



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:27 PM UTC

PDB ID : 7AOC / pdb_00007aoc
EMDB ID : EMD-11840
Title : Schizosaccharomyces pombe RNA polymerase I (monomer)
Authors : Heiss, F.; Daiss, J.; Becker, P.; Engel, C.
Deposited on : 2020-10-14
Resolution : 3.84 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

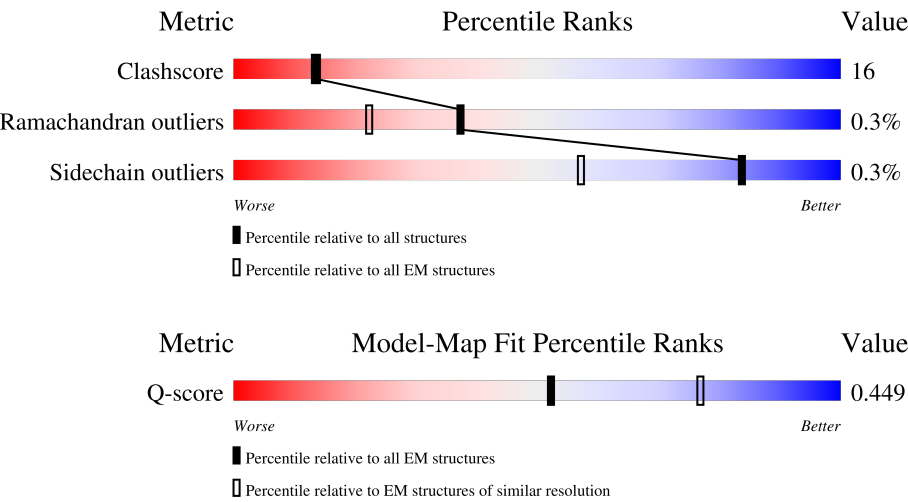
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.84 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	9033 (3.34 - 4.34)

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	1689	
2	B	1174	
3	C	348	
4	D	147	

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Mol	Chain	Length	Quality of chain
5	E	210	
6	F	142	
7	G	173	
8	H	125	
9	I	119	
10	J	71	
11	K	125	
12	L	63	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 29724 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 DNA-directed RNA polymerase I subunit rpa1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1394	Total	C	N	O	S	0	0
			11051	7009	1907	2076	59		

- Molecule 2 is a protein called Probable DNA-directed RNA polymerase I subunit RPA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1159	Total	C	N	O	S	0	0
			9148	5803	1595	1691	59		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	317	Total	C	N	O	S	0	0
			2533	1621	430	475	7		

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit rpa14.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	39	Total	C	N	O	S	0	0
			322	203	57	61	1		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	207	Total	C	N	O	S	0	0
			1663	1050	301	306	6		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			650	413	111	123	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit rpa43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	160	Total	C	N	O	S	0	0
			1267	817	210	236	4		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	123	Total	C	N	O	S	0	0
			990	628	166	193	3		

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	57	Total	C	N	O	S	0	0
			431	269	69	89	4		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	68	Total	C	N	O	S	0	0
			550	350	93	100	7		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	95	Total	C	N	O	S	0	0
			745	472	123	146	4		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			368	225	74	61	8		

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
13	A	2	Total	Zn	0
			2	2	
13	B	1	Total	Zn	0
			1	1	

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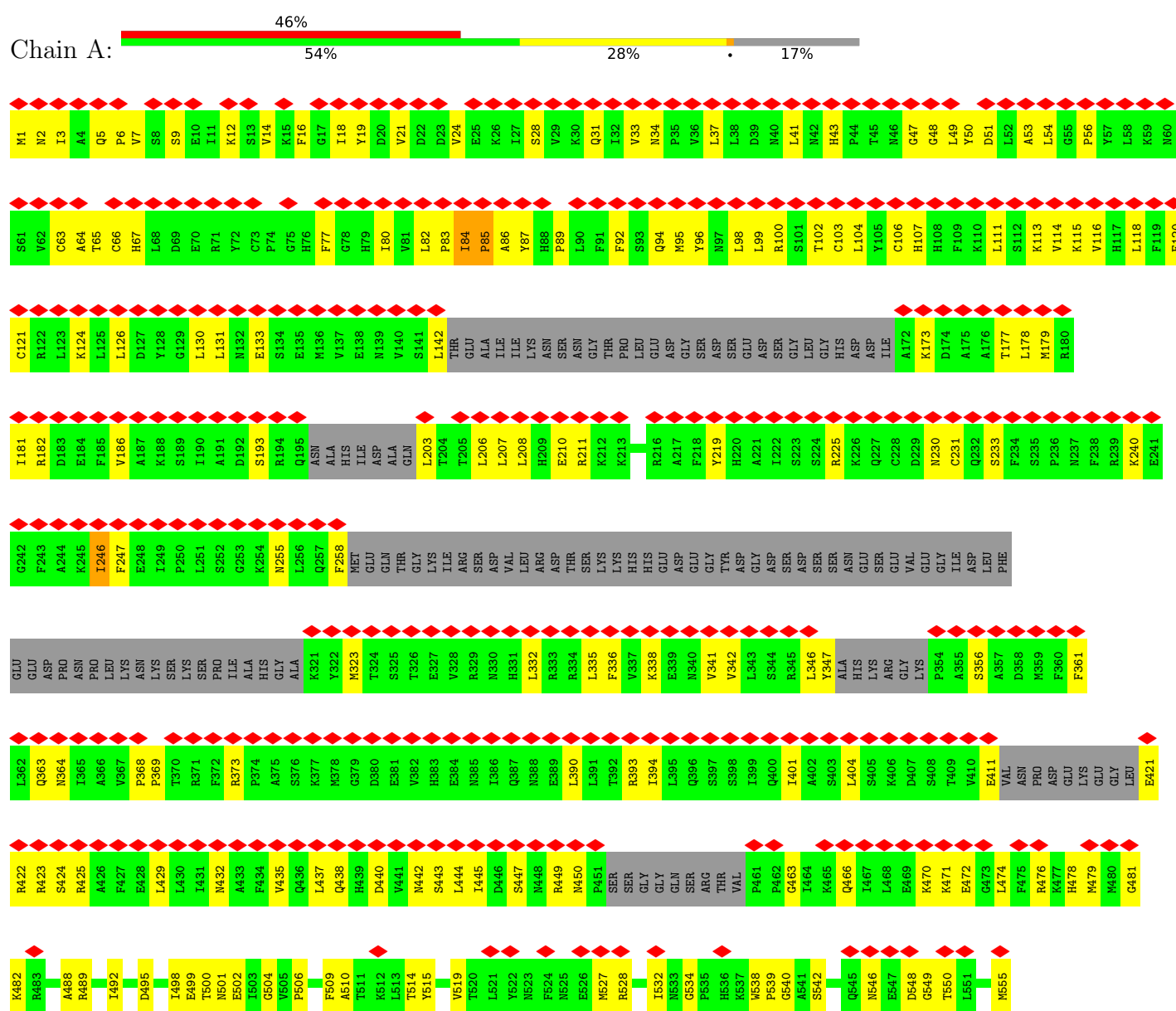
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Mol	Chain	Residues	Atoms		AltConf
13	I	1	Total 1	Zn 1	0
13	J	1	Total 1	Zn 1	0
13	L	1	Total 1	Zn 1	0

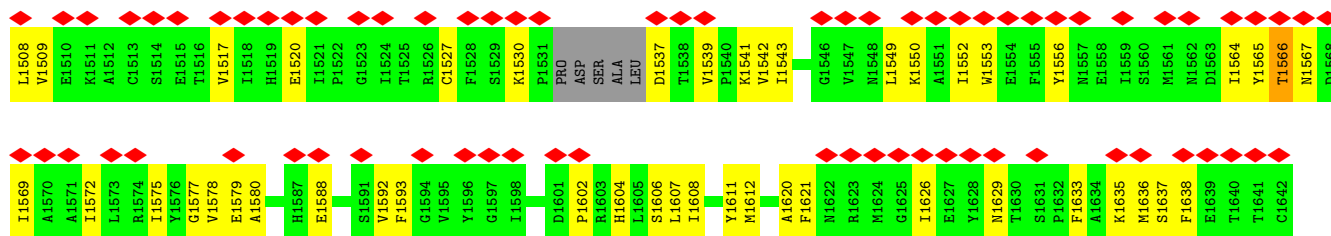
3 Residue-property plots

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.

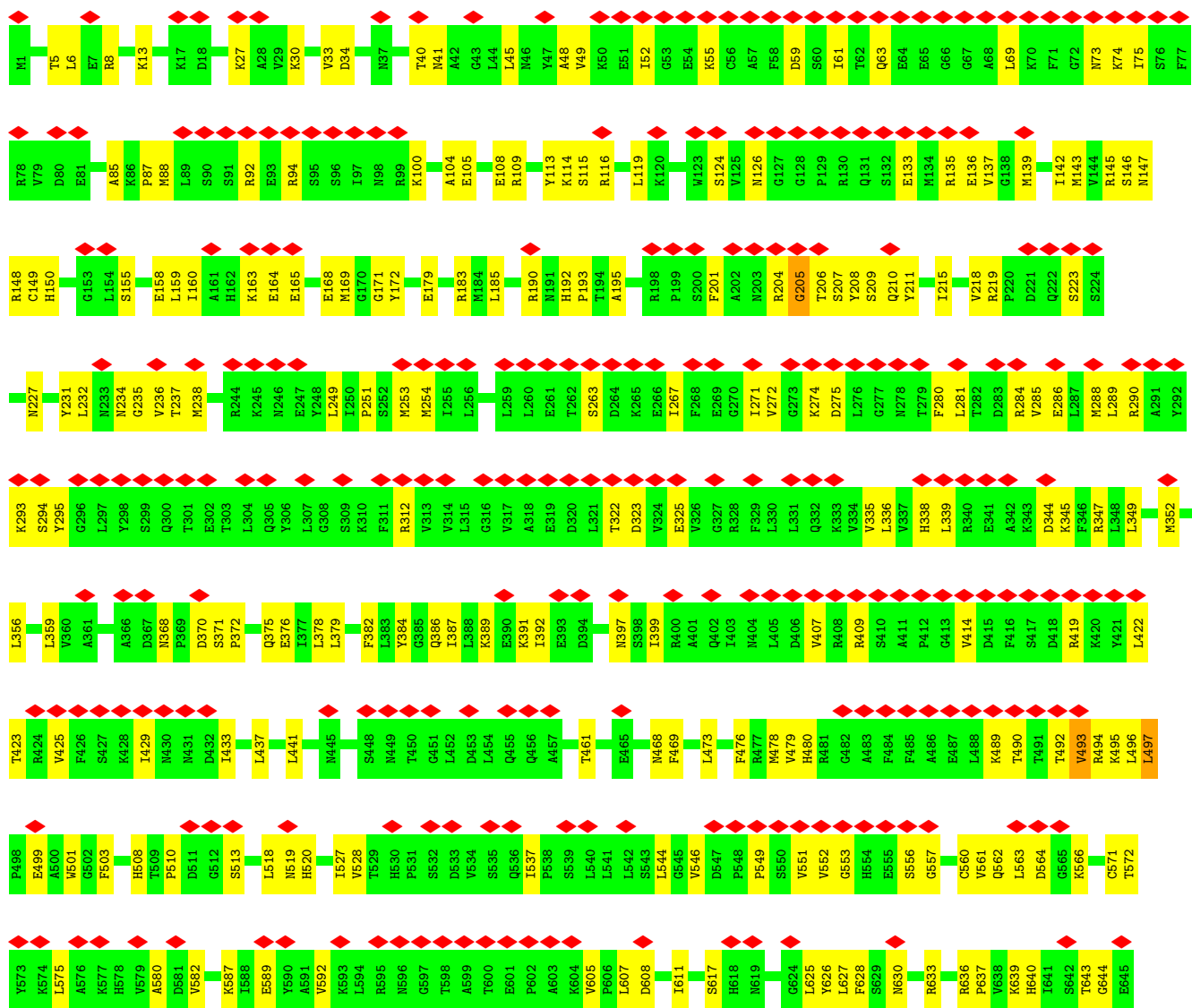
- Molecule 1: DNA-directed RNA polymerase I subunit rpa1

