100%)	0	100	100
2	E	70/342 (20%)	70 (100%)	0	100	100
2	F	42/342 (12%)	42 (100%)	0	100	100
All	All	2019/3729 (54%)	2010 (100%)	9 (0%)	81	82

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	421	LEU
1	A	423	LEU
1	A	426	ASN
1	A	689	TYR
1	A	1294	LEU
1	A	1373	CYS
1	A	1740	ILE
1	A	1743	ASN
1	A	1970	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	65	ASN
1	A	81	HIS
1	A	104	ASN
1	A	186	GLN
1	A	194	GLN
1	A	208	ASN
1	A	302	GLN

Continued on next page...

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Mol	Chain	Res	Type
1	A	315	HIS
1	A	368	HIS
1	A	403	HIS
1	A	414	HIS
1	A	436	ASN
1	A	531	GLN
1	A	583	HIS
1	A	591	ASN
1	A	774	ASN
1	A	775	GLN
1	A	849	ASN
1	A	892	ASN
1	A	925	HIS
1	A	941	ASN
1	A	1002	ASN
1	A	1027	ASN
1	A	1101	ASN
1	A	1109	ASN
1	A	1272	ASN
1	A	1289	ASN
1	A	1338	GLN
1	A	1366	HIS
1	A	1447	GLN
1	A	1622	HIS
1	A	1659	ASN
1	A	1688	ASN
1	A	1898	ASN
1	A	1919	ASN
1	A	1920	GLN
1	A	2024	ASN
1	A	2057	ASN
2	F	372	ASN
2	F	379	GLN
2	B	234	ASN
2	B	255	ASN
2	D	234	ASN
2	D	255	ASN

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

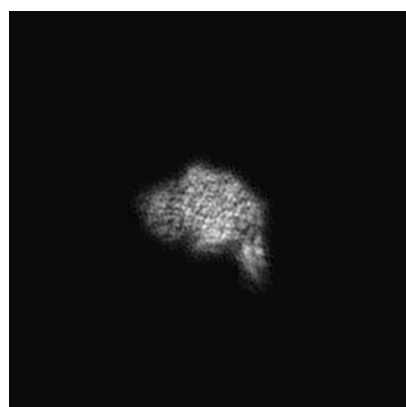
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21095. These allow visual inspection of the internal detail of the map and identification of artifacts.

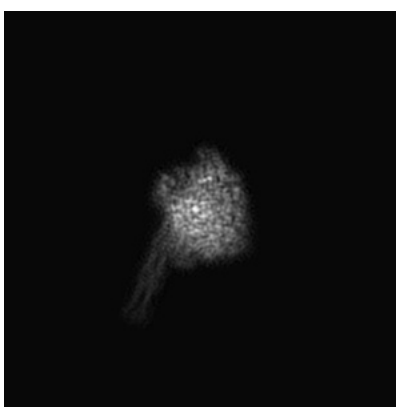
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

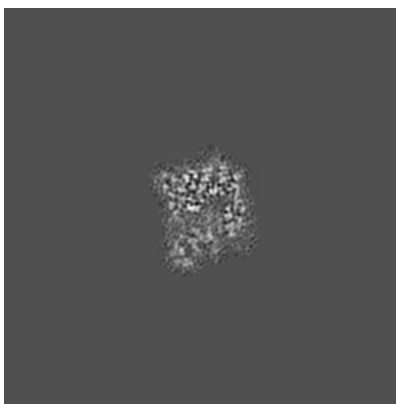
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

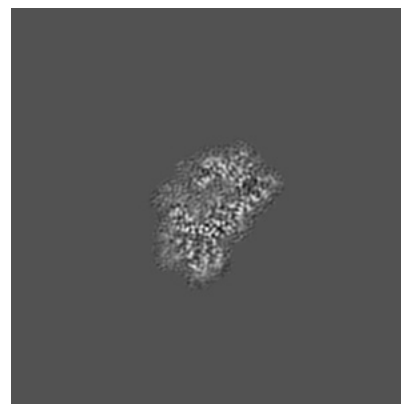
6.2.1 Primary map



X Index: 180



Y Index: 180



Z Index: 180

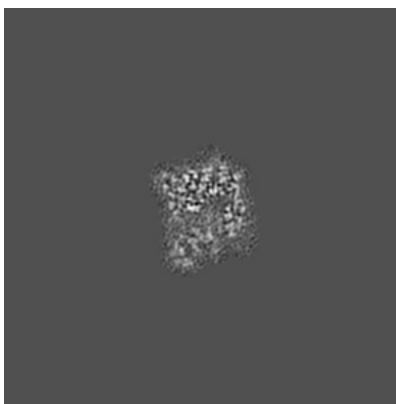
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

