



Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 02:27 PM EST

PDB ID : 6V86
EMDB ID : EMD-21096
Title : Parainfluenza virus 5 L-P complex with an alternate conformation of the CD-MTase-CTD module
Authors : Abdella, R.; He, Y.
Deposited on : 2019-12-10
Resolution : 4.63 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

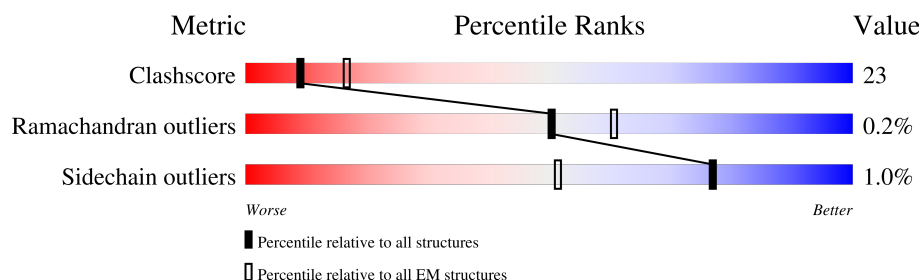
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.63 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	<div> <div>17%</div> <div>46%</div> <div>37%</div> <div>16%</div> </div>
2	B	392	<div> <div>14%</div> <div>10%</div> <div>9%</div> <div>82%</div> </div>
2	C	392	<div> <div>16%</div> <div>8%</div> <div>10%</div> <div>81%</div> </div>
2	D	392	<div> <div>15%</div> <div>9%</div> <div>9%</div> <div>82%</div> </div>
2	E	392	<div> <div>13%</div> <div>10%</div> <div>9%</div> <div>81%</div> </div>
2	F	392	<div> <div>8%</div> <div>88%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17781 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	1890	Total	C	N	O	S	0	0
			15103	9712	2555	2753	83		

- Molecule 2 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
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		
2	F	47	Total	C	N	O	S	0	0
			374	238	64	70	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

A1553	L1484	L1207	L1128	L1049	L967	M895	T523	I732	L660
P1554	D1485	D1208	K1129	L1050	I968	Q899	I824	P735	T661
ASN	F1488	N1209	M1131	D1051	K969	L900	I325	ARG	T662
ALA	M1489	P1210	T1132	R1052	S970	S901	S26	GLY	D63
HIS	C1491	P1211	E1133	E1053	G971	Y902	S827	G738	L664
PHE			E1134	V1054	C972	D903	H828		K665
A1561		Y1216	E1133	V1054	M973	F829	F829		K666
S1562		I1217	E1134	F1055	D974	I904	F830		Y667
L1563		G1218	C1136	F1056		I905	F831		C668
D1564		G1219	E1137	P1057	Y979	F906	F832		L669
		S1219	I1138	P1058	N980	A748	Y832		Q670
		ARG	D1139	V1059	L981	W747	S833		Q670
		THR	N1143	I1064	K985	T748	K834		W671
		ASP	K1146	E1065	S910	S751	R835		I677
		GLU		E1066	I911	I752	I836		P678
		ARG		T1067	P912	I755	F837		F679
		ARG	A1150	S1068	G987	I755	Y838		A880
		VAL	P1151	V1069	G988	I756	Q839		Q881
		ALA	L1152		G989	L757	G840		S682
		SER	L1153	R1072	W991	A758	R841		L683
		NET	G1154	Q1076	A995	A759	I842		N884
		ALA	G1155		D996	T760	L843		R685
		TYR	R1156	L1079	D997	T764	L847		Y689
		ILE	N1157	D1080	P998	R765	K848		P690
		ARG	L1158		Y999	S768	N849		H891
		ALA	E1159	L1083	N1002	I777	S851		L892
		S1236	L1161	S1084	N923	I777	K852		F993
		L1239	D1165	I1085	N923	I777	L853		E694
		K1240	P1166	M1086	N922	I777	L854		W895
		A1241	I1167	R1087	N922	I777	L855		I696
		V1242		K1088	N922	I777	L856		H697
		L1243	I1176	E1091	N922	I777	L857		L698
		R1244	G1177	P1094	N922	I777	L858		R699
		W1251	S1178	L1095	N922	I777	L859		R702
		A1252	G1179	L1096	N922	I777	L860		S703
		F1253	Y1180	S1096	N922	I777	L861		V707
		G1254	C1181	N1097	N922	I777	L862		GLY
			E1182	R1098	N922	I777	L863		ASP
		E1258	Q1183	L1098	N922	I777	L864		PRG
		N1259	C1184	M1101	N922	I777	L865		F711
		W1260	ALA	E1102	N922	I777	L866		N712
		I1261	ALA	N1107	N922	I777	L867		P713
		D1262	GLY		N922	I777	L868		P714
		A1263	ASP	Y1110	N922	I777	L869		A715
		L1264	ASN		N922	I777	L870		S718
		D1265	ARG	N1114	N922	I777	L871		Q719
		L1266	F1191	L1115	N922	I777	L872		D723
		S1267	L1196	L1118	N922	I777	L873		LYS
		H1268		L1119	N922	I777	L874		VAL
		T1269	E1201	N1120	N922	I777	L875		ILE
		R1270	I1202	A1121	N922	I777	L876		ASN
		V1271	G1203	E1122	N922	I777	L877		GLY
		N1272	D1204	E1123	N922	I777	L878		ASP
		I1273	L1274	T1126	N922	I777	L879		I730
		T1274	L1275	Y1127	N922	I777	L880		F731
		L1276	Q1277		N922	I777	L881		
					N922	I777	L882		
					N922	I777	L883		
					N922	I777	L884		
					N922	I777	L885		
					N922	I777	L886		
					N922	I777	L887		
					N922	I777	L888		
					N922	I777	L889		
					N922	I777	L890		
					N922	I777	L891		
					N922	I777	L892		
					N922	I777	L893		
					N922	I777	L894		
					N922	I777	L895		
					N922	I777	L896		
					N922	I777	L897		
					N922	I777	L898		
					N922	I777	L899		
					N922	I777	L900		
					N922	I777	L901		
					N922	I777	L902		
					N922	I777	L903		
					N922	I777	L904		
					N922	I777	L905		
					N922	I777	L906		
					N922	I777	L907		
					N922	I777	L908		
					N922	I777	L909		
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					N922	I777	L912		
					N922	I777	L913		
					N922	I777	L914		
					N922	I777	L915		
					N922	I777	L916		
					N922	I777	L917		
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					N922	I777	L919		
					N922	I777	L920		
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					N922	I777	L922		
					N922	I777	L923		
					N922	I777	L924		
					N922	I777	L925		
					N922	I777	L926		
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					N922	I777	L1012		
					N922	I777	L1013		
					N922	I777	L1014		
					N922	I777	L1015		
					N922	I777	L1016		
					N922	I777	L1017		
					N922	I777	L1018		
					N922	I777	L1019		
					N922	I777	L1020		
					N922	I777	L1021		
					N922	I777	L1022		
					N922	I777	L1023		
					N922	I777	L1024		
					N922	I777	L1025		</

[illegible]





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	78547	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	0.083	Depositor
Minimum map value	-0.039	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	0.28	0/15416	0.48	0/20905
2	B	0.26	0/575	0.47	0/776
2	C	0.25	0/588	0.46	0/794
2	D	0.25	0/575	0.45	0/776
2	E	0.24	0/588	0.48	0/794
2	F	0.24	0/375	0.42	0/498
All	All	0.27	0/18117	0.48	0/24543

There are no bond length outliers.

There are no bond angle outliers.

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	15103	0	15272	699	0
2	B	569	0	600	41	0
2	C	582	0	611	41	0
2	D	569	0	600	38	0
2	E	582	0	611	34	0
2	F	374	0	414	9	0
3	A	2	0	0	0	0
All	All	17781	0	18108	827	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 23.