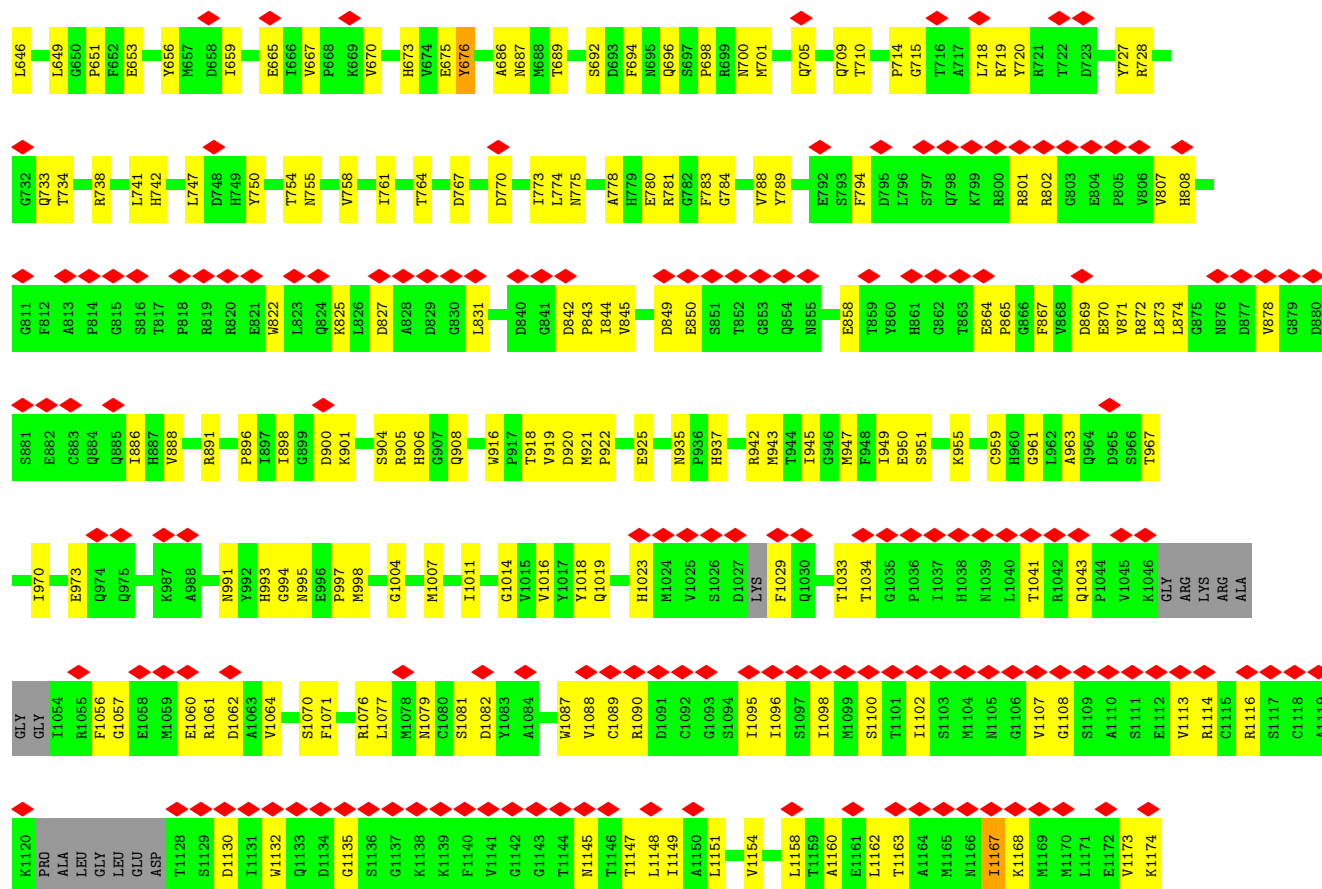


ALA	THR	F1328	V1267	S1206	Y1063	P971	N891	A803	D719	L624	P556
THR	ASN	L1329	N1268	T1207	G1064		L892	S804	E720	P625	L557
GLU	GLU	K1330	K1269	Q1208	E1065	S975	E893	H810	T721	G626	T558
LEU	LEU	L1331	L1270	M1209	D1066		E894	V811	G722	E827	I559
LYS	LYS	L1332	V1271	M1210	S1067	Y985	V895	V812	W723	K628	E560
GLN	VAL	L1333	V1272	L1211	L1068	E986	Y896	V813	W724	T629	Q561
ASN	ASN	M1333	L1273	L1212	D1069	T987	R897	H813	G725	T630	R562
THR	ARG	L1334	S1273	N1212	V1070	S988	D898	E814	K726	R631	T563
VAL	VAL	I1335	E1274	T1213	T1071	A989	D899	D819	P732	M632	A564
LYS	LYS				K1072		E900	A820	A733	H633	
ILE	ILE	PHE	R1277	PHE	Q1073	1995	E901	L820	T734	Y634	N567
GLN	HIS	HIS	Q1278	PHE	K1074		K901	A821	I734	Y640	Q568
SER	GLU	ALA	Q1278	ALA	L1075	R998	L902	G822	G735	L569	L570
GLU	SER	GLY	V1279	GLY	L1076	F999	Q903	L824	W741	N641	L571
ARG	ARG	LYS	R1280	PHE	T1077	L1000	G904	L824	T742	D643	T571
GLU	GLU	GLY	V1281	GLY	T1077	T1001	L905	L825	G743	P644	P672
LEU	GLY	ALA	T1282	ALA	E1080	M1013	D906	S826	K744	D645	Q573
LEU	LYS	LYS	E1283	LYS	F1081		A907	R830	S748	Q574	N575
ALA	ALA	N1223	K1284	N1223	K1084	R1016	A908	M838		S578	L576
ASP	ASP	V1224	ILE	V1224	N1085	E1017	M909	R839		R651	I577
GLU	GLU	T1225	GLY	T1225	Y1086	G1018	K910	G840	S757	M651	S579
ALA	ASP	L1226	GLY	L1226		L1019	F841	F841	D647	P653	P580
VAL	VAL					L1156	G911	T842	E648	N649	L576
LYS	LYS					I1157	K912		D758	N650	I577
GLY	GLY	P1229	GLY	P1229	K1094	T1020			L762	R651	S578
SER	SER	R1230	GLY	R1230	N1095	D1021			N763	M652	S579
LEU	LEU	L1231	GLY	L1231	K1096	T1022	T917	L850	K765	P653	P580
GLN	GLN	N1232	GLN	N1232	S1097	ALA	1920	D851	S766	S661	
LEU	LEU	E1233	LEU	E1233	V1098	VAL	K912	E852	K767		
LYS	LYS	T1234	LYS	T1234	L1099	LYS	1925	R859	V770		
ASN	ASN	I1235	ASN	I1235	S1100	THR	P926	G860			
VAL	VAL	M1236	VAL	M1236	A1101	ARG	D927	L861			
GLU	GLU	T1237	GLU	T1237	V1102	SER	G928	L862	K773		
VAL	VAL	A1298	VAL	A1298	D1103	G1030	L929	L862	Y774		
GLY	GLY	I1299	GLY	I1299	S1104	Y1031		E863			
ASP	ASP	R1300	ASP	R1300	E1105	L1032	K932	N864			
ALA	ALA	L1301	ALA	L1301		L1033	N936	G865			
LEU	LEU	N1241	LEU	N1241	S1109	R1034	T940	K866			
LYS	LYS	T1242	LYS	T1242				S867			
PRO	PRO	L1303	PRO	L1303	N1171	K1038	Q939	R868			
LEU	LEU	Y1304	LEU	Y1304	A1111		T940	G869			
GLU	GLU	S1305	GLU	S1305	K1112	E1041	V943	L870			
ASP	ASP	T1244	ASP	T1244	S1173	G1042	S944	L870			
ILE	ILE	P1245	ILE	P1245	K1113	L1043		E871			
ASP	ASP	T1246	ASP	T1246	F1175	L1043	S949	A872			
GLU	GLU	M1247	GLU	M1247	A1114	L1042	N950	N950			
ALA	ALA	L1248	ALA	L1248	L1175	Q1046	V951	A873			
ALA	ALA	E1308	ALA	E1308	A1177	Y1047	N952	S874			
LYS	LYS	I1309	LYS	I1309	K1116			E875			
PRO	PRO	Q1310	PRO	Q1310	K1117			G878			
ILE	ILE	L1251	ILE	L1251	P1118						
GLU	GLU	D1311	GLU	D1311	Y1119	H1048	S957	S874			
GLY	GLY	E1312	GLY	E1312	K1120	H1049	C958	L791			
ARG	ARG	L1313	ARG	L1313	K1121	T1050	L959	L792			
VAL	VAL	G1314	VAL	G1314	Y1121	V1051		G793			
ASP	ASP	V1255	ASP	V1255	P1122	D1052	Q963	G794			
ALA	ALA	S1256	ALA	S1256	D1122	D1053	D892	L795			
LEU	LEU	T1257	LEU	T1257	P1123	S1054	S883	L796			
GLU	GLU	K1258	GLU	K1258	V1124	D1055	L965	L797			
GLU	GLU	E1318	GLU	E1318	L1125		P884	D797			
ASP	ASP	R1259	ASP	R1259	D1126		E966				
ASN	ASN	A1260	ASN	A1260	K1127	T1058	R895	A896			
ASN	ASN	S1261	ASN	S1261	Y1128	V1059	G967	L887			
ASP	ASP	E1321	ASP	E1321	P1129	Q1060	R968				
GLU	GLU	S1322	GLU	S1322	P1130						
GLU	GLU	T1323	GLU	T1323	S1131						
GLU	GLU	F1324	GLU	F1324	P1205						
GLU	GLU	S1325	GLU	S1325							
GLU	GLU	N1326	GLU	N1326							
GLU	GLU	R1327	GLU	R1327							
ARG	LYS		LYS								
LYS	LEU		LEU								
LEU	LEU		LEU								
LEU	LEU		LEU								
LYS	LYS		LYS								
GLN	GLN		GLN								
VAL	VAL		VAL								
GLN	GLN		GLN								
THR	THR		THR								
ALA	ALA		ALA								
ASP	ASP		ASP								
LYS	LYS		LYS								
GLU	GLU		GLU								
VAL	VAL		VAL								
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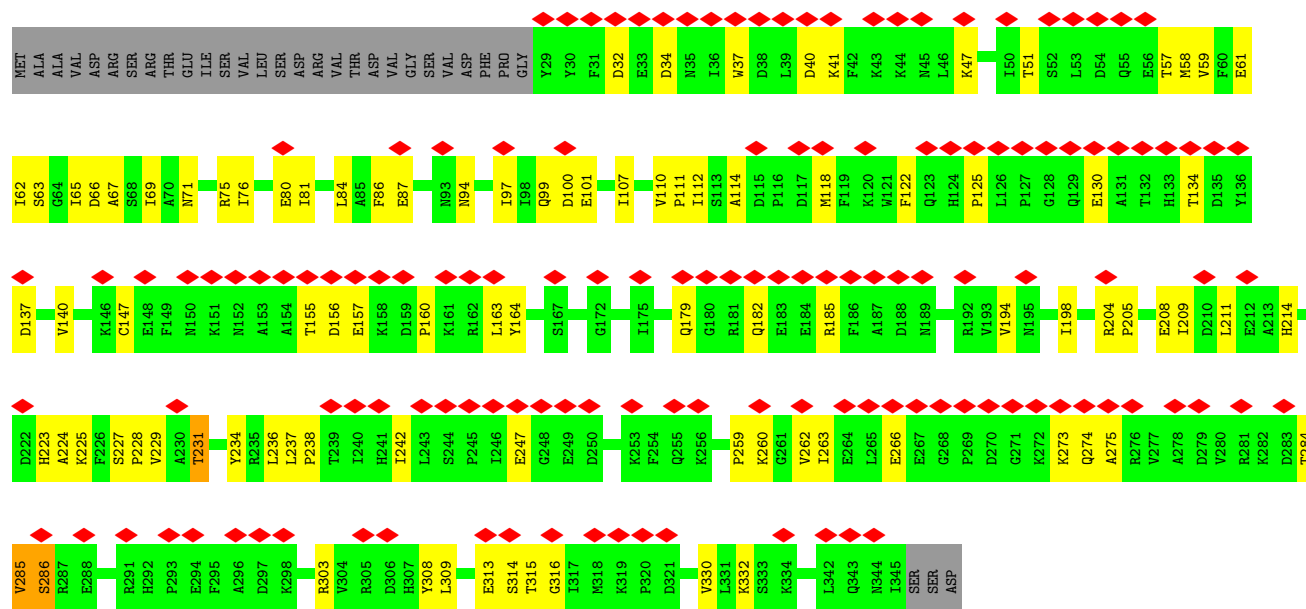
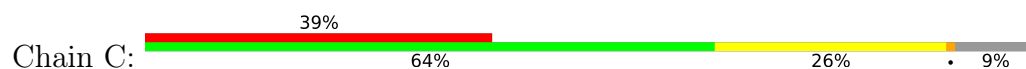


• Molecule 2: Probable DNA-directed RNA polymerase I subunit RPA2

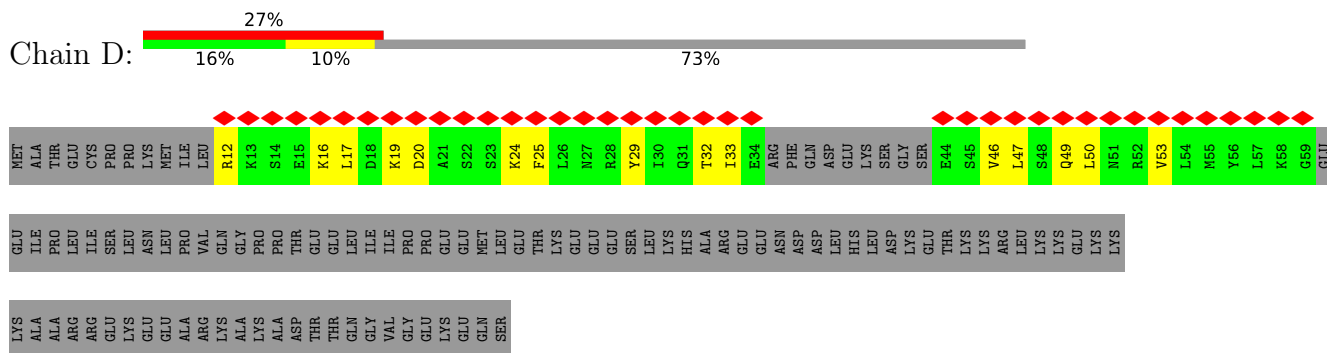




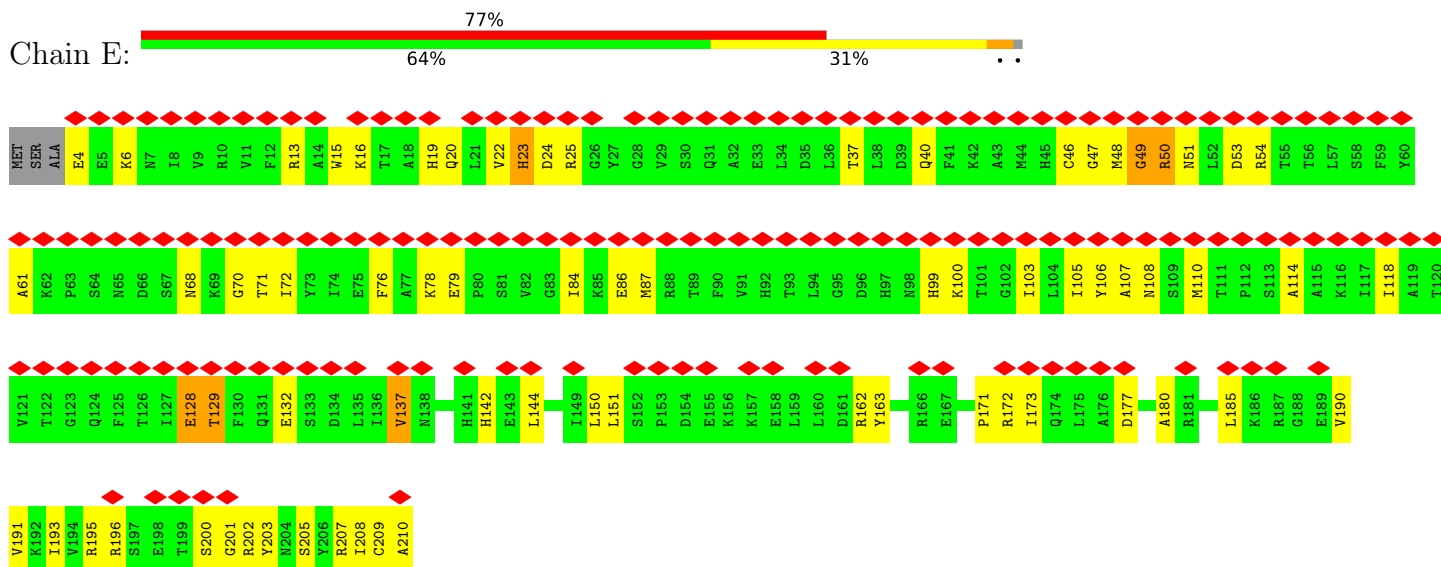
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



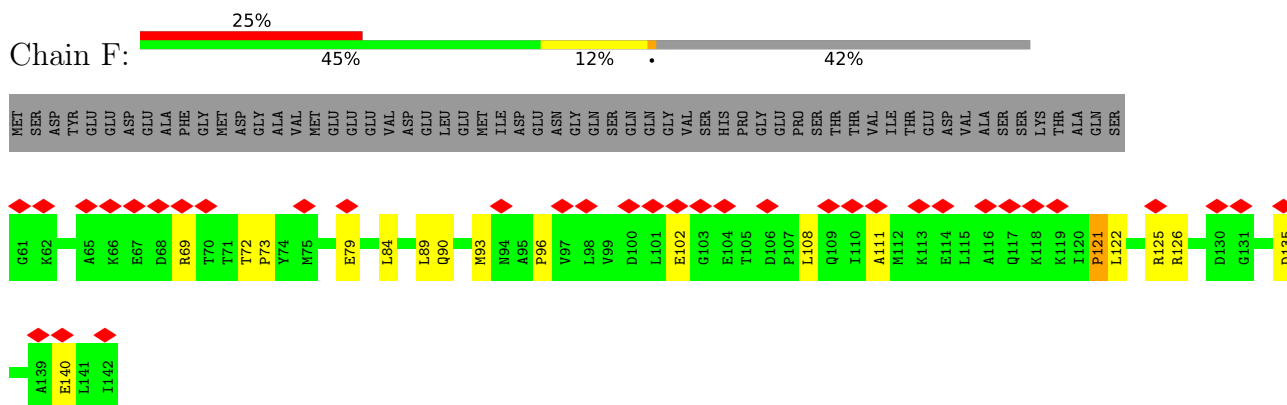
• Molecule 4: DNA-directed RNA polymerase I subunit rpa14



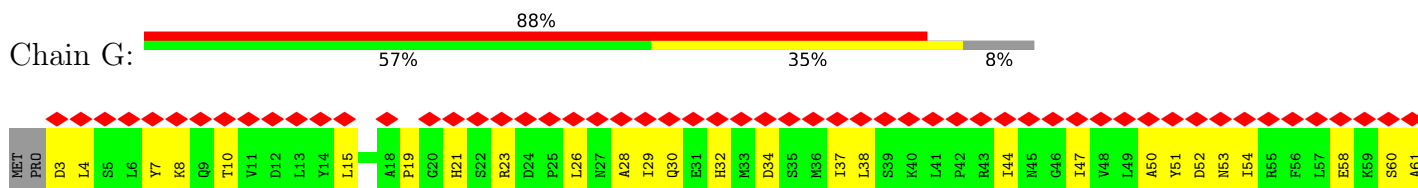
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

