



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:37 PM UTC

PDB ID : 7UFG / pdb_00007ufg
EMDB ID : EMD-26475
Title : Cryo-EM structure of PAPP-A in complex with IGFBP5
Authors : Judge, R.A.; Jain, R.; Hao, Q.; Ouch, C.; Sridar, J.; Smith, C.L.; Wang, J.C.K.; Eaton, D.
Deposited on : 2022-03-22
Resolution : 3.28 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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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

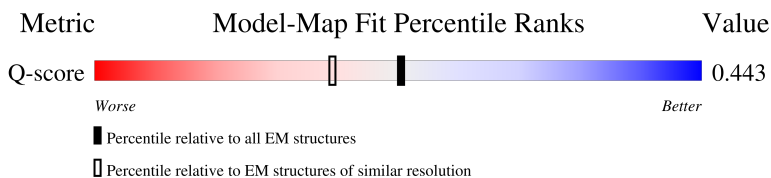
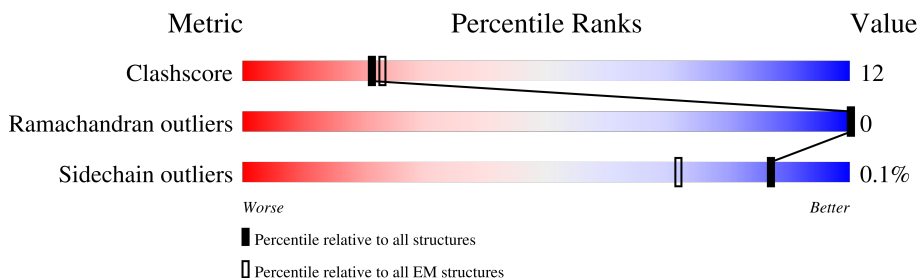
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.28 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	14492 (2.78 - 3.78)

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	1581	 56% 16% 27%
1	B	1581	 58% 16% 25%
2	C	272	 6% 93%
2	D	272	 8% 91%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33028 atoms, of which 14783 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 Pappalysin-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1151	Total	C	H	N	O	S	0	0
			15782	5542	7002	1505	1670	63		
1	B	1182	Total	C	H	N	O	S	0	0
			16506	5734	7411	1549	1746	66		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	483	ALA	GLU	engineered mutation	UNP Q13219
A	1144	TYR	SER	engineered mutation	UNP Q13219
A	1548	SER	-	expression tag	UNP Q13219
A	1549	GLY	-	expression tag	UNP Q13219
A	1550	PRO	-	expression tag	UNP Q13219
A	1551	THR	-	expression tag	UNP Q13219
A	1552	ARG	-	expression tag	UNP Q13219
A	1553	THR	-	expression tag	UNP Q13219
A	1554	ARG	-	expression tag	UNP Q13219
A	1555	PRO	-	expression tag	UNP Q13219
A	1556	LEU	-	expression tag	UNP Q13219
A	1557	GLU	-	expression tag	UNP Q13219
A	1558	GLN	-	expression tag	UNP Q13219
A	1559	LYS	-	expression tag	UNP Q13219
A	1560	LEU	-	expression tag	UNP Q13219
A	1561	ILE	-	expression tag	UNP Q13219
A	1562	SER	-	expression tag	UNP Q13219
A	1563	GLU	-	expression tag	UNP Q13219
A	1564	GLU	-	expression tag	UNP Q13219
A	1565	ASP	-	expression tag	UNP Q13219
A	1566	LEU	-	expression tag	UNP Q13219
A	1567	ALA	-	expression tag	UNP Q13219
A	1568	ALA	-	expression tag	UNP Q13219
A	1569	ASN	-	expression tag	UNP Q13219
A	1570	ASP	-	expression tag	UNP Q13219
A	1571	ILE	-	expression tag	UNP Q13219

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1572	LEU	-	expression tag	UNP Q13219
A	1573	ASP	-	expression tag	UNP Q13219
A	1574	TYR	-	expression tag	UNP Q13219
A	1575	LYS	-	expression tag	UNP Q13219
A	1576	ASP	-	expression tag	UNP Q13219
A	1577	ASP	-	expression tag	UNP Q13219
A	1578	ASP	-	expression tag	UNP Q13219
A	1579	ASP	-	expression tag	UNP Q13219
A	1580	LYS	-	expression tag	UNP Q13219
A	1581	VAL	-	expression tag	UNP Q13219
B	483	ALA	GLU	engineered mutation	UNP Q13219
B	1144	TYR	SER	engineered mutation	UNP Q13219
B	1548	SER	-	expression tag	UNP Q13219
B	1549	GLY	-	expression tag	UNP Q13219
B	1550	PRO	-	expression tag	UNP Q13219
B	1551	THR	-	expression tag	UNP Q13219
B	1552	ARG	-	expression tag	UNP Q13219
B	1553	THR	-	expression tag	UNP Q13219
B	1554	ARG	-	expression tag	UNP Q13219
B	1555	PRO	-	expression tag	UNP Q13219
B	1556	LEU	-	expression tag	UNP Q13219
B	1557	GLU	-	expression tag	UNP Q13219
B	1558	GLN	-	expression tag	UNP Q13219
B	1559	LYS	-	expression tag	UNP Q13219
B	1560	LEU	-	expression tag	UNP Q13219
B	1561	ILE	-	expression tag	UNP Q13219
B	1562	SER	-	expression tag	UNP Q13219
B	1563	GLU	-	expression tag	UNP Q13219
B	1564	GLU	-	expression tag	UNP Q13219
B	1565	ASP	-	expression tag	UNP Q13219
B	1566	LEU	-	expression tag	UNP Q13219
B	1567	ALA	-	expression tag	UNP Q13219
B	1568	ALA	-	expression tag	UNP Q13219
B	1569	ASN	-	expression tag	UNP Q13219
B	1570	ASP	-	expression tag	UNP Q13219
B	1571	ILE	-	expression tag	UNP Q13219
B	1572	LEU	-	expression tag	UNP Q13219
B	1573	ASP	-	expression tag	UNP Q13219
B	1574	TYR	-	expression tag	UNP Q13219
B	1575	LYS	-	expression tag	UNP Q13219
B	1576	ASP	-	expression tag	UNP Q13219
B	1577	ASP	-	expression tag	UNP Q13219

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1578	ASP	-	expression tag	UNP Q13219
B	1579	ASP	-	expression tag	UNP Q13219
B	1580	LYS	-	expression tag	UNP Q13219
B	1581	VAL	-	expression tag	UNP Q13219

- Molecule 2 is a protein called Insulin-like growth factor-binding protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	25	Total	C	H	N	O	0	0
			403	127	197	43	36		
2	C	20	Total	C	H	N	O	0	0
			335	100	173	32	30		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	HIS	-	expression tag	UNP P24593
D	-7	HIS	-	expression tag	UNP P24593
D	-6	HIS	-	expression tag	UNP P24593
D	-5	HIS	-	expression tag	UNP P24593
D	-4	HIS	-	expression tag	UNP P24593
D	-3	HIS	-	expression tag	UNP P24593
D	-2	ALA	-	expression tag	UNP P24593
D	-1	ALA	-	expression tag	UNP P24593
D	0	ALA	-	expression tag	UNP P24593
D	253	ALA	-	expression tag	UNP P24593
D	254	ALA	-	expression tag	UNP P24593
D	255	ALA	-	expression tag	UNP P24593
D	256	ASP	-	expression tag	UNP P24593
D	257	TYR	-	expression tag	UNP P24593
D	258	LYS	-	expression tag	UNP P24593
D	259	ASP	-	expression tag	UNP P24593
D	260	ASP	-	expression tag	UNP P24593
D	261	ASP	-	expression tag	UNP P24593
D	262	ASP	-	expression tag	UNP P24593
D	263	LYS	-	expression tag	UNP P24593
C	-8	HIS	-	expression tag	UNP P24593
C	-7	HIS	-	expression tag	UNP P24593
C	-6	HIS	-	expression tag	UNP P24593
C	-5	HIS	-	expression tag	UNP P24593
C	-4	HIS	-	expression tag	UNP P24593
C	-3	HIS	-	expression tag	UNP P24593

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	ALA	-	expression tag	UNP P24593
C	-1	ALA	-	expression tag	UNP P24593
C	0	ALA	-	expression tag	UNP P24593
C	253	ALA	-	expression tag	UNP P24593
C	254	ALA	-	expression tag	UNP P24593
C	255	ALA	-	expression tag	UNP P24593
C	256	ASP	-	expression tag	UNP P24593
C	257	TYR	-	expression tag	UNP P24593
C	258	LYS	-	expression tag	UNP P24593
C	259	ASP	-	expression tag	UNP P24593
C	260	ASP	-	expression tag	UNP P24593
C	261	ASP	-	expression tag	UNP P24593
C	262	ASP	-	expression tag	UNP P24593
C	263	LYS	-	expression tag	UNP P24593

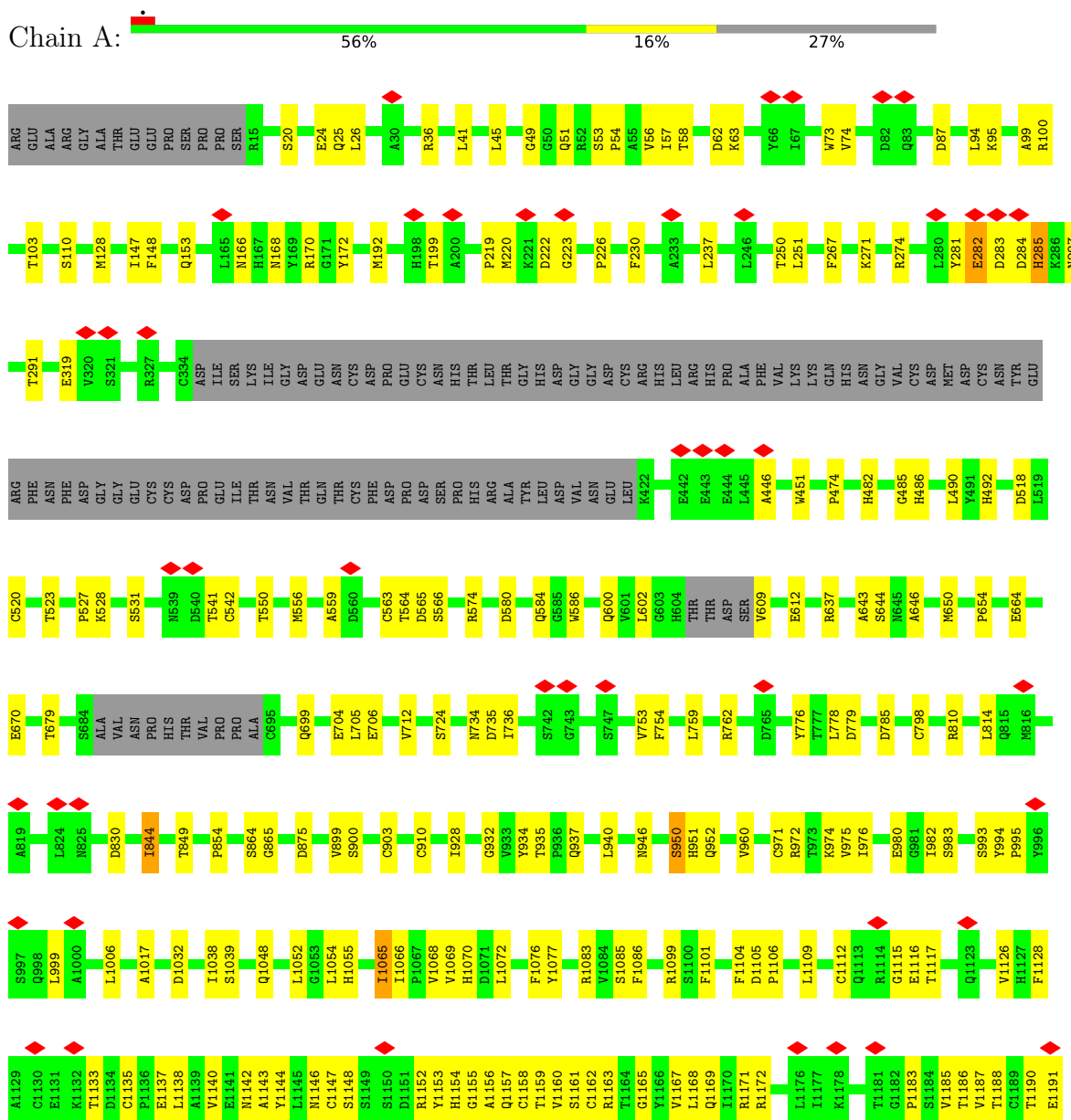
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Zn 1	0
3	B	1	Total 1	Zn 1	0