All (827) 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:1739:ILE:HD11	1:A:1972:VAL:CG1	1.47	1.43
1:A:1744:ALA:O	1:A:1964:TRP:CE2	1.89	1.25
1:A:1739:ILE:CD1	1:A:1972:VAL:HG12	1.69	1.22
1:A:1744:ALA:O	1:A:1964:TRP:CZ2	2.03	1.10
1:A:1971:THR:HG22	1:A:1988:ILE:HD13	1.34	1.09
1:A:1744:ALA:O	1:A:1964:TRP:NE1	1.89	1.06
1:A:1737:ILE:CG2	1:A:1972:VAL:CG1	2.34	1.05
1:A:1191:PHE:O	1:A:1321:GLU:HB2	1.57	1.05
1:A:1737:ILE:CG2	1:A:1972:VAL:HG12	1.88	1.03
1:A:1191:PHE:O	1:A:1321:GLU:CB	2.06	1.02
1:A:1737:ILE:HG23	1:A:1739:ILE:HD13	1.37	1.01
1:A:1954:THR:O	1:A:1958:THR:HG23	1.60	1.01
1:A:1739:ILE:HD11	1:A:1972:VAL:HG12	0.99	0.96
1:A:1956:PHE:O	1:A:1960:ILE:HG12	1.67	0.94
1:A:1619:LEU:O	1:A:1623:ASN:HB2	1.66	0.94
1:A:1971:THR:HG22	1:A:1988:ILE:CD1	1.98	0.94
1:A:211:GLY:HA2	1:A:223:PHE:O	1.67	0.94
1:A:1739:ILE:CD1	1:A:1972:VAL:CG1	2.37	0.92
1:A:1737:ILE:HG21	1:A:1972:VAL:CG1	2.02	0.88
1:A:1191:PHE:O	1:A:1321:GLU:CG	2.22	0.87
1:A:1745:ASN:HB3	1:A:1964:TRP:CZ2	2.09	0.86
1:A:1739:ILE:HD11	1:A:1972:VAL:HG11	1.55	0.86
1:A:1745:ASN:HB3	1:A:1964:TRP:CH2	2.10	0.85
1:A:1737:ILE:HG22	1:A:1972:VAL:CG1	2.06	0.85
1:A:457:LYS:H	1:A:685:ARG:HG2	1.40	0.85
1:A:1660:LEU:O	1:A:1663:PHE:HB2	1.78	0.84
1:A:1743:ASN:O	1:A:1743:ASN:ND2	2.09	0.83
1:A:1183:GLN:HE21	1:A:1183:GLN:HA	1.44	0.83
1:A:590:GLU:HG3	1:A:756:ILE:HD11	1.63	0.81
1:A:1030:LEU:HA	1:A:1033:ILE:HD13	1.62	0.80
1:A:1737:ILE:CG2	1:A:1972:VAL:HG13	2.13	0.78
1:A:332:PHE:HB3	1:A:336:GLU:HB2	1.66	0.78
1:A:1737:ILE:HG22	1:A:1972:VAL:HG13	1.66	0.78
1:A:1816:THR:HG22	1:A:1851:PHE:HD1	1.49	0.77
1:A:1737:ILE:HD11	1:A:2022:ARG:HB3	1.65	0.77
1:A:1971:THR:CG2	1:A:1988:ILE:HD13	2.14	0.76
1:A:418:TRP:O	1:A:420:PRO:HD3	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1181:CYS:SG	1:A:1368:HIS:NE2	2.58	0.76
1:A:1920:GLN:NE2	1:A:1922:CYS:SG	2.59	0.76
1:A:1737:ILE:CG2	1:A:1739:ILE:HD13	2.16	0.75
2:B:212:VAL:HG21	2:C:208:LEU:HD12	1.68	0.75
1:A:2158:GLN:O	1:A:2161:GLU:O	2.04	0.75
1:A:1737:ILE:HG23	1:A:1739:ILE:CD1	2.16	0.74
1:A:1243:LEU:HG	1:A:1285:PRO:HG3	1.68	0.74
1:A:10:PRO:O	1:A:188:ARG:NH2	2.20	0.73
1:A:1745:ASN:CA	1:A:1964:TRP:CZ2	2.71	0.73
1:A:1539:HIS:CE1	1:A:1766:LEU:H	2.05	0.73
1:A:514:LEU:O	1:A:518:PHE:HB3	1.88	0.73
1:A:1519:TYR:HB3	1:A:1523:ARG:HH21	1.54	0.73
1:A:1745:ASN:HA	1:A:1964:TRP:CZ2	2.24	0.72
2:F:386:ALA:O	2:F:390:SER:HB2	1.89	0.72
1:A:684:ASN:HD21	1:A:691:HIS:H	1.36	0.72
1:A:11:GLU:O	1:A:188:ARG:NH1	2.23	0.71
1:A:1897:ILE:O	1:A:1899:ARG:NH1	2.23	0.71
1:A:784:PRO:O	1:A:792:LYS:NZ	2.24	0.71
1:A:206:ILE:HB	1:A:213:ILE:HB	1.72	0.71
1:A:287:TYR:O	1:A:290:ILE:HB	1.91	0.71
2:F:355:LYS:HA	2:F:364:ARG:HD3	1.72	0.71
1:A:1500:SER:HA	1:A:1503:MET:HG2	1.73	0.70
1:A:1533:LEU:HD11	1:A:1565:TYR:HB3	1.72	0.70
1:A:1569:SER:O	1:A:1572:ALA:HB3	1.92	0.70
1:A:1254:GLY:O	1:A:1259:ASN:ND2	2.25	0.70
2:C:243:ILE:O	2:C:247:GLN:NE2	2.24	0.70
1:A:374:SER:OG	1:A:375:GLN:OE1	2.07	0.70
1:A:1744:ALA:H	1:A:1964:TRP:HE1	1.40	0.70
1:A:1768:ALA:HB3	1:A:1979:ASP:HB2	1.75	0.69
1:A:1744:ALA:C	1:A:1964:TRP:CZ2	2.66	0.69
1:A:346:SER:O	1:A:349:GLN:NE2	2.25	0.69
1:A:1537:LEU:O	1:A:1763:ASN:ND2	2.25	0.69
1:A:885:LYS:NZ	1:A:948:LEU:O	2.24	0.69
1:A:1183:GLN:HA	1:A:1183:GLN:NE2	2.06	0.69
1:A:2207:LEU:N	1:A:2207:LEU:HD23	2.08	0.69
1:A:92:PRO:HB2	1:A:95:LEU:HB2	1.75	0.68
1:A:82:TRP:HB3	1:A:85:TYR:HB3	1.74	0.68
1:A:847:LEU:O	1:A:850:ALA:HB3	1.93	0.68
1:A:1571:ASP:O	1:A:1574:LEU:HB3	1.91	0.68
1:A:307:ILE:HD12	1:A:308:PRO:HD2	1.76	0.68
1:A:257:VAL:HG11	1:A:887:ILE:HD12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:VAL:HG23	1:A:419:PRO:HD3	1.75	0.68
1:A:204:THR:HB	1:A:215:ILE:HB	1.76	0.68
1:A:1270:ARG:NH1	1:A:1270:ARG:O	2.27	0.68
1:A:323:LEU:HD13	1:A:337:LEU:HD21	1.75	0.68
1:A:1745:ASN:CB	1:A:1964:TRP:CZ2	2.78	0.68
1:A:1771:HIS:O	1:A:1775:ARG:NH1	2.27	0.68
1:A:1784:TRP:HB3	1:A:1814:SER:HA	1.75	0.68
1:A:1971:THR:H	1:A:1988:ILE:HG12	1.59	0.68
1:A:1446:ARG:NH1	1:A:1593:VAL:O	2.27	0.67
1:A:871:LEU:HD21	1:A:895:MET:HG3	1.76	0.67
1:A:1737:ILE:CG2	1:A:1739:ILE:CD1	2.73	0.67
1:A:1747:GLU:HG3	1:A:2016:THR:HG23	1.76	0.67
1:A:2158:GLN:O	1:A:2161:GLU:C	2.32	0.67
2:C:254:LYS:HA	2:C:257:ILE:HD12	1.77	0.67
2:B:219:VAL:HG21	2:C:215:LEU:HD12	1.75	0.67
1:A:11:GLU:HA	1:A:859:VAL:HG23	1.77	0.67
1:A:1731:CYS:N	1:A:1785:TYR:HH	1.93	0.67
1:A:1827:ILE:HD13	1:A:1851:PHE:CE2	2.29	0.67
1:A:1501:TYR:HB2	1:A:1614:LEU:HG	1.75	0.67
2:D:251:GLN:O	2:D:255:ASN:ND2	2.28	0.66
1:A:1191:PHE:C	1:A:1321:GLU:HB2	2.14	0.66
1:A:1680:TYR:HB3	1:A:1684:ARG:HH21	1.60	0.66
1:A:189:GLN:HE22	1:A:193:ARG:HE	1.42	0.66
1:A:1629:LYS:NZ	1:A:1630:ILE:O	2.28	0.66
1:A:864:THR:H	1:A:1107:ASN:HD21	1.41	0.66
1:A:196:ASP:O	1:A:197:HIS:ND1	2.29	0.66
1:A:1534:ALA:HB2	1:A:1760:ASN:HB2	1.78	0.66
1:A:1745:ASN:CB	1:A:1964:TRP:CH2	2.78	0.66
2:B:258:VAL:HA	2:B:261:LYS:HE2	1.78	0.66
1:A:684:ASN:ND2	1:A:691:HIS:H	1.94	0.65
1:A:1739:ILE:HD11	1:A:1972:VAL:CB	2.26	0.65
1:A:1750:PRO:HA	1:A:2017:LEU:HB2	1.78	0.65
1:A:880:GLU:HG3	1:A:1308:SER:HB3	1.78	0.65
1:A:980:ASN:HD21	1:A:1120:ASN:HA	1.62	0.65
1:A:658:SER:OG	1:A:779:VAL:O	2.14	0.65
1:A:2225:CYS:SG	1:A:2226:HIS:N	2.70	0.65
1:A:1905:CYS:HB2	1:A:1933:THR:HA	1.79	0.65
2:D:200:LEU:HD21	2:E:200:LEU:H	1.62	0.65
1:A:413:LYS:O	1:A:414:HIS:ND1	2.31	0.64
1:A:1743:ASN:HD22	1:A:1743:ASN:C	2.01	0.64
1:A:1021:LEU:HD23	1:A:1079:LEU:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1476:ILE:O	1:A:1535:SER:OG	2.11	0.64
1:A:1943:VAL:HG11	1:A:1988:ILE:HD12	1.79	0.64
1:A:400:ALA:HB1	1:A:452:GLU:HG2	1.79	0.64
1:A:476:ASP:HB2	1:A:515:LEU:HB2	1.79	0.64
1:A:1731:CYS:SG	1:A:1733:ASN:ND2	2.70	0.64
1:A:856:THR:HG22	1:A:857:ALA:H	1.61	0.64
1:A:1129:LYS:HA	1:A:1132:THR:HG22	1.79	0.63
1:A:1741:GLU:HG3	1:A:1744:ALA:HB2	1.80	0.63
2:D:257:ILE:HG13	2:E:256:ASP:HB3	1.80	0.63
1:A:137:TYR:HD1	1:A:141:GLY:HA2	1.62	0.63
1:A:1744:ALA:N	1:A:1964:TRP:HE1	1.95	0.63
1:A:258:SER:HA	1:A:261:LEU:HD13	1.79	0.63
1:A:2208:THR:OG1	1:A:2210:PRO:HD2	1.98	0.63
1:A:1284:LEU:O	1:A:1681:TYR:OH	2.16	0.63
1:A:876:MET:O	1:A:879:THR:OG1	2.12	0.63
1:A:31:ASN:O	1:A:67:ARG:NH2	2.30	0.62
1:A:1762:HIS:ND1	1:A:1762:HIS:O	2.31	0.62
1:A:447:LEU:HD22	1:A:760:THR:HG22	1.81	0.62
1:A:299:ALA:O	1:A:302:GLN:HB3	1.99	0.62
1:A:1030:LEU:O	1:A:1033:ILE:HB	2.00	0.62
1:A:1746:LEU:CB	1:A:1748:LYS:NZ	2.63	0.62
1:A:695:TRP:O	1:A:698:LEU:HB3	2.00	0.62
1:A:1331:ALA:HA	1:A:1334:ASN:HB2	1.81	0.62
2:C:257:ILE:HD13	2:D:253:ILE:HG12	1.82	0.62
2:D:200:LEU:HD13	2:D:202:GLN:HB2	1.81	0.62
2:D:205:LEU:HD13	2:D:208:LEU:HD12	1.82	0.62
1:A:838:TYR:HB3	1:A:843:LEU:HD21	1.81	0.62
1:A:1042:GLU:HG2	1:A:1064:ILE:HD11	1.81	0.62
1:A:1054:VAL:H	1:A:1383:LEU:HD13	1.65	0.61
1:A:1136:CYS:SG	1:A:1374:CYS:HB3	2.39	0.61
1:A:1210:PRO:HG2	1:A:1211:PRO:HD3	1.82	0.61
1:A:1854:SER:O	1:A:1858:LYS:NZ	2.33	0.61
1:A:399:LEU:HD13	1:A:678:PRO:HB2	1.82	0.61
2:E:218:ASN:O	2:E:222:ILE:HG12	2.00	0.61
1:A:519:LEU:O	1:A:1027:ASN:ND2	2.32	0.61
1:A:806:ARG:O	1:A:810:ASN:ND2	2.34	0.61
1:A:411:ARG:NH1	1:A:415:HIS:O	2.34	0.61
2:D:248:SER:HB3	2:D:251:GLN:HE21	1.64	0.61
1:A:1613:LYS:NZ	1:A:1634:SER:O	2.28	0.61
2:E:253:ILE:O	2:E:257:ILE:HG12	2.00	0.60
1:A:768:SER:HB2	1:A:777:ILE:HG13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:ALA:HB1	1:A:827:SER:HB2	1.82	0.60
1:A:986:PRO:HB2	1:A:1151:PRO:HG3	1.83	0.60
1:A:332:PHE:HE2	1:A:335:ASP:HB2	1.65	0.60
1:A:904:ILE:HD11	1:A:917:THR:HA	1.81	0.60
1:A:1028:PRO:O	1:A:1030:LEU:N	2.34	0.60
2:C:213:GLN:O	2:C:217:LEU:HG	2.01	0.60
1:A:381:ARG:NE	1:A:723:ASP:OD2	2.35	0.60
1:A:476:ASP:OD1	1:A:477:LYS:N	2.34	0.60
1:A:945:CYS:O	1:A:948:LEU:CB	2.50	0.60
1:A:1541:LYS:O	1:A:1545:ARG:N	2.27	0.60
1:A:192:VAL:O	1:A:195:THR:OG1	2.17	0.60
1:A:287:TYR:HD1	1:A:290:ILE:HD12	1.66	0.60
1:A:549:SER:OG	1:A:564:LYS:NZ	2.34	0.60
1:A:1820:TYR:CZ	1:A:2060:ILE:HB	2.37	0.60
1:A:1272:ASN:HB3	1:A:1395:VAL:O	2.01	0.60
1:A:1022:MET:HG3	1:A:1076:GLN:HG2	1.83	0.60
1:A:1181:CYS:HG	1:A:1368:HIS:CD2	2.20	0.60
2:E:216:ALA:O	2:E:220[B]:ASN:ND2	2.35	0.60
1:A:130:GLN:O	1:A:134:ASN:ND2	2.35	0.59
1:A:235:PHE:O	1:A:238:VAL:HG22	2.02	0.59
1:A:964:LEU:O	1:A:968:ILE:HG12	2.02	0.59
2:B:261:LYS:NZ	2:C:256:ASP:OD1	2.34	0.59
1:A:914:ASP:OD1	1:A:915:GLN:N	2.35	0.59
1:A:1772:HIS:HA	1:A:1775:ARG:HH22	1.67	0.59
1:A:1739:ILE:HD13	1:A:1972:VAL:HG12	1.78	0.59
1:A:1201:GLU:HG3	1:A:1202:ILE:H	1.67	0.59
1:A:251:ILE:HG21	1:A:362:ILE:HG21	1.83	0.59
1:A:418:TRP:NE1	1:A:437:ASP:OD1	2.35	0.59
1:A:433:GLU:HG3	1:A:438:ASN:HD22	1.68	0.59
1:A:1191:PHE:O	1:A:1321:GLU:HG3	2.02	0.59
1:A:216:THR:OG1	1:A:219:LEU:N	2.36	0.58
2:E:222:ILE:O	2:E:226:VAL:HG23	2.03	0.58
1:A:184:LYS:O	1:A:188:ARG:HG3	2.03	0.58
1:A:12:VAL:O	1:A:13:HIS:ND1	2.36	0.58
1:A:875:VAL:O	1:A:878:LEU:HB3	2.03	0.58
1:A:78:ARG:NH2	1:A:79:LYS:O	2.37	0.58
1:A:384:MET:HG3	1:A:385:CYS:H	1.68	0.58
1:A:1564:ASP:OD1	1:A:1565:TYR:N	2.36	0.58
1:A:457:LYS:O	1:A:685:ARG:NE	2.37	0.58
1:A:536:GLY:O	1:A:540:HIS:N	2.37	0.58
1:A:2100:ILE:HD11	1:A:2192:ALA:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:240:VAL:HA	2:E:243:ILE:HG22	1.84	0.58
1:A:298:TYR:O	1:A:302:GLN:N	2.36	0.58
1:A:319:CYS:O	1:A:323:LEU:HG	2.03	0.58
1:A:901:SER:O	1:A:905:ILE:HG12	2.03	0.58
1:A:1045:LEU:HD22	1:A:1064:ILE:HD12	1.86	0.58