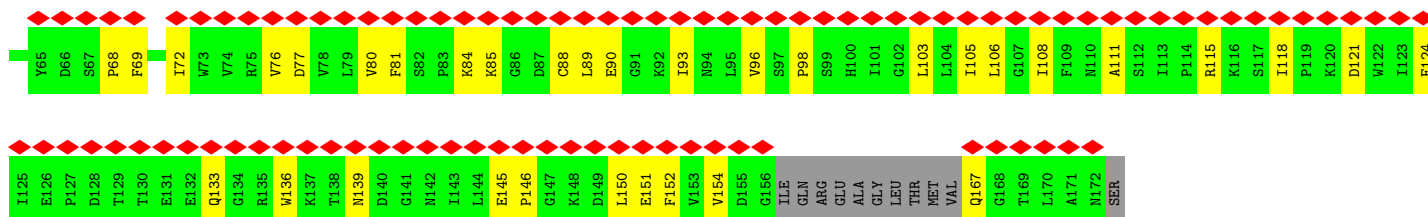


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

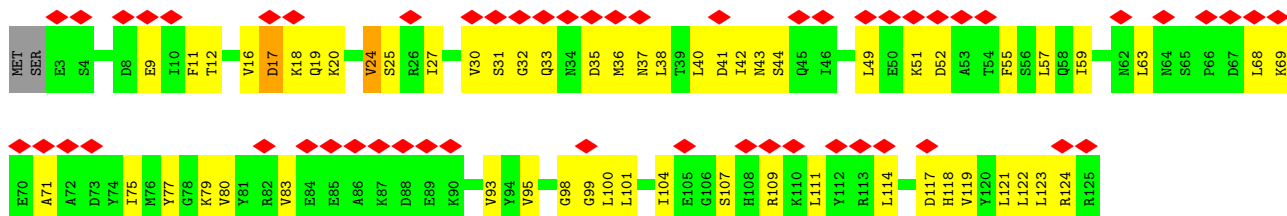
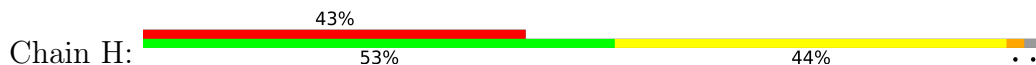


- Molecule 7: DNA-directed RNA polymerase I subunit rpa43

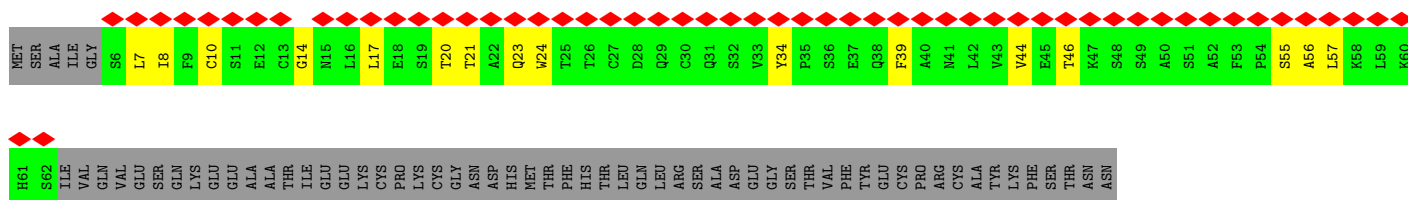
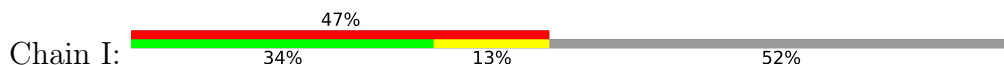




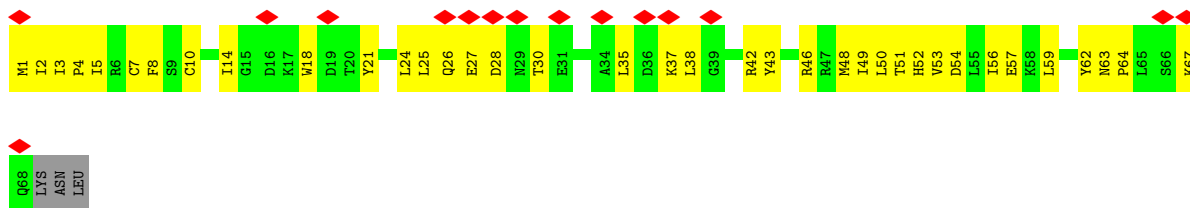
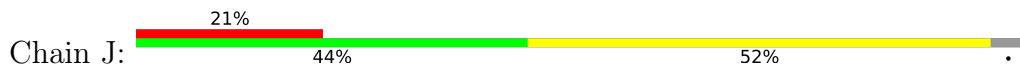
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



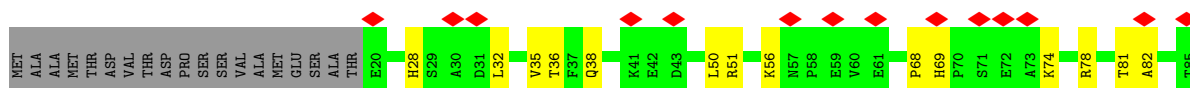
• Molecule 9: DNA-directed RNA polymerase I subunit RPA12

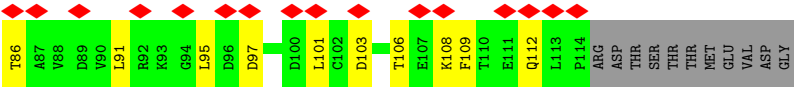


• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

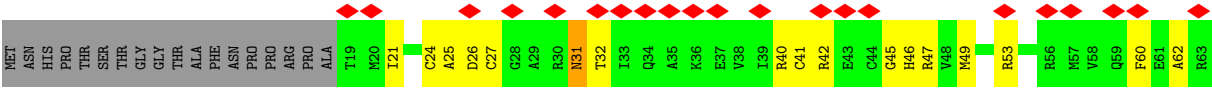


• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2





- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79313	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	86.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.501	Depositor
Minimum map value	-0.291	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.11	Depositor
Map size ($\text{\AA}$)	233.97002, 233.97002, 233.97002	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0635, 1.0635, 1.0635	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	0.32	0/11271	0.53	1/15226 (0.0%)
2	B	0.36	0/9353	0.53	0/12644
3	C	0.32	0/2588	0.49	0/3505
4	D	0.18	0/323	0.41	0/427
5	E	0.26	0/1695	0.63	3/2287 (0.1%)
6	F	0.32	0/660	0.47	0/893
7	G	0.20	0/1295	0.46	0/1755
8	H	0.30	0/1004	0.63	2/1355 (0.1%)
9	I	0.22	0/439	0.53	0/596
10	J	0.41	0/558	0.55	0/751
11	K	0.36	0/759	0.42	0/1030
12	L	0.30	0/371	0.55	0/491
All	All	0.33	0/30316	0.53	6/40960 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
2	B	0	2
5	E	0	5
All	All	0	14

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	24	ASP	N-CA-C	7.23	126.20	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	49	GLY	CA-C-N	5.87	132.26	121.70
5	E	49	GLY	C-N-CA	5.87	132.26	121.70
1	A	1066	ASP	N-CA-C	5.33	122.16	110.80
8	H	17	ASP	CA-C-N	5.11	130.90	121.70
8	H	17	ASP	C-N-CA	5.11	130.90	121.70

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1065	GLU	Peptide
1	A	1066	ASP	Peptide
1	A	1566	THR	Peptide
1	A	1656	ASP	Peptide
1	A	246	ILE	Peptide
1	A	84	ILE	Peptide
1	A	896	TYR	Peptide
2	B	205	GLY	Peptide
2	B	409	ARG	Peptide
5	E	128	GLU	Peptide
5	E	129	THR	Peptide
5	E	23	HIS	Peptide
5	E	50	ARG	Peptide
5	E	68	ASN	Peptide

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	11051	0	11047	391	0
2	B	9148	0	9109	328	0
3	C	2533	0	2540	74	0
4	D	322	0	338	19	0
5	E	1663	0	1684	60	0
6	F	650	0	674	19	0
7	G	1267	0	1278	53	0
8	H	990	0	1001	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	431	0	410	14	0
10	J	550	0	566	38	0
11	K	745	0	745	22	0
12	L	368	0	377	17	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	I	1	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
All	All	29724	0	29769	944	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 16.