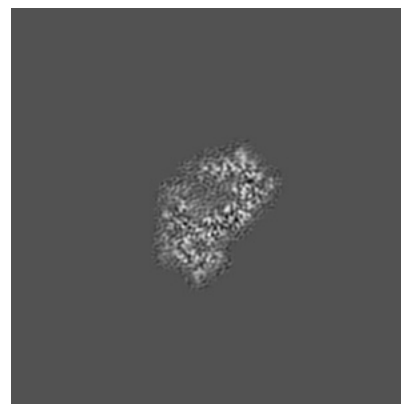
6.3.1 Primary map



X Index: 180



Y Index: 180

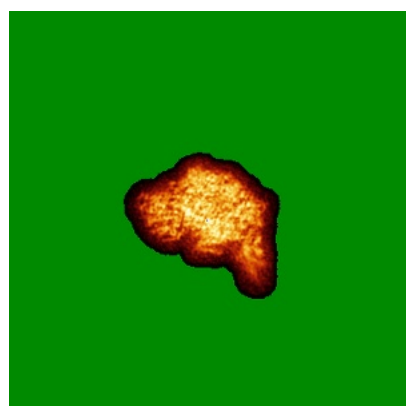


Z Index: 185

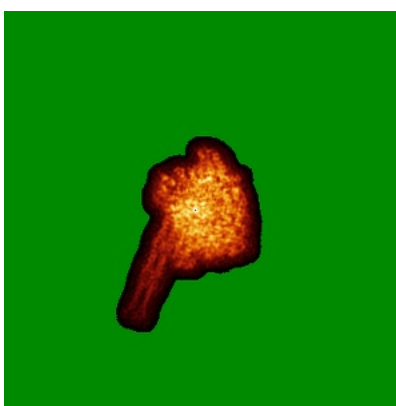
The images above show the largest variance slices of the map in three orthogonal directions.

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

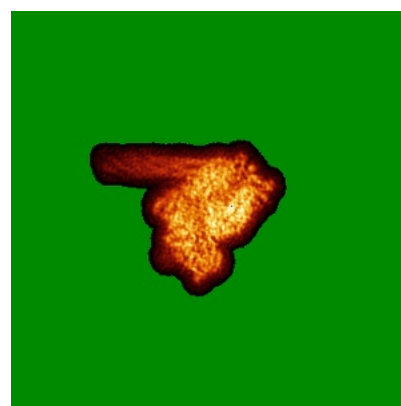
6.4.1 Primary map



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 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