3 Residue-property plots

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

• Molecule 1: Pappalysin-1



C1266	LEU	SER	PRO	GLY	GLN	C1266	G1192
	ALA	THR	HIS	SER	GLU		LEU
	ALA	VAL	TRP	PHE	GLY		ALA
	ASN	LYS	ASN	HIS	ALA		PRO
	ASP	THR	ASN	VAL	CYS		PRO
	ILE	LYS	PRO	CYS	VAL		PRO
	LEU	LYS	THR	GLN	PRO		VAL
	ASP	VAL	ARG	GLU	VAL		ASN
	THR	THR	VAL	MET	THR		ASN
	LYS	THR	GLU	GLN	CYS		ALA
F1202	ASP	PHE	ARG	GLY	ASP	ASP	F1202
	ASP	PRO	VAL	GLN	PRO	LEU	V1203
	ASP	MET	VAL	CYS	PRO	GLN	D1204
	ASP	THR	VAL	SER	PRO	THR	C1205
	ASP	CYS	THR	VAL	PRO	ALA	F1208
	ASP	ASP	ALA	PRO	LYS	ARG	D1209
	GLN	LEU	GLY	ASN	PHE	CYS	H1210
	GLY	LEU	LEU	GLU	HIS	ARG	H1211
	GLY	LYS	LEU	LEU	GLY	GLU	V1212
	CYS	THR	TRP	SER	TYR	ASN	H1213
A1216	CYS	CYS	HIS	LEU	GLN	LYS	A1216
	ARG	ASP	PRO	LYS	THR	VAL	S1217
	ASP	ALA	PRO	LEU	ASN	GLY	F1218
	GLN	PRO	LEU	GLN	GLY	SER	F1225
	ILE	ILE	ILE	CYS	PHE	PHE	F1226
	GLN	GLN	HIS	PRO	GLN	CYS	G1227
	GLN	CYS	ASN	ASP	PHE	LYS	S1228
	GLU	VAL	VAL	GLY	ASN	TYR	Q1229
	LYS	LYS	LYS	TYR	SER	CYS	F1233
	GLY	GLY	GLY	ILE	GLU	VAL	C1234
H1235	ASP	ASP	PRO	SER	ILE	GLY	R1235
	LEU	PHE	LEU	GLU	LYS	TYR	H1236
	ARG	MET	ASP	CYS	CYS	HIS	F1237
	GLY	GLY	GLY	ALA	GLU	VAL	A1238
	THR	THR	ASP	THR	ASP	PRO	Q1239
	ASN	SER	SER	SER	SER	GLY	L1240
	HIS	TYR	TYR	CYS	ASP	SER	K1241
	GLY	CYS	CYS	LEU	ALA	SER	G1242
	ASP	ASP	ASP	ASP	ARG	ARG	S1245
	GLY	GLY	ALA	HIS	GLN	LYS	L1246
H1250	THR	THR	PRO	ASN	SER	LEU	L1247
	ARG	ARG	ASN	GLU	GLY	LYS	M1250
	THR	THR	ARG	SER	SER	ARG	E1251
	ALA	ALA	ALA	ILE	ASN	ALA	D1252
	PRO	PHE	PHE	ILE	VAL	PHE	L1252
	THR	CYS	CYS	LEU	ILE	LYS	F1255
	GLU	GLU	ASN	PRO	HIS	THR	S1255
	GLN	GLN	TYR	MET	CYS	GLN	W1255
	LYS	LYS	ASP	ASN	ARG	CYS	A1260
	GLY	GLY	GLY	VAL	LYS	THR	L1261
C1262	ILE	ILE	THR	THR	GLY	ASP	C1262
	SER	SER	ASP	VAL	GLY	GLY	E1263
	GLU	GLU	CYS	ARG	THR	GLY	F1263
	ASP	GLU	CYS	ASP	TRP	SER	L1264
	GLU	ASP	THR	TYR	ASN	THR	W1265
	THR	THR	THR	THR	THR	THR	F1265
	THR	THR	THR	THR	THR	THR	F1265
	THR	THR	THR	THR	THR	THR	F1265
	THR	THR	THR	THR	THR	THR	F1265
	THR	THR	THR	THR	THR	THR	F1265

- Molecule 1: Pappalysin-1



A1156	Q1157	C1158	T1159	V1160	S1161	V1084	C932	T679	L421	CYS	L165	ARG
Q1157	S1085	F1086	T1159	V1160	S1161	S1085	T935	H689	L433	ARG	N166	GLU
T1159	I1093	I1093	D941	G942	G943	D941	D941	T690	L445	LEU	N167	ALA
S1161	A1097	A1097	G942	G942	G943	G942	G942	V691	T477	HIS	R170	ARG
G1165	L1098	L1098	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
V1167	R1099	R1099	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
L1168	F1104	F1104	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
Q1169	D1105	D1105	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
T1170	P1106	P1106	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
R1171	V1107	V1107	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
R1172	T1108	T1108	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
ASP	L1109	L1109	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
ASP	S1110	S1110	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
GLU	G1111	G1111	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
LEU	C1112	C1112	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
ILE	Q1113	Q1113	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
LYS	R1114	R1114	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
GLN	G1115	G1115	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
THR	E1116	E1116	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
GLY	T1117	T1117	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
PRO	S1119	S1119	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
S1184	P1120	P1120	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
V1185	E1121	E1121	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
T1186	Q1122	Q1122	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
V1187	R1123	R1123	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
T1188	C1124	C1124	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
C1189	V1125	V1125	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
T1190	C1126	C1126	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
K1193	H1127	H1127	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
W1194	F1128	F1128	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
V1198	C1130	C1130	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
A1199	E1131	E1131	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
C1200	K1132	K1132	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
E1201	T1133	T1133	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
V1203	D1134	D1134	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
D1204	C1135	C1135	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
C1205	P1136	P1136	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
S1206	E1137	E1137	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
T1207	L1138	L1138	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
P1208	A1139	A1139	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
D1209	V1140	V1140	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
H1210	A1143	A1143	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
H1211	Y1144	Y1144	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
Q1212	L1145	L1145	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
V1213	N1146	N1146	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
Y1214	C1147	C1147	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
A1215	S1150	S1150	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
A1216	D1151	D1151	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
S1217	F1218	F1218	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
F1219	Y1153	Y1153	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
A1156	Q1157	C1158	T1159	V1160	S1161	V1084	C932	T679	L421	CYS	L165	ARG
Q1157	S1085	F1086	T1159	V1160	S1161	S1085	T935	H689	L433	ARG	N166	GLU
T1159	I1093	I1093	D941	G942	G943	D941	D941	T690	L445	LEU	N167	ALA
S1161	A1097	A1097	G942	G942	G943	G942	G942	V691	T477	HIS	R170	ARG
G1165	L1098	L1098	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
V1167	R1099	R1099	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
L1168	F1104	F1104	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
Q1169	D1105	D1105	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
T1170	P1106	P1106	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
R1171	V1107	V1107	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
R1172	T1108	T1108	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
ASP	L1109	L1109	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
ASP	S1110	S1110	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
GLU	G1111	G1111	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
LEU	C1112	C1112	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
ILE	Q1113	Q1113	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
LYS	R1114	R1114	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
GLN	G1115	G1115	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
THR	E1116	E1116	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
GLY	T1117	T1117	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
PRO	S1119	S1119	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
S1184	P1120	P1120	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
V1185	E1121	E1121	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
T1186	Q1122	Q1122	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
V1187	R1123	R1123	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
T1188	C1124	C1124	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
C1189	V1125	V1125	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
T1190	C1126	C1126	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
K1193	H1127	H1127	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
W1194	F1128	F1128	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
V1198	C1130	C1130	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
A1199	E1131	E1131	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
C1200	K1132	K1132	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
E1201	T1133	T1133	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
V1203	D1134	D1134	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
D1204	C1135	C1135	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
C1205	P1136	P1136	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
S1206	E1137	E1137	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
T1207	L1138	L1138	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
P1208	A1139	A1139	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
D1209	V1140	V1140	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
H1210	A1143	A1143	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
H1211	Y1144	Y1144	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
Q1212	L1145	L1145	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
V1213	N1146	N1146	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
Y1214	C1147	C1147	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
A1215	S1150	S1150	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
A1216	D1151	D1151	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
S1217	F1218	F1218	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA
F1219	Y1153	Y1153	A947	P691	A947	A947	A947	P692	T477	HIS	R170	ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	245018	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.691	Depositor
Minimum map value	-1.645	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.2305	Depositor
Map size (Å)	365.19998, 365.19998, 365.19998	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.10	0/9019	0.72	56/12321 (0.5%)
1	B	0.10	0/9343	0.39	12/12757 (0.1%)
2	C	0.08	0/161	0.18	0/210
2	D	0.08	0/207	0.17	0/271
All	All	0.10	0/18730	0.57	68/25559 (0.3%)

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	875	ASP	CA-C-N	10.68	142.33	121.18
1	A	875	ASP	C-N-CA	10.68	142.33	121.18
1	A	1077	TYR	CA-C-N	10.57	139.18	122.26
1	A	1077	TYR	C-N-CA	10.57	139.18	122.26
1	A	474	PRO	CA-C-N	10.43	142.17	121.93
1	A	474	PRO	C-N-CA	10.43	142.17	121.93
1	A	946	ASN	CA-C-N	10.23	139.59	120.97
1	A	946	ASN	C-N-CA	10.23	139.59	120.97
1	A	284	ASP	CA-C-N	10.10	144.35	125.66
1	A	284	ASP	C-N-CA	10.10	144.35	125.66
1	B	542	CYS	CA-C-N	9.91	140.83	121.41
1	B	542	CYS	C-N-CA	9.91	140.83	121.41
1	A	285	HIS	CA-C-N	9.86	138.44	121.29
1	A	285	HIS	C-N-CA	9.86	138.44	121.29
1	A	283	ASP	CA-C-N	9.85	138.38	121.14
1	A	283	ASP	C-N-CA	9.85	138.38	121.14
1	B	1015	VAL	CA-C-N	9.76	139.50	122.32
1	B	1015	VAL	C-N-CA	9.76	139.50	122.32
1	A	230	PHE	CA-C-N	9.65	138.66	121.97
1	A	230	PHE	C-N-CA	9.65	138.66	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1065	ILE	CA-C-N	9.63	141.16	123.34
1	A	1065	ILE	C-N-CA	9.63	141.16	123.34
1	A	952	GLN	CA-C-N	9.49	138.64	121.94
1	A	952	GLN	C-N-CA	9.49	138.64	121.94
1	A	983	SER	CA-C-N	9.30	135.48	120.60
1	A	983	SER	C-N-CA	9.30	135.48	120.60
1	A	1054	LEU	CA-C-N	8.64	136.38	122.81
1	A	1054	LEU	C-N-CA	8.64	136.38	122.81
1	B	1046	LYS	CA-C-N	8.57	135.27	122.68
1	B	1046	LYS	C-N-CA	8.57	135.27	122.68
1	B	949	VAL	CA-C-N	8.56	132.44	120.29
1	B	949	VAL	C-N-CA	8.56	132.44	120.29
1	A	654	PRO	CA-C-N	8.55	132.60	120.28
1	A	654	PRO	C-N-CA	8.55	132.60	120.28
1	A	937	GLN	CA-C-N	8.49	134.85	122.46
1	A	937	GLN	C-N-CA	8.49	134.85	122.46
1	A	849	THR	CA-C-N	8.48	132.75	120.71
1	A	849	THR	C-N-CA	8.48	132.75	120.71
1	B	1078	HIS	CA-C-N	8.47	132.90	120.87
1	B	1078	HIS	C-N-CA	8.47	132.90	120.87
1	A	446	ALA	CA-C-N	8.27	132.33	120.91
1	A	446	ALA	C-N-CA	8.27	132.33	120.91
1	A	982	ILE	CA-C-N	8.27	131.71	120.38
1	A	982	ILE	C-N-CA	8.27	131.71	120.38
1	A	934	TYR	CA-C-N	8.20	135.11	123.30
1	A	934	TYR	C-N-CA	8.20	135.11	123.30
1	B	338	LYS	CD-CE-NZ	-8.14	85.85	111.90
1	A	282	GLU	CA-C-N	8.07	131.44	120.38
1	A	282	GLU	C-N-CA	8.07	131.44	120.38
1	A	1006	LEU	CA-C-N	7.89	133.89	123.00
1	A	1006	LEU	C-N-CA	7.89	133.89	123.00
1	A	975	VAL	CA-C-N	7.78	130.36	120.56
1	A	975	VAL	C-N-CA	7.78	130.36	120.56
1	A	319	GLU	CA-C-N	7.71	133.24	123.14
1	A	319	GLU	C-N-CA	7.71	133.24	123.14
1	A	940	LEU	CA-C-N	7.67	132.97	122.77
1	A	940	LEU	C-N-CA	7.67	132.97	122.77
1	A	950	SER	CA-C-N	7.62	132.90	122.77
1	A	950	SER	C-N-CA	7.62	132.90	122.77
1	A	1083	ARG	CA-C-N	7.43	132.29	122.93
1	A	1083	ARG	C-N-CA	7.43	132.29	122.93
1	A	192	MET	CB-CG-SD	7.35	134.75	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	550	THR	OG1-CB-CG2	5.74	120.78	109.30
1	A	199	THR	OG1-CB-CG2	5.62	120.54	109.30
1	A	935	THR	OG1-CB-CG2	5.55	120.41	109.30
1	B	80	ILE	CG1-CB-CG2	5.26	126.50	110.70
1	A	844	ILE	CG1-CB-CG2	5.11	126.02	110.70
1	A	976	ILE	CG1-CB-CG2	5.02	125.77	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8780	7002	8123	199	0
1	B	9095	7411	8490	229	0
2	C	162	173	183	2	0
2	D	206	197	231	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	18245	14783	17027	416	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 12.