All (944) 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)
5:E:23:HIS:HA	5:E:25:ARG:H	1.27	0.97
1:A:1324:PHE:O	1:A:1328:PHE:HB3	1.72	0.90
1:A:103:CYS:SG	1:A:106:CYS:HB3	1.86	0.90
8:H:17:ASP:HA	8:H:18:LYS:HB2	1.58	0.84
1:A:56:PRO:HG3	1:A:63:CYS:HB2	1.58	0.84
1:A:103:CYS:CB	1:A:106:CYS:HB3	2.07	0.83
7:G:96:VAL:H	7:G:133:GLN:HE22	1.28	0.81
2:B:1041:THR:HB	2:B:1154:VAL:HG22	1.63	0.81
1:A:1:MET:SD	2:B:1079:ASN:ND2	2.55	0.80
1:A:597:VAL:HG12	1:A:653:PHE:HE1	1.45	0.80
2:B:227:ASN:ND2	2:B:335:VAL:O	2.15	0.80
2:B:920:ASP:OD1	3:C:75:ARG:NH2	2.14	0.79
1:A:842:THR:HG21	2:B:1011:ILE:HA	1.63	0.79
6:F:93:MET:HG3	7:G:68:PRO:HG3	1.65	0.79
5:E:84:ILE:HG13	5:E:114:ALA:HB2	1.66	0.78
1:A:606:ASN:ND2	2:B:1060:GLU:OE1	2.16	0.78
2:B:190:ARG:HD3	2:B:218:VAL:HG11	1.65	0.78
2:B:494:ARG:NH2	2:B:513:SER:O	2.17	0.78
1:A:1567:ASN:HB2	1:A:1569:ILE:HG23	1.66	0.77
7:G:19:PRO:HD3	7:G:69:PHE:HB3	1.66	0.77
2:B:831:LEU:HD22	2:B:886:ILE:HD12	1.64	0.77
5:E:46:CYS:SG	5:E:47:GLY:N	2.58	0.77
2:B:105:GLU:OE2	2:B:109:ARG:NH2	2.18	0.76
1:A:103:CYS:HB3	1:A:106:CYS:HB3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:LYS:HG3	1:A:614:PRO:HD3	1.67	0.75
2:B:761:ILE:HD12	2:B:1011:ILE:HD13	1.68	0.75
1:A:120:PHE:HB2	1:A:342:VAL:HG22	1.69	0.75
7:G:10:THR:HG22	7:G:77:ASP:HB3	1.68	0.75
6:F:96:PRO:HG3	7:G:23:ARG:HG2	1.67	0.74
4:D:17:LEU:HD11	7:G:7:TYR:HD1	1.50	0.74
1:A:679:GLY:HA3	1:A:1074:LYS:HD3	1.70	0.74
1:A:1086:TYR:HD1	1:A:1178:LEU:HD22	1.52	0.74
10:J:3:ILE:HD11	10:J:49:ILE:HG22	1.69	0.73
2:B:235:GLY:HA2	2:B:284:ARG:HH11	1.54	0.73
3:C:229:VAL:HA	3:C:314:SER:HA	1.71	0.73
1:A:1553:TRP:CZ3	5:E:137:VAL:HG22	2.24	0.72
3:C:61:GLU:HG2	3:C:309:LEU:HD22	1.71	0.72
2:B:347:ARG:NH2	2:B:549:PRO:O	2.22	0.72
1:A:94:GLN:NE2	1:A:347:TYR:OH	2.22	0.72
1:A:770:VAL:HG11	1:A:795:ILE:HD11	1.72	0.72
12:L:24:CYS:HB3	12:L:27:CYS:SG	2.29	0.72
2:B:709:GLN:OE1	2:B:1023:HIS:NE2	2.24	0.71
5:E:190:VAL:HG22	5:E:208:ILE:HG22	1.72	0.71
3:C:266:GLU:HB2	3:C:274:GLN:HB2	1.73	0.71
1:A:540:GLY:O	1:A:596:HIS:ND1	2.23	0.71
2:B:263:SER:HB3	9:I:14:GLY:HA3	1.73	0.70
7:G:34:ASP:OD2	7:G:51:TYR:OH	2.08	0.70
3:C:57:THR:HG22	3:C:313:GLU:HG2	1.73	0.70
1:A:917:THR:HG23	1:A:959:LEU:HD21	1.73	0.70
12:L:24:CYS:CB	12:L:27:CYS:SG	2.80	0.70
2:B:767:ASP:O	2:B:935:ASN:ND2	2.24	0.70
2:B:1163:THR:HG23	2:B:1168:LYS:HD2	1.74	0.70
2:B:961:GLY:HA2	10:J:50:LEU:HD11	1.74	0.69
1:A:765:LYS:HD2	1:A:785:LEU:HD12	1.74	0.69
4:D:29:TYR:HA	4:D:32:THR:HG22	1.74	0.69
1:A:597:VAL:HG12	1:A:653:PHE:CE1	2.27	0.69
1:A:1069:ASP:OD2	1:A:1604:HIS:NE2	2.26	0.69
2:B:63:GLN:HB3	2:B:69:LEU:HB3	1.74	0.69
1:A:121:CYS:HB3	1:A:186:VAL:HG21	1.75	0.69
1:A:514:THR:HG21	1:A:542:SER:HB2	1.72	0.69
5:E:87:MET:HG2	5:E:118:ILE:HG21	1.75	0.69
1:A:1052:ARG:HG2	1:A:1058:ILE:HD13	1.75	0.68
1:A:99:LEU:O	1:A:102:THR:OG1	2.11	0.68
4:D:19:LYS:HD2	7:G:4:LEU:HD22	1.75	0.68
2:B:1088:VAL:HG11	2:B:1173:VAL:HG21	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:8:ILE:HG13	9:I:17:LEU:HD12	1.76	0.68
1:A:1636:MET:HE2	1:A:1645:LEU:HA	1.75	0.68
2:B:1081:SER:OG	2:B:1082:ASP:OD1	2.10	0.68
1:A:788:ASP:OD2	8:H:79:LYS:NZ	2.27	0.68
1:A:1235:ILE:HG13	1:A:1612:MET:HE1	1.76	0.68
1:A:1239:SER:OG	1:A:1240:ALA:O	2.12	0.68
1:A:131:LEU:HD12	1:A:210:GLU:HG3	1.74	0.67
2:B:770:ASP:OD1	2:B:942:ARG:NH2	2.28	0.67
4:D:53:VAL:HG23	7:G:106:LEU:HB3	1.77	0.67
1:A:1251:LEU:HD12	1:A:1255:VAL:HG21	1.77	0.67
1:A:498:ILE:HG13	1:A:499:GLU:H	1.60	0.67
1:A:1068:LEU:HD23	1:A:1072:LYS:HB2	1.76	0.67
1:A:763:ASN:HA	1:A:786:PHE:O	1.95	0.67
2:B:906:HIS:NE2	2:B:950:GLU:OE1	2.26	0.67
5:E:61:ALA:O	5:E:71:THR:OG1	2.11	0.67
1:A:781:GLU:O	1:A:783:SER:N	2.26	0.67
2:B:775:ASN:HD22	2:B:921:MET:HG3	1.60	0.67
1:A:1146:ASP:OD1	1:A:1176:LYS:NZ	2.23	0.66
2:B:209:SER:OG	2:B:231:TYR:O	2.12	0.66
2:B:696:GLN:HG2	2:B:698:PRO:HD2	1.78	0.66
2:B:734:THR:O	10:J:51:THR:OG1	2.13	0.66
5:E:49:GLY:HA2	5:E:50:ARG:HB2	1.77	0.66
1:A:952:ASN:HA	2:B:943:MET:HE1	1.77	0.66
3:C:198:ILE:HG21	10:J:5:ILE:HD12	1.77	0.66
1:A:1068:LEU:HD13	1:A:1188:VAL:HA	1.76	0.66
1:A:18:ILE:HD13	2:B:1167:ILE:HG22	1.78	0.66
2:B:871:VAL:HG12	2:B:888:VAL:HG13	1.78	0.65
5:E:128:GLU:HA	5:E:129:THR:HG23	1.79	0.65
1:A:726:ARG:HA	11:K:78:ARG:NH2	2.11	0.65
1:A:481:GLY:HA2	2:B:1057:GLY:HA3	1.79	0.65
2:B:687:ASN:ND2	2:B:741:LEU:HD12	2.12	0.65
1:A:606:ASN:HD22	1:A:616:MET:HG3	1.60	0.65
2:B:967:THR:HB	2:B:970:ILE:HD11	1.79	0.65
8:H:16:VAL:HG22	8:H:27:ILE:HG22	1.79	0.65
1:A:546:ASN:ND2	1:A:550:THR:OG1	2.27	0.65
1:A:2:ASN:HB3	1:A:5:GLN:HG2	1.79	0.64
2:B:1145:ASN:HD21	4:D:12:ARG:HH12	1.44	0.64
3:C:122:PHE:HE2	3:C:125:PRO:HD3	1.62	0.64
2:B:205:GLY:O	2:B:207:SER:N	2.30	0.64
9:I:23:GLN:HG3	9:I:24:TRP:H	1.61	0.64
1:A:595:ARG:NH2	1:A:601:ASP:OD2	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:ARG:HH22	2:B:249:LEU:HD11	1.62	0.64
1:A:1281:VAL:HG13	9:I:46:THR:HB	1.80	0.64
1:A:744:LYS:NZ	1:A:794:GLY:O	2.31	0.64
2:B:183:ARG:HD2	2:B:478:MET:HE3	1.80	0.64
2:B:692:SER:OG	2:B:700:ASN:ND2	2.31	0.64
1:A:630:ILE:HG21	1:A:651:MET:HE1	1.80	0.63
1:A:597:VAL:HG23	1:A:623:ILE:HD11	1.81	0.63
1:A:748:SER:HB2	1:A:790:GLU:HA	1.79	0.63
2:B:1100:SER:HA	2:B:1113:VAL:HG12	1.81	0.63
1:A:206:LEU:HD22	5:E:172:ARG:HD3	1.80	0.63
1:A:1066:ASP:N	1:A:1066:ASP:OD1	2.30	0.63
2:B:143:MET:HB3	2:B:146:SER:HB2	1.81	0.63
1:A:678:SER:HA	1:A:1070:VAL:HG11	1.81	0.63
1:A:515:TYR:HE1	1:A:595:ARG:CZ	2.12	0.62
2:B:773:ILE:HG21	2:B:916:TRP:HB2	1.80	0.62
2:B:849:ASP:OD1	2:B:850:GLU:N	2.33	0.62
1:A:103:CYS:SG	1:A:106:CYS:N	2.65	0.62
8:H:63:LEU:HD21	8:H:75:ILE:HD13	1.82	0.62
12:L:24:CYS:CB	12:L:41:CYS:SG	2.84	0.62
2:B:231:TYR:OH	2:B:284:ARG:NH1	2.32	0.62
2:B:236:VAL:HG13	2:B:288:MET:HG3	1.82	0.61
1:A:603:LEU:HD22	1:A:621:ALA:HB2	1.80	0.61
2:B:85:ALA:O	2:B:115:SER:OG	2.13	0.61
2:B:908:GLN:HE22	2:B:942:ARG:HD2	1.65	0.61
4:D:47:LEU:HA	4:D:50:LEU:HD12	1.81	0.61
1:A:546:ASN:HD22	1:A:550:THR:HG1	1.48	0.61
2:B:728:ARG:NH2	2:B:789:TYR:OH	2.33	0.61
2:B:1056:PHE:HA	2:B:1060:GLU:HG3	1.82	0.61
3:C:97:ILE:HG21	10:J:59:LEU:HD22	1.82	0.61
6:F:69:ARG:NH2	6:F:140:GLU:OE2	2.33	0.61
2:B:94:ARG:HD2	2:B:878:VAL:HG23	1.81	0.61
8:H:59:ILE:HD11	8:H:114:LEU:HD21	1.81	0.61
2:B:734:THR:HG23	10:J:53:VAL:HG22	1.80	0.61
1:A:500:THR:HB	1:A:683:ARG:NH2	2.16	0.61
1:A:19:TYR:CG	2:B:1168:LYS:HD3	2.36	0.61
8:H:38:LEU:HD12	8:H:104:ILE:HD13	1.82	0.61
8:H:63:LEU:HG	8:H:68:LEU:HD12	1.83	0.61
1:A:1549:LEU:HD13	1:A:1575:ILE:HD11	1.83	0.61
3:C:65:ILE:HG23	3:C:69:ILE:HB	1.83	0.61
2:B:116:ARG:NH1	2:B:136:GLU:OE2	2.33	0.60
5:E:49:GLY:HA3	5:E:51:ASN:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:845:VAL:HG12	2:B:858:GLU:HB2	1.82	0.60
2:B:959:CYS:O	10:J:46:ARG:NH2	2.30	0.60
1:A:661:SER:HB2	6:F:108:LEU:HD11	1.82	0.60
1:A:1309:TYR:O	1:A:1313:TYR:HB2	2.00	0.60
1:A:92:PHE:HA	1:A:95:MET:HE3	1.83	0.60
1:A:675:VAL:HG13	1:A:682:LEU:HB3	1.81	0.60
3:C:37:TRP:HB2	11:K:56:LYS:HB3	1.82	0.60
3:C:231:THR:HG21	10:J:42:ARG:HH12	1.65	0.60
1:A:519:VAL:HG21	1:A:569:LEU:HD21	1.82	0.60
5:E:23:HIS:HA	5:E:25:ARG:N	2.08	0.60
5:E:142:HIS:CD2	5:E:144:LEU:H	2.20	0.60
8:H:24:VAL:HG12	8:H:43:ASN:HA	1.83	0.60
5:E:180:ALA:HA	5:E:185:LEU:HD12	1.84	0.60
2:B:192:HIS:HB2	2:B:628:PHE:HZ	1.66	0.60
7:G:98:PRO:O	7:G:115:ARG:NH1	2.34	0.60
1:A:1553:TRP:HZ3	5:E:137:VAL:HG22	1.67	0.59
1:A:142:LEU:HD22	1:A:178:LEU:HB2	1.84	0.59
5:E:103:ILE:HA	5:E:128:GLU:O	2.03	0.59
1:A:893:GLU:OE2	2:B:617:SER:OG	2.19	0.59
1:A:1230:ARG:NH2	1:A:1588:GLU:OE2	2.34	0.59
2:B:92:ARG:HH11	2:B:878:VAL:HG11	1.67	0.59
1:A:102:THR:HG22	1:A:335:LEU:HD22	1.84	0.59
8:H:57:LEU:HD12	8:H:123:LEU:HD21	1.84	0.59
1:A:1038:LYS:HB2	1:A:1638:PHE:CE1	2.37	0.59
5:E:53:ASP:HB2	5:E:54:ARG:HH11	1.68	0.59
1:A:797:ASP:N	1:A:797:ASP:OD1	2.32	0.59
1:A:1279:VAL:HG21	1:A:1509:VAL:HG11	1.85	0.59
2:B:508:HIS:HB2	2:B:686:ALA:HB2	1.85	0.58
7:G:90:GLU:HB3	7:G:151:GLU:HG2	1.85	0.58
1:A:1336:ILE:HD11	1:A:1505:MET:HE1	1.84	0.58
2:B:204:ARG:HH12	2:B:249:LEU:HD11	1.69	0.58
1:A:732:PRO:HG2	1:A:735:GLN:HG2	1.84	0.58
8:H:38:LEU:HD21	8:H:40:LEU:HD22	1.85	0.58
8:H:19:GLN:OE1	8:H:19:GLN:N	2.36	0.58
1:A:422:ARG:HA	1:A:425:ARG:HE	1.67	0.58
1:A:1230:ARG:NH2	1:A:1567:ASN:OD1	2.33	0.58
2:B:94:ARG:HH12	12:L:40:ARG:HE	1.51	0.58
1:A:77:PHE:CD2	2:B:1096:ILE:HG12	2.39	0.58
1:A:726:ARG:HA	11:K:78:ARG:HH21	1.68	0.58
1:A:1046:GLN:HG3	1:A:1052:ARG:HD2	1.86	0.57
5:E:54:ARG:HB3	5:E:78:LYS:HG2	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:150:LEU:HD23	5:E:191:VAL:HG12	1.86	0.57
1:A:96:TYR:OH	1:A:100:ARG:NH2	2.23	0.57
1:A:77:PHE:CD1	1:A:369:PRO:HD3	2.40	0.57
1:A:612:HIS:CD2	1:A:614:PRO:HD2	2.40	0.57
1:A:67:HIS:CE1	2:B:1102:ILE:HD11	2.38	0.57
1:A:1171:ASN:HB2	1:A:1174:LYS:HB2	1.86	0.57
2:B:285:VAL:O	2:B:289:LEU:HG	2.05	0.57
1:A:687:GLN:HB3	2:B:937:HIS:CD2	2.40	0.57
1:A:940:THR:O	1:A:944:SER:HB3	2.04	0.57
1:A:1251:LEU:HD21	1:A:1542:VAL:HG23	1.86	0.57
3:C:81:ILE:HD11	3:C:228:PRO:HG3	1.87	0.57
2:B:219:ARG:NH1	2:B:223:SER:O	2.38	0.57
2:B:955:LYS:NZ	2:B:994:GLY:O	2.38	0.57
2:B:195:ALA:HB1	2:B:359:LEU:HD22	1.86	0.57
2:B:6:LEU:HD21	10:J:25:LEU:HB2	1.87	0.57
10:J:21:TYR:HB2	10:J:38:LEU:HD21	1.85	0.57
1:A:1306:ARG:HD3	1:A:1317:GLN:NE2	2.20	0.57
3:C:332:LYS:NZ	11:K:103:ASP:OD1	2.22	0.57
1:A:606:ASN:OD1	1:A:607:ARG:N	2.38	0.57
8:H:17:ASP:N	8:H:17:ASP:OD1	2.36	0.57
2:B:715:GLY:HA2	2:B:750:TYR:HE1	1.70	0.56
2:B:842:ASP:OD1	2:B:843:PRO:HD2	2.05	0.56
1:A:3:ILE:HG21	6:F:89:LEU:HD11	1.87	0.56
1:A:1038:LYS:HB2	1:A:1638:PHE:CD1	2.41	0.56
11:K:50:LEU:HD21	11:K:91:LEU:HD11	1.87	0.56
2:B:164:GLU:OE1	2:B:164:GLU:N	2.39	0.56
2:B:1090:ARG:HB3	2:B:1145:ASN:HB3	1.87	0.56
3:C:76:ILE:HG23	3:C:80:GLU:HB2	1.87	0.56
2:B:904:SER:OG	2:B:905:ARG:N	2.36	0.56
2:B:643:THR:HG22	2:B:644:GLY:H	1.69	0.56
1:A:975:SER:HB2	2:B:656:TYR:CE2	2.42	0.55
1:A:1154:ASP:N	1:A:1154:ASP:OD1	2.37	0.55
1:A:1517:VAL:HG21	1:A:1520:GLU:HB3	1.88	0.55
1:A:126:LEU:HD21	1:A:211:ARG:HB2	1.87	0.55
1:A:527:MET:HE1	1:A:595:ARG:HB3	1.87	0.55
2:B:891:ARG:NH1	3:C:101:GLU:OE1	2.40	0.55
5:E:171:PRO:HB2	5:E:207:ARG:HG2	1.88	0.55
2:B:468:ASN:OD1	2:B:469:PHE:N	2.38	0.55
7:G:96:VAL:H	7:G:133:GLN:NE2	2.00	0.55
2:B:546:VAL:HG12	2:B:571:CYS:HB3	1.88	0.55
1:A:1320:ILE:O	1:A:1324:PHE:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1579:GLU:OE2	5:E:193:ILE:HD12	2.07	0.55
1:A:442:ASN:HD21	1:A:449:ARG:HG2	1.71	0.55
2:B:687:ASN:HD21	2:B:741:LEU:HD12	1.70	0.55
1:A:501:ASN:HA	1:A:669:THR:HG21	1.89	0.55
1:A:607:ARG:HD2	1:A:649:MET:HE2	1.89	0.55
1:A:77:PHE:CE1	1:A:369:PRO:HD3	2.42	0.54
1:A:98:LEU:O	1:A:102:THR:HG23	2.08	0.54
1:A:786:PHE:HB3	1:A:791:LEU:HA	1.88	0.54
3:C:204:ARG:HB2	10:J:63:ASN:HD21	1.70	0.54
10:J:3:ILE:HD13	10:J:18:TRP:HB2	1.90	0.54
1:A:177:THR:O	1:A:181:ILE:HG13	2.08	0.54
2:B:49:VAL:HA	2:B:52:ILE:HD12	1.89	0.54
2:B:422:LEU:HA	2:B:425:VAL:HG12	1.89	0.54
7:G:52:ASP:OD2	7:G:53:ASN:N	2.33	0.54
1:A:113:LYS:HG3	1:A:179:MET:HE1	1.89	0.54
2:B:1147:THR:HG22	2:B:1148:LEU:H	1.72	0.54
1:A:1001:THR:HG21	2:B:973:GLU:HG3	1.88	0.54
1:A:1675:GLY:N	2:B:1070:SER:OG	2.40	0.54
2:B:94:ARG:NE	2:B:878:VAL:O	2.41	0.54
2:B:510:PRO:HA	2:B:705:GLN:HG3	1.90	0.54
2:B:870:GLU:OE2	2:B:872:ARG:NH2	2.41	0.54
2:B:1113:VAL:O	2:B:1114:ARG:NH1	2.35	0.54
1:A:120:PHE:CE2	1:A:124:LYS:HD2	2.42	0.54
1:A:231:CYS:SG	1:A:233:SER:OG	2.63	0.54
2:B:232:LEU:HD23	2:B:238:MET:HG2	1.88	0.54
2:B:715:GLY:HA2	2:B:750:TYR:CE1	2.43	0.54
2:B:947:MET:HE3	2:B:1016:VAL:HG11	1.90	0.54
1:A:120:PHE:CZ	1:A:124:LYS:HD2	2.43	0.54
3:C:204:ARG:CB	10:J:63:ASN:HD21	2.21	0.54
8:H:31:SER:OG	8:H:32:GLY:N	2.41	0.54
1:A:2:ASN:OD1	1:A:3:ILE:N	2.41	0.54
1:A:130:LEU:HD21	1:A:193:SER:HB2	1.89	0.54
1:A:1537:ASP:HB2	1:A:1539:VAL:HG22	1.90	0.54
1:A:1549:LEU:HD12	1:A:1549:LEU:H	1.72	0.54
2:B:59:ASP:OD2	2:B:73:ASN:ND2	2.40	0.53
1:A:510:ALA:HA	1:A:597:VAL:HG22	1.89	0.53
2:B:168:GLU:OE2	2:B:172:TYR:OH	2.25	0.53
2:B:773:ILE:HG22	2:B:774:LEU:H	1.73	0.53
2:B:146:SER:OG	2:B:147:ASN:N	2.42	0.53
2:B:280:PHE:O	2:B:284:ARG:HG2	2.08	0.53
2:B:518:LEU:H	2:B:518:LEU:HD23	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:LYS:NZ	2:B:397:ASN:OD1	2.41	0.53
5:E:70:GLY:H	5:E:100:LYS:HB2	1.72	0.53
5:E:76:PHE:HD1	5:E:105:ILE:HD13	1.71	0.53
1:A:390:LEU:HD13	1:A:444:LEU:HA	1.90	0.53
1:A:1051:VAL:CG1	1:A:1060:GLN:HB2	2.39	0.53
1:A:1247:MET:HE1	1:A:1552:ILE:HG13	1.91	0.53
1:A:1602:PRO:O	1:A:1606:SER:OG	2.21	0.53
3:C:62:ILE:HG21	3:C:65:ILE:HD12	1.89	0.53
3:C:118:MET:HB3	3:C:185:ARG:HH22	1.74	0.53
7:G:29:ILE:HG21	7:G:54:ILE:HD11	1.89	0.53
8:H:11:PHE:HB2	8:H:55:PHE:HB2	1.90	0.53
10:J:7:CYS:HB2	10:J:48:MET:HG3	1.90	0.53
1:A:41:LEU:HB3	1:A:43:HIS:HD2	1.74	0.53
1:A:1242:ILE:HD11	1:A:1245:PRO:HA	1.90	0.53
2:B:94:ARG:NH1	12:L:40:ARG:HE	2.07	0.53
10:J:2:ILE:HG22	10:J:3:ILE:H	1.73	0.53
1:A:616:MET:HE1	2:B:1064:VAL:HG12	1.89	0.53
1:A:1304:TYR:CZ	9:I:57:LEU:HD11	2.44	0.53
3:C:140:VAL:HG22	3:C:214:HIS:ND1	2.23	0.53
1:A:82:LEU:HD12	1:A:437:LEU:HD21	1.91	0.53
1:A:949:SER:OG	1:A:950:ASN:N	2.42	0.53
1:A:1231:LEU:HA	1:A:1234:ILE:HG22	1.90	0.53
2:B:1082:ASP:OD1	2:B:1082:ASP:N	2.39	0.53
7:G:26:LEU:HA	7:G:29:ILE:HD12	1.90	0.53
8:H:80:VAL:HB	8:H:95:VAL:HG22	1.90	0.53
12:L:31:ASN:ND2	12:L:42:ARG:HG3	2.24	0.53
1:A:130:LEU:HB3	1:A:133:GLU:HB2	1.92	0.52
1:A:762:LEU:O	1:A:789:GLY:N	2.39	0.52
1:A:1569:ILE:HA	1:A:1572:ILE:HG22	1.89	0.52
2:B:636:ARG:NH1	2:B:675:GLU:OE1	2.35	0.52
7:G:88:CYS:HA	7:G:152:PHE:O	2.08	0.52
2:B:473:LEU:O	2:B:476:PHE:N	2.42	0.52
8:H:42:ILE:HD13	8:H:49:LEU:HD12	1.90	0.52
8:H:59:ILE:HB	8:H:119:VAL:HG13	1.91	0.52
1:A:247:PHE:CE2	1:A:323:MET:HB2	2.44	0.52
2:B:272:VAL:HA	2:B:274:LYS:HZ3	1.75	0.52
2:B:692:SER:O	2:B:700:ASN:ND2	2.39	0.52
1:A:1539:VAL:O	1:A:1541:LYS:HG3	2.10	0.52
2:B:335:VAL:HG13	2:B:336:LEU:H	1.75	0.52
7:G:124:PHE:HB2	7:G:136:TRP:CE3	2.44	0.52
1:A:447:SER:HB2	1:A:466:GLN:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:867:PHE:HE1	12:L:60:PHE:CE2	2.27	0.52
7:G:85:LYS:HA	7:G:154:VAL:HB	1.92	0.52
9:I:10:CYS:HB2	9:I:17:LEU:HD21	1.90	0.52
1:A:77:PHE:CE1	1:A:368:PRO:HA	2.45	0.52
2:B:714:PRO:HG2	2:B:718:LEU:HD21	1.91	0.52
4:D:32:THR:HG23	4:D:33:ILE:HD12	1.92	0.52