1:A:1745:ASN:HB3	1:A:1964:TRP:HZ2	1.67	0.58
1:A:99:PRO:HB3	1:A:102:LYS:HD3	1.85	0.57
1:A:286:VAL:HA	1:A:289:ILE:HG12	1.85	0.57
1:A:989:GLY:HA3	1:A:1002:ASN:HD21	1.68	0.57
1:A:1136:CYS:SG	1:A:1373:CYS:SG	3.01	0.57
2:C:215:LEU:O	2:C:219:VAL:HG23	2.04	0.57
1:A:219:LEU:HD11	1:A:232:TYR:HB3	1.86	0.57
1:A:166:ALA:O	1:A:170:ASP:N	2.37	0.57
1:A:1539:HIS:CE1	1:A:1763:ASN:HA	2.40	0.57
1:A:1793:TYR:OH	1:A:1971:THR:HG21	2.04	0.57
1:A:2148:LEU:HB2	1:A:2153:ARG:HH11	1.68	0.57
1:A:1816:THR:HG22	1:A:1851:PHE:CD1	2.37	0.57
1:A:1959:LEU:HD23	1:A:1959:LEU:O	2.04	0.57
2:B:200:LEU:HD11	2:C:200:LEU:HD22	1.87	0.57
1:A:1737:ILE:HG23	1:A:1972:VAL:HG12	1.84	0.57
1:A:1832:LEU:HB2	1:A:1887:ILE:HG13	1.87	0.57
1:A:595:MET:HG2	1:A:599:SER:HB2	1.87	0.57
1:A:1177:GLY:HA2	1:A:1919:ASN:HD21	1.69	0.57
1:A:1746:LEU:HB2	1:A:1748:LYS:NZ	2.20	0.57
1:A:892:ASN:ND2	1:A:944:SER:OG	2.38	0.57
1:A:991:TRP:NE1	1:A:1152:LEU:HD11	2.20	0.57
1:A:1265:ASP:OD2	1:A:1390:LYS:NZ	2.35	0.57
1:A:925:HIS:HE1	1:A:929:ARG:HE	1.50	0.56
1:A:593:VAL:HG21	1:A:771:GLN:HE21	1.70	0.56
1:A:468:GLU:OE1	1:A:468:GLU:N	2.38	0.56
1:A:1911:ASP:OD1	1:A:1911:ASP:N	2.38	0.56
1:A:1951:LEU:HB3	1:A:1952:PRO:HD3	1.86	0.56
1:A:71:ILE:HD13	1:A:74:ILE:HD11	1.87	0.56
1:A:1538:SER:HA	1:A:1763:ASN:ND2	2.20	0.56
1:A:1138:ILE:HD12	1:A:1138:ILE:H	1.71	0.56
1:A:1507:ARG:NH2	1:A:1621:HIS:O	2.35	0.56
1:A:2001:SER:HB3	1:A:2004:THR:HG23	1.88	0.56
1:A:1807:ILE:HB	1:A:1910:VAL:HG12	1.87	0.56
2:B:249:LEU:O	2:B:253:ILE:HG12	2.06	0.56
1:A:137:TYR:HA	1:A:141:GLY:HA2	1.86	0.56
1:A:1499:LEU:HD11	1:A:1517:TYR:HE2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ARG:HH21	1:A:368:HIS:CE1	2.24	0.56
2:E:230:ASP:O	2:E:233:MET:HG3	2.05	0.56
1:A:9:LEU:HD12	1:A:188:ARG:HE	1.72	0.55
1:A:1068:SER:OG	1:A:1072:ARG:NH2	2.39	0.55
1:A:411:ARG:HD3	1:A:418:TRP:CD1	2.42	0.55
1:A:1115:LEU:O	1:A:1118:LEU:HB2	2.06	0.55
1:A:1497:LEU:HB3	1:A:1614:LEU:HD23	1.86	0.55
1:A:1734:ASP:HB2	1:A:1974:ARG:HG3	1.89	0.55
1:A:1158:LEU:H	1:A:1158:LEU:HD23	1.71	0.55
2:B:229:LEU:O	2:B:233:MET:HG3	2.07	0.55
1:A:1745:ASN:HB3	1:A:1964:TRP:HH2	1.65	0.55
1:A:160:ASP:OD1	1:A:161:LEU:N	2.37	0.55
1:A:1920:GLN:OE1	1:A:1923:LEU:N	2.40	0.55
1:A:1052:ARG:NH1	1:A:1386:ALA:O	2.39	0.55
1:A:400:ALA:O	1:A:404:THR:HG23	2.07	0.55
1:A:542:ASP:OD1	1:A:542:ASP:N	2.40	0.55
1:A:544:PHE:CZ	1:A:699:ARG:HB3	2.42	0.55
1:A:789:THR:O	1:A:793:LYS:HG2	2.07	0.55
1:A:1769:PRO:HB2	1:A:2216:TRP:CD1	2.42	0.55
1:A:113:TRP:CH2	1:A:902:TYR:HB2	2.42	0.55
1:A:1539:HIS:NE2	1:A:1763:ASN:HA	2.21	0.55
1:A:1658:GLU:O	1:A:1661:SER:OG	2.15	0.54
1:A:1849:THR:O	1:A:1853:GLU:HG2	2.08	0.54
1:A:955:ASP:OD2	1:A:958:VAL:N	2.30	0.54
1:A:864:THR:H	1:A:1107:ASN:ND2	2.04	0.54
1:A:1499:LEU:HD21	1:A:1517:TYR:HD2	1.72	0.54
2:D:253:ILE:HG21	2:E:253:ILE:HG23	1.88	0.54
1:A:31:ASN:HB2	1:A:67:ARG:HD2	1.89	0.54
1:A:469:GLU:OE1	1:A:582:ASN:ND2	2.40	0.54
1:A:1827:ILE:HD13	1:A:1851:PHE:HE2	1.71	0.54
1:A:1963:LEU:HD23	1:A:1970:ILE:HD12	1.90	0.54
2:D:250:ILE:HD12	2:E:249:LEU:HD22	1.88	0.54
1:A:49:TRP:CE3	1:A:52:ILE:HD11	2.43	0.54
1:A:476:ASP:OD1	1:A:514:LEU:HB3	2.07	0.54
1:A:1744:ALA:C	1:A:1964:TRP:HZ2	2.10	0.54
1:A:472:ILE:HG21	1:A:578:SER:HB3	1.89	0.54
1:A:2029:GLY:HA2	1:A:2032:LYS:HD2	1.90	0.54
2:C:251:GLN:O	2:C:254:LYS:HG2	2.07	0.54
1:A:2096:LEU:HD11	1:A:2188:ALA:HB1	1.89	0.54
2:C:232:ARG:HH21	2:C:236:LEU:HD23	1.71	0.54
2:E:237:GLU:HA	2:E:240:VAL:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:ILE:HG13	1:A:1158:LEU:HA	1.89	0.54
2:E:202:GLN:HB2	2:E:206:ASN:OD1	2.07	0.54
1:A:1509:VAL:H	1:A:1513:ASN:HB2	1.72	0.53
1:A:1619:LEU:O	1:A:1623:ASN:CB	2.48	0.53
2:B:248:SER:O	2:B:252:THR:HG23	2.08	0.53
1:A:353:PRO:HB2	1:A:843:LEU:HD11	1.90	0.53
1:A:580:LEU:HD22	1:A:745:LYS:HB2	1.88	0.53
1:A:1530:LEU:HG	1:A:1760:ASN:HB3	1.90	0.53
1:A:1532:ASN:O	1:A:1536:THR:HG22	2.08	0.53
1:A:2041:ILE:O	1:A:2045:VAL:HG23	2.08	0.53
1:A:886:ASP:OD1	1:A:887:ILE:N	2.40	0.53
1:A:956:PRO:O	1:A:960:ALA:N	2.35	0.53
1:A:1605:ARG:HA	1:A:1608:ASN:ND2	2.23	0.53
1:A:1632:GLY:H	1:A:1638:LYS:HZ2	1.54	0.53
1:A:272:LEU:HA	1:A:366:TRP:HZ2	1.73	0.53
1:A:1852:ILE:HG13	1:A:1856:PRO:HG3	1.90	0.53
1:A:2054:SER:HA	1:A:2057:ASN:ND2	2.23	0.53
2:D:225:THR:O	2:D:228[A]:ASN:ND2	2.41	0.53
1:A:247:GLY:O	1:A:251:ILE:HG12	2.08	0.53
1:A:224:ASN:OD1	1:A:229:THR:OG1	2.26	0.53
1:A:332:PHE:CE2	1:A:335:ASP:HB2	2.43	0.53
1:A:358:GLU:CD	1:A:847:LEU:H	2.10	0.53
1:A:1115:LEU:HD12	1:A:1118:LEU:HD13	1.90	0.53
1:A:580:LEU:HB3	1:A:745:LYS:HD2	1.90	0.53
1:A:2024:ASN:OD1	1:A:2025:GLN:N	2.42	0.53
1:A:375:GLN:OE1	1:A:375:GLN:N	2.40	0.53
1:A:476:ASP:OD2	1:A:515:LEU:N	2.38	0.53
1:A:518:PHE:CD2	1:A:519:LEU:HD12	2.44	0.53
2:B:215:LEU:O	2:B:219:VAL:HG22	2.09	0.53
2:D:248:SER:O	2:D:252:THR:HG23	2.09	0.53
1:A:411:ARG:HD3	1:A:418:TRP:HD1	1.73	0.52
2:B:251:GLN:O	2:B:255:ASN:ND2	2.41	0.52
1:A:95:LEU:O	1:A:98:ILE:HB	2.10	0.52
1:A:381:ARG:HB2	1:A:732:ILE:HG12	1.89	0.52
1:A:1056:PHE:HB2	1:A:1059:VAL:HG12	1.91	0.52
1:A:1745:ASN:CA	1:A:1964:TRP:HZ2	2.20	0.52
2:B:254:LYS:O	2:B:258:VAL:HG23	2.09	0.52
2:D:249:LEU:O	2:D:253:ILE:HG13	2.09	0.52
1:A:517:ASN:OD1	1:A:518:PHE:N	2.42	0.52
2:F:358:ILE:O	2:F:364:ARG:NH1	2.30	0.52
1:A:671:TRP:CH2	1:A:747:TRP:HA	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1516:ASP:O	1:A:1520:MET:HG2	2.09	0.52
1:A:1737:ILE:HG22	1:A:1972:VAL:HG12	1.73	0.52
1:A:1745:ASN:HA	1:A:1964:TRP:CH2	2.45	0.52
2:C:230:ASP:OD1	2:D:225:THR:HG23	2.10	0.52
2:C:250:ILE:O	2:C:253:ILE:HG22	2.09	0.52
1:A:411:ARG:HD2	1:A:416:GLY:HA3	1.90	0.52
1:A:1731:CYS:N	1:A:1785:TYR:OH	2.41	0.52
1:A:1740:ILE:HD13	1:A:1741:GLU:H	1.75	0.52
2:B:234:ASN:OD1	2:B:235:GLN:N	2.42	0.52
1:A:945:CYS:O	1:A:948:LEU:HB2	2.09	0.52
1:A:967:LEU:O	1:A:971:GLY:N	2.39	0.52
2:B:219:VAL:HA	2:B:222:ILE:HG22	1.90	0.52
2:C:205:LEU:HD21	2:D:205:LEU:HD11	1.92	0.52
1:A:76:ASP:HA	1:A:79:LYS:HE3	1.91	0.52
1:A:472:ILE:HG13	1:A:473:PHE:H	1.74	0.52
1:A:567:LYS:HG3	1:A:568:ARG:N	2.24	0.52
1:A:831:VAL:HG13	1:A:836:ILE:HG22	1.92	0.52
2:C:258:VAL:HA	2:C:261:LYS:HE3	1.91	0.52
1:A:427:ALA:HB1	1:A:430:GLY:H	1.75	0.52
1:A:481:ALA:HB2	1:A:510:PHE:CE1	2.45	0.52
1:A:671:TRP:NE1	1:A:816:HIS:HE1	2.08	0.52
1:A:1971:THR:HG23	1:A:1988:ILE:HG21	1.92	0.52
1:A:11:GLU:OE1	1:A:1083:ARG:NH2	2.35	0.51
1:A:1637:GLU:HG3	1:A:1638:LYS:HD3	1.91	0.51
1:A:1068:SER:HB3	1:A:1269:THR:HG22	1.90	0.51
1:A:2148:LEU:HD13	1:A:2153:ARG:NH1	2.25	0.51
1:A:1972:VAL:HG22	1:A:1985:VAL:HG22	1.92	0.51
1:A:480:SER:HB3	1:A:564:LYS:HG3	1.92	0.51
1:A:830:PHE:HB3	1:A:837:PHE:HB2	1.93	0.51
1:A:1953:PHE:HZ	1:A:2019:SER:HB2	1.76	0.51
2:B:218:ASN:ND2	2:E:220[B]:ASN:HD21	2.08	0.51
2:C:204:ASP:O	2:C:208:LEU:HB2	2.09	0.51
2:F:368:LEU:HA	2:F:371:ILE:HG22	1.93	0.51
1:A:62:ARG:NH2	1:A:194:GLN:OE1	2.26	0.51
1:A:172:ASP:HB3	1:A:173:TRP:CE3	2.45	0.51
1:A:837:PHE:CE1	1:A:842:ILE:HG12	2.45	0.51
1:A:1971:THR:HG23	1:A:1988:ILE:CG2	2.41	0.51
1:A:1485:ASP:HB2	1:A:1575:TRP:CH2	2.45	0.51
1:A:1606:SER:OG	1:A:1607:MET:SD	2.68	0.51
1:A:1915:SER:O	1:A:1955:ARG:NH1	2.39	0.51
1:A:65:ASN:HD21	1:A:203:ILE:HD11	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:HB2	1:A:110:LEU:HD13	1.93	0.51
2:C:258:VAL:O	2:C:261:LYS:HG2	2.10	0.51
1:A:442:SER:O	1:A:446:THR:HG23	2.11	0.51
1:A:1343:THR:O	1:A:1347:ILE:HG12	2.11	0.51
1:A:2208:THR:HG23	1:A:2211:ILE:HG12	1.93	0.51
1:A:459:LYS:HG3	1:A:460:LYS:HG2	1.92	0.51
1:A:789:THR:O	1:A:792:LYS:HB2	2.11	0.51
1:A:1339:GLN:HA	1:A:1342:ILE:HD12	1.93	0.51
1:A:287:TYR:CD2	1:A:369:PRO:HB3	2.46	0.51
1:A:1745:ASN:CB	1:A:1964:TRP:HH2	2.21	0.51
1:A:245:TYR:HD1	1:A:248:ARG:HD2	1.75	0.50
1:A:1127:TYR:HA	1:A:1130:ALA:HB3	1.91	0.50
2:B:249:LEU:HD22	2:E:254:LYS:HD3	1.93	0.50
2:D:215:LEU:O	2:D:219:VAL:HG23	2.11	0.50
1:A:364:ARG:HH21	1:A:368:HIS:HE1	1.60	0.50
1:A:1136:CYS:SG	1:A:1373:CYS:HB2	2.51	0.50
1:A:1920:GLN:OE1	1:A:1922:CYS:N	2.45	0.50
2:C:237:GLU:HA	2:D:236:LEU:HD21	1.92	0.50
1:A:580:LEU:HD22	1:A:745:LYS:HD2	1.93	0.50
1:A:867:SER:OG	1:A:868:CYS:N	2.44	0.50
2:B:257:ILE:HG23	2:B:261:LYS:HZ1	1.76	0.50
1:A:214:ILE:O	1:A:220:VAL:HA	2.11	0.50
1:A:359:LEU:HD23	1:A:363:MET:HG3	1.94	0.50
1:A:1690:ILE:HG23	1:A:1691:ARG:HE	1.76	0.50
1:A:332:PHE:HD2	1:A:336:GLU:H	1.60	0.50
1:A:589:LYS:O	1:A:591:ASN:ND2	2.45	0.50
1:A:751:SER:O	1:A:755:ILE:HG12	2.12	0.50
2:D:219:VAL:HB	2:E:215:LEU:HD12	1.94	0.50
1:A:667:TYR:OH	1:A:751:SER:OG	2.21	0.50
1:A:826:SER:OG	1:A:827:SER:N	2.44	0.50
1:A:1118:LEU:HG	1:A:1119:LYS:H	1.75	0.50
1:A:1772:HIS:HA	1:A:1775:ARG:NH2	2.26	0.50
1:A:2219:LEU:O	1:A:2223:VAL:HG23	2.12	0.50
2:C:261:LYS:HA	2:C:264:MET:HG2	1.94	0.50
1:A:771:GLN:HB2	1:A:832:TYR:OH	2.12	0.50
1:A:945:CYS:O	1:A:948:LEU:HB3	2.11	0.50
1:A:968:ILE:HD12	1:A:974:ASP:O	2.11	0.50
1:A:998:PRO:HB3	1:A:1057:PRO:HB2	1.94	0.50
1:A:1980:PRO:HB3	1:A:2034:GLU:HG3	1.94	0.50
1:A:2207:LEU:N	1:A:2207:LEU:CD2	2.73	0.50
1:A:474:MET:HA	1:A:518:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:GLY:HA2	1:A:526:PRO:HG2	1.94	0.49
1:A:1540:PRO:HG3	1:A:2162:PHE:CD2	2.47	0.49
2:B:254:LYS:NZ	2:C:256:ASP:OD2	2.32	0.49
1:A:28:LEU:HB3	1:A:49:TRP:CH2	2.47	0.49
2:E:234:ASN:O	2:E:237:GLU:HG2	2.13	0.49
1:A:296:PHE:O	1:A:299:ALA:HB3	2.13	0.49
1:A:567:LYS:HG3	1:A:568:ARG:H	1.76	0.49
1:A:1616:LEU:HD22	1:A:1642:LEU:HB2	1.94	0.49