All (416) 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:1147:CYS:HA	1:A:1158:CYS:HA	1.39	1.03
1:A:1137:GLU:HA	1:A:1152:ARG:HD2	1.43	1.00
1:B:1144:TYR:HB2	1:B:1161:SER:HB3	1.41	0.99
1:B:1118:TYR:H	1:B:1126:VAL:HG12	1.25	0.99
1:A:1135:CYS:HA	1:A:1192:GLY:HA2	1.43	0.98
1:B:1238:ALA:HB1	1:B:1262:CYS:HB2	1.45	0.98
1:B:87:ASP:OD1	1:B:110:SER:OG	1.90	0.88
1:B:302:LEU:HD11	1:B:480:MET:HE1	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1160:VAL:HG21	1:B:1198:VAL:HG21	1.57	0.87
1:B:1247:LEU:HD21	1:B:1258:PRO:HA	1.55	0.87
1:A:1105:ASP:HB2	1:A:1106:PRO:HD2	1.55	0.86
1:A:1133:THR:HG22	1:A:1191:GLU:HB3	1.56	0.86
1:A:45:LEU:HD22	1:A:57:ILE:HD13	1.59	0.85
1:A:1171:ARG:O	1:A:1197:GLN:N	2.12	0.81
1:B:1074:GLN:HB3	1:B:1075:PRO:HD2	1.63	0.79
1:B:1116:GLU:HG2	1:B:1127:HIS:HA	1.63	0.79
1:B:1108:THR:HA	1:B:1112:CYS:HB2	1.66	0.78
1:B:1116:GLU:HA	1:B:1126:VAL:O	1.84	0.78
1:A:518:ASP:OD2	1:A:523:THR:OG1	2.02	0.77
1:A:1128:PHE:HE1	1:A:1154:HIS:HB3	1.49	0.76
1:B:1190:THR:OG1	1:B:1193:LYS:O	2.04	0.76
1:B:495:ARG:NH1	1:B:517:GLY:O	2.20	0.75
1:B:174:GLU:OE2	1:B:195:HIS:NE2	2.20	0.74
1:A:1144:TYR:N	1:A:1161:SER:O	2.15	0.74
1:B:935:THR:OG1	1:B:941:ASP:OD2	2.03	0.73
1:A:100:ARG:NH1	1:B:1212:GLN:OE1	2.20	0.73
1:A:1160:VAL:HG11	1:A:1198:VAL:HG21	1.70	0.73
1:B:1152:ARG:HD3	1:B:1194:TRP:HZ2	1.52	0.73
1:A:974:LYS:NZ	1:A:1032:ASP:O	2.22	0.73
1:A:609:VAL:N	1:A:830:ASP:O	2.22	0.72
1:B:1160:VAL:N	1:B:1185:VAL:O	2.21	0.72
1:B:1144:TYR:O	1:B:1161:SER:N	2.17	0.71
1:A:147:ILE:HG22	1:A:148:PHE:H	1.54	0.71
1:B:723:VAL:HG22	1:B:726:ASP:HB2	1.72	0.71
1:B:670:GLU:OE1	1:B:670:GLU:N	2.23	0.71
1:B:1147:CYS:HA	1:B:1158:CYS:HA	1.73	0.71
1:A:1250:MET:HE2	1:A:1256:SER:HB2	1.72	0.70
1:A:1133:THR:HA	1:A:1191:GLU:HA	1.74	0.69
1:A:1217:SER:N	1:A:1233:GLN:O	2.22	0.69
1:B:1213:VAL:HG23	1:B:1216:ALA:HB3	1.75	0.69
1:B:677:VAL:HG22	2:D:135:ASP:OD2	1.93	0.69
1:A:451:TRP:NE1	2:C:142:GLN:OE1	2.25	0.69
1:A:1148:SER:N	1:A:1157:GLN:O	2.23	0.68
1:B:489:GLY:O	1:B:574:ARG:NH1	2.25	0.68
1:A:679:THR:HG22	1:A:785:ASP:HA	1.75	0.68
1:A:87:ASP:OD1	1:A:110:SER:OG	2.10	0.68
1:B:482:HIS:CE1	1:B:492:HIS:HE2	2.10	0.68
1:B:1146:ASN:HB3	1:B:1159:THR:HB	1.76	0.68
1:A:643:ALA:HB1	1:A:705:LEU:HD12	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1208:PRO:HB2	1:A:1218:PHE:CD2	2.30	0.67
1:A:646:ALA:N	1:A:664:GLU:OE2	2.28	0.66
1:A:1128:PHE:HZ	1:A:1153:TYR:HB2	1.61	0.66
1:A:1165:GLY:HA3	1:A:1226:PHE:CE2	2.31	0.66
1:B:328:ARG:NH1	1:B:413:ARG:O	2.29	0.66
1:A:950:SER:OG	1:A:951:HIS:ND1	2.25	0.65
1:A:485:GLY:HA3	1:A:556:MET:HE1	1.78	0.65
1:B:45:LEU:HD22	1:B:57:ILE:HD13	1.79	0.65
1:A:1252:ASP:OD2	1:B:98:ARG:NH2	2.30	0.65
1:B:1070:HIS:CE1	1:B:1076:PHE:HA	2.31	0.65
1:A:1225:THR:O	1:A:1228:SER:OG	2.14	0.65
1:A:580:ASP:O	1:A:584:GLN:NE2	2.30	0.64
1:A:62:ASP:OD1	1:A:63:LYS:N	2.31	0.64
1:A:1216:ALA:HA	1:A:1234:CYS:HA	1.80	0.64
1:B:237:LEU:HB3	1:B:602:LEU:HD11	1.80	0.64
1:A:1160:VAL:HB	1:A:1185:VAL:HG12	1.80	0.64
1:B:54:PRO:HB3	1:B:78:HIS:HB2	1.80	0.64
1:B:953:ASP:OD1	1:B:954:GLN:N	2.32	0.63
1:A:1133:THR:HG22	1:A:1191:GLU:CB	2.28	0.63
1:B:1208:PRO:HB2	1:B:1218:PHE:CG	2.33	0.63
1:A:1237:PRO:HD2	1:A:1264:LEU:HD11	1.80	0.63
1:B:1216:ALA:HB2	1:B:1234:CYS:SG	2.39	0.62
1:A:1208:PRO:HB2	1:A:1218:PHE:CG	2.35	0.62
1:B:543:GLY:O	1:B:545:HIS:ND1	2.27	0.62
1:B:1206:SER:O	1:B:1255:TRP:NE1	2.31	0.62
1:A:971:CYS:SG	1:A:972:ARG:N	2.72	0.62
1:B:1144:TYR:N	1:B:1161:SER:O	2.26	0.62
1:A:26:LEU:HD11	1:A:226:PRO:HG3	1.81	0.62
1:A:724:SER:HB2	1:A:779:ASP:OD2	2.00	0.62
1:A:1187:VAL:CG2	1:A:1194:TRP:HB3	2.30	0.62
1:B:1239:GLN:O	1:B:1262:CYS:HA	2.00	0.61
1:A:222:ASP:OD1	1:A:223:GLY:N	2.34	0.61
1:A:637:ARG:NH1	1:A:798:CYS:O	2.33	0.61
1:A:1070:HIS:NE2	1:A:1076:PHE:HA	2.14	0.61
1:B:1216:ALA:HA	1:B:1234:CYS:HA	1.81	0.61
1:B:253:ASP:OD1	1:B:574:ARG:NH2	2.33	0.61
1:A:41:LEU:HD21	1:A:58:THR:HG21	1.83	0.61
1:A:267:PHE:O	1:A:271:LYS:NZ	2.34	0.61
1:A:1104:PHE:CZ	1:B:1109:LEU:HB2	2.35	0.61
1:A:1241:LYS:O	1:A:1260:ALA:HB1	2.01	0.61
1:A:1160:VAL:HB	1:A:1185:VAL:CG1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1128:PHE:CZ	1:A:1153:TYR:HB2	2.36	0.60
1:B:1167:VAL:N	1:B:1201:GLU:O	2.27	0.60
1:B:1251:GLU:OE1	1:B:1251:GLU:N	2.28	0.60
1:B:1119:SER:HB2	1:B:1124:SER:O	2.01	0.60
1:A:1190:THR:N	1:A:1193:LYS:O	2.33	0.60
1:B:1218:PHE:CE1	1:B:1247:LEU:HD12	2.37	0.60
1:B:1167:VAL:HG12	1:B:1201:GLU:O	2.02	0.60
1:B:1156:ALA:H	1:B:1189:CYS:HB3	1.65	0.59
1:B:42:GLN:NE2	1:B:118:TYR:OH	2.34	0.59
1:B:1245:SER:C	1:B:1246:LEU:HD12	2.28	0.59
1:B:838:VAL:HG22	1:B:861:ILE:HG12	1.84	0.59
1:B:999:LEU:HD12	1:B:1000:ALA:N	2.18	0.59
1:B:1126:VAL:HG13	1:B:1129:ALA:HB2	1.82	0.59
1:B:733:VAL:HG12	1:B:733:VAL:O	2.02	0.59
1:A:518:ASP:O	1:A:574:ARG:NH2	2.34	0.59
1:B:1208:PRO:HB2	1:B:1218:PHE:CD2	2.38	0.59
1:B:165:LEU:HD23	1:B:165:LEU:O	2.04	0.58
1:B:553:ASN:O	1:B:565:ASP:N	2.31	0.58
1:B:971:CYS:SG	1:B:972:ARG:N	2.75	0.58
1:B:25:GLN:OE1	1:B:166:ASN:ND2	2.35	0.58
1:B:54:PRO:HD2	1:B:167:HIS:CE1	2.39	0.58
1:A:1137:GLU:HA	1:A:1152:ARG:CD	2.25	0.57
1:A:1172:ARG:HA	1:A:1196:LYS:HA	1.86	0.57
1:B:613:TRP:O	1:B:826:ARG:NH1	2.37	0.57
1:A:220:MET:O	1:A:220:MET:HG2	2.05	0.57
1:B:1106:PRO:O	1:B:1110:SER:N	2.37	0.57
1:A:95:LYS:NZ	1:A:100:ARG:O	2.32	0.57
1:B:1118:TYR:N	1:B:1126:VAL:HG12	2.08	0.57
1:B:1238:ALA:HA	1:B:1263:GLU:O	2.05	0.57
1:A:1165:GLY:O	1:A:1203:VAL:HG23	2.05	0.57
1:A:1229:GLN:HB2	1:A:1247:LEU:O	2.05	0.57
1:A:1143:ALA:HB2	1:A:1200:CYS:SG	2.45	0.57
1:B:974:LYS:NZ	1:B:1032:ASP:O	2.35	0.57
1:B:697:GLU:N	1:B:697:GLU:OE1	2.37	0.56
1:B:1118:TYR:HA	1:B:1125:CYS:HA	1.87	0.56
1:B:646:ALA:N	1:B:664:GLU:OE2	2.38	0.56
1:A:600:GLN:N	1:A:612:GLU:O	2.37	0.56
1:B:45:LEU:CD2	1:B:57:ILE:HD13	2.34	0.56
1:A:753:VAL:HG22	1:A:759:LEU:HD12	1.88	0.56
1:B:54:PRO:HB3	1:B:78:HIS:CB	2.35	0.56
1:B:334:CYS:SG	1:B:335:ASP:N	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1187:VAL:HG21	1:B:1194:TRP:HB3	1.88	0.56
1:B:1156:ALA:N	1:B:1189:CYS:HB3	2.20	0.56
1:A:1128:PHE:CE1	1:A:1154:HIS:HB3	2.36	0.56
1:A:1239:GLN:O	1:A:1262:CYS:HA	2.06	0.56
1:A:1142:ASN:C	1:A:1163:ARG:HD3	2.30	0.56
1:A:274:ARG:NE	1:A:586:TRP:O	2.35	0.55
1:B:823:HIS:ND1	1:B:827:LYS:O	2.34	0.55
1:B:1204:ASP:HA	1:B:1225:THR:HA	1.88	0.55
1:B:1217:SER:N	1:B:1233:GLN:O	2.32	0.55
1:A:1109:LEU:HD13	1:B:1104:PHE:HE2	1.71	0.55
1:A:1138:LEU:HB3	1:A:1152:ARG:NH1	2.21	0.55
1:B:302:LEU:CD1	1:B:480:MET:HE1	2.33	0.55
1:A:1017:ALA:HA	1:B:1072:LEU:HD22	1.88	0.55