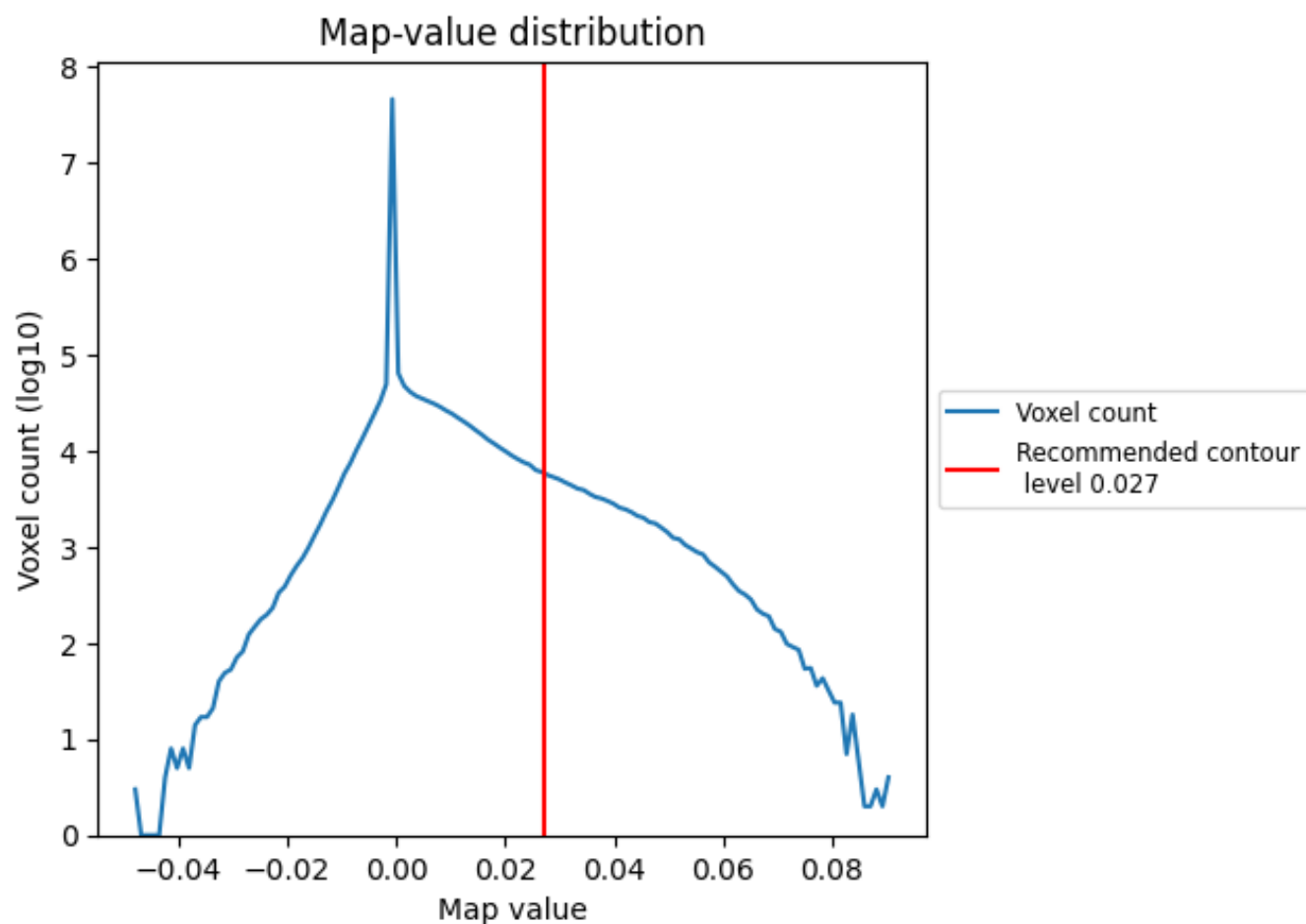
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