1:A:77:PHE:CE2	2:B:1096:ILE:HG12	2.45	0.52
2:B:719:ARG:HH21	10:J:64:PRO:HG3	1.74	0.52
1:A:1068:LEU:HG	1:A:1069:ASP:O	2.10	0.52
1:A:1110:TYR:CD2	1:A:1124:VAL:HG12	2.45	0.52
2:B:137:VAL:HG12	2:B:433:ILE:HG12	1.90	0.52
2:B:208:TYR:CD1	2:B:232:LEU:HB3	2.44	0.52
2:B:231:TYR:HB2	2:B:356:LEU:HD21	1.91	0.52
2:B:869:ASP:CG	2:B:891:ARG:HE	2.18	0.52
5:E:22:VAL:O	5:E:25:ARG:HB2	2.10	0.52
5:E:71:THR:HG23	5:E:99:HIS:HD2	1.75	0.52
4:D:49:GLN:O	7:G:108:ILE:HD11	2.10	0.51
1:A:528:ARG:O	1:A:532:ILE:HG12	2.11	0.51
1:A:219:TYR:HE2	1:A:346:LEU:HD21	1.76	0.51
1:A:718:PRO:O	1:A:722:GLY:N	2.34	0.51
1:A:1140:LYS:HE3	5:E:200:SER:HA	1.91	0.51
5:E:22:VAL:HG23	5:E:23:HIS:ND1	2.26	0.51
12:L:31:ASN:HD22	12:L:42:ARG:HG3	1.76	0.51
1:A:742:THR:HG21	8:H:98:GLY:O	2.11	0.51
1:A:774:TYR:O	8:H:20:LYS:NZ	2.36	0.51
2:B:290:ARG:O	2:B:290:ARG:NH1	2.43	0.51
2:B:637:PRO:HB2	2:B:646:LEU:HD11	1.92	0.51
3:C:194:VAL:HG11	3:C:316:GLY:HA3	1.92	0.51
1:A:411:GLU:OE2	1:A:423:ARG:NH1	2.44	0.51
1:A:538:TRP:CD1	1:A:539:PRO:HA	2.45	0.51
1:A:1669:VAL:HG11	2:B:1071:PHE:HE1	1.75	0.51
3:C:237:LEU:HD12	3:C:238:PRO:HD2	1.92	0.51
1:A:63:CYS:HB3	1:A:66:CYS:SG	2.50	0.51
1:A:87:TYR:HA	1:A:361:PHE:HA	1.93	0.51
1:A:861:LEU:HD13	1:A:920:ILE:HG22	1.93	0.51
1:A:1539:VAL:HG23	1:A:1541:LYS:HE2	1.92	0.51
2:B:192:HIS:HB2	2:B:628:PHE:CZ	2.45	0.51
2:B:286:GLU:HG3	9:I:7:LEU:HD21	1.92	0.51
2:B:738:ARG:HD3	2:B:963:ALA:HB1	1.92	0.51
1:A:653:PHE:O	2:B:1076:ARG:NH2	2.44	0.51
1:A:763:ASN:OD1	1:A:1085:ASN:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1110:TYR:HD2	1:A:1124:VAL:HG12	1.76	0.51
1:A:1139:GLU:O	1:A:1143:ARG:HG2	2.10	0.51
2:B:636:ARG:NH2	2:B:675:GLU:OE2	2.44	0.50
2:B:251:PRO:HG2	2:B:254:MET:HB2	1.93	0.50
1:A:85:PRO:HG3	1:A:363:GLN:HG3	1.93	0.50
2:B:951:SER:OG	2:B:1014:GLY:HA3	2.10	0.50
1:A:826:SER:OG	1:A:830:ARG:NH1	2.42	0.50
3:C:285:VAL:HG21	3:C:303:ARG:NH2	2.26	0.50
1:A:178:LEU:HA	1:A:181:ILE:HD12	1.93	0.50
1:A:1137:VAL:HG23	1:A:1183:TYR:CG	2.47	0.50
1:A:1656:ASP:O	1:A:1657:LEU:HG	2.11	0.50
5:E:76:PHE:HA	5:E:105:ILE:HG12	1.94	0.50
7:G:21:HIS:HB2	7:G:28:ALA:HB2	1.92	0.50
7:G:103:LEU:HB2	7:G:111:ALA:HB3	1.92	0.50
1:A:96:TYR:CZ	1:A:240:LYS:HG2	2.47	0.50
1:A:576:LEU:HG	1:A:578:SER:H	1.77	0.50
1:A:634:TYR:HB3	1:A:686:ILE:HD11	1.94	0.50
2:B:323:ASP:OD1	2:B:323:ASP:N	2.43	0.50
8:H:107:SER:C	8:H:109:ARG:H	2.19	0.50
1:A:1205:PRO:HA	1:A:1208:GLN:HB2	1.92	0.50
2:B:733:GLN:HA	10:J:53:VAL:HG23	1.94	0.50
1:A:84:ILE:HD11	1:A:401:ILE:HG21	1.93	0.50
1:A:1530:LYS:HB2	1:A:1543:ILE:HD13	1.93	0.50
2:B:794:PHE:HB2	2:B:886:ILE:HG22	1.93	0.50
2:B:998:MET:HB2	2:B:1011:ILE:HD12	1.93	0.50
1:A:920:ILE:HD11	1:A:959:LEU:HD22	1.94	0.50
2:B:172:TYR:CD2	2:B:179:GLU:HB3	2.46	0.50
5:E:70:GLY:H	5:E:100:LYS:CB	2.25	0.50
7:G:121:ASP:OD1	7:G:121:ASP:N	2.43	0.50
10:J:51:THR:OG1	10:J:51:THR:O	2.30	0.50
1:A:404:LEU:HD21	1:A:429:LEU:HG	1.94	0.49
1:A:1235:ILE:HD11	1:A:1608:ILE:HG21	1.93	0.49
1:A:1339:TYR:CE2	1:A:1508:LEU:HD21	2.47	0.49
1:A:107:HIS:HB3	1:A:338:LYS:HD2	1.93	0.49
1:A:706:ASP:HB3	11:K:51:ARG:HH12	1.77	0.49
1:A:1038:LYS:HZ2	1:A:1626:ILE:HG23	1.77	0.49
2:B:312:ARG:HH12	2:B:323:ASP:HA	1.78	0.49
2:B:925:GLU:OE1	2:B:997:PRO:HB2	2.12	0.49
3:C:51:THR:OG1	3:C:59:VAL:O	2.23	0.49
3:C:236:LEU:HD21	3:C:308:TYR:CZ	2.47	0.49
7:G:93:ILE:HG23	7:G:150:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:VAL:HG12	1:A:342:VAL:HG21	1.95	0.49
1:A:1270:LEU:HD22	1:A:1313:TYR:CD1	2.47	0.49
2:B:653:GLU:N	2:B:653:GLU:OE1	2.45	0.49
4:D:47:LEU:HD23	4:D:50:LEU:HD12	1.93	0.49
1:A:12:LYS:HD2	2:B:1174:LYS:HB2	1.95	0.49
1:A:103:CYS:O	1:A:107:HIS:N	2.43	0.49
1:A:1248:THR:HB	1:A:1564:ILE:HB	1.93	0.49
1:A:1268:ASN:OD1	1:A:1269:LYS:N	2.45	0.49
1:A:492:ILE:HG22	1:A:630:ILE:HD11	1.94	0.49
1:A:502:GLU:OE1	1:A:622:ARG:HB2	2.12	0.49
1:A:1034:ARG:HG2	1:A:1638:PHE:CE1	2.47	0.49
1:A:1645:LEU:HD11	2:B:1162:LEU:HD11	1.93	0.49
1:A:1131:SER:HB3	6:F:72:THR:HB	1.95	0.49
2:B:719:ARG:O	2:B:872:ARG:NH2	2.45	0.49
5:E:185:LEU:HD13	5:E:209:CYS:SG	2.53	0.49
1:A:432:ASN:O	1:A:435:VAL:HG12	2.13	0.49
8:H:99:GLY:O	8:H:101:LEU:HD12	2.12	0.49
9:I:55:SER:OG	9:I:56:ALA:N	2.46	0.49
1:A:34:ASN:OD1	1:A:48:GLY:HA2	2.12	0.49
3:C:37:TRP:HB2	11:K:56:LYS:CB	2.42	0.49
12:L:24:CYS:HB2	12:L:41:CYS:SG	2.51	0.49
1:A:676:PRO:O	1:A:1604:HIS:HE1	1.95	0.49
1:A:734:ILE:HG12	1:A:740:TYR:HB2	1.95	0.49
2:B:781:ARG:NH1	10:J:10:CYS:O	2.46	0.49
7:G:103:LEU:HD21	7:G:150:LEU:HB2	1.95	0.49
1:A:28:SER:O	2:B:1116:ARG:NH2	2.46	0.48
1:A:31:GLN:HG2	1:A:33:VAL:HG13	1.95	0.48
1:A:631:ARG:NH2	2:B:898:ILE:HD13	2.28	0.48
1:A:1134:LEU:HD11	1:A:1181:LEU:HA	1.94	0.48
1:A:1283:GLU:HB2	9:I:44:VAL:HB	1.95	0.48
3:C:130:GLU:CD	3:C:130:GLU:H	2.21	0.48
6:F:72:THR:HG23	6:F:126:ARG:HH12	1.78	0.48
8:H:83:VAL:HG22	8:H:93:VAL:HG22	1.94	0.48
1:A:873:ALA:HB2	1:A:909:MET:HE1	1.94	0.48
1:A:1679:ILE:HD11	6:F:122:LEU:HD23	1.94	0.48
2:B:149:CYS:SG	2:B:150:HIS:N	2.87	0.48
2:B:253:MET:HE1	2:B:267:ILE:HG13	1.96	0.48
2:B:639:LYS:HB2	2:B:676:TYR:CE1	2.48	0.48
7:G:26:LEU:O	7:G:30:GLN:HG3	2.13	0.48
8:H:59:ILE:HG13	8:H:59:ILE:O	2.13	0.48
1:A:840:GLY:HA3	2:B:1007:MET:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:THR:HG22	2:B:8:ARG:NH2	2.28	0.48
2:B:104:ALA:HB1	2:B:163:LYS:HE2	1.95	0.48
2:B:825:LYS:HE3	2:B:842:ASP:OD2	2.13	0.48
7:G:51:TYR:HA	7:G:77:ASP:O	2.14	0.48
2:B:205:GLY:HA3	2:B:208:TYR:CD2	2.47	0.48
7:G:115:ARG:HA	7:G:118:ILE:HD12	1.95	0.48
1:A:118:LEU:HB2	1:A:182:ARG:NH1	2.28	0.48
1:A:504:GLY:HA2	1:A:622:ARG:O	2.13	0.48
2:B:232:LEU:HD12	2:B:235:GLY:H	1.79	0.48
2:B:560:CYS:SG	2:B:561:VAL:N	2.87	0.48
8:H:41:ASP:HB2	8:H:100:LEU:HB3	1.95	0.48
11:K:36:THR:CG2	11:K:78:ARG:HD3	2.44	0.48
1:A:83:PRO:C	1:A:85:PRO:HD3	2.39	0.48
1:A:1103:ASP:O	1:A:1134:LEU:N	2.39	0.48
2:B:492:THR:O	2:B:494:ARG:N	2.47	0.48
2:B:528:VAL:HG21	2:B:608:ASP:HB2	1.95	0.48
1:A:598:ARG:O	1:A:600:GLY:N	2.46	0.48
7:G:77:ASP:OD1	7:G:77:ASP:N	2.38	0.48
7:G:98:PRO:HG3	7:G:124:PHE:CD2	2.49	0.48
8:H:17:ASP:HA	8:H:18:LYS:CB	2.38	0.48
6:F:121:PRO:O	6:F:122:LEU:HB2	2.14	0.48
8:H:109:ARG:C	8:H:111:LEU:H	2.20	0.48
10:J:26:GLN:HG3	10:J:27:GLU:HG2	1.95	0.48
1:A:704:THR:HG22	1:A:705:ARG:H	1.77	0.48
10:J:30:THR:HG21	10:J:37:LYS:NZ	2.28	0.48
1:A:77:PHE:CD1	1:A:368:PRO:HA	2.48	0.48
1:A:1060:GLN:NE2	1:A:1607:LEU:HA	2.29	0.48
2:B:163:LYS:HD2	2:B:720:TYR:CD2	2.49	0.48
2:B:649:LEU:HD11	2:B:659:ILE:HD11	1.94	0.48
5:E:196:ARG:HA	5:E:202:ARG:HB2	1.95	0.48
1:A:846:ASP:HB3	2:B:993:HIS:CG	2.48	0.47
2:B:728:ARG:HH22	3:C:99:GLN:CD	2.22	0.47
7:G:105:ILE:HG12	7:G:106:LEU:HG	1.96	0.47
12:L:25:ALA:HB3	12:L:46:HIS:CD2	2.48	0.47
1:A:120:PHE:CE1	1:A:341:VAL:HB	2.49	0.47
1:A:447:SER:OG	1:A:463:GLY:N	2.47	0.47
1:A:602:MET:HE2	1:A:602:MET:HB2	1.71	0.47
1:A:1102:VAL:HG12	6:F:73:PRO:HG2	1.95	0.47
2:B:271:ILE:HG22	2:B:272:VAL:HG13	1.95	0.47
3:C:179:GLN:H	3:C:182:GLN:NE2	2.13	0.47
1:A:368:PRO:O	1:A:373:ARG:NE	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:HIS:NE2	1:A:640:TYR:OH	2.45	0.47
2:B:294:SER:OG	2:B:295:TYR:N	2.47	0.47
3:C:259:PRO:O	3:C:262:VAL:HG12	2.14	0.47
1:A:393:ARG:HG2	1:A:440:ASP:OD2	2.15	0.47
2:B:208:TYR:HD1	2:B:232:LEU:HB3	1.79	0.47
2:B:755:ASN:ND2	10:J:51:THR:HG21	2.29	0.47
2:B:1107:VAL:HG23	2:B:1108:GLY:H	1.80	0.47
10:J:54:ASP:OD2	10:J:57:GLU:HG3	2.14	0.47
1:A:16:PHE:CE2	1:A:1636:MET:HE1	2.50	0.47
1:A:111:LEU:HD23	1:A:225:ARG:HG2	1.97	0.47
1:A:481:GLY:CA	2:B:1057:GLY:HA3	2.43	0.47
1:A:534:GLY:O	1:A:540:GLY:HA3	2.15	0.47
1:A:939:GLN:O	1:A:943:VAL:HG12	2.14	0.47
1:A:963:GLN:HE21	1:A:995:ILE:HD11	1.78	0.47
1:A:1140:LYS:HB2	5:E:201:GLY:H	1.80	0.47
2:B:1004:GLY:HA2	3:C:71:ASN:HD22	1.80	0.47
4:D:46:VAL:HG11	7:G:37:ILE:HG23	1.96	0.47
7:G:15:LEU:HD22	7:G:32:HIS:NE2	2.30	0.47
2:B:478:MET:HB3	2:B:520:HIS:CD2	2.50	0.47
3:C:32:ASP:C	3:C:34:ASP:H	2.23	0.47
1:A:1204:GLU:HB3	1:A:1205:PRO:HD3	1.97	0.47
1:A:1324:PHE:O	1:A:1328:PHE:CB	2.54	0.47
2:B:864:GLU:HG3	2:B:865:PRO:HD2	1.97	0.47
5:E:128:GLU:HA	5:E:129:THR:CG2	2.43	0.47
9:I:24:TRP:NE1	9:I:34:TYR:O	2.48	0.47
1:A:1157:ILE:HD12	1:A:1166:ASP:HA	1.96	0.47
1:A:1337:LYS:HE3	1:A:1341:ALA:HB2	1.97	0.47
2:B:143:MET:SD	2:B:171:GLY:HA2	2.55	0.47
2:B:587:LYS:HD2	2:B:607:LEU:HA	1.96	0.47
8:H:71:ALA:HB1	8:H:124:ARG:HE	1.80	0.47
1:A:77:PHE:HZ	2:B:1160:ALA:HA	1.79	0.46
1:A:80:ILE:HG13	1:A:80:ILE:O	2.16	0.46
1:A:470:LYS:O	1:A:471:LYS:HG2	2.15	0.46
1:A:510:ALA:HB1	1:A:538:TRP:CD1	2.50	0.46
1:A:999:PHE:HB3	2:B:945:ILE:HG21	1.98	0.46
2:B:387:ILE:O	2:B:391:LYS:HG2	2.15	0.46
2:B:74:LYS:H	2:B:126:ASN:ND2	2.13	0.46
2:B:155:SER:OG	2:B:158:GLU:OE2	2.24	0.46
2:B:290:ARG:HH11	2:B:293:LYS:HB3	1.80	0.46
2:B:336:LEU:HB2	2:B:345:LYS:HD3	1.98	0.46
2:B:719:ARG:NH2	10:J:64:PRO:HG3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:51:THR:OG1	3:C:59:VAL:HG23	2.15	0.46
3:C:284:THR:C	3:C:286:SER:H	2.23	0.46
5:E:48:MET:HG2	5:E:49:GLY:H	1.80	0.46
5:E:195:ARG:HH21	5:E:205:SER:CB	2.28	0.46
10:J:2:ILE:HG22	10:J:3:ILE:N	2.30	0.46
11:K:38:GLN:NE2	11:K:74:LYS:HD3	2.30	0.46
2:B:312:ARG:NH2	2:B:322:THR:O	2.48	0.46
2:B:490:THR:HB	2:B:492:THR:HG22	1.98	0.46
1:A:498:ILE:HG13	1:A:499:GLU:N	2.27	0.46
1:A:1297:TYR:HE2	1:A:1505:MET:HE2	1.81	0.46
3:C:94:ASN:H	12:L:53:ARG:NH1	2.13	0.46
5:E:16:LYS:O	5:E:20:GLN:HG3	2.15	0.46
8:H:80:VAL:HG12	8:H:117:ASP:O	2.15	0.46
1:A:687:GLN:H	1:A:687:GLN:HG3	1.47	0.46
1:A:1068:LEU:HD12	1:A:1069:ASP:H	1.79	0.46
2:B:480:HIS:HD2	2:B:518:LEU:HB3	1.80	0.46
5:E:15:TRP:O	5:E:19:HIS:N	2.46	0.46
1:A:1680:PHE:CZ	6:F:125:ARG:HD2	2.50	0.46
2:B:630:ASN:O	2:B:633:ARG:NH1	2.49	0.46
8:H:30:VAL:HG12	8:H:37:ASN:HA	1.98	0.46
1:A:479:MET:HE2	2:B:1154:VAL:HG12	1.97	0.46
1:A:555:MET:HE2	1:A:555:MET:HB3	1.83	0.46
1:A:1550:LYS:HA	1:A:1553:TRP:CD1	2.51	0.46
2:B:75:ILE:HA	2:B:124:SER:O	2.16	0.46
2:B:232:LEU:HG	2:B:236:VAL:O	2.16	0.46
2:B:497:LEU:HD12	2:B:497:LEU:O	2.15	0.46
2:B:544:LEU:HD21	2:B:582:VAL:HG11	1.96	0.46
3:C:260:LYS:HA	3:C:260:LYS:HD3	1.73	0.46
1:A:336:PHE:CD1	1:A:356:SER:HB2	2.50	0.46
1:A:390:LEU:O	1:A:394:ILE:HG23	2.16	0.46
1:A:1038:LYS:NZ	1:A:1629:ASN:HD22	2.14	0.46
2:B:48:ALA:O	2:B:52:ILE:HG13	2.16	0.46
2:B:211:TYR:HD1	2:B:359:LEU:HG	1.80	0.46
5:E:195:ARG:HH21	5:E:205:SER:HB3	1.81	0.46
1:A:1327:ARG:NH1	1:A:1517:VAL:O	2.48	0.46
3:C:147:CYS:O	3:C:205:PRO:HA	2.16	0.46
5:E:173:ILE:N	5:E:208:ILE:O	2.48	0.46
1:A:443:SER:HB2	1:A:450:ASN:HD22	1.80	0.46
3:C:107:ILE:HD13	3:C:211:LEU:HD11	1.98	0.46
1:A:6:PRO:HA	7:G:69:PHE:CE2	2.50	0.45
1:A:1645:LEU:HD21	2:B:1167:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:THR:HG23	2:B:41:ASN:H	1.81	0.45
2:B:142:ILE:HD13	2:B:148:ARG:HB3	1.96	0.45
2:B:561:VAL:HG23	2:B:625:LEU:HD23	1.99	0.45
2:B:701:MET:HE3	2:B:701:MET:HB2	1.87	0.45
1:A:960:LEU:HD21	1:A:999:PHE:CE1	2.51	0.45
1:A:1043:LEU:HD12	1:A:1607:LEU:HD11	1.98	0.45
2:B:549:PRO:HB2	2:B:551:VAL:O	2.15	0.45
1:A:65:THR:HA	2:B:1135:GLY:HA3	1.98	0.45
1:A:920:ILE:HD11	1:A:959:LEU:HD13	1.98	0.45
1:A:1267:VAL:HG13	1:A:1527:CYS:SG	2.55	0.45
2:B:169:MET:HE2	2:B:169:MET:HB3	1.81	0.45
5:E:106:TYR:CD2	5:E:110:MET:HB2	2.52	0.45
8:H:9:GLU:HB2	8:H:11:PHE:CE2	2.51	0.45
12:L:49:MET:HE3	12:L:49:MET:HB3	1.83	0.45
1:A:84:ILE:HD12	1:A:84:ILE:H	1.82	0.45
1:A:652:HIS:HB3	2:B:1076:ARG:HH21	1.81	0.45
2:B:193:PRO:HB3	2:B:352:MET:HE2	1.97	0.45
2:B:501:TRP:NE1	2:B:675:GLU:OE2	2.48	0.45
3:C:76:ILE:HA	3:C:80:GLU:HG2	1.99	0.45
1:A:173:LYS:O	1:A:177:THR:HG23	2.15	0.45
1:A:1635:LYS:HB3	1:A:1644:PHE:CD2	2.51	0.45
2:B:869:ASP:OD1	2:B:891:ARG:NE	2.39	0.45
3:C:100:ASP:CG	12:L:60:PHE:HE1	2.24	0.45
7:G:81:PHE:CE1	7:G:106:LEU:HD11	2.51	0.45
10:J:24:LEU:O	10:J:28:ASP:HB2	2.17	0.45
1:A:49:LEU:HG	1:A:373:ARG:HH12	1.82	0.45
1:A:115:LYS:HE3	1:A:115:LYS:HB2	1.79	0.45
1:A:130:LEU:HD23	1:A:133:GLU:HG3	1.99	0.45
1:A:968:ARG:H	1:A:968:ARG:HG2	1.57	0.45
2:B:48:ALA:HB1	2:B:389:LYS:HG3	1.99	0.45
4:D:17:LEU:HD11	7:G:7:TYR:CD1	2.41	0.45
7:G:58:GLU:OE2	7:G:60:SER:N	2.47	0.45
1:A:19:TYR:HD2	1:A:24:VAL:HG22	1.82	0.45
1:A:482:LYS:HG2	2:B:1043:GLN:NE2	2.31	0.45
1:A:694:VAL:HG21	1:A:944:SER:HB2	1.98	0.45
1:A:1236:MET:O	1:A:1620:ALA:HB1	2.16	0.45
2:B:508:HIS:CE1	2:B:520:HIS:CG	3.05	0.45
2:B:781:ARG:NH1	10:J:8:PHE:O	2.44	0.45
1:A:682:LEU:H	1:A:682:LEU:HD23	1.81	0.45
1:A:702:PHE:HB3	1:A:740:TYR:HD2	1.82	0.45
1:A:925:ILE:O	1:A:929:LEU:HD22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1065:GLU:HB3	5:E:200:SER:OG	2.17	0.45
2:B:370:ASP:HB3	2:B:493:VAL:HB	1.98	0.45
2:B:1033:THR:HG23	2:B:1034:THR:H	1.81	0.45
5:E:4:GLU:N	5:E:6:LYS:HE2	2.32	0.45
9:I:55:SER:OG	9:I:57:LEU:N	2.47	0.45
1:A:500:THR:HB	1:A:683:ARG:HH21	1.80	0.45
1:A:763:ASN:HB3	1:A:787:ASP:HA	1.99	0.45
1:A:1063:TYR:CE1	1:A:1194:VAL:HG11	2.52	0.45
3:C:262:VAL:HG13	3:C:263:ILE:HG12	1.99	0.45
12:L:21:ILE:HD13	12:L:32:THR:HG22	1.98	0.45
1:A:1205:PRO:HB2	1:A:1593:PHE:HE1	1.82	0.45
1:A:1504:LEU:HD21	2:B:284:ARG:CZ	2.47	0.45
2:B:322:THR:HG23	2:B:325:GLU:HB3	1.99	0.45
2:B:479:VAL:HG22	2:B:519:ASN:O	2.17	0.45
2:B:640:HIS:HA	2:B:673:HIS:HD2	1.82	0.45
2:B:727:TYR:CD1	2:B:788:VAL:HG22	2.51	0.45
2:B:778:ALA:O	2:B:783:PHE:HB2	2.16	0.45
2:B:844:ILE:HG22	2:B:858:GLU:O	2.17	0.45
3:C:84:LEU:HD12	3:C:114:ALA:HB3	1.99	0.45
8:H:33:GLN:C	8:H:35:ASP:H	2.25	0.45
1:A:53:ALA:HB2	1:A:64:ALA:HB3	2.00	0.44
1:A:691:VAL:HG11	1:A:841:PHE:CZ	2.52	0.44
1:A:720:GLU:OE1	11:K:68:PRO:HG3	2.17	0.44
1:A:1225:THR:O	1:A:1226:LEU:HD23	2.17	0.44
2:B:873:LEU:HD23	2:B:873:LEU:HA	1.79	0.44
1:A:41:LEU:HB3	1:A:43:HIS:CD2	2.52	0.44
1:A:506:PRO:HB3	1:A:627:GLU:O	2.17	0.44
1:A:786:PHE:CB	1:A:791:LEU:HA	2.48	0.44
1:A:1556:TYR:OH	5:E:13:ARG:HG3	2.17	0.44
1:A:1664:LEU:HD11	2:B:1077:LEU:HD13	1.98	0.44
2:B:689:THR:HB	2:B:692:SER:HB2	1.98	0.44
2:B:925:GLU:OE1	3:C:303:ARG:NH2	2.35	0.44
7:G:47:ILE:O	7:G:80:VAL:HA	2.17	0.44
1:A:975:SER:O	1:A:975:SER:OG	2.30	0.44
2:B:160:ILE:HG23	10:J:62:TYR:CE1	2.52	0.44
2:B:227:ASN:OD1	2:B:227:ASN:N	2.50	0.44
2:B:1004:GLY:O	3:C:234:TYR:OH	2.30	0.44
6:F:79:GLU:OE2	6:F:126:ARG:NE	2.51	0.44
6:F:90:GLN:HE22	6:F:122:LEU:HD11	1.82	0.44
1:A:476:ARG:NH1	1:A:1638:PHE:O	2.49	0.44