1:B:1105:ASP:HB3	1:B:1106:PRO:HD2	1.87	0.55
1:A:1117:THR:N	1:A:1126:VAL:O	2.39	0.55
1:B:1208:PRO:HG3	1:B:1255:TRP:NE1	2.22	0.55
1:A:1152:ARG:NH1	1:A:1158:CYS:SG	2.80	0.55
1:A:1101:PHE:CZ	1:B:1072:LEU:HD21	2.42	0.55
1:A:1142:ASN:HA	1:A:1163:ARG:NH1	2.21	0.55
1:A:1245:SER:C	1:A:1246:LEU:HD12	2.31	0.55
1:A:1261:LEU:HD23	1:B:151:LEU:HD13	1.87	0.55
1:B:947:ALA:HB1	1:B:961:ILE:HD11	1.89	0.55
1:B:1040:VAL:HG22	1:B:1084:VAL:HG22	1.88	0.55
1:B:279:ASN:HB3	1:B:290:VAL:HG12	1.88	0.55
1:B:1169:GLN:O	1:B:1198:VAL:HA	2.07	0.55
1:B:1108:THR:HA	1:B:1112:CYS:CB	2.36	0.54
1:B:677:VAL:HG23	1:B:678:ARG:HD2	1.89	0.54
1:B:1119:SER:HB3	1:B:1120:PRO:HD2	1.90	0.54
1:A:1160:VAL:CG1	1:A:1198:VAL:HG21	2.38	0.54
1:A:1210:HIS:HA	1:A:1213:VAL:O	2.07	0.54
1:B:198:HIS:ND1	1:B:199:THR:O	2.41	0.54
1:A:1116:GLU:HB2	1:A:1126:VAL:O	2.08	0.54
1:A:281:TYR:OH	1:A:291:THR:HG21	2.08	0.54
1:A:735:ASP:OD1	1:A:736:ILE:N	2.41	0.54
1:A:1133:THR:O	1:A:1154:HIS:HB2	2.08	0.53
1:B:1126:VAL:CG1	1:B:1129:ALA:HB2	2.38	0.53
1:A:903:CYS:SG	1:A:910:CYS:N	2.81	0.53
1:B:1140:VAL:HG21	1:B:1198:VAL:HG23	1.89	0.53
1:B:928:ILE:O	1:B:932:GLY:N	2.41	0.53
1:A:1216:ALA:HB2	1:A:1234:CYS:SG	2.49	0.53
1:A:1155:GLY:HA2	1:A:1188:THR:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:HIS:O	1:B:195:HIS:ND1	2.42	0.53
1:A:670:GLU:N	1:A:670:GLU:OE1	2.42	0.53
1:B:1240:LEU:HA	1:B:1261:LEU:O	2.09	0.52
1:A:1052:LEU:O	1:A:1052:LEU:HG	2.08	0.52
1:A:1162:CYS:SG	1:A:1168:LEU:HA	2.49	0.52
1:A:679:THR:HG22	1:A:785:ASP:CA	2.38	0.52
1:A:1105:ASP:HB2	1:A:1106:PRO:CD	2.33	0.52
1:A:1187:VAL:HG22	1:A:1194:TRP:CE3	2.45	0.52
1:A:103:THR:HB	1:A:128:MET:HE1	1.92	0.52
1:A:1205:CYS:HB3	1:A:1255:TRP:CD1	2.45	0.52
1:A:1133:THR:CA	1:A:1191:GLU:HA	2.40	0.52
1:A:51:GLN:NE2	1:A:170:ARG:O	2.38	0.52
1:B:51:GLN:NE2	1:B:170:ARG:O	2.37	0.52
1:A:1152:ARG:HD3	1:A:1194:TRP:HZ2	1.74	0.51
1:A:520:CYS:SG	1:A:574:ARG:NH2	2.83	0.51
1:A:166:ASN:OD1	1:A:168:ASN:ND2	2.43	0.51
1:B:237:LEU:HD22	1:B:602:LEU:HD21	1.91	0.51
1:B:49:GLY:O	1:B:170:ARG:NH2	2.43	0.51
1:A:1072:LEU:HB2	1:B:1068:VAL:HG23	1.93	0.51
1:B:183:ARG:NH1	1:B:187:GLU:OE2	2.44	0.51
1:B:1165:GLY:O	1:B:1203:VAL:HG23	2.11	0.51
1:A:482:HIS:CE1	1:A:492:HIS:HE2	2.28	0.51
1:A:864:SER:OG	1:A:865:GLY:N	2.43	0.51
1:A:960:VAL:HG23	1:A:960:VAL:O	2.09	0.51
1:A:1167:VAL:HG12	1:A:1201:GLU:O	2.10	0.51
1:A:20:SER:OG	1:A:24:GLU:OE2	2.27	0.51
1:A:1052:LEU:HD11	1:A:1068:VAL:HG22	1.92	0.51
1:B:1132:LYS:O	1:B:1153:TYR:HA	2.11	0.51
1:B:1205:CYS:O	1:B:1206:SER:OG	2.22	0.51
1:A:1055:HIS:NE2	1:A:1066:ILE:HG23	2.27	0.50
1:B:723:VAL:CG2	1:B:726:ASP:HB2	2.41	0.50
1:B:1237:PRO:HD2	1:B:1264:LEU:HD12	1.93	0.50
1:B:607:ASP:OD1	1:B:607:ASP:N	2.43	0.50
1:A:1112:CYS:HA	1:A:1116:GLU:OE2	2.12	0.50
1:B:712:VAL:O	1:B:712:VAL:HG13	2.12	0.50
1:A:1115:GLY:HA2	1:A:1154:HIS:CE1	2.47	0.49
1:A:993:SER:OG	1:A:994:TYR:N	2.43	0.49
1:B:602:LEU:HD22	1:B:612:GLU:OE1	2.12	0.49
1:B:1042:LEU:C	1:B:1043:LEU:HD23	2.38	0.49
1:B:1132:LYS:HA	1:B:1153:TYR:HB2	1.94	0.49
1:A:899:VAL:O	1:A:900:SER:OG	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1076:PHE:HB2	1:A:1106:PRO:HB3	1.94	0.49
1:A:1250:MET:CE	1:A:1256:SER:HB2	2.41	0.49
1:A:1156:ALA:O	1:A:1188:THR:HA	2.13	0.49
1:A:1160:VAL:HG11	1:A:1198:VAL:CG2	2.41	0.49
1:B:339:ILE:HG13	1:B:415:TYR:OH	2.13	0.48
1:A:1187:VAL:HG22	1:A:1194:TRP:HE3	1.77	0.48
1:B:334:CYS:HB2	1:B:348:CYS:HA	1.94	0.48
1:B:1159:THR:HA	1:B:1186:THR:HA	1.95	0.48
1:B:1217:SER:O	1:B:1232:PHE:HA	2.11	0.48
1:B:433:LEU:HD23	1:B:433:LEU:O	2.13	0.48
1:A:49:GLY:O	1:A:170:ARG:NH2	2.47	0.48
1:B:1145:LEU:CD2	1:B:1160:VAL:HG13	2.43	0.48
1:B:1157:GLN:HA	1:B:1187:VAL:O	2.12	0.48
1:A:1052:LEU:CD1	1:A:1068:VAL:HG22	2.44	0.48
1:A:1146:ASN:HB3	1:A:1159:THR:HB	1.94	0.48
1:B:1042:LEU:CD1	1:B:1052:LEU:HD22	2.43	0.48
1:B:1187:VAL:CG2	1:B:1194:TRP:HB3	2.43	0.48
1:A:650:MET:HE2	1:A:650:MET:HA	1.94	0.48
1:A:1144:TYR:HB2	1:A:1161:SER:HB3	1.96	0.48
1:A:1155:GLY:HA2	1:A:1188:THR:CG2	2.44	0.48
1:A:486:HIS:CE1	1:A:492:HIS:NE2	2.81	0.48
1:B:252:CYS:SG	1:B:581:LEU:HD13	2.54	0.48
1:B:1137:GLU:HA	1:B:1152:ARG:NE	2.29	0.48
1:B:1219:SER:O	1:B:1230:CYS:HB3	2.13	0.48
1:B:542:CYS:SG	1:B:1056:VAL:HG11	2.54	0.47
1:A:1208:PRO:HB2	1:A:1218:PHE:CE2	2.49	0.47
1:A:960:VAL:O	1:A:960:VAL:CG2	2.62	0.47
1:B:1119:SER:HB3	1:B:1120:PRO:CD	2.44	0.47
1:B:1207:ILE:HG13	1:B:1207:ILE:O	2.13	0.47
1:B:418:VAL:O	1:B:421:LEU:N	2.48	0.47
1:B:679:THR:OG1	1:B:783:GLU:OE1	2.31	0.47
1:B:1016:ALA:O	1:B:1068:VAL:HG21	2.15	0.47
1:B:1131:GLU:HG3	1:B:1134:ASP:OD2	2.15	0.47
1:B:1126:VAL:O	1:B:1126:VAL:HG13	2.15	0.47
1:A:1161:SER:HA	1:A:1183:PRO:O	2.14	0.47
1:A:1213:VAL:HG23	1:A:1216:ALA:HB3	1.96	0.47
1:B:1015:VAL:HG22	1:B:1106:PRO:HD3	1.97	0.47
1:B:1165:GLY:C	1:B:1203:VAL:HG23	2.40	0.47
1:B:1145:LEU:HD23	1:B:1160:VAL:HG13	1.97	0.47
1:A:1205:CYS:HB3	1:A:1255:TRP:NE1	2.30	0.46
1:B:734:ASN:C	1:B:734:ASN:HD22	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1190:THR:O	1:A:1191:GLU:HG2	2.16	0.46
1:A:485:GLY:HA2	1:A:490:LEU:HD12	1.96	0.46
1:A:753:VAL:HG12	1:A:754:PHE:O	2.16	0.46
1:A:250:THR:HG22	1:A:251:LEU:N	2.29	0.46
1:B:1155:GLY:HA2	1:B:1189:CYS:O	2.15	0.46
1:A:1251:GLU:OE1	1:A:1251:GLU:N	2.33	0.46
1:B:999:LEU:HD12	1:B:1000:ALA:HB2	1.98	0.46
1:B:1109:LEU:O	1:B:1109:LEU:HD12	2.15	0.46
1:A:237:LEU:CD2	1:A:602:LEU:HD11	2.46	0.45
1:B:71:ARG:NH1	1:B:97:ASP:O	2.48	0.45
1:B:994:TYR:N	1:B:995:PRO:HD2	2.31	0.45
1:B:250:THR:HG22	1:B:251:LEU:N	2.31	0.45
1:B:1108:THR:O	1:B:1112:CYS:HB3	2.15	0.45
1:B:1218:PHE:CZ	1:B:1247:LEU:HD12	2.52	0.45
1:A:1138:LEU:HB2	1:A:1194:TRP:NE1	2.31	0.45
1:A:1209:ASP:OD1	1:A:1211:HIS:HB2	2.15	0.45
1:B:711:LEU:HD13	1:B:791:SER:HB2	1.99	0.45
1:B:1074:GLN:HB3	1:B:1075:PRO:CD	2.40	0.45
1:B:1218:PHE:HE1	1:B:1247:LEU:HD12	1.79	0.45
1:B:1226:PHE:HA	1:B:1249:CYS:SG	2.56	0.45
1:A:1140:VAL:HG21	1:A:1198:VAL:CG2	2.47	0.45
1:B:691:VAL:CG1	1:B:692:PRO:HD2	2.45	0.45
1:B:1017:ALA:N	1:B:1099:ARG:O	2.45	0.45
1:B:1152:ARG:NH1	1:B:1158:CYS:SG	2.89	0.45
1:B:1247:LEU:HD21	1:B:1258:PRO:CA	2.36	0.45
1:A:1101:PHE:HZ	1:B:1072:LEU:HD21	1.79	0.45
1:A:1140:VAL:HG21	1:A:1198:VAL:HG23	1.99	0.45
1:B:53:SER:HA	1:B:54:PRO:HA	1.69	0.45
1:B:529:HIS:ND1	1:B:531:SER:OG	2.42	0.45
1:B:1158:CYS:C	1:B:1186:THR:HG23	2.41	0.45
1:A:1226:PHE:CE2	1:A:1251:GLU:HA	2.52	0.45
1:A:565:ASP:OD1	1:A:566:SER:N	2.43	0.45
1:B:1119:SER:OG	1:B:1126:VAL:HA	2.17	0.45
1:A:1048:GLN:OE1	1:A:1048:GLN:HA	2.16	0.45
1:B:160:LEU:HD11	1:B:173:ILE:HD13	1.99	0.45