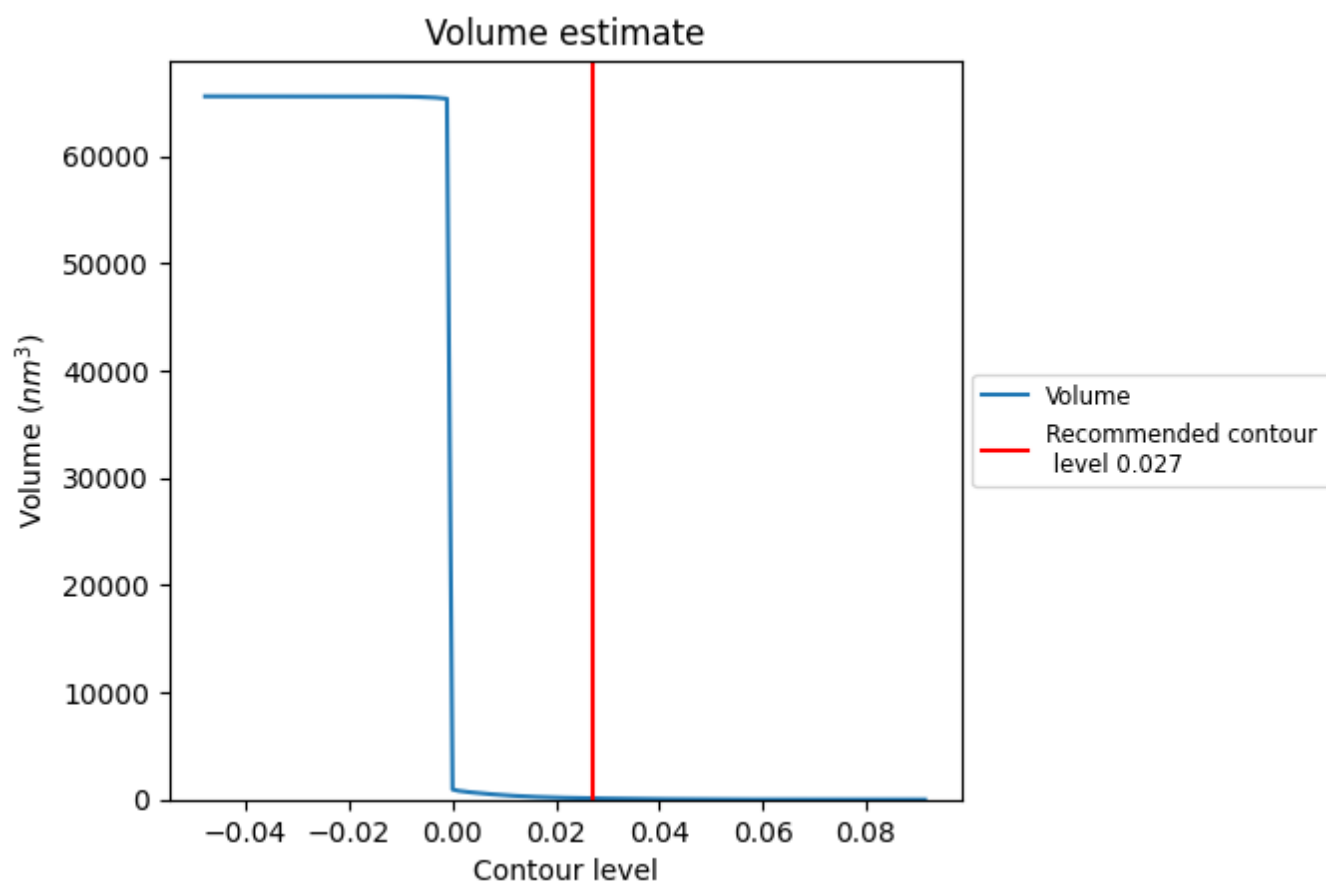
This section contains the results of statistical analysis of the map.

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.