1:A:1735:TYR:HB2	1:A:1974:ARG:HH12	1.77	0.49
1:A:1849:THR:O	1:A:1852:ILE:HG22	2.12	0.49
1:A:1779:LEU:HD11	1:A:1850:GLN:HG3	1.95	0.49
1:A:1947:LYS:HB2	1:A:1986:TYR:CE1	2.47	0.49
1:A:2054:SER:HA	1:A:2057:ASN:HD21	1.78	0.49
1:A:1139:ASP:O	1:A:1143:ASN:ND2	2.38	0.49
1:A:1856:PRO:HB2	1:A:1860:TRP:CZ2	2.48	0.49
1:A:1894:GLU:O	1:A:1897:ILE:HG22	2.13	0.49
2:B:234:ASN:HA	2:B:237:GLU:HG3	1.93	0.49
1:A:299:ALA:HB1	1:A:315:HIS:HA	1.95	0.49
1:A:513:ARG:CZ	1:A:1084:SER:HB3	2.43	0.49
1:A:1180:TYR:OH	1:A:1921:GLN:O	2.21	0.49
1:A:81:HIS:CE1	1:A:83:GLN:HG3	2.48	0.49
1:A:1334:ASN:HA	1:A:1337:TYR:HB3	1.94	0.49
1:A:8:LEU:HD11	1:A:860:LEU:HA	1.94	0.49
1:A:348:PHE:CE1	1:A:359:LEU:HD22	2.48	0.49
1:A:1478:GLU:C	1:A:1480:MET:H	2.16	0.49
2:B:252:THR:HA	2:B:255:ASN:HD21	1.78	0.49
2:C:223:LEU:HA	2:C:226:VAL:HG12	1.93	0.49
1:A:315:HIS:CE1	2:F:352:GLN:HE22	2.30	0.49
1:A:744:GLN:HA	1:A:747:TRP:HB2	1.94	0.49
1:A:2152:LEU:HD11	1:A:2168:THR:HG22	1.94	0.49
1:A:297:VAL:HG11	1:A:360:LEU:HB2	1.93	0.48
1:A:352:THR:HB	1:A:353:PRO:HD2	1.94	0.48
1:A:361:CYS:HB2	1:A:848:LYS:HB2	1.95	0.48
1:A:1015:ARG:O	1:A:1018:GLN:NE2	2.46	0.48
1:A:251:ILE:HD12	1:A:847:LEU:HG	1.95	0.48
1:A:515:LEU:HD23	1:A:1085:ILE:HG12	1.95	0.48
1:A:1929:ASN:HA	1:A:1932:ILE:HG22	1.94	0.48
2:C:222:ILE:HA	2:C:225:THR:HG22	1.95	0.48
1:A:364:ARG:O	1:A:364:ARG:HD3	2.13	0.48
1:A:918:LEU:HA	1:A:921:ILE:HG22	1.95	0.48
1:A:1362:GLU:H	1:A:1362:GLU:CD	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:ILE:HG13	2:B:251:GLN:N	2.28	0.48
2:D:234:ASN:O	2:D:237:GLU:HG2	2.12	0.48
1:A:513:ARG:HH12	1:A:1088:LYS:HB2	1.79	0.48
1:A:677:ILE:N	1:A:678:PRO:HD2	2.27	0.48
1:A:110:LEU:O	1:A:113:TRP:HB3	2.14	0.48
1:A:113:TRP:O	1:A:117:VAL:HG22	2.13	0.48
1:A:1808:ALA:N	1:A:1830:ASN:OD1	2.46	0.48
1:A:2090:THR:O	1:A:2094:THR:HG23	2.13	0.48
2:C:240:VAL:HG21	2:D:236:LEU:HD13	1.94	0.48
2:B:247:GLN:O	2:B:250:ILE:HG12	2.14	0.48
1:A:478:ALA:O	1:A:570:ARG:NH1	2.47	0.48
1:A:1806:TYR:CZ	1:A:1815:MET:HB2	2.49	0.48
1:A:44:LEU:HD23	1:A:44:LEU:H	1.78	0.48
1:A:261:LEU:HG	1:A:262:ASN:H	1.78	0.48
1:A:289:ILE:O	1:A:293:LEU:N	2.46	0.48
1:A:667:TYR:HB3	1:A:773:ASP:OD2	2.12	0.48
1:A:1353:ASN:N	1:A:1354:PRO:HD3	2.29	0.48
2:C:262:ALA:O	2:C:266:THR:HG23	2.14	0.48
1:A:911:ILE:HG12	1:A:913:GLY:H	1.79	0.48
1:A:1216:TYR:OH	1:A:1338:GLN:NE2	2.47	0.48
2:B:246:SER:O	2:B:249:LEU:HG	2.14	0.48
1:A:130:GLN:HG3	1:A:134:ASN:HD21	1.78	0.48
1:A:271:LEU:HD21	1:A:363:MET:HG2	1.96	0.48
1:A:1146:LYS:HG3	1:A:1157:ASN:HB3	1.96	0.48
1:A:1793:TYR:OH	1:A:1971:THR:CG2	2.61	0.48
1:A:2167:ILE:HD12	1:A:2199:ILE:HA	1.96	0.48
2:B:257:ILE:HG12	2:B:261:LYS:NZ	2.29	0.48
2:E:240:VAL:O	2:E:244:LEU:HD23	2.14	0.48
1:A:1088:LYS:O	1:A:1091:GLU:HB3	2.14	0.47
1:A:1165:ASP:OD1	1:A:1166:PRO:HD2	2.14	0.47
1:A:1304:THR:OG1	1:A:1305:PRO:HD3	2.14	0.47
1:A:2159:ASP:HB3	1:A:2165:PHE:H	1.79	0.47
2:D:216:ALA:HA	2:E:215:LEU:HG	1.95	0.47
1:A:71:ILE:HD12	1:A:77:LEU:HB2	1.95	0.47
1:A:263:PRO:O	1:A:267:ARG:HG2	2.14	0.47
1:A:535:SER:OG	1:A:536:GLY:N	2.48	0.47
1:A:1563:LEU:HB3	1:A:2027:TRP:CZ2	2.49	0.47
1:A:1739:ILE:HD13	1:A:1739:ILE:H	1.79	0.47
1:A:1818:ILE:O	1:A:1822:PHE:N	2.47	0.47
1:A:2084:PHE:HA	1:A:2087:LEU:HB3	1.97	0.47
1:A:548:TYR:HD1	1:A:563:ALA:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1290:LEU:HD21	1:A:1328:ASP:HB2	1.94	0.47
1:A:1589:ASP:O	1:A:1590:LEU:HG	2.15	0.47
1:A:244:MET:HG3	1:A:365:LEU:O	2.14	0.47
1:A:1658:GLU:HG2	1:A:1659:ASN:N	2.30	0.47
2:C:233:MET:HG2	2:D:229:LEU:HD22	1.97	0.47
1:A:575:ILE:O	1:A:579:LEU:HG	2.15	0.47
1:A:1563:LEU:HG	1:A:1755:PRO:HG2	1.95	0.47
1:A:1739:ILE:HB	1:A:1970:ILE:HG12	1.96	0.47
1:A:301:LEU:HD11	1:A:353:PRO:HB3	1.96	0.47
1:A:1893:VAL:HB	1:A:1928:ILE:HD11	1.96	0.47
1:A:1924:SER:O	1:A:1928:ILE:HG12	2.15	0.47
1:A:1949:SER:HB2	1:A:1984:GLU:HA	1.96	0.47
1:A:238:VAL:HA	1:A:241:VAL:HG12	1.97	0.47
1:A:376:ALA:HA	1:A:379:LYS:HD2	1.96	0.47
1:A:1211:PRO:HG2	1:A:1314:PHE:CG	2.50	0.47
1:A:1608:ASN:OD1	1:A:1609:LEU:N	2.48	0.47
1:A:1735:TYR:HB2	1:A:1974:ARG:NH1	2.30	0.47
2:C:207:ALA:O	2:C:210:THR:HG22	2.14	0.47
1:A:210:GLU:HG3	1:A:224:ASN:HB2	1.97	0.47
1:A:1126:THR:OG1	1:A:1127:TYR:N	2.47	0.47
1:A:1506:LEU:O	1:A:1508:VAL:HG23	2.15	0.47
1:A:2170:ILE:HG22	1:A:2199:ILE:HG21	1.96	0.47
2:B:210:THR:O	2:B:213:GLN:HG3	2.14	0.47
1:A:867:SER:OG	1:A:899:GLN:NE2	2.48	0.46
1:A:1580:VAL:O	1:A:1583:VAL:HB	2.15	0.46
1:A:1750:PRO:O	1:A:2017:LEU:HD12	2.14	0.46
1:A:1779:LEU:HG	1:A:1784:TRP:CH2	2.50	0.46
2:B:222:ILE:HD12	2:E:223:LEU:HB3	1.97	0.46
1:A:359:LEU:O	1:A:363:MET:HG3	2.15	0.46
1:A:1067:THR:HG23	1:A:1069:VAL:HG22	1.96	0.46
1:A:1320:ASP:OD1	1:A:1320:ASP:N	2.47	0.46
1:A:1437:LEU:HG	1:A:1690:ILE:HD12	1.98	0.46
1:A:1783:ALA:O	1:A:1786:LYS:HG2	2.15	0.46
1:A:2015:PHE:O	1:A:2016:THR:OG1	2.32	0.46
2:C:242:ARG:O	2:C:245:SER:OG	2.26	0.46
2:D:209:VAL:O	2:D:212:VAL:HG22	2.16	0.46
2:E:246:SER:O	2:E:250:ILE:HG12	2.15	0.46
1:A:57:SER:C	1:A:59:LEU:H	2.19	0.46
1:A:1267:SER:O	1:A:1271:VAL:HB	2.16	0.46
1:A:1950:TRP:HD1	1:A:1950:TRP:O	1.98	0.46
1:A:2170:ILE:HG13	1:A:2171:LEU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ASN:O	1:A:72:THR:HG23	2.14	0.46
1:A:98:ILE:O	1:A:100:ASP:N	2.49	0.46
1:A:183:ILE:O	1:A:187:MET:HG3	2.15	0.46
1:A:448:LYS:O	1:A:449:HIS:ND1	2.48	0.46
1:A:694:GLU:OE1	1:A:694:GLU:N	2.49	0.46
1:A:1752:PRO:HB3	1:A:2017:LEU:HD11	1.97	0.46
1:A:658:SER:HB2	1:A:800:CYS:HB3	1.97	0.46
1:A:1048:PHE:CD2	1:A:1389:VAL:HG12	2.50	0.46
1:A:1150:ALA:O	1:A:1154:GLY:N	2.46	0.46
1:A:1643:THR:O	1:A:1647:ARG:HG2	2.14	0.46
1:A:1950:TRP:HB2	1:A:1953:PHE:HA	1.97	0.46
1:A:2051:LEU:HG	1:A:2052:PHE:H	1.79	0.46
2:B:250:ILE:HG22	2:C:250:ILE:HD11	1.97	0.46
1:A:312:GLY:HA3	2:F:384:LYS:NZ	2.31	0.46
1:A:353:PRO:HG3	1:A:838:TYR:CE1	2.50	0.46
1:A:985:LYS:HD3	1:A:986:PRO:HD2	1.97	0.46
1:A:1386:ALA:O	1:A:1387:LEU:HD22	2.16	0.46
1:A:1981:ALA:H	1:A:2030:HIS:HE1	1.63	0.46
1:A:142:ARG:NH1	1:A:143:GLY:O	2.49	0.46
1:A:1352:ASN:HB3	1:A:1356:ILE:HD13	1.98	0.46
2:C:210:THR:O	2:C:213:GLN:HG2	2.16	0.46
2:E:248:SER:O	2:E:251:GLN:HG3	2.15	0.46
2:E:215:LEU:HD13	2:E:218:ASN:HD22	1.81	0.46
2:D:235:GLN:O	2:D:239:LYS:HG2	2.16	0.45
2:D:257:ILE:HD11	2:E:257:ILE:HD13	1.97	0.45
1:A:390:LEU:HD23	1:A:390:LEU:H	1.81	0.45
1:A:404:THR:HG21	1:A:446:THR:HG21	1.98	0.45
1:A:595:MET:SD	1:A:598:LEU:HB3	2.56	0.45
1:A:607:MET:HA	1:A:610:ILE:HG12	1.98	0.45
1:A:997:ASP:OD2	1:A:1007:TYR:OH	2.34	0.45
1:A:1052:ARG:HG3	1:A:1385:GLU:HA	1.98	0.45
1:A:1097:ASN:OD1	1:A:1101:ASN:ND2	2.44	0.45
1:A:1136:CYS:HB2	1:A:1139:ASP:OD2	2.17	0.45
1:A:1210:PRO:CG	1:A:1211:PRO:HD3	2.44	0.45
1:A:1826:LYS:HA	1:A:1826:LYS:HD2	1.78	0.45
2:B:223:LEU:HD23	2:C:218:ASN:HD21	1.81	0.45
2:D:232:ARG:O	2:D:236:LEU:HG	2.16	0.45
1:A:284:ASP:O	1:A:287:TYR:HB2	2.16	0.45
1:A:935:SER:OG	1:A:941:ASN:N	2.50	0.45
1:A:1633:PHE:O	1:A:1637:GLU:HB3	2.16	0.45
1:A:1889:MET:SD	1:A:1889:MET:N	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:LEU:HD22	1:A:1086:MET:SD	2.56	0.45
1:A:2041:ILE:HA	1:A:2044:VAL:HG22	1.98	0.45
1:A:46:ASN:N	1:A:47:GLN:OE1	2.49	0.45
1:A:1123:GLU:N	1:A:1123:GLU:OE1	2.49	0.45
1:A:1150:ALA:N	1:A:1151:PRO:HD2	2.32	0.45
1:A:2130:VAL:O	1:A:2134:THR:HG23	2.16	0.45
1:A:1095:LEU:HG	1:A:1096:SER:H	1.82	0.45
1:A:1443:PHE:HB3	1:A:1683:THR:HG22	1.99	0.45
2:C:261:LYS:O	2:C:264:MET:HG2	2.17	0.45
1:A:189:GLN:NE2	1:A:193:ARG:HE	2.13	0.45
1:A:295:SER:HA	1:A:298:TYR:CD1	2.52	0.45
1:A:298:TYR:HD2	1:A:829:PHE:CZ	2.34	0.45
1:A:569:MET:HE3	1:A:696:ILE:HG23	1.98	0.45
1:A:1067:THR:OG1	1:A:1068:SER:N	2.49	0.45
1:A:1956:PHE:CE1	1:A:1960:ILE:HD11	2.52	0.45
2:E:244:LEU:HA	2:E:247:GLN:HG2	1.99	0.45
1:A:110:LEU:HD23	1:A:178:ASP:HB3	1.99	0.45
1:A:187:MET:SD	1:A:238:VAL:HG21	2.57	0.45
1:A:383:SER:OG	1:A:669:LEU:O	2.35	0.45
1:A:600:LEU:HD21	1:A:1302:LYS:HZ3	1.82	0.45
1:A:1749:TYR:CE2	1:A:1751:ILE:HB	2.52	0.45
2:B:208:LEU:HG	2:C:208:LEU:HG	1.99	0.45
1:A:1736:ILE:HD12	1:A:1738:TRP:HB3	1.99	0.45
1:A:702:ARG:O	1:A:703:SER:OG	2.26	0.45
1:A:1509:VAL:O	1:A:1514:ILE:HG12	2.17	0.45
1:A:1851:PHE:O	1:A:1855:VAL:HG12	2.16	0.45
1:A:2164:ILE:HD12	1:A:2164:ILE:H	1.81	0.45
1:A:695:TRP:HE1	1:A:699:ARG:NE	2.15	0.44
1:A:510:PHE:CG	1:A:511:ASN:N	2.85	0.44
1:A:1390:LYS:O	1:A:1392:HIS:NE2	2.49	0.44
1:A:1529:ALA:HB1	1:A:1566:ILE:HD11	1.98	0.44
1:A:1584:LEU:HD21	1:A:1619:LEU:HA	1.99	0.44
1:A:1745:ASN:CB	1:A:1964:TRP:HZ2	2.24	0.44
2:C:239:LYS:O	2:C:243:ILE:HG23	2.17	0.44
1:A:1767:ASN:OD1	1:A:1767:ASN:N	2.50	0.44
1:A:1950:TRP:O	1:A:1950:TRP:CD1	2.70	0.44
1:A:2167:ILE:HB	1:A:2199:ILE:HG23	1.97	0.44
2:D:225:THR:O	2:D:229:LEU:HG	2.18	0.44
1:A:19:VAL:HA	1:A:371:LEU:H	1.82	0.44
1:A:514:LEU:O	1:A:518:PHE:CB	2.60	0.44
1:A:677:ILE:HD12	1:A:680:ALA:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:ASN:O	1:A:714:PRO:HD3	2.18	0.44
1:A:1003:ILE:HG22	1:A:1004:GLU:H	1.82	0.44
1:A:1805:LEU:HA	1:A:1828:TYR:O	2.17	0.44
1:A:2035:ARG:HD3	1:A:2035:ARG:HA	1.72	0.44
1:A:2051:LEU:HD12	1:A:2054:SER:HB2	2.00	0.44
1:A:24:TYR:HA	1:A:27:ILE:HG12	1.99	0.44
1:A:1374:CYS:HB2	1:A:1376:ARG:HG2	2.00	0.44
1:A:836:ILE:O	1:A:843:LEU:HD23	2.18	0.44
1:A:1279:GLN:HE22	1:A:1282:THR:N	2.16	0.44
1:A:70:LEU:O	1:A:74:ILE:N	2.51	0.44
1:A:660:LEU:HB2	1:A:825:ILE:HG22	1.99	0.44
1:A:1052:ARG:HE	1:A:1386:ALA:H	1.66	0.44