1:B:331:LEU:HD13	1:B:334:CYS:HB3	1.99	0.45
1:B:1015:VAL:CG2	1:B:1106:PRO:HD3	2.47	0.45
1:A:282:GLU:OE2	1:A:287:ASN:ND2	2.48	0.44
1:A:1072:LEU:HD21	1:B:1076:PHE:HE1	1.82	0.44
1:A:1133:THR:HB	1:A:1191:GLU:H	1.82	0.44
1:B:250:THR:N	1:B:253:ASP:OD2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:ILE:HD13	1:A:854:PRO:HA	2.00	0.44
1:B:1138:LEU:HD22	1:B:1194:TRP:CD1	2.52	0.44
1:A:172:TYR:OH	1:A:762:ARG:NE	2.50	0.44
1:B:1038:ILE:HG22	1:B:1086:PHE:HB3	1.98	0.44
1:B:33:GLU:O	1:B:205:LEU:HD11	2.16	0.44
1:A:237:LEU:HD23	1:A:602:LEU:HD11	1.99	0.44
1:A:1039:SER:OG	1:A:1085:SER:OG	2.33	0.44
1:A:734:ASN:HB2	1:A:778:LEU:HD23	2.00	0.44
1:A:1169:GLN:OE1	1:A:1171:ARG:NH2	2.51	0.44
1:A:1242:GLY:HA3	1:A:1260:ALA:HB2	2.00	0.44
1:B:1138:LEU:HB2	1:B:1194:TRP:NE1	2.33	0.44
1:B:1145:LEU:HA	1:B:1159:THR:O	2.16	0.44
1:A:1069:VAL:HG12	1:B:1071:ASP:HA	1.99	0.44
1:A:41:LEU:HD21	1:A:58:THR:CG2	2.47	0.44
1:A:1070:HIS:CE1	1:A:1076:PHE:HA	2.52	0.44
1:B:17:LEU:HD23	1:B:19:PHE:CE1	2.53	0.44
1:B:943:TRP:CE3	1:B:1097:ALA:HB2	2.52	0.44
1:A:147:ILE:HG22	1:A:148:PHE:N	2.25	0.44
1:A:1038:ILE:HG22	1:A:1086:PHE:HB3	1.99	0.44
1:B:602:LEU:HD13	1:B:612:GLU:OE1	2.17	0.44
1:B:1120:PRO:O	1:B:1122:GLU:N	2.51	0.44
1:B:1129:ALA:O	1:B:1130:CYS:HB2	2.18	0.44
1:B:1152:ARG:HD3	1:B:1194:TRP:CZ2	2.42	0.44
1:A:650:MET:HE2	1:A:650:MET:CA	2.48	0.43
1:A:699:GLN:HE22	1:A:776:TYR:HE1	1.65	0.43
1:B:733:VAL:CG2	1:B:753:VAL:HG11	2.48	0.43
1:B:1138:LEU:HB2	1:B:1194:TRP:HE1	1.82	0.43
1:B:58:THR:HB	1:B:160:LEU:HD12	2.00	0.43
1:B:1234:CYS:HB3	1:B:1238:ALA:HB3	2.00	0.43
1:A:99:ALA:N	1:B:1254:LEU:HD13	2.33	0.43
1:A:1187:VAL:HG21	1:A:1194:TRP:HB3	1.98	0.43
1:B:70:ASP:OD1	1:B:70:ASP:N	2.44	0.43
1:A:41:LEU:HD22	1:A:73:TRP:CZ3	2.53	0.43
1:A:563:CYS:O	1:A:564:THR:C	2.61	0.43
1:B:691:VAL:HG13	1:B:692:PRO:HD2	2.00	0.43
1:B:1042:LEU:HD11	1:B:1052:LEU:HD22	1.99	0.43
1:B:1070:HIS:O	1:B:1070:HIS:CG	2.71	0.43
1:B:1237:PRO:HD2	1:B:1264:LEU:CD1	2.48	0.43
1:B:673:CYS:N	1:B:721:THR:O	2.50	0.43
1:B:1247:LEU:CD2	1:B:1258:PRO:HA	2.39	0.43
1:A:541:THR:OG1	1:A:542:CYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:GLN:NE2	1:B:477:THR:OG1	2.52	0.43
1:A:527:PRO:O	1:A:528:LYS:C	2.60	0.43
1:B:1131:GLU:O	1:B:1154:HIS:HB2	2.19	0.43
1:B:1224:THR:HG22	1:B:1255:TRP:HZ2	1.83	0.43
1:A:1251:GLU:HG2	1:A:1252:ASP:N	2.34	0.43
1:B:417:ASP:O	1:B:418:VAL:C	2.62	0.43
1:B:734:ASN:O	1:B:734:ASN:ND2	2.50	0.43
1:A:704:GLU:C	1:A:705:LEU:HD22	2.44	0.43
1:A:928:ILE:O	1:A:932:GLY:N	2.51	0.43
1:B:1143:ALA:HB2	1:B:1200:CYS:SG	2.59	0.43
2:C:125:SER:OG	2:C:128:LYS:HD3	2.18	0.43
1:B:1072:LEU:HD23	1:B:1072:LEU:O	2.19	0.42
1:B:1105:ASP:HB2	1:B:1107:VAL:HG22	2.01	0.42
1:A:644:SER:HG	1:A:706:GLU:C	2.27	0.42
1:A:1142:ASN:HA	1:A:1163:ARG:HH11	1.84	0.42
1:B:69:ARG:O	1:B:69:ARG:HG2	2.20	0.42
1:B:1146:ASN:N	1:B:1159:THR:O	2.37	0.42
1:B:906:GLU:HB3	1:B:907:PRO:HD3	2.00	0.42
1:A:650:MET:HE2	1:A:650:MET:N	2.34	0.42
1:A:1186:THR:O	1:A:1196:LYS:HD2	2.19	0.42
1:B:186:ARG:NH1	1:B:905:ASP:OD2	2.52	0.42
1:A:753:VAL:CG2	1:A:759:LEU:HD12	2.49	0.42
1:A:995:PRO:HD2	1:A:999:LEU:HD21	2.00	0.42
1:B:279:ASN:CB	1:B:290:VAL:HG12	2.50	0.42
1:A:1065:ILE:O	1:A:1065:ILE:HG23	2.19	0.42
1:B:298:GLN:CG	1:B:480:MET:HE3	2.48	0.42
1:A:810:ARG:CZ	1:A:814:LEU:HD23	2.49	0.42
1:A:1052:LEU:CD2	1:A:1066:ILE:HG21	2.50	0.42
1:A:36:ARG:NH2	1:A:153:GLN:OE1	2.52	0.42
1:A:1135:CYS:CA	1:A:1192:GLY:HA2	2.31	0.42
1:B:961:ILE:HG22	1:B:1093:ILE:O	2.20	0.42
1:B:1070:HIS:NE2	1:B:1076:PHE:HA	2.35	0.42
1:B:1069:VAL:HG23	1:B:1070:HIS:N	2.35	0.41
1:A:1235:ARG:O	1:A:1238:ALA:HB3	2.20	0.41
1:B:613:TRP:CE3	1:B:843:VAL:HG21	2.55	0.41
1:A:73:TRP:HB3	1:A:94:LEU:HD13	2.02	0.41
1:A:1144:TYR:CE2	1:A:1163:ARG:HG3	2.55	0.41
1:B:17:LEU:HD23	1:B:19:PHE:CZ	2.56	0.41
1:B:699:GLN:HG2	1:B:700:GLY:N	2.36	0.41
1:B:1210:HIS:HA	1:B:1213:VAL:O	2.20	0.41
1:B:1234:CYS:HB3	1:B:1238:ALA:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:SER:C	1:A:559:ALA:HB1	2.45	0.41
1:A:712:VAL:O	1:A:712:VAL:HG13	2.21	0.41
1:B:1253:GLY:O	1:B:1254:LEU:HD23	2.20	0.41
1:A:1138:LEU:HD12	1:A:1194:TRP:CD1	2.56	0.41
1:A:1239:GLN:N	1:A:1263:GLU:O	2.40	0.41
1:B:711:LEU:C	1:B:711:LEU:HD12	2.45	0.41
1:A:282:GLU:O	1:A:285:HIS:HA	2.21	0.41
1:A:1017:ALA:N	1:A:1099:ARG:O	2.53	0.41
1:A:1105:ASP:OD1	1:A:1105:ASP:N	2.49	0.41
1:A:1238:ALA:HA	1:A:1263:GLU:O	2.20	0.41
1:B:844:ILE:HD13	1:B:854:PRO:HA	2.03	0.41
1:B:1225:THR:O	1:B:1228:SER:OG	2.36	0.41
1:A:1070:HIS:CE1	1:A:1076:PHE:HD1	2.38	0.41
1:B:1145:LEU:HD22	1:B:1160:VAL:HG22	2.02	0.41
1:A:25:GLN:C	1:A:26:LEU:HD12	2.46	0.41
1:A:1104:PHE:O	1:A:1104:PHE:CD2	2.74	0.41
1:A:1168:LEU:HD22	1:A:1183:PRO:O	2.20	0.41
1:B:445:LEU:HD23	1:B:445:LEU:O	2.21	0.41
1:B:724:SER:OG	1:B:779:ASP:OD1	2.39	0.41
1:B:735:ASP:OD1	1:B:736:ILE:N	2.53	0.41
1:B:482:HIS:CE1	1:B:492:HIS:NE2	2.83	0.41
1:B:734:ASN:C	1:B:734:ASN:ND2	2.79	0.41
1:A:980:GLU:OE1	1:A:980:GLU:N	2.54	0.40
1:A:1165:GLY:HA3	1:A:1226:PHE:HE2	1.80	0.40
1:B:250:THR:HG22	1:B:251:LEU:H	1.86	0.40
1:B:1137:GLU:HA	1:B:1152:ARG:HD2	2.02	0.40
1:A:219:PRO:O	1:A:220:MET:HB3	2.21	0.40
1:A:1138:LEU:HD21	1:A:1140:VAL:HG23	2.03	0.40
1:B:57:ILE:HD11	1:B:77:ILE:HD11	2.04	0.40
1:B:102:VAL:O	1:B:102:VAL:HG13	2.20	0.40
1:B:298:GLN:HE21	1:B:480:MET:HE3	1.86	0.40
1:B:953:ASP:OD2	1:B:955:GLN:NE2	2.55	0.40
1:B:1131:GLU:HB3	1:B:1154:HIS:HB2	2.04	0.40
1:B:1138:LEU:H	1:B:1152:ARG:CZ	2.35	0.40
1:A:53:SER:HA	1:A:54:PRO:HA	1.83	0.40
1:A:56:VAL:HG13	1:A:74:VAL:CG2	2.52	0.40
1:A:1104:PHE:CE1	1:B:1109:LEU:HB2	2.56	0.40
1:B:500:ILE:HD12	1:B:503:CYS:HA	2.03	0.40
1:B:899:VAL:HG13	1:B:900:SER:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1143/1581 (72%)	1077 (94%)	66 (6%)	0	100	100
1	B	1176/1581 (74%)	1101 (94%)	75 (6%)	0	100	100
2	C	18/272 (7%)	18 (100%)	0	0	100	100
2	D	23/272 (8%)	21 (91%)	2 (9%)	0	100	100
All	All	2360/3706 (64%)	2217 (94%)	143 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	938/1386 (68%)	938 (100%)	0	100	100
1	B	993/1386 (72%)	993 (100%)	0	100	100
2	C	18/234 (8%)	18 (100%)	0	100	100
2	D	23/234 (10%)	22 (96%)	1 (4%)	26	54
All	All	1972/3240 (61%)	1971 (100%)	1 (0%)	87	91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	143	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	195	HIS
1	A	529	HIS
1	A	937	GLN
1	A	1033	GLN
1	A	1154	HIS
1	A	1195	ASN
1	A	1211	HIS
1	A	1239	GLN
1	B	25	GLN
1	B	42	GLN
1	B	115	GLN
1	B	166	ASN
1	B	168	ASN
1	B	215	HIS
1	B	310	ASN
1	B	774	GLN
1	B	969	GLN
1	B	1050	HIS