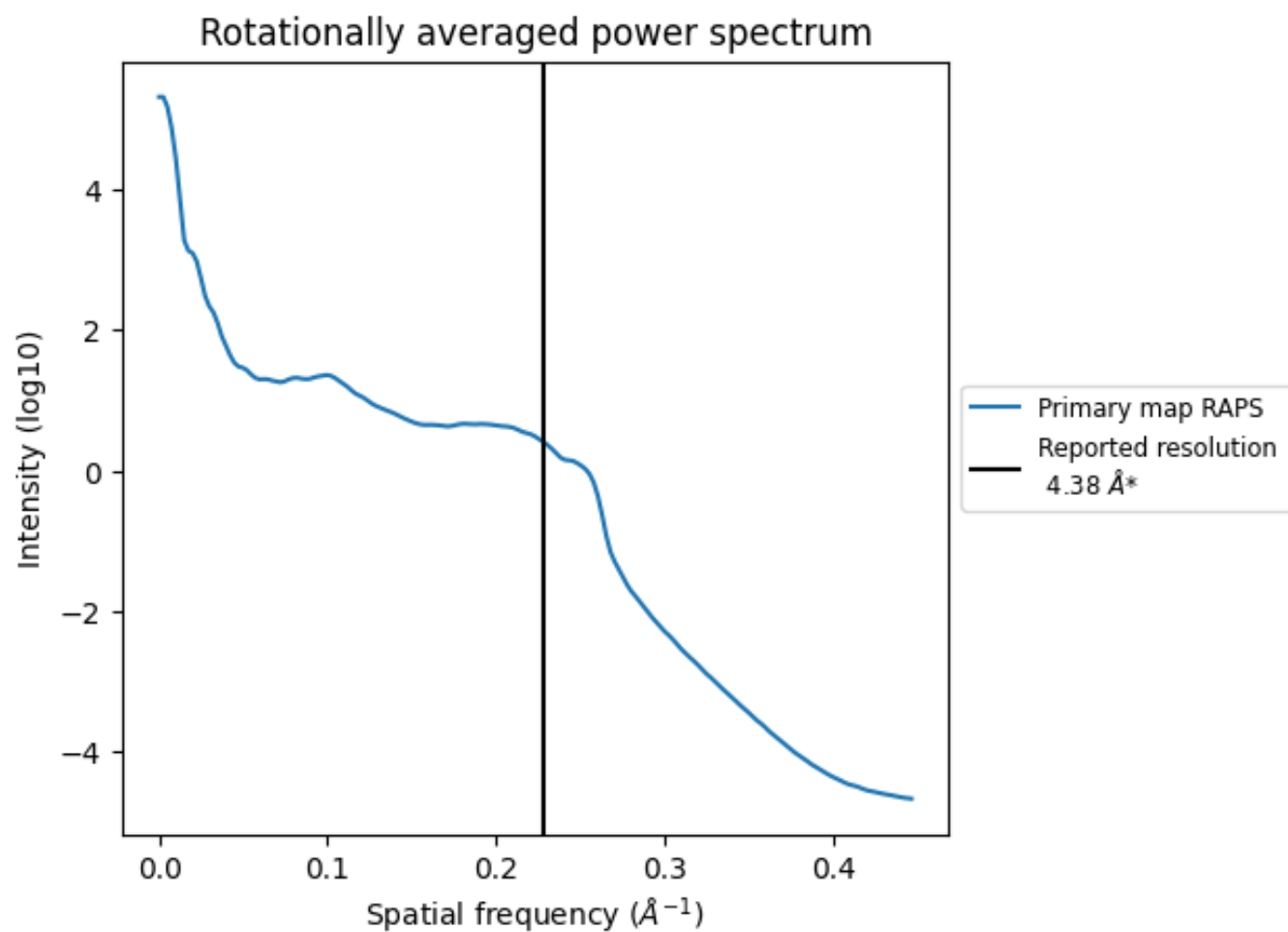
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 116 nm^3 ; this corresponds to an approximate mass of 105 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 ⓘ