1:A:495:ASP:OD2	11:K:69:HIS:NE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:THR:OG1	1:A:683:ARG:NH1	2.50	0.44
1:A:893:GLU:HB2	1:A:985:TYR:CZ	2.53	0.44
2:B:45:LEU:O	2:B:49:VAL:HG22	2.17	0.44
2:B:754:THR:OG1	2:B:755:ASN:N	2.51	0.44
4:D:16:LYS:NZ	4:D:17:LEU:O	2.42	0.44
5:E:151:LEU:HD12	5:E:190:VAL:HG12	1.98	0.44
6:F:79:GLU:OE1	6:F:126:ARG:NH2	2.43	0.44
7:G:167:GLN:N	7:G:167:GLN:OE1	2.50	0.44
10:J:7:CYS:HB3	10:J:14:ILE:HD13	1.98	0.44
1:A:1637:SER:OG	1:A:1638:PHE:HD2	2.00	0.44
2:B:272:VAL:HG11	2:B:281:LEU:HB3	2.00	0.44
2:B:896:PRO:HA	2:B:900:ASP:OD1	2.18	0.44
2:B:1158:LEU:O	2:B:1162:LEU:HB2	2.17	0.44
3:C:314:SER:OG	3:C:315:THR:N	2.50	0.44
5:E:37:THR:OG1	5:E:40:GLN:HB2	2.18	0.44
10:J:43:TYR:HA	10:J:46:ARG:HB3	2.00	0.44
1:A:744:LYS:HD2	8:H:99:GLY:CA	2.47	0.44
1:A:1086:TYR:CD1	1:A:1178:LEU:HD22	2.43	0.44
3:C:86:PHE:CZ	3:C:112:ILE:HD11	2.52	0.44
7:G:23:ARG:HD2	7:G:23:ARG:HA	1.72	0.44
7:G:44:ILE:HG22	7:G:80:VAL:HG21	1.99	0.44
1:A:784:VAL:HA	1:A:793:CYS:O	2.17	0.44
1:A:1123:PRO:HG2	5:E:203:TYR:HA	2.00	0.44
1:A:1577:GLY:HA2	5:E:177:ASP:OD1	2.17	0.44
2:B:503:PHE:CE2	2:B:651:PRO:HB3	2.52	0.44
3:C:81:ILE:HG22	3:C:330:VAL:HG21	1.99	0.44
1:A:478:HIS:HA	2:B:1043:GLN:HE22	1.83	0.44
2:B:190:ARG:HG3	2:B:376:GLU:OE1	2.18	0.44
2:B:563:LEU:HG	2:B:564:ASP:OD1	2.18	0.44
2:B:580:ALA:HA	2:B:611:ILE:HG21	2.00	0.44
3:C:163:LEU:HG	3:C:164:TYR:CE1	2.52	0.44
3:C:266:GLU:N	3:C:274:GLN:O	2.46	0.44
8:H:9:GLU:HG3	8:H:36:MET:HE3	2.00	0.44
1:A:116:VAL:CG1	1:A:342:VAL:HG21	2.48	0.44
1:A:850:LEU:HD21	1:A:957:SER:HB3	1.99	0.44
1:A:936:ASN:OD1	1:A:939:GLN:N	2.42	0.44
1:A:1115:LEU:HA	1:A:1115:LEU:HD23	1.68	0.44
1:A:1498:ILE:HG21	9:I:21:THR:HB	2.00	0.44
2:B:190:ARG:HD2	2:B:630:ASN:HB2	2.00	0.44
2:B:734:THR:OG1	10:J:51:THR:OG1	2.19	0.44
2:B:807:VAL:HG23	2:B:808:HIS:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1061:ARG:HA	2:B:1064:VAL:HG22	1.99	0.44
3:C:32:ASP:O	3:C:34:ASP:N	2.51	0.44
7:G:89:LEU:HD12	7:G:154:VAL:HG21	1.98	0.44
1:A:421:GLU:HB2	1:A:424:SER:HB3	2.00	0.43
1:A:812:VAL:HG21	1:A:824:LEU:HD13	2.00	0.43
2:B:572:THR:HG23	2:B:575:LEU:H	1.83	0.43
1:A:1119:TYR:HD1	1:A:1120:LYS:HG3	1.83	0.43
1:A:1611:TYR:HE2	1:A:1621:PHE:HE1	1.66	0.43
2:B:493:VAL:C	2:B:495:LYS:H	2.26	0.43
2:B:758:VAL:HG21	2:B:1018:TYR:HE2	1.83	0.43
2:B:780:GLU:HB3	3:C:223:HIS:CE1	2.53	0.43
2:B:1089:CYS:H	2:B:1098:ILE:HD11	1.82	0.43
10:J:35:LEU:HD21	10:J:50:LEU:HD12	1.99	0.43
1:A:488:ALA:HB1	1:A:509:PHE:CZ	2.53	0.43
1:A:514:THR:HG22	1:A:596:HIS:HD2	1.83	0.43
2:B:274:LYS:O	2:B:275:ASP:C	2.61	0.43
2:B:676:TYR:HD1	2:B:676:TYR:HA	1.68	0.43
2:B:998:MET:HE2	2:B:998:MET:HB3	1.85	0.43
1:A:1066:ASP:O	1:A:1067:SER:C	2.61	0.43
2:B:384:TYR:CZ	2:B:437:LEU:HD23	2.54	0.43
7:G:38:LEU:HG	7:G:38:LEU:O	2.18	0.43
1:A:786:PHE:HB2	1:A:790:GLU:O	2.18	0.43
2:B:88:MET:HE1	2:B:100:LYS:HG2	2.00	0.43
2:B:322:THR:OG1	2:B:323:ASP:N	2.47	0.43
2:B:419:ARG:O	2:B:423:THR:HG23	2.18	0.43
2:B:441:LEU:HD23	2:B:461:THR:HG21	2.00	0.43
2:B:489:LYS:HD2	2:B:489:LYS:HA	1.91	0.43
3:C:157:GLU:O	3:C:157:GLU:HG2	2.18	0.43
6:F:125:ARG:HG2	6:F:135:ASP:OD1	2.19	0.43
1:A:131:LEU:HD21	1:A:207:LEU:HD12	1.99	0.43
1:A:564:ALA:O	1:A:568:GLN:HG2	2.18	0.43
1:A:810:HIS:CE1	1:A:1075:HIS:HE1	2.35	0.43
1:A:1184:GLN:O	1:A:1187:LEU:HD23	2.19	0.43
2:B:232:LEU:HD13	2:B:234:ASN:HB3	2.01	0.43
2:B:371:SER:HA	2:B:497:LEU:HD11	2.00	0.43
4:D:17:LEU:HD22	7:G:8:LYS:O	2.18	0.43
10:J:1:MET:HB3	10:J:56:ILE:HD12	2.01	0.43
1:A:9:SER:CB	2:B:1149:ILE:HG22	2.49	0.43
1:A:1085:ASN:OD1	1:A:1086:TYR:N	2.42	0.43
1:A:1550:LYS:HA	1:A:1553:TRP:HD1	1.84	0.43
2:B:145:ARG:O	2:B:145:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:ARG:NH2	2:B:249:LEU:HD11	2.30	0.43
2:B:1130:ASP:O	2:B:1132:TRP:HD1	2.01	0.43
4:D:29:TYR:CD2	7:G:50:ALA:HA	2.54	0.43
5:E:105:ILE:HD12	5:E:132:GLU:CD	2.44	0.43
11:K:81:THR:OG1	11:K:82:ALA:N	2.50	0.43
1:A:653:PHE:H	2:B:1076:ARG:NH2	2.16	0.43
2:B:104:ALA:O	2:B:108:GLU:HG2	2.19	0.43
2:B:335:VAL:HG13	2:B:336:LEU:N	2.33	0.43
2:B:589:GLU:O	2:B:592:VAL:HG12	2.19	0.43
2:B:738:ARG:NH2	2:B:742:HIS:HD2	2.16	0.43
2:B:764:THR:HG21	2:B:773:ILE:HG13	2.01	0.43
2:B:822:TRP:CD1	2:B:822:TRP:N	2.86	0.43
2:B:831:LEU:HD22	2:B:886:ILE:CD1	2.44	0.43
2:B:901:LYS:HD3	2:B:1023:HIS:HB2	2.01	0.43
2:B:991:ASN:HD22	2:B:995:ASN:HB2	1.84	0.43
3:C:37:TRP:HH2	11:K:101:LEU:HB2	1.83	0.43
3:C:247:GLU:HA	3:C:273:LYS:O	2.19	0.43
8:H:77:TYR:CE2	8:H:118:HIS:HD2	2.37	0.43
1:A:104:LEU:HD23	1:A:104:LEU:HA	1.77	0.43
1:A:838:MET:HE2	1:A:838:MET:HB3	1.76	0.43
1:A:1259:ARG:HD2	1:A:1259:ARG:HA	1.84	0.43
2:B:236:VAL:HG12	2:B:237:THR:H	1.83	0.43
2:B:551:VAL:HG12	2:B:552:VAL:H	1.83	0.43
3:C:285:VAL:HG12	3:C:285:VAL:O	2.18	0.43
6:F:108:LEU:O	6:F:111:ALA:N	2.50	0.43
1:A:684:GLY:HA3	1:A:802:GLY:HA2	2.01	0.43
1:A:902:LEU:HD23	1:A:902:LEU:HA	1.81	0.43
1:A:1063:TYR:O	1:A:1066:ASP:HA	2.19	0.43
2:B:667:VAL:HG13	2:B:670:VAL:HG23	1.99	0.43
2:B:801:ARG:O	2:B:802:ARG:HG2	2.18	0.43
3:C:160:PRO:HB2	3:C:164:TYR:CD2	2.54	0.43
1:A:86:ALA:HB1	1:A:438:GLN:OE1	2.19	0.42
1:A:820:ILE:HD13	1:A:823:ARG:HD3	2.01	0.42
1:A:1041:GLU:HB3	1:A:1660:PRO:HD2	2.01	0.42
1:A:1579:GLU:CD	5:E:193:ILE:HD12	2.44	0.42
2:B:61:ILE:O	2:B:69:LEU:HB2	2.19	0.42
2:B:767:ASP:OD1	2:B:935:ASN:ND2	2.52	0.42
3:C:223:HIS:CD2	3:C:225:LYS:HG2	2.53	0.42
5:E:23:HIS:O	5:E:23:HIS:CG	2.72	0.42
7:G:15:LEU:HD13	7:G:32:HIS:CE1	2.54	0.42
1:A:1098:VAL:HG11	1:A:1181:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:PHE:HB2	2:B:210:GLN:HA	2.01	0.42
2:B:728:ARG:HE	2:B:728:ARG:HB3	1.45	0.42
2:B:922:PRO:HB2	2:B:998:MET:HE2	2.01	0.42
1:A:51:ASP:HB3	1:A:54:LEU:HB2	2.02	0.42
2:B:109:ARG:HA	2:B:874:LEU:HG	2.01	0.42
2:B:493:VAL:C	2:B:495:LYS:N	2.76	0.42
7:G:51:TYR:HB2	7:G:76:VAL:HG22	2.01	0.42
1:A:346:LEU:HD12	1:A:346:LEU:HA	1.84	0.42
1:A:1224:VAL:HG12	1:A:1244:THR:OG1	2.20	0.42
1:A:1231:LEU:O	1:A:1235:ILE:HG22	2.19	0.42
2:B:165:GLU:HA	10:J:62:TYR:OH	2.19	0.42
7:G:121:ASP:HB2	7:G:139:ASN:HB2	2.01	0.42
8:H:36:MET:SD	8:H:104:ILE:HD11	2.59	0.42
1:A:394:ILE:HG22	1:A:440:ASP:OD1	2.19	0.42
1:A:1663:ARG:NE	1:A:1668:ARG:HH21	2.17	0.42
1:A:1680:PHE:CE1	6:F:125:ARG:HD2	2.55	0.42
2:B:40:THR:HG21	2:B:147:ASN:HB3	2.01	0.42
2:B:382:PHE:O	2:B:386:GLN:HG3	2.19	0.42
2:B:694:PHE:CD2	2:B:949:ILE:HG13	2.55	0.42
2:B:1095:ILE:HD12	2:B:1151:LEU:HD21	2.00	0.42
1:A:82:LEU:HB2	1:A:84:ILE:HD13	2.02	0.42
1:A:850:LEU:HD13	1:A:929:LEU:HA	2.02	0.42
1:A:896:TYR:HB3	1:A:902:LEU:HD21	2.00	0.42
2:B:30:LYS:O	2:B:34:ASP:HB2	2.18	0.42
2:B:492:THR:OG1	2:B:493:VAL:N	2.36	0.42
5:E:171:PRO:O	5:E:208:ILE:HG12	2.20	0.42
1:A:255:ASN:HA	1:A:258:PHE:CD2	2.54	0.42
2:B:919:VAL:CG2	3:C:75:ARG:HG2	2.50	0.42
2:B:1087:TRP:CD1	2:B:1113:VAL:HG21	2.55	0.42
3:C:224:ALA:O	3:C:227:SER:OG	2.35	0.42
6:F:102:GLU:N	6:F:102:GLU:OE2	2.53	0.42
12:L:45:GLY:O	12:L:47:ARG:NH1	2.53	0.42
1:A:1553:TRP:CE3	5:E:137:VAL:HG22	2.55	0.42
2:B:27:LYS:HE3	2:B:27:LYS:HB3	1.89	0.42
2:B:537:ILE:HD11	2:B:605:VAL:HG13	2.02	0.42
7:G:84:LYS:O	7:G:85:LYS:HG2	2.20	0.42
8:H:24:VAL:HA	8:H:42:ILE:O	2.19	0.42
8:H:25:SER:OG	8:H:44:SER:OG	2.19	0.42
10:J:59:LEU:O	10:J:59:LEU:HD23	2.20	0.42
11:K:36:THR:HG23	11:K:78:ARG:HD3	2.01	0.42
1:A:470:LYS:C	1:A:472:GLU:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1669:VAL:HG11	2:B:1071:PHE:CE1	2.55	0.42
2:B:92:ARG:HG3	2:B:92:ARG:O	2.20	0.42
2:B:133:GLU:OE2	2:B:135:ARG:HD3	2.19	0.42
3:C:223:HIS:HD2	3:C:225:LYS:HG2	1.85	0.42
6:F:84:LEU:HA	6:F:84:LEU:HD23	1.85	0.42
8:H:9:GLU:HB2	8:H:11:PHE:HE2	1.84	0.42
8:H:69:LYS:HD3	8:H:69:LYS:HA	1.80	0.42
1:A:247:PHE:CD2	1:A:323:MET:HB2	2.54	0.42
1:A:438:GLN:O	1:A:438:GLN:NE2	2.53	0.42
1:A:643:ASP:OD1	1:A:645:ASP:HB2	2.20	0.42
1:A:1163:SER:HA	1:A:1166:ASP:OD2	2.20	0.42
2:B:562:GLN:HB3	2:B:626:TYR:HD1	1.85	0.42
2:B:780:GLU:OE1	3:C:223:HIS:HA	2.20	0.42
2:B:1043:GLN:HE21	2:B:1154:VAL:HG21	1.85	0.42
3:C:47:LYS:O	3:C:63:SER:OG	2.24	0.42
4:D:46:VAL:O	4:D:50:LEU:HG	2.20	0.42
1:A:784:VAL:HG11	1:A:796:LEU:HD23	2.00	0.41
1:A:912:LYS:HA	1:A:912:LYS:HD3	1.89	0.41
8:H:51:LYS:HG2	8:H:52:ASP:OD1	2.19	0.41
8:H:121:LEU:O	8:H:122:LEU:HD23	2.20	0.41
1:A:203:LEU:HD21	1:A:208:LEU:HD12	2.03	0.41
1:A:548:ASP:OD1	1:A:549:GLY:N	2.53	0.41
1:A:1580:ALA:HA	5:E:144:LEU:O	2.20	0.41
2:B:114:LYS:HB2	2:B:139:MET:HB3	2.01	0.41
2:B:564:ASP:N	2:B:627:LEU:O	2.45	0.41
4:D:29:TYR:CG	7:G:50:ALA:HA	2.55	0.41
5:E:193:ILE:H	5:E:193:ILE:HG12	1.71	0.41
1:A:106:CYS:SG	1:A:230:ASN:HB2	2.59	0.41
1:A:793:CYS:HB2	8:H:101:LEU:HD11	2.02	0.41
2:B:379:LEU:HD21	2:B:527:ILE:HG21	2.01	0.41
2:B:399:ILE:HG22	2:B:429:ILE:HG21	2.03	0.41
2:B:747:LEU:HD13	2:B:747:LEU:HA	1.88	0.41
3:C:37:TRP:NE1	11:K:97:ASP:OD1	2.53	0.41
1:A:500:THR:HG21	1:A:825:LEU:HB3	2.01	0.41
1:A:632:MET:HE1	1:A:640:TYR:HD2	1.85	0.41
1:A:1297:TYR:OH	1:A:1505:MET:HB2	2.19	0.41
2:B:33:VAL:HG23	2:B:146:SER:HA	2.03	0.41
2:B:338:HIS:NE2	2:B:339:LEU:HG	2.35	0.41
2:B:349:LEU:HD12	2:B:349:LEU:HA	1.91	0.41
3:C:208:GLU:HG2	3:C:209:ILE:N	2.35	0.41
4:D:20:ASP:O	4:D:24:LYS:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:12:THR:HG22	8:H:31:SER:HB2	2.02	0.41
1:A:246:ILE:O	1:A:247:PHE:CG	2.73	0.41
1:A:489:ARG:O	2:B:1029:PHE:HA	2.20	0.41
1:A:542:SER:HB3	1:A:594:TYR:HB2	2.01	0.41
1:A:671:SER:O	1:A:671:SER:OG	2.38	0.41
1:A:1309:TYR:OH	1:A:1315:VAL:O	2.31	0.41
1:A:1329:LEU:HD11	1:A:1480:LEU:HD13	2.02	0.41
2:B:87:PRO:HG3	2:B:113:TYR:CE2	2.55	0.41
2:B:104:ALA:HB1	2:B:163:LYS:HB2	2.03	0.41
3:C:155:THR:OG1	3:C:156:ASP:N	2.54	0.41
7:G:61:ALA:HB2	7:G:72:ILE:HD12	2.01	0.41
1:A:6:PRO:O	1:A:7:VAL:C	2.64	0.41
1:A:19:TYR:CD1	2:B:1168:LYS:HD3	2.56	0.41
1:A:89:PRO:HG2	1:A:445:ILE:HB	2.01	0.41
1:A:474:LEU:HD23	1:A:478:HIS:HB2	2.02	0.41
3:C:40:ASP:OD1	3:C:41:LYS:N	2.54	0.41
3:C:242:ILE:HD13	3:C:275:ALA:O	2.20	0.41
10:J:67:LYS:HD3	10:J:67:LYS:HA	1.90	0.41
11:K:95:LEU:HD23	11:K:95:LEU:HA	1.90	0.41
12:L:31:ASN:CB	12:L:49:MET:HE1	2.51	0.41
1:A:1566:THR:O	1:A:1567:ASN:C	2.62	0.41
2:B:549:PRO:HG3	2:B:553:GLY:H	1.85	0.41
5:E:71:THR:OG1	5:E:72:ILE:N	2.54	0.41
5:E:162:ARG:HD2	5:E:163:TYR:CE2	2.56	0.41
1:A:957:SER:O	1:A:998:ARG:HD2	2.21	0.41
1:A:1508:LEU:HA	1:A:1508:LEU:HD23	1.78	0.41
2:B:274:LYS:HG3	2:B:275:ASP:OD1	2.20	0.41
2:B:1077:LEU:HD23	2:B:1077:LEU:HA	1.82	0.41
5:E:172:ARG:NE	5:E:210:ALA:HB3	2.36	0.41
1:A:47:GLY:N	1:A:51:ASP:OD1	2.45	0.41
1:A:240:LYS:HA	1:A:246:ILE:HG22	2.02	0.41
1:A:702:PHE:HZ	8:H:100:LEU:HD11	1.85	0.41
1:A:1094:LYS:O	1:A:1098:VAL:HG23	2.20	0.41
1:A:1130:PRO:HA	1:A:1136:SER:OG	2.21	0.41
1:A:1578:VAL:HG23	5:E:177:ASP:OD2	2.20	0.41
2:B:293:LYS:O	2:B:293:LYS:HG3	2.21	0.41
2:B:312:ARG:NH1	2:B:322:THR:O	2.51	0.41
2:B:338:HIS:CD2	2:B:339:LEU:HG	2.56	0.41
2:B:665:GLU:O	2:B:665:GLU:HG3	2.21	0.41
3:C:58:MET:HE1	11:K:109:PHE:CZ	2.56	0.41
3:C:66:ASP:OD2	3:C:67:ALA:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:111:PRO:HB2	3:C:194:VAL:HG12	2.03	0.41
3:C:134:THR:HG22	3:C:137:ASP:HB2	2.01	0.41
5:E:79:GLU:HB2	5:E:86:GLU:OE1	2.21	0.41
7:G:3:ASP:HB2	7:G:4:LEU:H	1.73	0.41
10:J:4:PRO:HD3	10:J:52:HIS:CD2	2.55	0.41
11:K:68:PRO:HD2	11:K:74:LYS:O	2.21	0.41
1:A:861:LEU:HD23	1:A:861:LEU:HA	1.93	0.41
1:A:1277:ARG:HB3	1:A:1302:ASP:HB3	2.03	0.41
2:B:556:SER:OG	2:B:557:GLY:N	2.54	0.41
2:B:908:GLN:HE22	2:B:942:ARG:CD	2.33	0.41
4:D:46:VAL:HG23	4:D:47:LEU:N	2.36	0.41
7:G:145:GLU:HB3	7:G:146:PRO:HD3	2.03	0.41
1:A:1:MET:HG2	1:A:2:ASN:N	2.36	0.40
1:A:21:VAL:HG23	1:A:364:ASN:HD21	1.86	0.40
1:A:825:LEU:HA	1:A:825:LEU:HD12	1.87	0.40
1:A:1539:VAL:O	1:A:1539:VAL:HG23	2.21	0.40
2:B:368:ASN:O	2:B:371:SER:OG	2.38	0.40
11:K:28:HIS:HB3	11:K:35:VAL:HG23	2.02	0.40
1:A:770:VAL:O	1:A:770:VAL:HG13	2.22	0.40
1:A:1013:MET:HE3	2:B:496:LEU:O	2.21	0.40
1:A:1200:GLN:HE21	2:B:1062:ASP:HB3	1.86	0.40
2:B:159:LEU:HD23	2:B:159:LEU:HA	1.93	0.40
2:B:867:PHE:CD2	2:B:867:PHE:N	2.88	0.40
2:B:1162:LEU:HG	2:B:1167:ILE:O	2.21	0.40
11:K:32:LEU:O	11:K:86:THR:OG1	2.37	0.40
11:K:103:ASP:O	11:K:106:THR:HG22	2.22	0.40
1:A:114:VAL:HG21	1:A:178:LEU:HD23	2.03	0.40
1:A:509:PHE:HD1	1:A:509:PHE:HA	1.74	0.40
1:A:1053:ASP:OD1	1:A:1054:SER:N	2.54	0.40
1:A:1129:PRO:HD2	1:A:1133:TYR:CE1	2.57	0.40
1:A:1164:LYS:HG3	1:A:1165:LEU:N	2.36	0.40
2:B:13:LYS:NZ	10:J:57:GLU:OE1	2.48	0.40
2:B:185:LEU:HD12	2:B:378:LEU:HD21	2.02	0.40
2:B:236:VAL:HG22	2:B:288:MET:HA	2.03	0.40
2:B:407:VAL:HG22	2:B:414:VAL:HG12	2.03	0.40
2:B:473:LEU:HD23	2:B:473:LEU:HA	1.96	0.40
2:B:775:ASN:ND2	2:B:918:THR:HA	2.36	0.40
4:D:25:PHE:HZ	7:G:52:ASP:N	2.19	0.40
9:I:7:LEU:HD23	9:I:7:LEU:HA	1.79	0.40
1:A:910:LYS:HB2	1:A:910:LYS:HE3	1.69	0.40
1:A:1172:GLU:OE2	1:A:1176:LYS:HE3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1549:LEU:HG	1:A:1565:TYR:OH	2.21	0.40
2:B:119:LEU:HD11	2:B:392:ILE:HD12	2.02	0.40
2:B:344:ASP:OD1	2:B:566:LYS:HE3	2.21	0.40
2:B:372:PRO:HA	2:B:375:GLN:HB2	2.03	0.40
3:C:84:LEU:HA	3:C:84:LEU:HD23	1.87	0.40
5:E:107:ALA:HA	5:E:108:ASN:HA	1.64	0.40
9:I:20:THR:HG21	9:I:39:PHE:HE2	1.85	0.40
11:K:108:LYS:O	11:K:112:GLN:HG2	2.21	0.40
1:A:14:VAL:HG21	1:A:1633:PHE:HE2	1.85	0.40
1:A:37:LEU:HD21	1:A:50:TYR:CE2	2.56	0.40
1:A:332:LEU:HA	1:A:332:LEU:HD23	1.82	0.40
1:A:1588:GLU:O	1:A:1592:VAL:HG23	2.22	0.40
2:B:552:VAL:O	2:B:552:VAL:HG23	2.22	0.40
2:B:710:THR:HG21	2:B:1019:GLN:HB2	2.04	0.40
2:B:783:PHE:O	2:B:784:GLY:C	2.64	0.40
2:B:1007:MET:H	2:B:1007:MET:HG2	1.71	0.40
3:C:87:GLU:O	12:L:62:ALA:N	2.35	0.40
3:C:236:LEU:HD23	3:C:236:LEU:HA	1.85	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	1368/1689 (81%)	1235 (90%)	130 (10%)	3 (0%)	43	74
2	B	1151/1174 (98%)	993 (86%)	155 (14%)	3 (0%)	36	69
3	C	315/348 (90%)	290 (92%)	23 (7%)	2 (1%)	21	55
4	D	35/147 (24%)	35 (100%)	0	0	100	100
5	E	205/210 (98%)	176 (86%)	29 (14%)	0	100	100
6	F	80/142 (56%)	74 (92%)	5 (6%)	1 (1%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	156/173 (90%)	141 (90%)	15 (10%)	0	100	100
8	H	121/125 (97%)	94 (78%)	26 (22%)	1 (1%)	16	50
9	I	55/119 (46%)	51 (93%)	4 (7%)	0	100	100
10	J	66/71 (93%)	50 (76%)	16 (24%)	0	100	100
11	K	93/125 (74%)	84 (90%)	9 (10%)	0	100	100
12	L	43/63 (68%)	42 (98%)	1 (2%)	0	100	100
All	All	3688/4386 (84%)	3265 (88%)	413 (11%)	10 (0%)	37	69