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 ⓘ

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

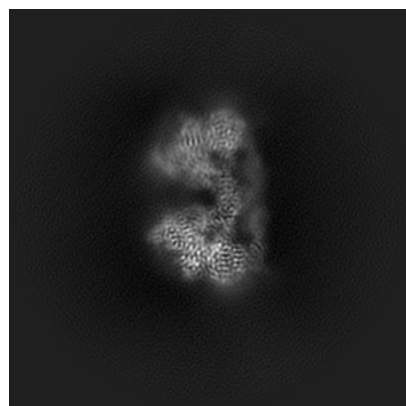
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26475. These allow visual inspection of the internal detail of the map and identification of artifacts.

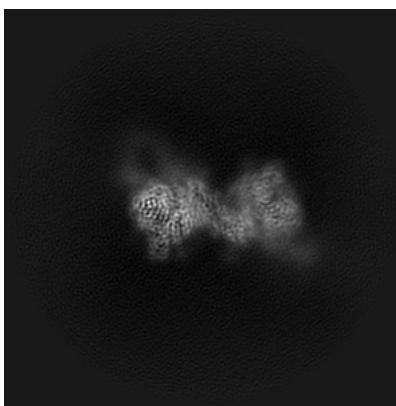
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

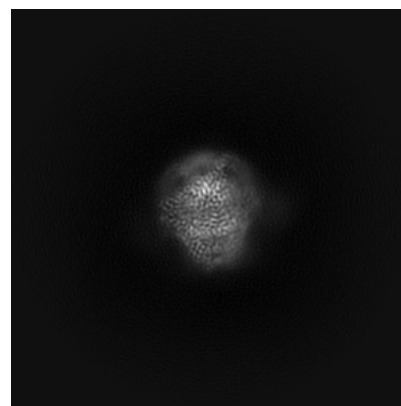
6.1.1 Primary map



X

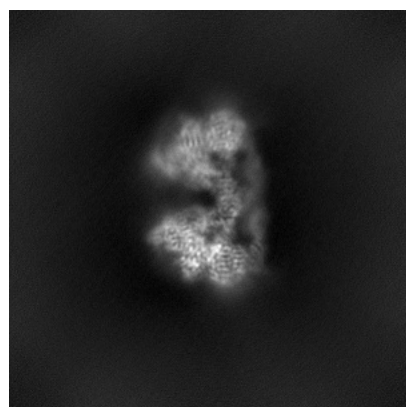


Y

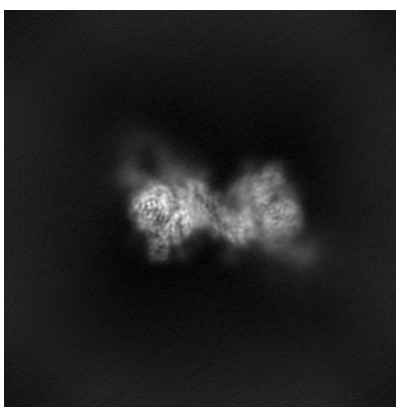


Z

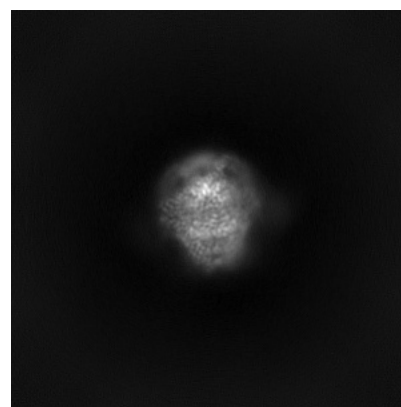
6.1.2 Raw map



X



Y

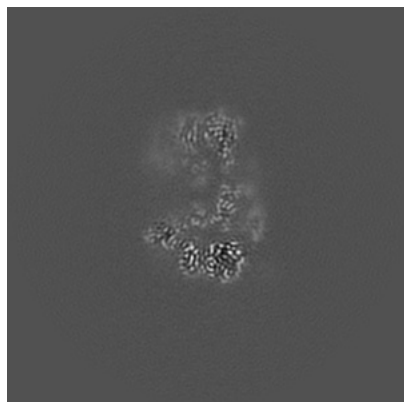


Z

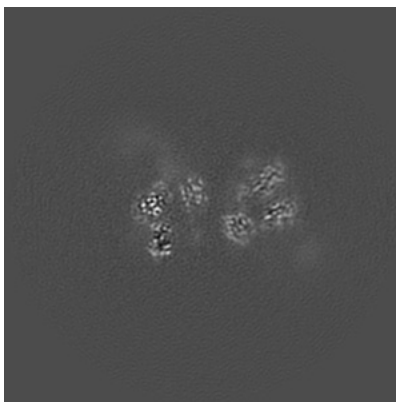
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

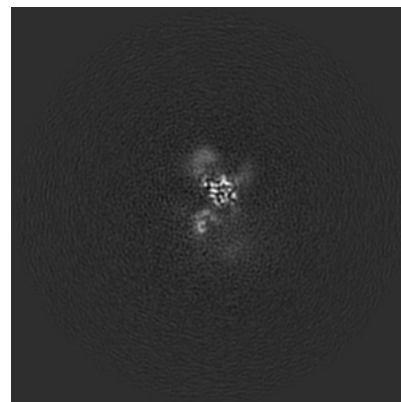
6.2.1 Primary map



X Index: 220

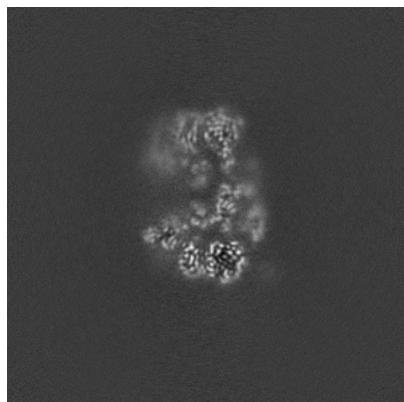


Y Index: 220

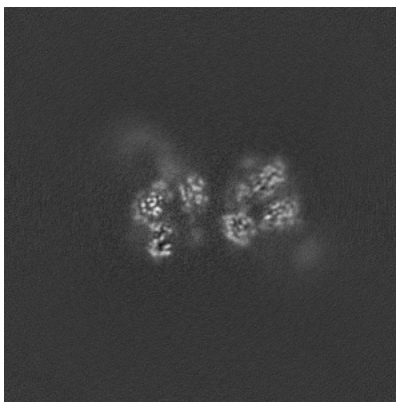


Z Index: 220

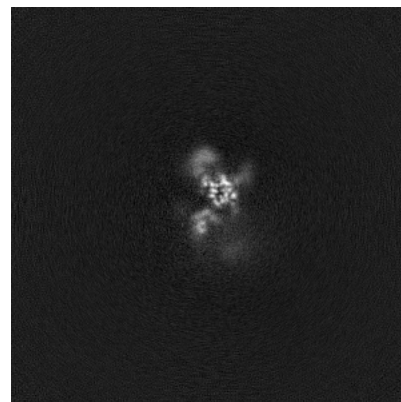
6.2.2 Raw map



X Index: 220



Y Index: 220

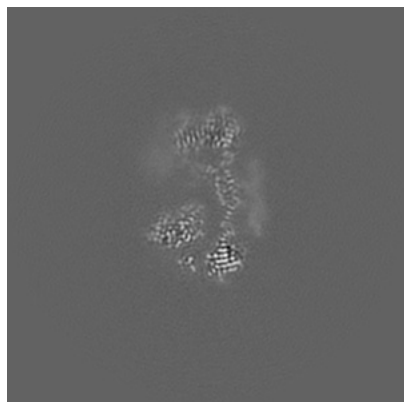


Z Index: 220

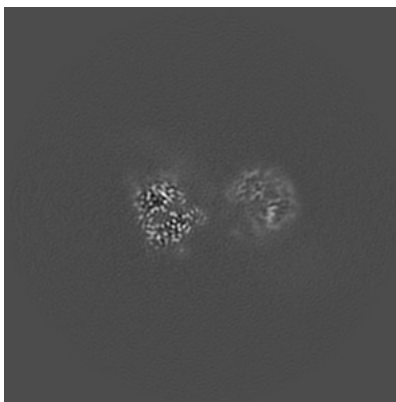
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

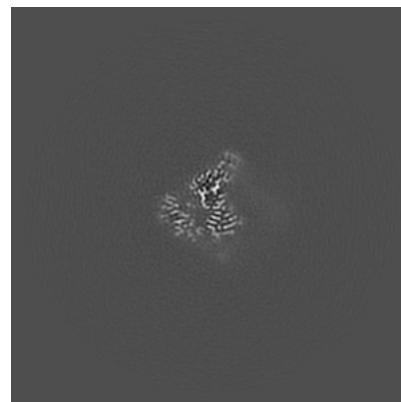
6.3.1 Primary map



X Index: 212

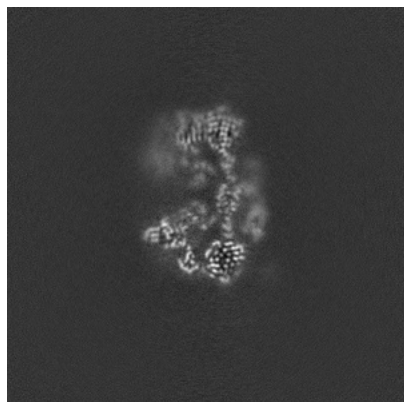


Y Index: 199

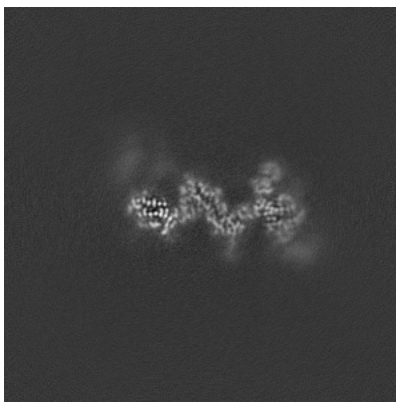


Z Index: 165

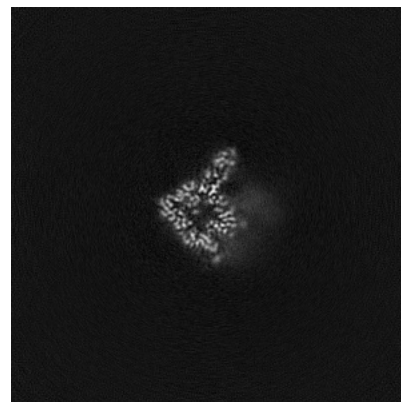
6.3.2 Raw map



X Index: 217



Y Index: 240

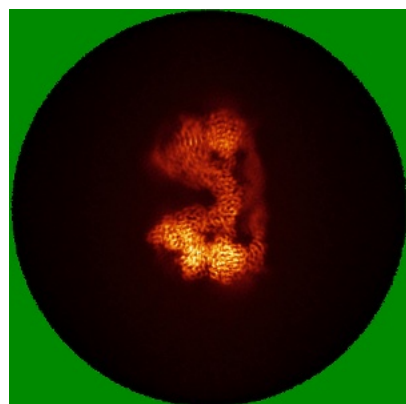


Z Index: 177

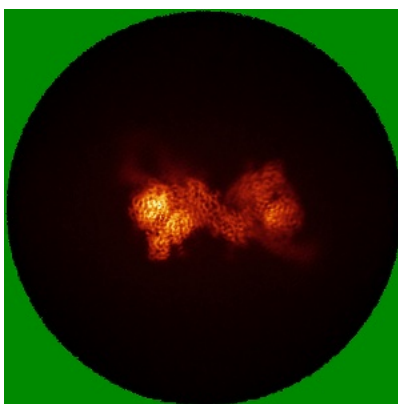
The images above show the largest variance slices of the map in three orthogonal directions.

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

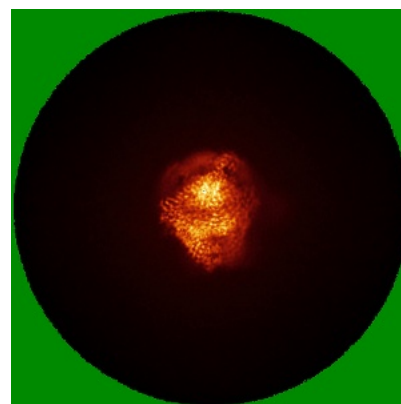
6.4.1 Primary map



X

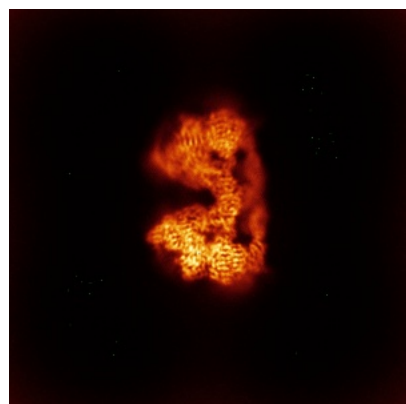


Y

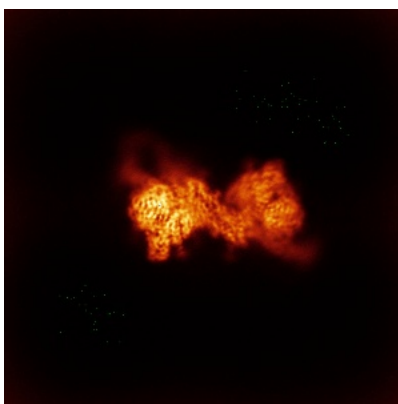


Z

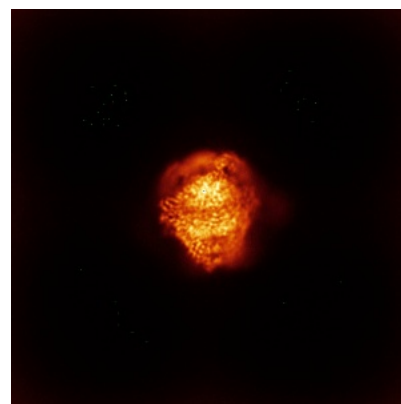
6.4.2 Raw map



X



Y

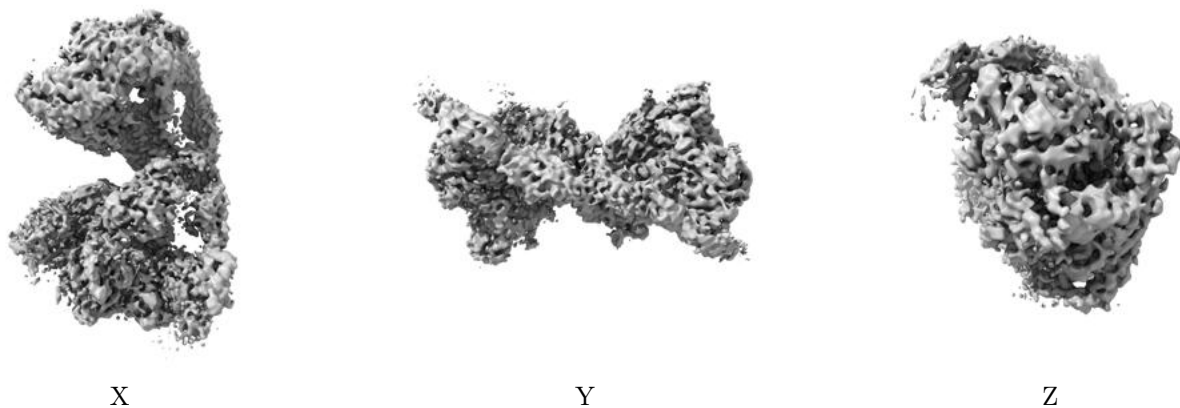


Z

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.