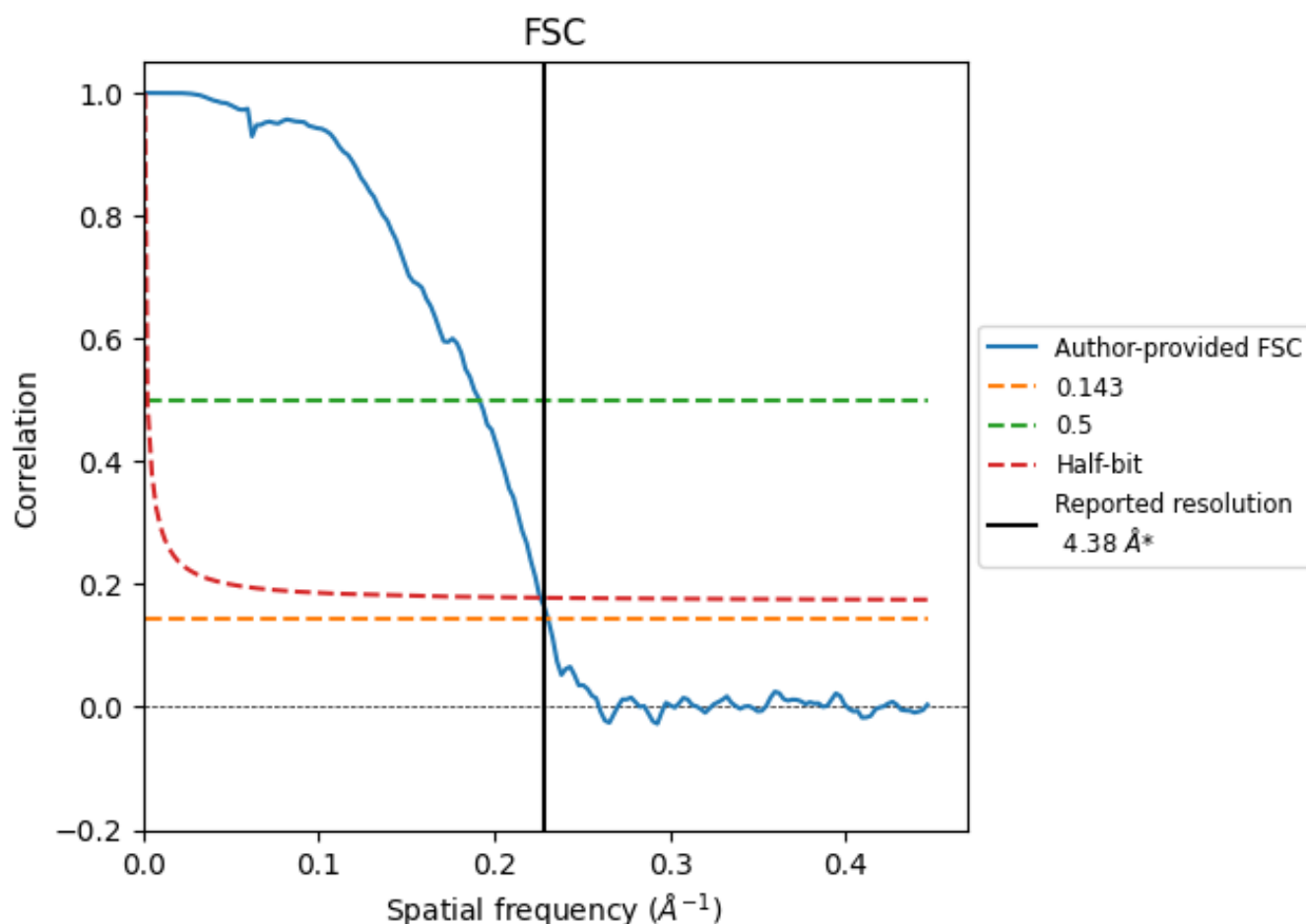


*Reported resolution corresponds to spatial frequency of 0.228 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.228 Å⁻¹

8.2 Resolution estimates [i](#)

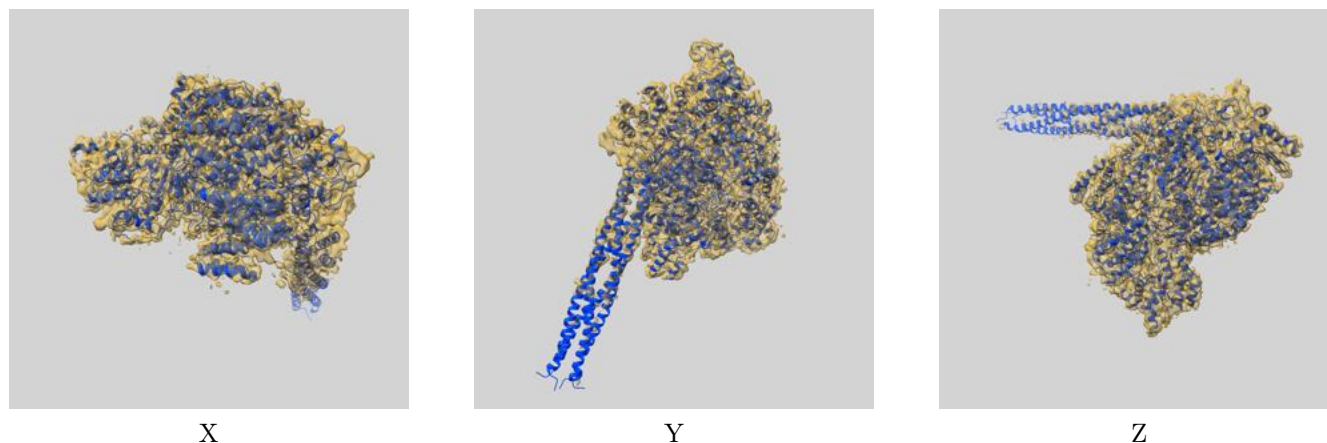
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.38	-	-
Author-provided FSC curve	4.34	5.23	4.43
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