1:A:1983:HIS:HE1	1:A:2033:GLN:HE22	1.65	0.44
2:D:200:LEU:HD11	2:E:200:LEU:HB2	1.99	0.44
1:A:62:ARG:HA	1:A:65:ASN:ND2	2.33	0.44
1:A:422:ASN:OD1	1:A:457:LYS:NZ	2.51	0.44
1:A:666:LYS:HG3	1:A:669:LEU:HD11	1.98	0.44
1:A:1005:TYR:HD2	1:A:1110:TYR:HA	1.83	0.44
1:A:1889:MET:HG2	1:A:1890:THR:N	2.32	0.44
1:A:2089:CYS:O	1:A:2092:LEU:HG	2.17	0.44
2:B:208:LEU:O	2:B:212:VAL:HG23	2.18	0.44
1:A:18:ILE:HD13	1:A:236:GLU:HB2	1.98	0.43
1:A:28:LEU:HB3	1:A:49:TRP:CZ2	2.53	0.43
1:A:131:CYS:HA	1:A:970:SER:HB2	2.00	0.43
1:A:287:TYR:CD1	1:A:290:ILE:HD12	2.50	0.43
1:A:510:PHE:O	1:A:512:ARG:HD3	2.18	0.43
1:A:1033:ILE:O	1:A:1072:ARG:HG2	2.18	0.43
1:A:1488:PHE:HA	1:A:1491:CYS:SG	2.58	0.43
1:A:1639:CYS:O	1:A:1643:THR:HG23	2.18	0.43
2:C:250:ILE:HA	2:C:253:ILE:HG22	2.00	0.43
1:A:530:LEU:HD13	1:A:530:LEU:HA	1.81	0.43
1:A:915:GLN:HG3	1:A:918:LEU:HD21	2.00	0.43
1:A:1326:ILE:HD12	1:A:1477:SER:OG	2.18	0.43
1:A:1659:ASN:HA	1:A:1662:ASN:HD22	1.82	0.43
2:E:208:LEU:O	2:E:212:VAL:HG22	2.18	0.43
1:A:936:GLN:O	1:A:1006:GLN:NE2	2.51	0.43
1:A:1307:SER:OG	1:A:1308:SER:N	2.51	0.43
1:A:1734:ASP:HB2	1:A:1974:ARG:O	2.18	0.43
1:A:1747:GLU:HG2	1:A:2017:LEU:O	2.19	0.43
2:E:206:ASN:HA	2:E:209:VAL:HB	2.00	0.43
1:A:955:ASP:OD1	1:A:999:TYR:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1119:LYS:HD2	1:A:1120:ASN:H	1.82	0.43
2:F:376:SER:HB3	2:F:379:GLN:HB2	2.00	0.43
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.84	0.43
1:A:338:ARG:HD2	2:F:348:ILE:HD11	2.01	0.43
1:A:411:ARG:HG2	1:A:439:THR:HA	2.01	0.43
1:A:1920:GLN:CD	1:A:1922:CYS:H	2.22	0.43
2:B:222:ILE:O	2:B:226:VAL:HG13	2.18	0.43
1:A:360:LEU:HD23	1:A:361:CYS:N	2.34	0.43
1:A:428:SER:O	1:A:431:LEU:HB3	2.19	0.43
1:A:879:THR:HG22	1:A:888:CYS:SG	2.59	0.43
1:A:965:LYS:HE2	1:A:1134:GLU:HB2	2.01	0.43
1:A:1889:MET:HG2	1:A:1890:THR:H	1.83	0.43
1:A:310:LEU:HD21	1:A:797:PHE:CE1	2.54	0.43
1:A:847:LEU:HD12	1:A:847:LEU:HA	1.83	0.43
1:A:1636:ASP:HA	1:A:1639:CYS:SG	2.59	0.43
1:A:2208:THR:CG2	1:A:2211:ILE:HG12	2.47	0.43
1:A:943:LEU:HB3	1:A:947:ARG:HD2	2.00	0.43
1:A:1291:THR:HG21	1:A:1330:THR:O	2.19	0.43
1:A:1965:CYS:SG	1:A:1966:TYR:N	2.88	0.43
1:A:1974:ARG:HD3	1:A:2033:GLN:OE1	2.19	0.43
1:A:451:LYS:HD2	1:A:451:LYS:HA	1.77	0.43
1:A:797:PHE:HA	1:A:800:CYS:SG	2.58	0.43
1:A:1849:THR:OG1	1:A:1850:GLN:N	2.52	0.43
2:D:226:VAL:HB	2:E:226:VAL:HG22	2.00	0.43
1:A:10:PRO:C	1:A:188:ARG:HH22	2.23	0.43
1:A:236:GLU:HA	1:A:239:LEU:HD13	2.01	0.43
1:A:476:ASP:N	1:A:1080:ASP:OD2	2.36	0.43
1:A:532:TYR:CD2	1:A:568:ARG:HG2	2.54	0.43
1:A:884:GLU:HG3	1:A:887:ILE:HG22	2.01	0.43
1:A:1239:LEU:O	1:A:1242:VAL:HG12	2.19	0.43
1:A:1805:LEU:HB3	1:A:1908:VAL:HG13	2.01	0.43
1:A:1954:THR:O	1:A:1958:THR:CG2	2.49	0.43
1:A:2018:ILE:O	1:A:2020:PRO:HD3	2.19	0.43
1:A:2163:GLY:H	1:A:2164:ILE:HD12	1.84	0.43
2:B:250:ILE:HG13	2:B:251:GLN:H	1.84	0.43
1:A:422:ASN:HB3	1:A:423:LEU:H	1.69	0.42
1:A:517:ASN:O	1:A:521:ASP:N	2.52	0.42
1:A:604:LEU:HB3	1:A:837:PHE:HE2	1.84	0.42
1:A:608:SER:OG	1:A:840:GLY:HA2	2.19	0.42
1:A:1770:SER:OG	1:A:1771:HIS:N	2.51	0.42
2:B:257:ILE:HG12	2:B:261:LYS:HZ3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:PRO:CB	1:A:102:LYS:HB2	2.49	0.42
1:A:267:ARG:HD2	1:A:347:PRO:HA	2.01	0.42
1:A:748:THR:O	1:A:752:ILE:HG13	2.19	0.42
1:A:923:ASN:ND2	1:A:926:LEU:HB2	2.34	0.42
1:A:997:ASP:OD1	1:A:997:ASP:N	2.52	0.42
1:A:1745:ASN:N	1:A:1745:ASN:OD1	2.53	0.42
1:A:180:TRP:CD1	1:A:245:TYR:HD2	2.37	0.42
1:A:1196:LEU:HB2	1:A:1348:LEU:HD21	2.01	0.42
1:A:411:ARG:NH1	1:A:416:GLY:HA3	2.34	0.42
1:A:580:LEU:HD12	1:A:693:PHE:CE2	2.55	0.42
1:A:1271:VAL:HG11	1:A:1277:GLN:HG2	2.01	0.42
1:A:1504:TYR:HD1	1:A:1504:TYR:HA	1.74	0.42
1:A:1549:LEU:HD23	1:A:1551:ILE:HD11	2.01	0.42
1:A:81:HIS:HE1	1:A:83:GLN:HG3	1.85	0.42
1:A:130:GLN:HG3	1:A:134:ASN:ND2	2.34	0.42
1:A:301:LEU:HD23	1:A:829:PHE:HE1	1.85	0.42
1:A:806:ARG:HG3	1:A:810:ASN:HD21	1.83	0.42
1:A:1349:GLU:O	1:A:1353:ASN:N	2.52	0.42
1:A:1737:ILE:HG21	1:A:1972:VAL:HG13	1.87	0.42
1:A:2038:ALA:HA	1:A:2041:ILE:HD12	2.01	0.42
1:A:2159:ASP:HB3	1:A:2165:PHE:N	2.34	0.42
1:A:515:LEU:HD12	1:A:515:LEU:HA	1.88	0.42
1:A:667:TYR:HB3	1:A:773:ASP:CG	2.40	0.42
1:A:443:TYR:O	1:A:446:THR:OG1	2.24	0.42
1:A:1390:LYS:HB2	1:A:1392:HIS:CE1	2.55	0.42
1:A:1522:LEU:HD12	1:A:1570:VAL:HG23	2.01	0.42
1:A:1740:ILE:HD12	1:A:1744:ALA:HB3	2.02	0.42
1:A:1974:ARG:HA	1:A:1985:VAL:HG23	2.02	0.42
2:D:222:ILE:HD12	2:E:222:ILE:HG21	2.02	0.42
1:A:875:VAL:O	1:A:879:THR:HG23	2.19	0.42
1:A:1251:TRP:HD1	1:A:1289:ASN:HD21	1.67	0.42
1:A:174:LYS:HE2	1:A:174:LYS:HB3	1.89	0.42
1:A:309:GLU:O	1:A:313:GLN:HB2	2.20	0.42
1:A:755:ILE:O	1:A:758:SER:OG	2.32	0.42
1:A:787:LEU:O	1:A:792:LYS:HE2	2.20	0.42
1:A:1815:MET:SD	1:A:1815:MET:N	2.93	0.42
1:A:1911:ASP:HB2	1:A:1947:LYS:HD2	2.02	0.42
1:A:1973:LEU:HD23	1:A:1974:ARG:O	2.19	0.42
1:A:1983:HIS:NE2	1:A:2033:GLN:OE1	2.51	0.42
1:A:2095:HIS:CG	1:A:2133:LEU:HD13	2.55	0.42
1:A:1983:HIS:CE1	1:A:2033:GLN:HE22	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2012:ASP:HB3	1:A:2016:THR:HB	2.02	0.42
1:A:2095:HIS:O	1:A:2099:ILE:HG12	2.20	0.42
2:E:202:GLN:HA	2:E:205:LEU:HB3	2.02	0.42
1:A:8:LEU:HD13	1:A:861:GLY:H	1.85	0.41
1:A:107:LEU:HD13	1:A:182:MET:HG2	2.02	0.41
1:A:245:TYR:HD1	1:A:245:TYR:HA	1.76	0.41
1:A:1205:ASP:HB2	1:A:1208:ASP:HB3	2.01	0.41
1:A:1739:ILE:CD1	1:A:1972:VAL:HG11	2.33	0.41
1:A:245:TYR:CD1	1:A:248:ARG:HD2	2.54	0.41
1:A:900:LEU:HD23	1:A:927:VAL:HG23	2.01	0.41
1:A:907:PRO:O	1:A:910:SER:OG	2.25	0.41
2:D:237:GLU:HA	2:D:240:VAL:HG12	2.02	0.41
1:A:392:PHE:HA	1:A:395:ILE:HG22	2.02	0.41
2:D:206:ASN:O	2:D:210:THR:HG22	2.20	0.41
1:A:392:PHE:N	1:A:393:PRO:HD2	2.35	0.41
1:A:925:HIS:CE1	1:A:929:ARG:HE	2.36	0.41
2:B:211[A]:SER:OG	2:E:212:VAL:HG23	2.21	0.41
2:B:223:LEU:HA	2:B:226:VAL:HG22	2.03	0.41
1:A:69:PHE:HB3	1:A:205:TYR:CE1	2.56	0.41
1:A:373:ALA:O	1:A:377:ALA:HB3	2.20	0.41
1:A:695:TRP:HE1	1:A:699:ARG:CZ	2.34	0.41
1:A:793:LYS:HG2	1:A:793:LYS:H	1.63	0.41
1:A:979:TYR:OH	1:A:1132:THR:OG1	2.22	0.41
1:A:1446:ARG:O	1:A:1450:ASN:HB2	2.21	0.41
1:A:1509:VAL:N	1:A:1513:ASN:HB2	2.35	0.41
2:B:233:MET:O	2:B:237:GLU:HG3	2.21	0.41
2:B:235:GLN:O	2:B:238:THR:OG1	2.31	0.41
2:C:226:VAL:HG22	2:D:225:THR:HG21	2.03	0.41
2:C:232:ARG:NH2	2:C:235[A]:GLN:HB3	2.35	0.41
2:D:230:ASP:OD1	2:E:229:LEU:HD13	2.21	0.41
1:A:1495:LEU:HD11	1:A:1522:LEU:HD21	2.03	0.41
1:A:1851:PHE:CE2	1:A:1855:VAL:HG11	2.56	0.41
2:C:220[B]:ASN:OD1	2:D:218:ASN:ND2	2.54	0.41
1:A:1021:LEU:HD12	1:A:1021:LEU:HA	1.78	0.41
1:A:1265:ASP:O	1:A:1269:THR:OG1	2.28	0.41
1:A:1325:THR:OG1	1:A:1327:ASN:ND2	2.54	0.41
1:A:1632:GLY:H	1:A:1638:LYS:NZ	2.19	0.41
2:C:208:LEU:HD13	2:C:208:LEU:HA	1.98	0.41
1:A:9:LEU:CG	1:A:188:ARG:HH21	2.34	0.41
1:A:102:LYS:HE3	1:A:175:ARG:HD2	2.01	0.41
1:A:300:GLN:O	1:A:303:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1928:ILE:HD13	1:A:1928:ILE:HA	1.97	0.41
1:A:2033:GLN:O	1:A:2037:VAL:HG13	2.20	0.41
1:A:2081:PHE:CE2	1:A:2083:GLU:HB2	2.55	0.41
2:B:234:ASN:O	2:B:238:THR:HG23	2.20	0.41
2:C:240:VAL:O	2:C:244:LEU:HD23	2.21	0.41
2:C:255:ASN:HA	2:C:258:VAL:HG22	2.03	0.41
2:F:377:GLU:HA	2:F:380:LEU:HG	2.03	0.41
1:A:62:ARG:O	1:A:66:VAL:HG23	2.21	0.41
1:A:1745:ASN:CA	1:A:1964:TRP:CH2	3.04	0.41
1:A:1947:LYS:HB2	1:A:1986:TYR:HE1	1.85	0.41
1:A:2128:THR:O	1:A:2131:ARG:HG2	2.20	0.41
2:B:226:VAL:HG21	2:C:222:ILE:HG23	2.03	0.41
1:A:94:ILE:HG13	1:A:95:LEU:HD22	2.03	0.40
1:A:1816:THR:HG21	1:A:1850:GLN:NE2	2.36	0.40
1:A:1893:VAL:HG11	1:A:1924:SER:HB2	2.03	0.40
1:A:2025:GLN:HA	1:A:2028:ASP:OD2	2.21	0.40
1:A:2214:GLN:O	1:A:2217:LYS:HG2	2.22	0.40
2:D:208:LEU:H	2:D:208:LEU:HG	1.74	0.40
2:D:257:ILE:HG22	2:D:261:LYS:HE2	2.03	0.40
1:A:331:SER:OG	1:A:332:PHE:N	2.53	0.40
1:A:770:VAL:O	1:A:771:GLN:HG2	2.21	0.40
1:A:1175:ILE:HD12	1:A:1179:GLY:C	2.42	0.40
1:A:1259:ASN:OD1	1:A:1260:TRP:N	2.54	0.40
1:A:1632:GLY:CA	1:A:1637:GLU:HG2	2.51	0.40
1:A:2085:GLU:HG2	1:A:2086:GLN:H	1.86	0.40
1:A:2148:LEU:HD12	1:A:2148:LEU:O	2.21	0.40
1:A:302:GLN:HG3	1:A:302:GLN:O	2.22	0.40
1:A:768:SER:OG	1:A:769:MET:N	2.54	0.40
1:A:1447:GLN:NE2	1:A:1679:ASN:HB3	2.37	0.40
1:A:1499:LEU:HD21	1:A:1517:TYR:CD2	2.54	0.40
1:A:1545:ARG:HH21	1:A:1700:VAL:HB	1.86	0.40
2:B:236:LEU:HA	2:B:239:LYS:HD2	2.03	0.40
1:A:9:LEU:HA	1:A:10:PRO:HD3	1.93	0.40
1:A:493:SER:OG	1:A:494:LEU:N	2.54	0.40
1:A:691:HIS:ND1	1:A:694:GLU:OE2	2.55	0.40
1:A:1209:ASN:HB3	1:A:1314:PHE:CZ	2.56	0.40
2:B:223:LEU:O	2:B:227:ARG:HG2	2.21	0.40
1:A:266:LYS:HA	1:A:269:THR:HG22	2.04	0.40
1:A:319:CYS:O	1:A:322:ILE:HG22	2.21	0.40
1:A:852:LYS:HD3	1:A:852:LYS:HA	1.86	0.40
1:A:1028:PRO:C	1:A:1030:LEU:H	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1629:LYS:HD2	1:A:1629:LYS:HA	1.87	0.40
1:A:1644:GLU:O	1:A:1648:LYS:HG3	2.22	0.40
1:A:1771:HIS:NE2	1:A:1977:TYR:O	2.54	0.40
1:A:1851:PHE:CZ	1:A:1855:VAL:HG11	2.57	0.40
1:A:1917:SER:OG	1:A:1919:ASN:OD1	2.39	0.40
1:A:1929:ASN:ND2	1:A:1944:LEU:HB3	2.36	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	1832/2255 (81%)	1555 (85%)	272 (15%)	5 (0%)	41	76
2	B	74/392 (19%)	71 (96%)	3 (4%)	0	100	100
2	C	76/392 (19%)	74 (97%)	2 (3%)	0	100	100
2	D	74/392 (19%)	72 (97%)	2 (3%)	0	100	100
2	E	76/392 (19%)	72 (95%)	4 (5%)	0	100	100
2	F	45/392 (12%)	44 (98%)	1 (2%)	0	100	100
All	All	2177/4215 (52%)	1888 (87%)	284 (13%)	5 (0%)	50	81