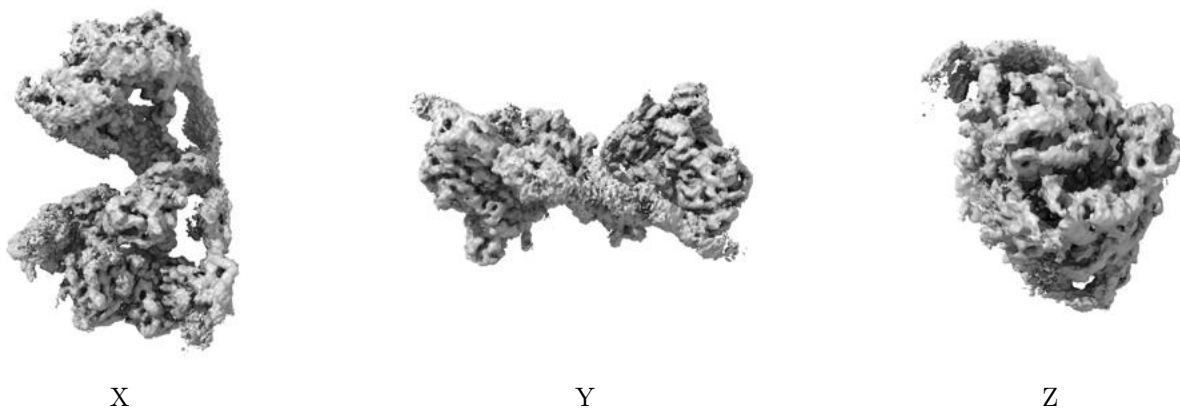
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2305. 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.

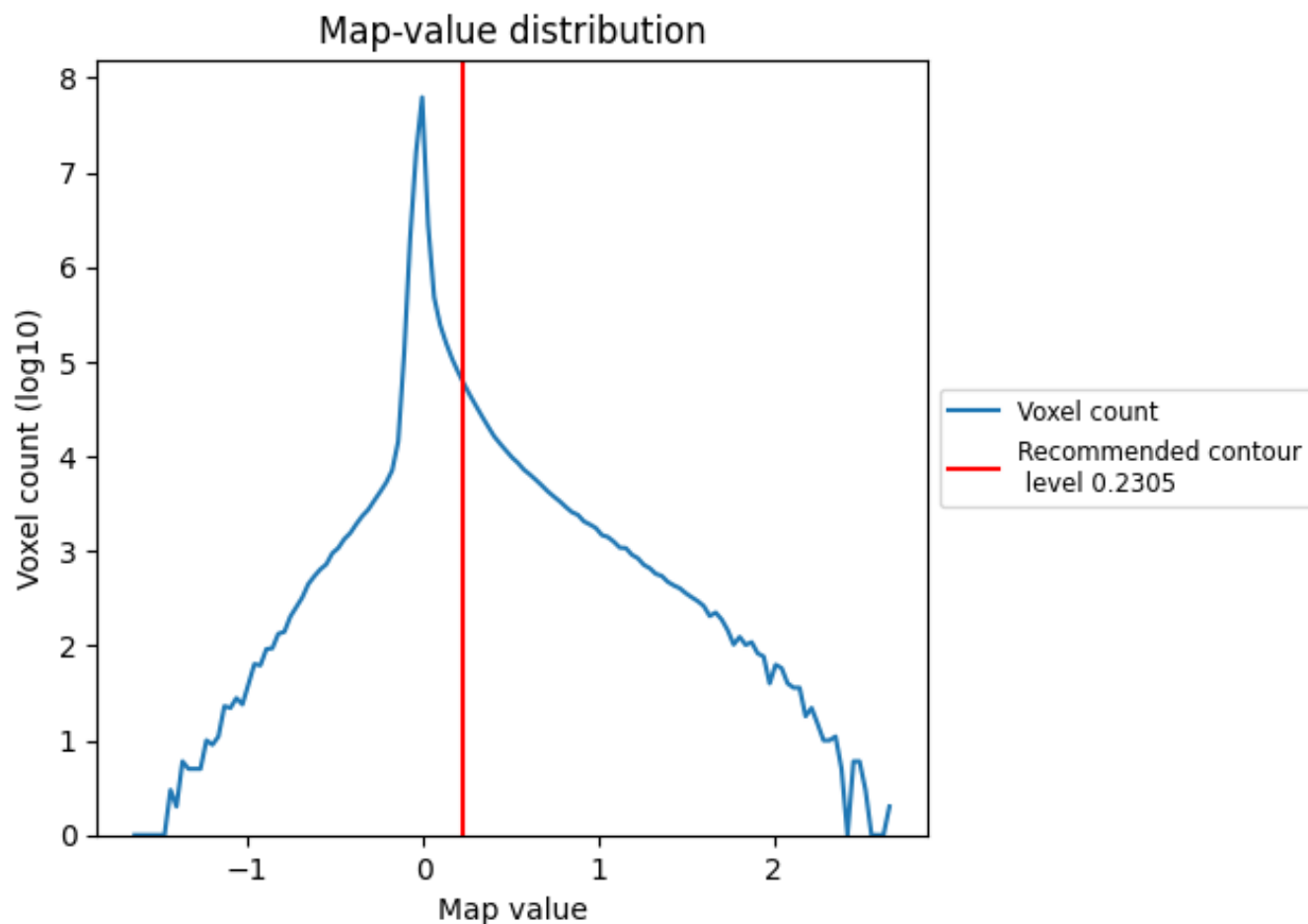
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

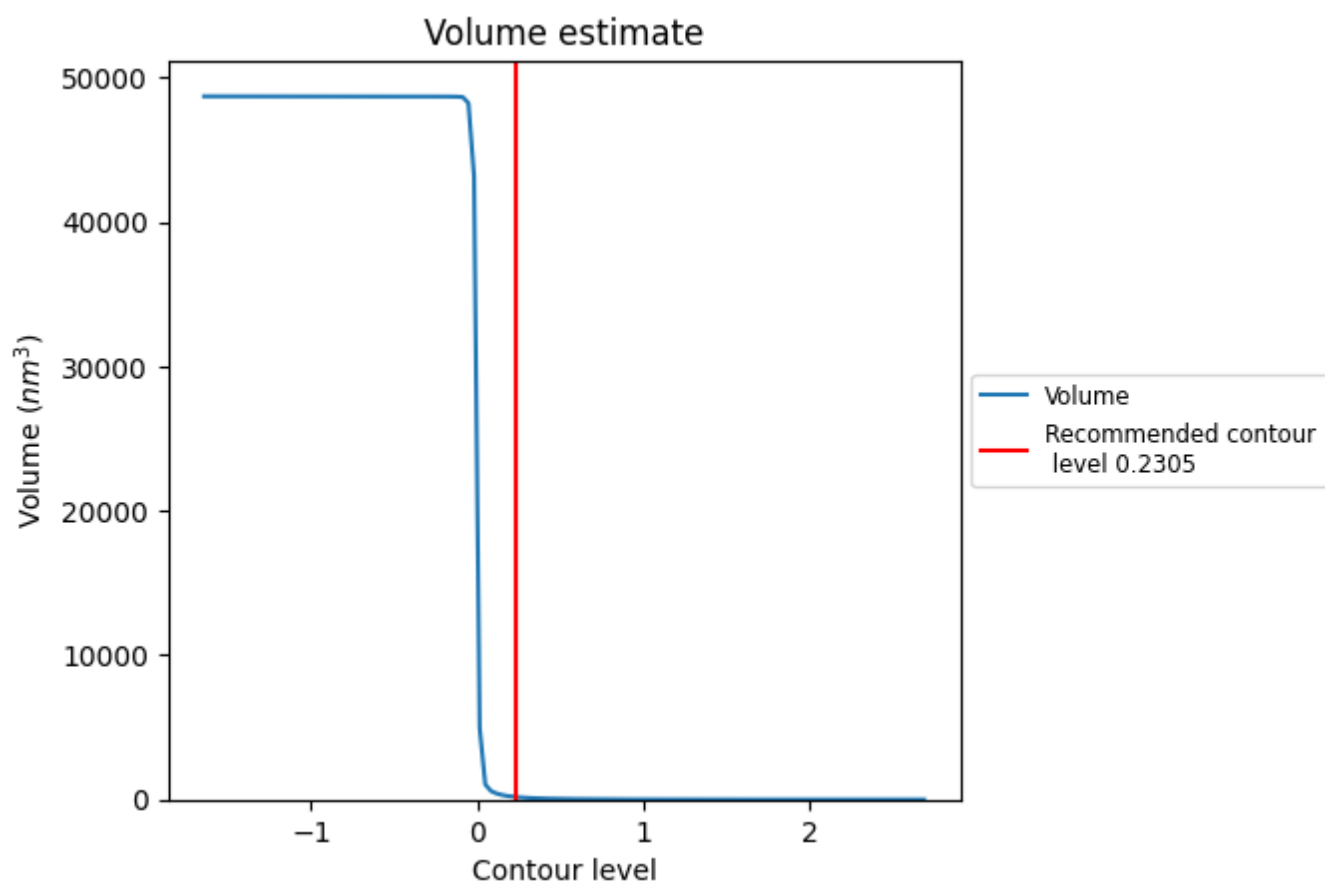
This section contains the results of statistical analysis of the map.

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.

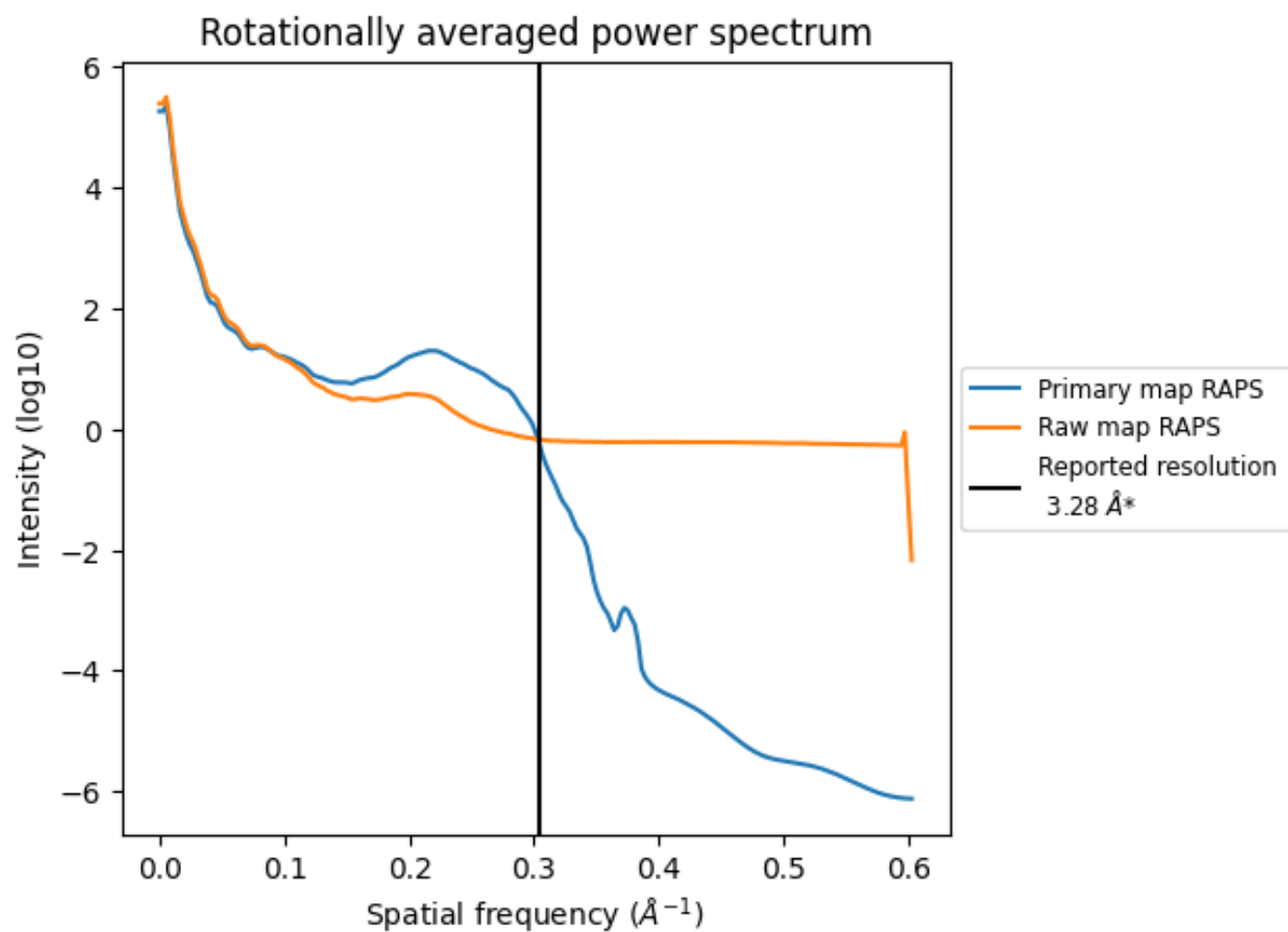
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 180 nm³; this corresponds to an approximate mass of 163 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 ⓘ