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	206	THR
2	B	493	VAL
1	A	782	GLY
3	C	286	SER
1	A	968	ARG
2	B	827	ASP
1	A	85	PRO
6	F	121	PRO
3	C	285	VAL
8	H	24	VAL

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	1233/1484 (83%)	1232 (100%)	1 (0%)	88	89
2	B	1004/1013 (99%)	999 (100%)	5 (0%)	81	81
3	C	281/308 (91%)	279 (99%)	2 (1%)	76	78
4	D	37/134 (28%)	37 (100%)	0	100	100
5	E	182/184 (99%)	181 (100%)	1 (0%)	81	81
6	F	70/121 (58%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	143/154 (93%)	143 (100%)	0	100	100
8	H	112/114 (98%)	112 (100%)	0	100	100
9	I	51/105 (49%)	51 (100%)	0	100	100
10	J	63/66 (96%)	63 (100%)	0	100	100
11	K	86/111 (78%)	86 (100%)	0	100	100
12	L	39/53 (74%)	37 (95%)	2 (5%)	21	47
All	All	3301/3847 (86%)	3290 (100%)	11 (0%)	84	85

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	786	PHE
2	B	215	ILE
2	B	497	LEU
2	B	499	GLU
2	B	676	TYR
2	B	1167	ILE
3	C	110	VAL
3	C	231	THR
5	E	137	VAL
12	L	26	ASP
12	L	31	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	60	ASN
1	A	67	HIS
1	A	94	GLN
1	A	107	HIS
1	A	117	HIS
1	A	230	ASN
1	A	232	GLN
1	A	257	GLN
1	A	330	ASN
1	A	364	ASN
1	A	432	ASN
1	A	439	HIS