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1739	ILE
1	A	1029	MET
1	A	1028	PRO
1	A	1218	GLY
1	A	1827	ILE

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	1692/2019 (84%)	1677 (99%)	15 (1%)	78	87
2	B	68/342 (20%)	68 (100%)	0	100	100
2	C	70/342 (20%)	68 (97%)	2 (3%)	42	64
2	D	68/342 (20%)	64 (94%)	4 (6%)	19	46
2	E	70/342 (20%)	68 (97%)	2 (3%)	42	64
2	F	42/342 (12%)	42 (100%)	0	100	100
All	All	2010/3729 (54%)	1987 (99%)	23 (1%)	77	85

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	142	ARG
1	A	364	ARG
1	A	512	ARG
1	A	1156	ARG
1	A	1483	LYS
1	A	1504	TYR
1	A	1740	ILE
1	A	1743	ASN
1	A	1775	ARG
1	A	1829	TYR
1	A	1950	TRP
1	A	1966	TYR
1	A	1967	PHE
1	A	1970	ILE
2	C	235[A]	GLN
2	C	235[B]	GLN
2	D	217[A]	LEU
2	D	217[B]	LEU
2	D	228[A]	ASN
2	D	228[B]	ASN
2	E	231[A]	SER

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Mol	Chain	Res	Type
2	E	231[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	81	HIS
1	A	134	ASN
1	A	315	HIS
1	A	368	HIS
1	A	609	GLN
1	A	771	GLN
1	A	810	ASN
1	A	816	HIS
1	A	817	HIS
1	A	892	ASN
1	A	925	HIS
1	A	980	ASN
1	A	1044	ASN
1	A	1107	ASN
1	A	1183	GLN
1	A	1289	ASN
1	A	1327	ASN
1	A	1338	GLN
1	A	1352	ASN
1	A	1447	GLN
1	A	1539	HIS
1	A	1733	ASN
1	A	1804	HIS
1	A	2030	HIS
2	B	201	GLN
2	B	255	ASN
2	C	218	ASN
2	C	247	GLN
2	C	251	GLN
2	D	202	GLN
2	D	251	GLN
2	E	218	ASN
2	E	247	GLN
2	E	255	ASN

5.3.3 RNA [i](#)

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 monosaccharides 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.

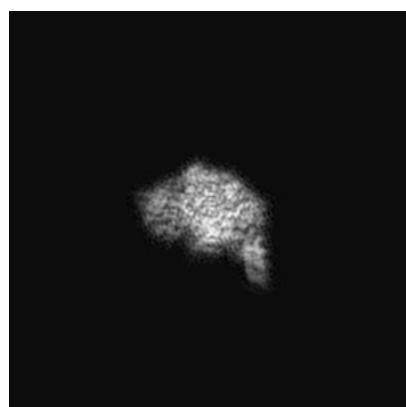
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21096. These allow visual inspection of the internal detail of the map and identification of artifacts.