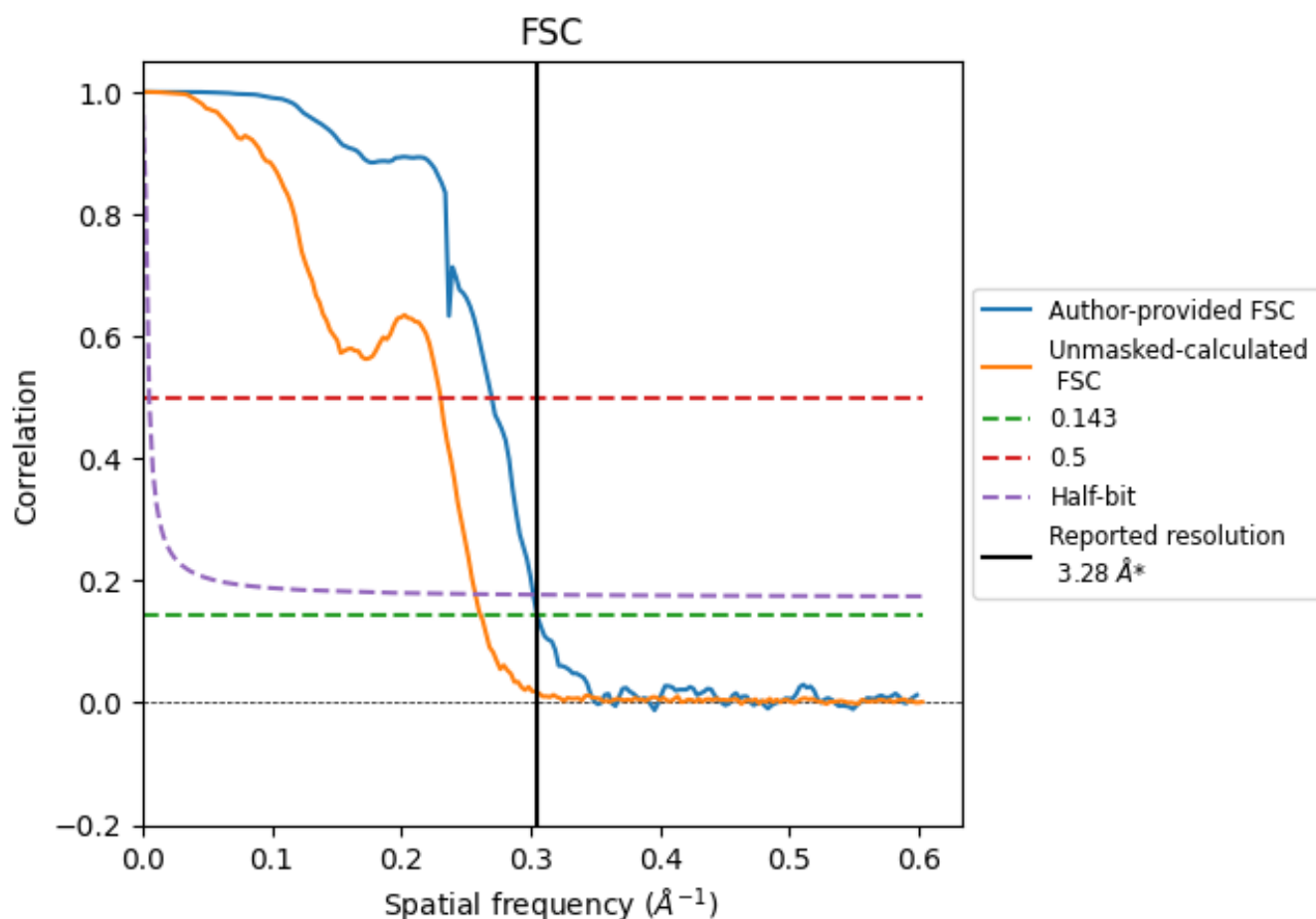


*Reported resolution corresponds to spatial frequency of 0.305 Å⁻¹

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 0.305 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

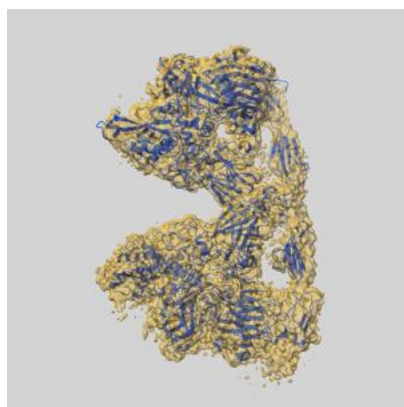
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	3.28	3.71	3.31
Unmasked-calculated*	3.82	4.34	3.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.82 differs from the reported value 3.28 by more than 10 %

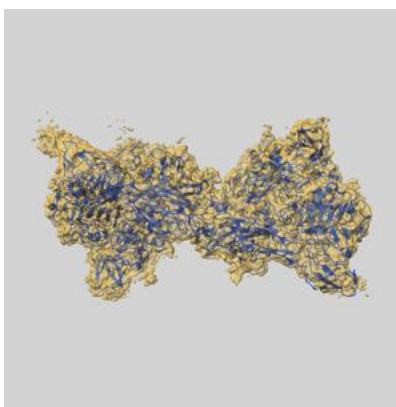
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26475 and PDB model 7UFG. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

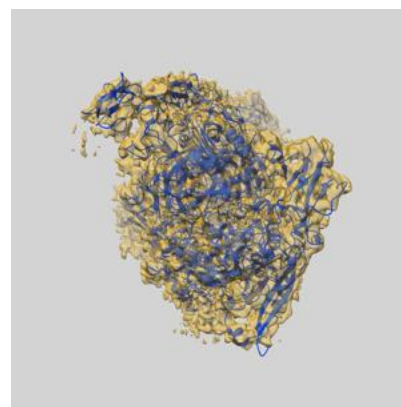
9.1 Map-model overlay [i](#)



X



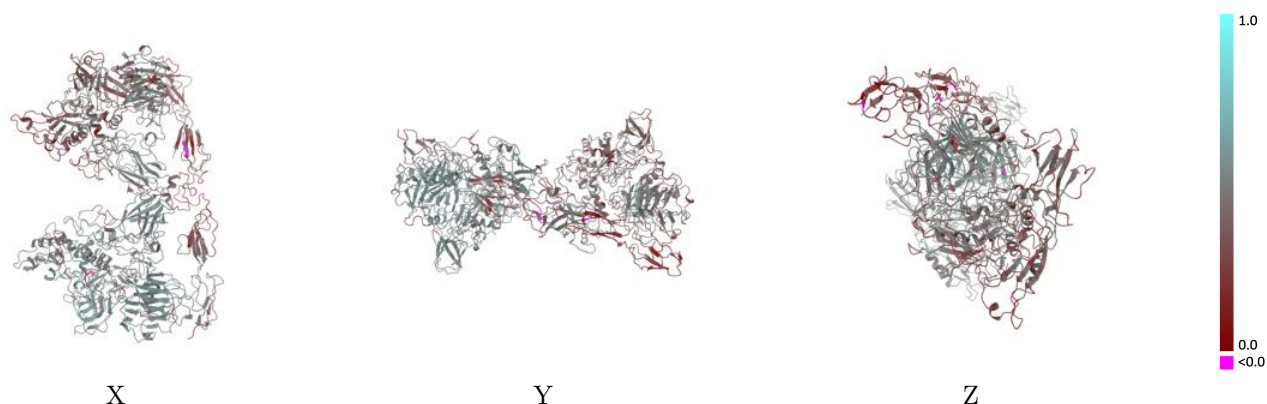
Y



Z

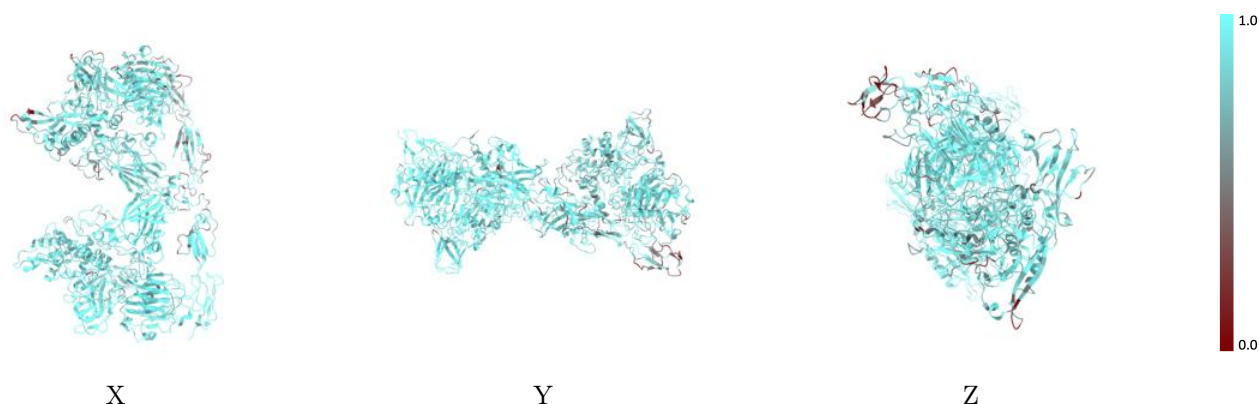
The images above show the 3D surface view of the map at the recommended contour level 0.2305 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



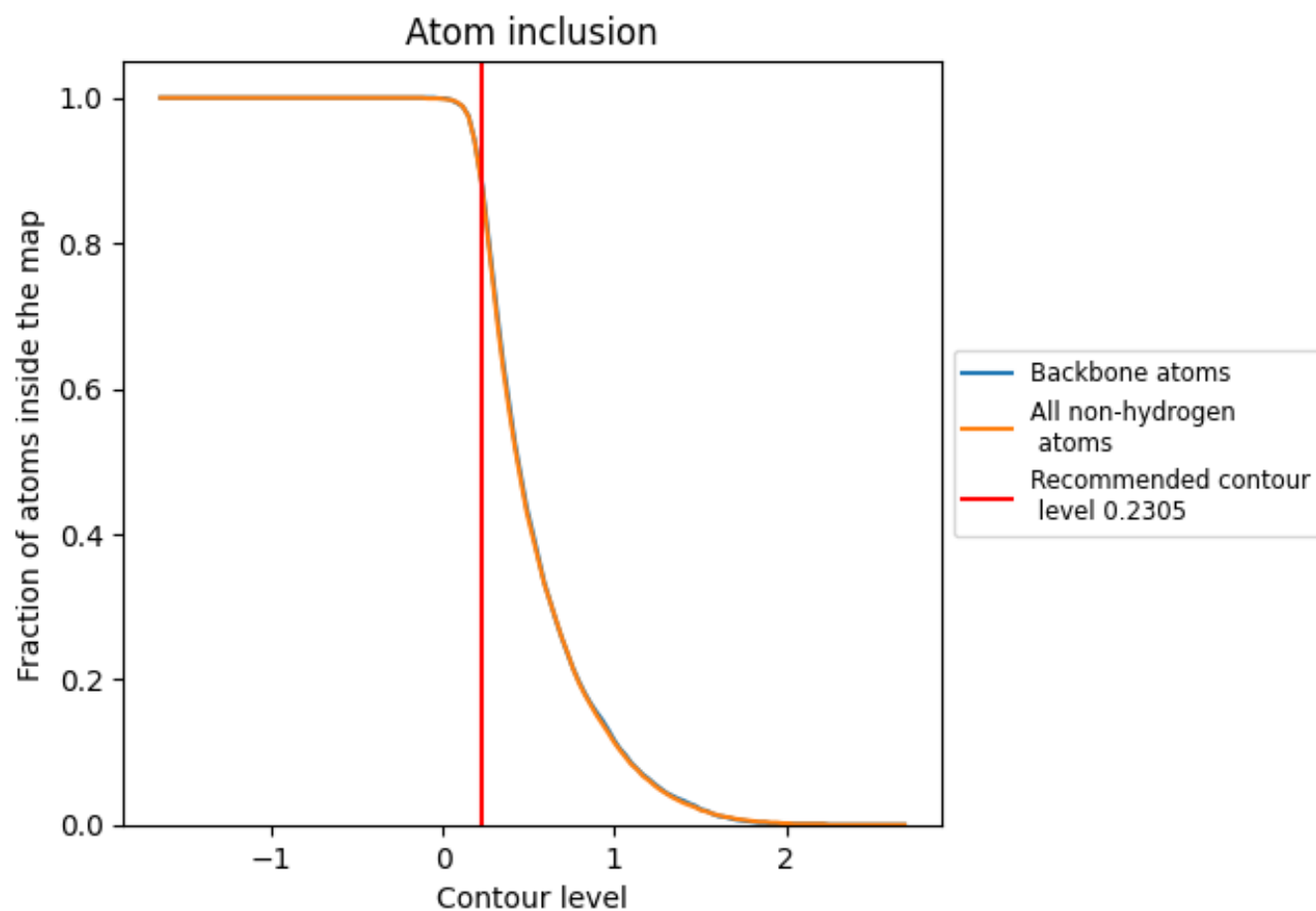
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2305).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.2305) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8750	0.4430
A	0.8450	0.4040
B	0.9020	0.4810
C	0.6830	0.3650
D	0.9000	0.4870