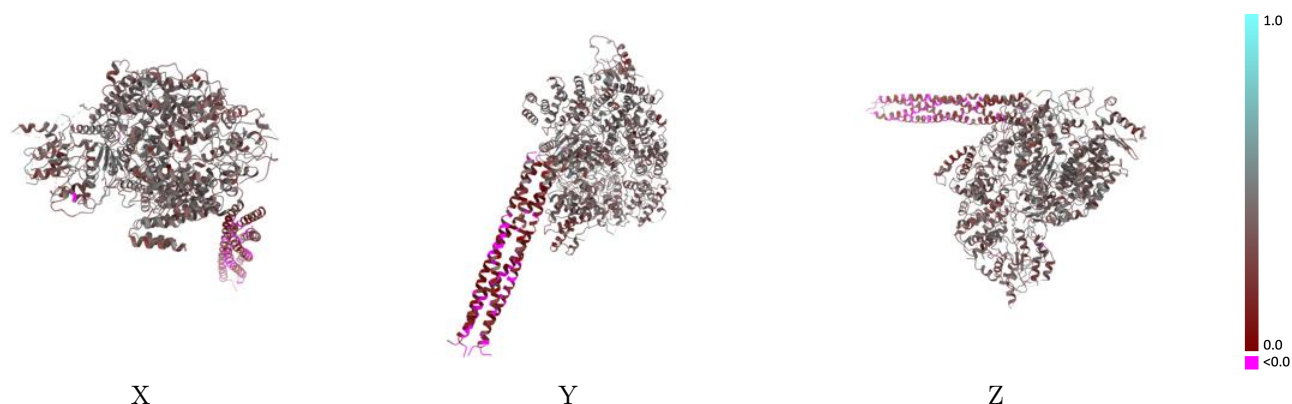
This section contains information regarding the fit between EMDB map EMD-21095 and PDB model 6V85. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



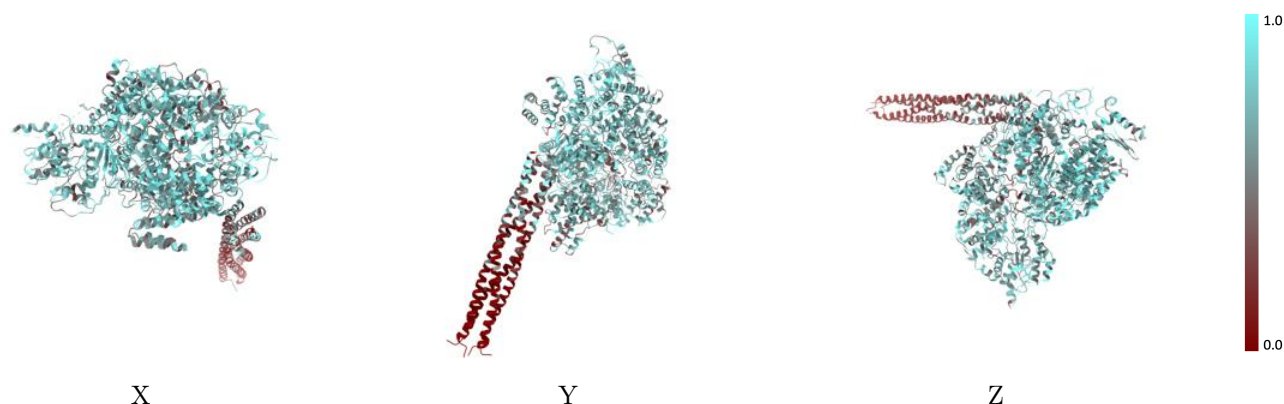
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