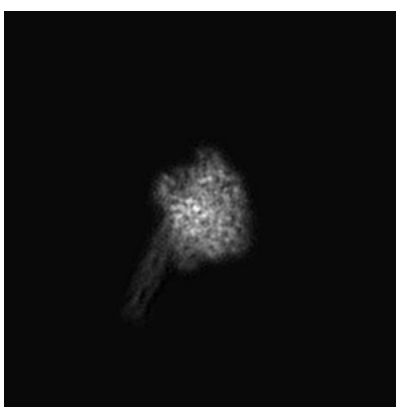
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

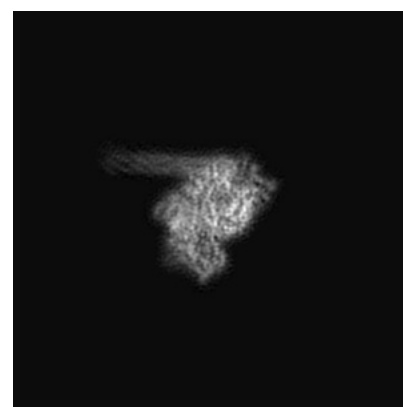
6.1.1 Primary map



X



Y



Z

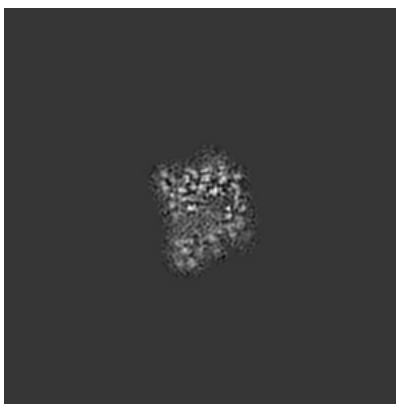
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

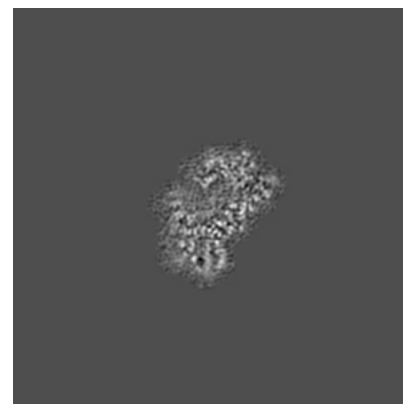
6.2.1 Primary map



X Index: 180



Y Index: 180

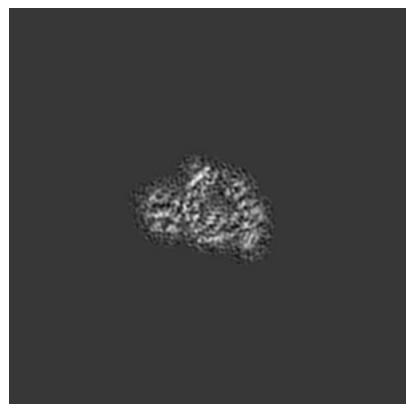


Z Index: 180

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

6.3 Largest variance slices [i](#)

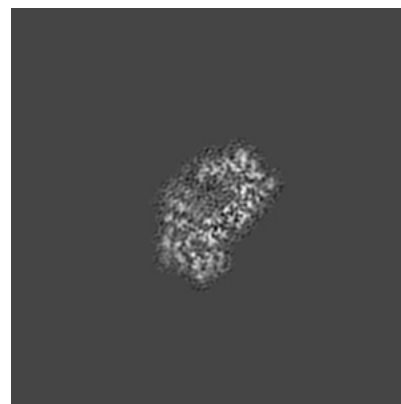
6.3.1 Primary map



X Index: 181



Y Index: 181

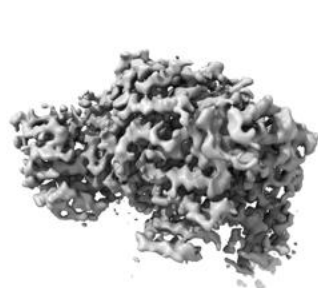


Z Index: 185

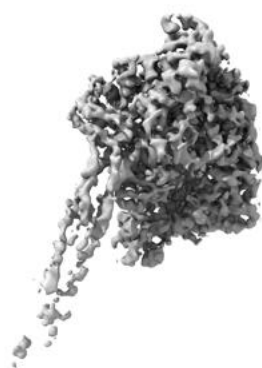
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

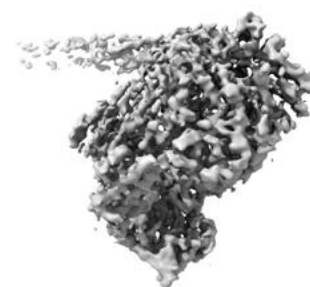
6.4.1 Primary map



X



Y



Z

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.

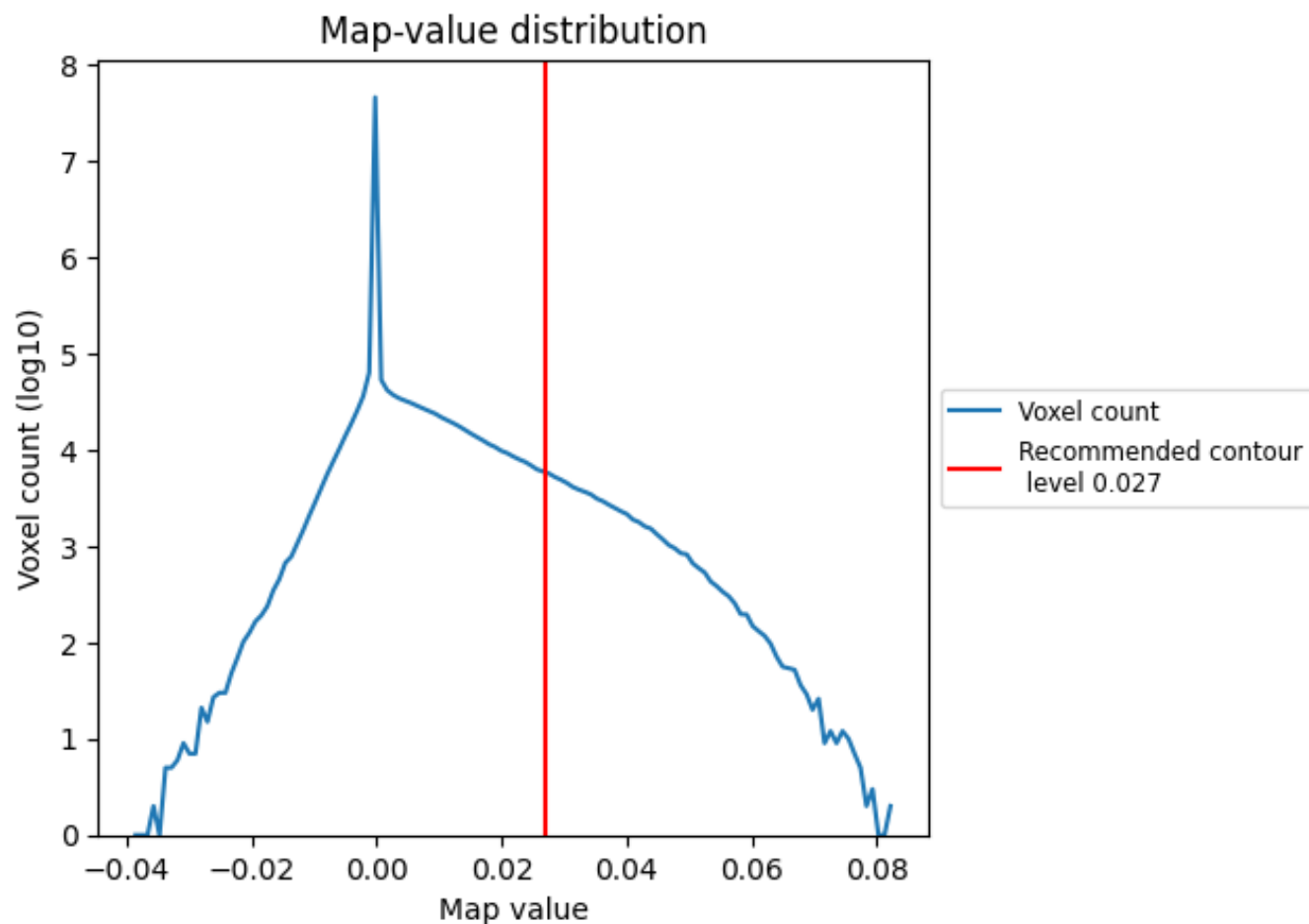
6.5 Mask visualisation

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

7 Map analysis [i](#)

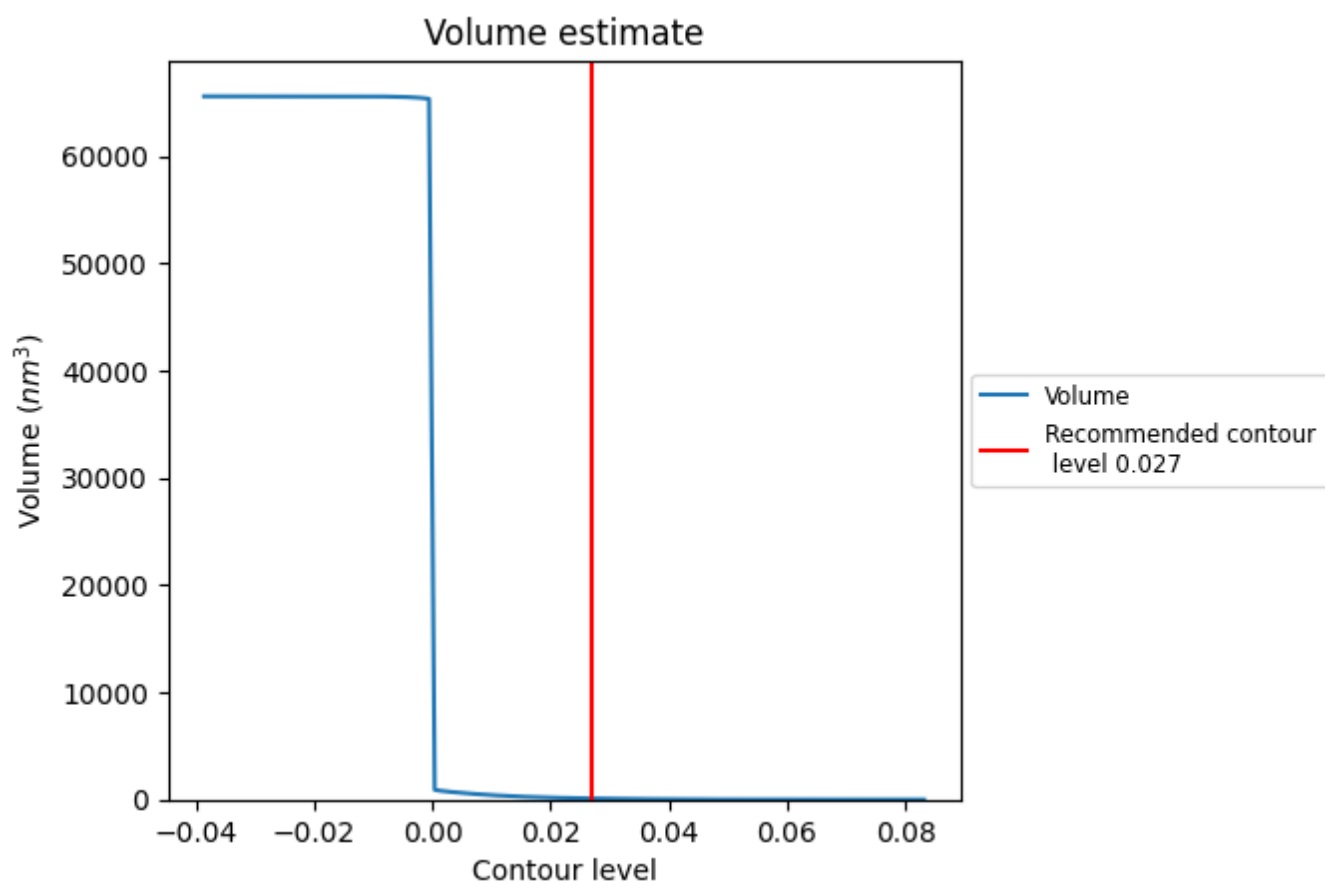
This section contains the results of statistical analysis of the map.

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.

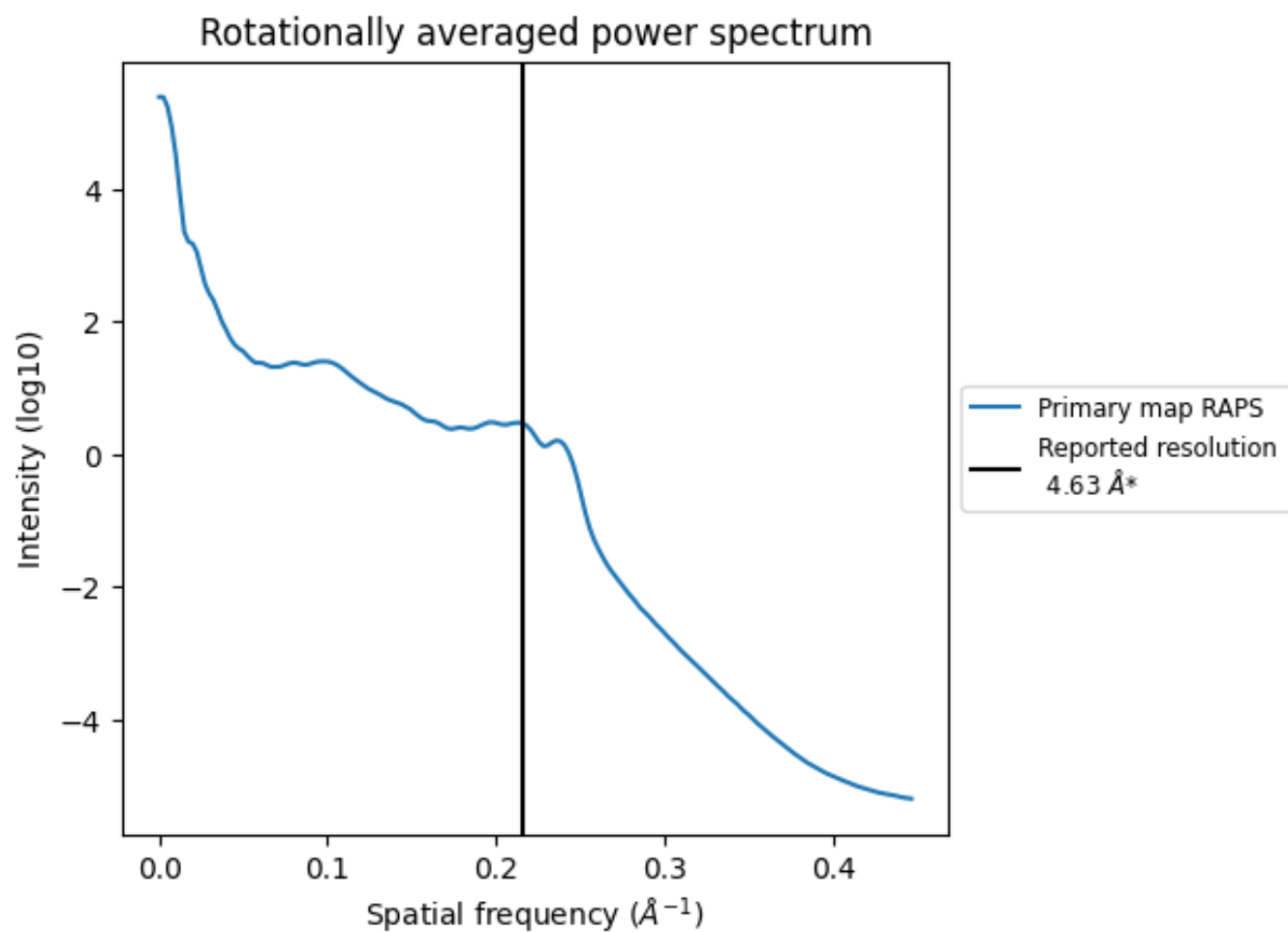
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 102 nm³; this corresponds to an approximate mass of 92 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 ⓘ