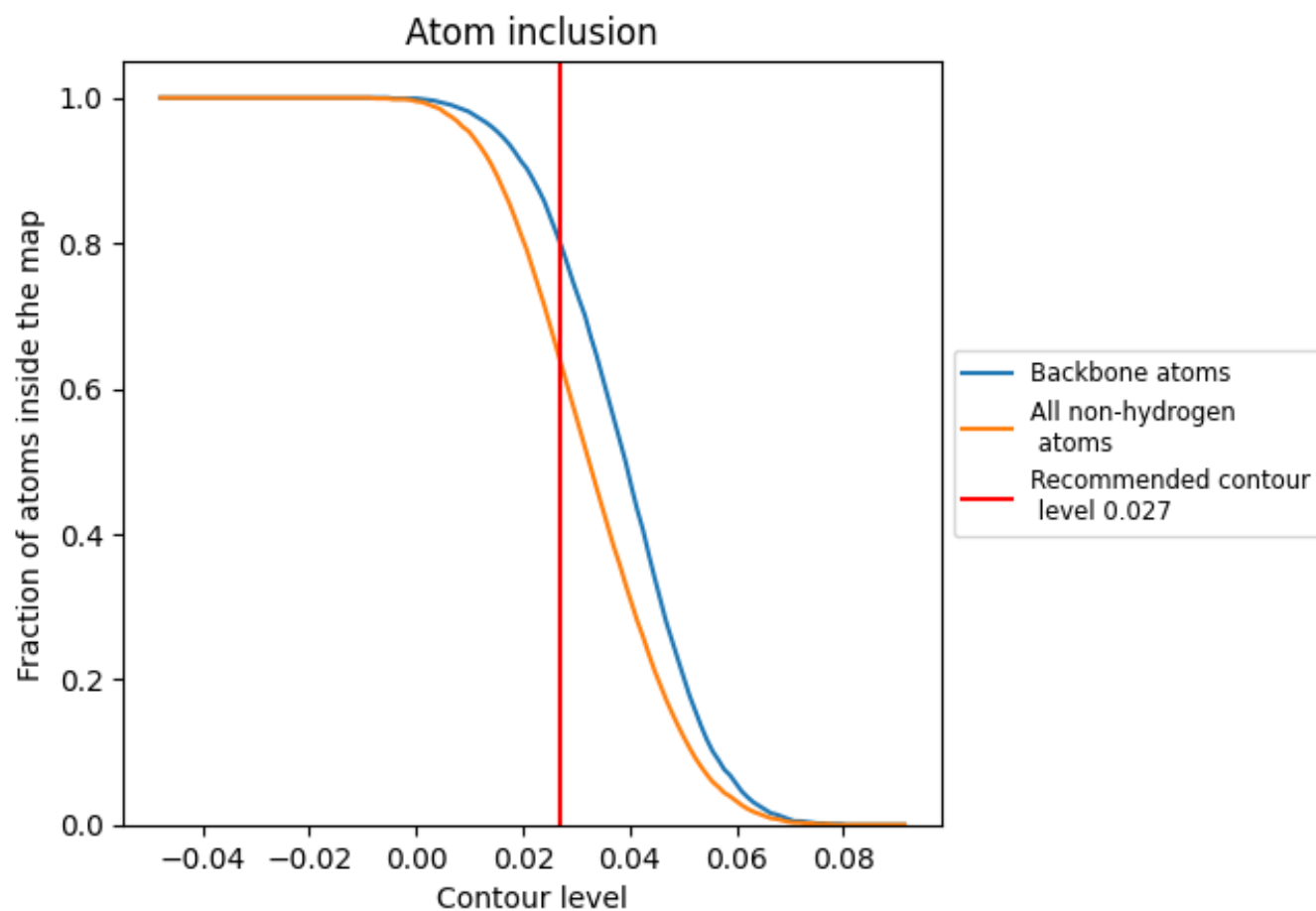
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.027).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 64% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6370	0.3600
A	0.7000	0.3960
B	0.1910	0.1040
C	0.2170	0.0960
D	0.1870	0.1180
E	0.2130	0.1110
F	0.6260	0.3970

1.0

0.0

<0.0