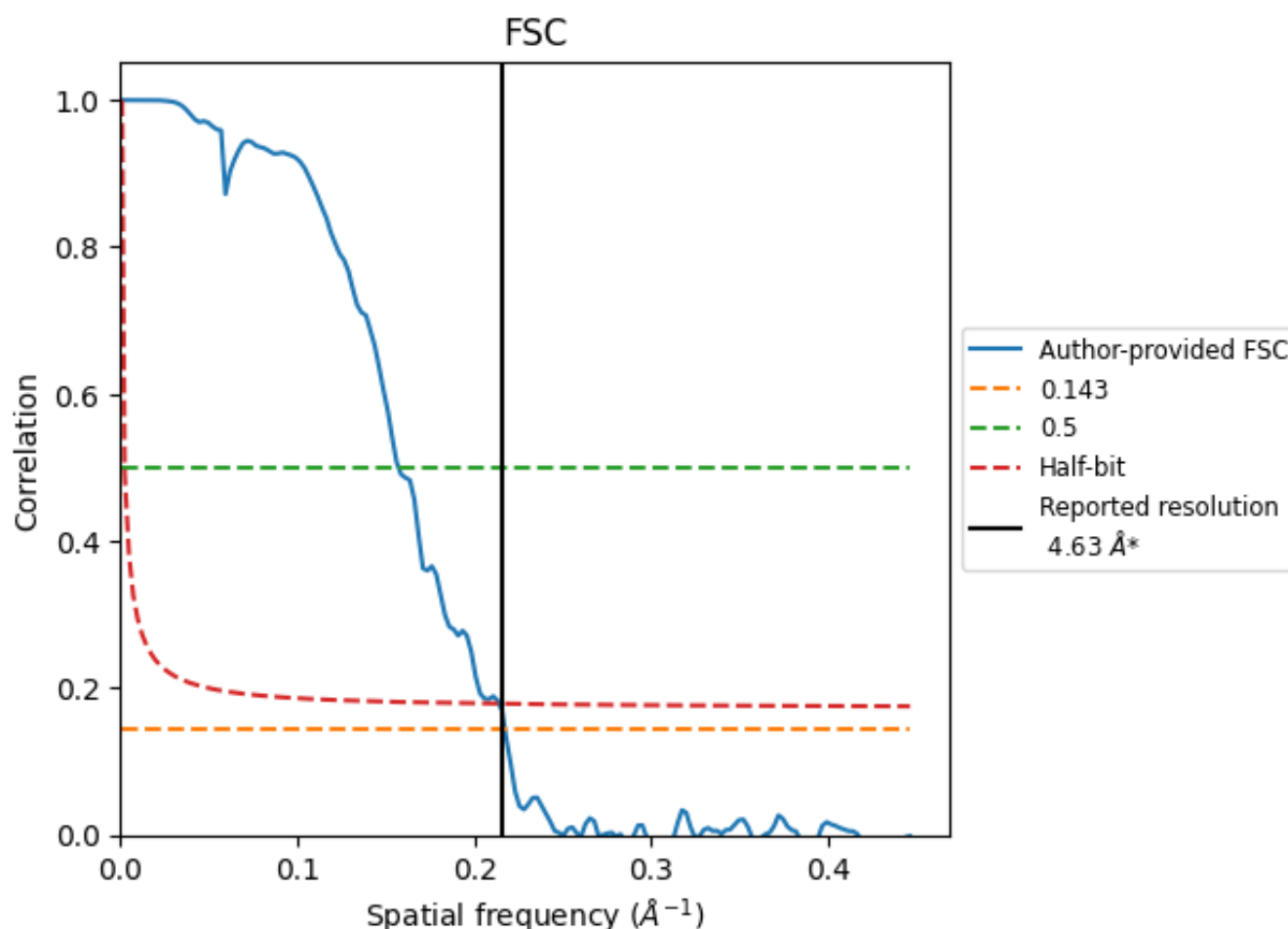


*Reported resolution corresponds to spatial frequency of 0.216 Å⁻¹

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 0.216 Å⁻¹

8.2 Resolution estimates [i](#)

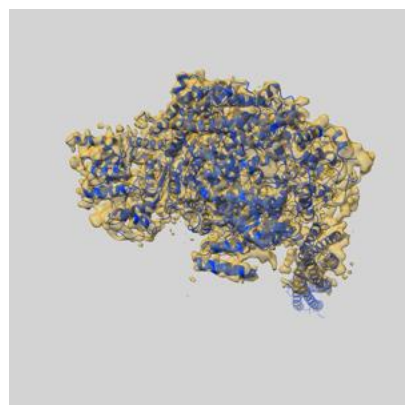
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.63	-	-
Author-provided FSC curve	4.60	6.36	4.67
Unmasked-calculated*	-	-	-

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

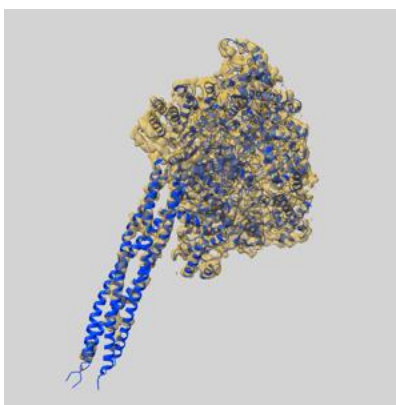
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21096 and PDB model 6V86. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

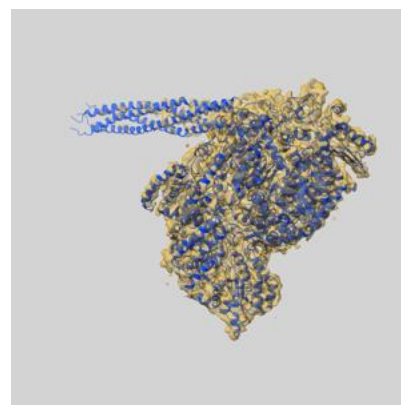
9.1 Map-model overlay [i](#)



X



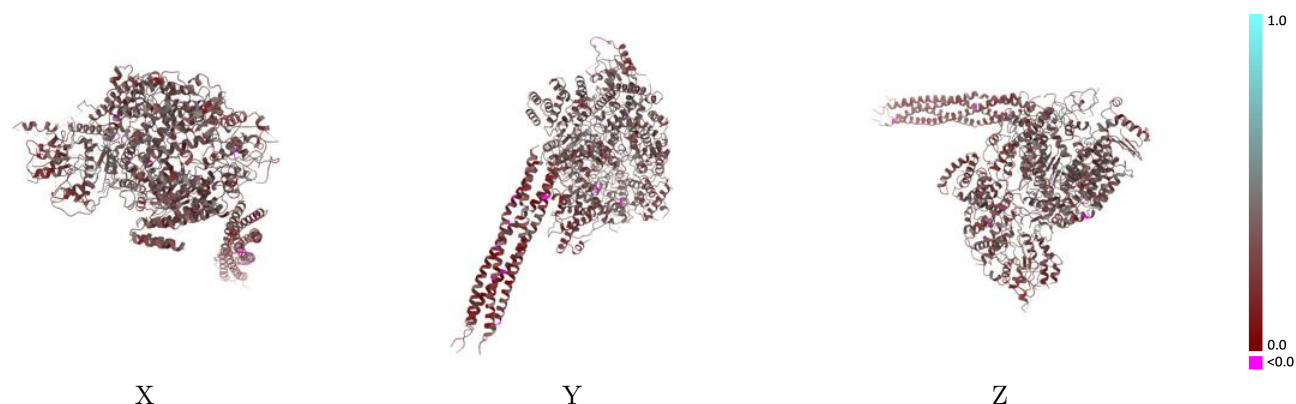
Y



Z

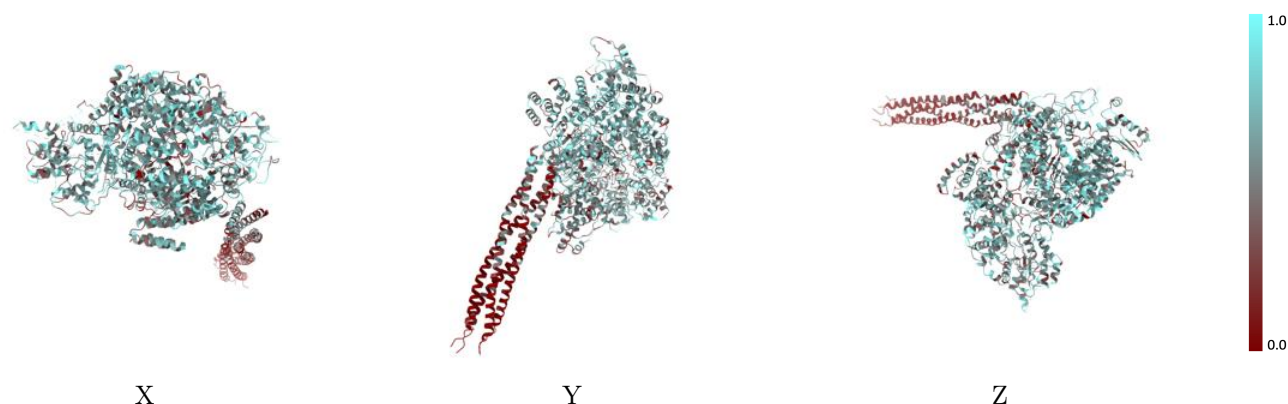
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



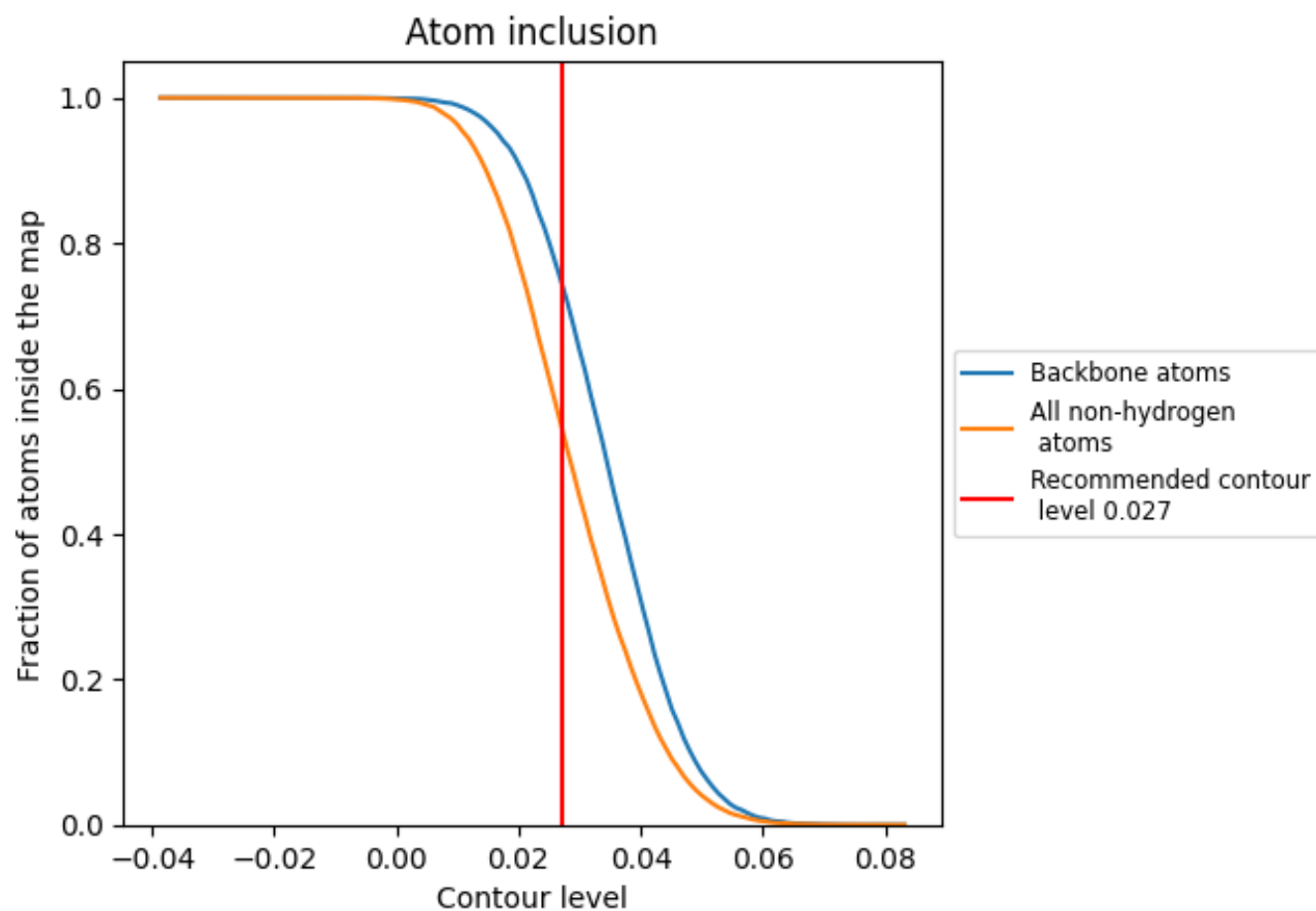
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 75% of all backbone atoms, 55% 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	<div></div> 0.5477	<div></div> 0.3350
A	<div></div> 0.5999	<div></div> 0.3490
B	<div></div> 0.1911	<div></div> 0.2510
C	<div></div> 0.1664	<div></div> 0.2210
D	<div></div> 0.1763	<div></div> 0.2470
E	<div></div> 0.2459	<div></div> 0.2260
F	<div></div> 0.5393	<div></div> 0.3330

1.0

0.0

<0.0