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Mol	Chain	Res	Type
1	A	442	ASN
1	A	450	ASN
1	A	536	HIS
1	A	543	HIS
1	A	599	ASN
1	A	606	ASN
1	A	608	GLN
1	A	655	GLN
1	A	672	GLN
1	A	710	GLN
1	A	735	GLN
1	A	860	GLN
1	A	963	GLN
1	A	1075	HIS
1	A	1476	ASN
1	A	1587	HIS
1	A	1629	ASN
1	A	1643	HIS
2	B	26	GLN
2	B	32	HIS
2	B	98	ASN
2	B	126	ASN
2	B	150	HIS
2	B	176	ASN
2	B	233	ASN
2	B	300	GLN
2	B	373	GLN
2	B	375	GLN
2	B	386	GLN
2	B	402	GLN
2	B	508	HIS
2	B	530	HIS
2	B	640	HIS
2	B	695	ASN
2	B	700	ASN
2	B	742	HIS
2	B	749	HIS
2	B	752	ASN
2	B	808	HIS
2	B	887	HIS
2	B	908	GLN
2	B	937	HIS

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Mol	Chain	Res	Type
2	B	993	HIS
2	B	1038	HIS
2	B	1043	GLN
2	B	1067	HIS
2	B	1145	ASN
3	C	55	GLN
3	C	150	ASN
3	C	182	GLN
3	C	207	GLN
3	C	223	HIS
3	C	300	GLN
4	D	51	ASN
5	E	19	HIS
5	E	98	ASN
5	E	99	HIS
5	E	141	HIS
5	E	142	HIS
5	E	204	ASN
6	F	94	ASN
7	G	30	GLN
7	G	133	GLN
7	G	167	GLN
8	H	37	ASN
8	H	118	HIS
9	I	41	ASN
10	J	63	ASN
11	K	38	GLN
11	K	40	GLN
11	K	76	ASN
12	L	31	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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.

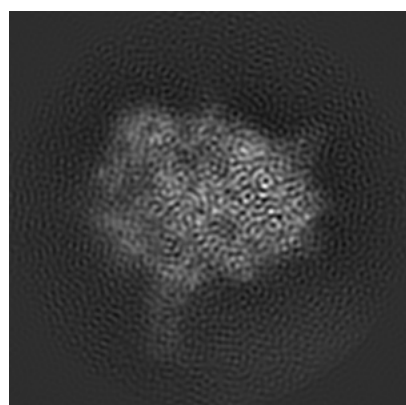
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11840. These allow visual inspection of the internal detail of the map and identification of artifacts.

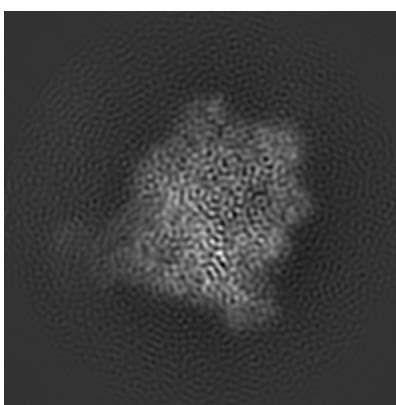
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

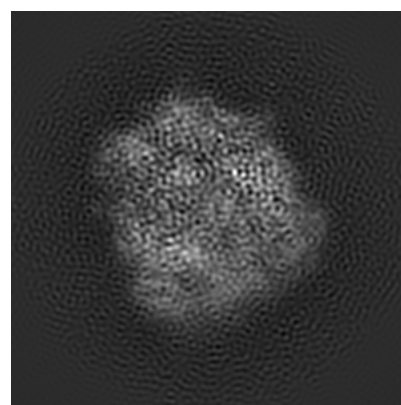
6.1.1 Primary map



X



Y

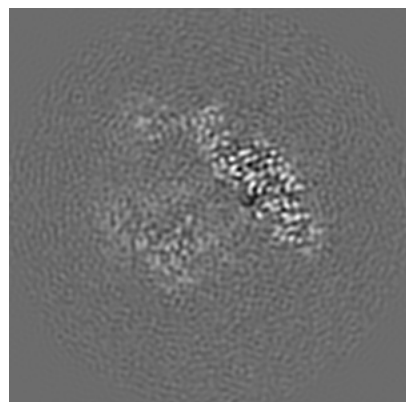


Z

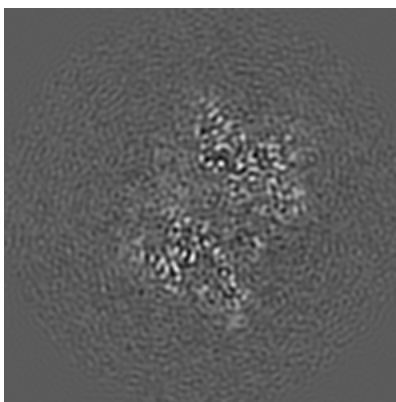
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

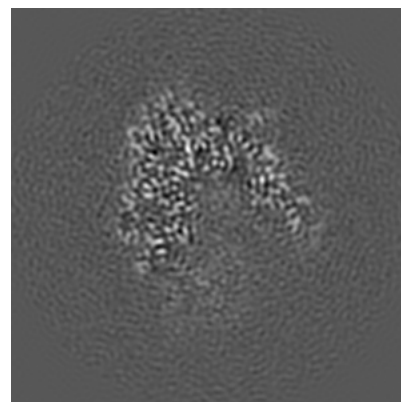
6.2.1 Primary map



X Index: 110



Y Index: 110

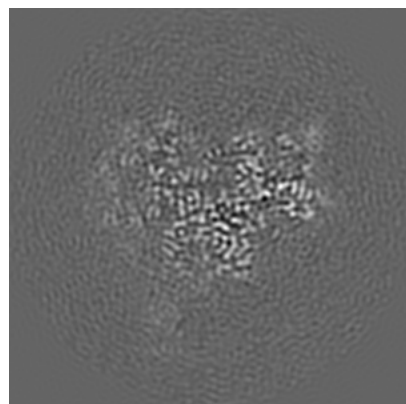


Z Index: 110

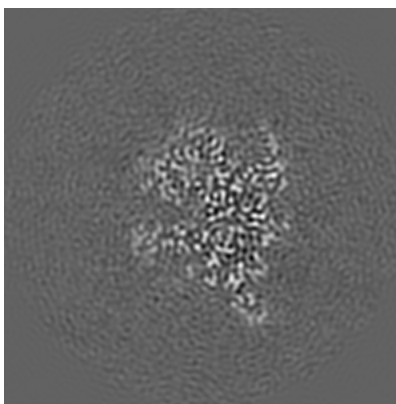
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

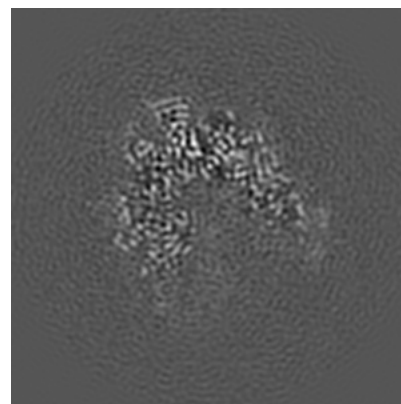
6.3.1 Primary map



X Index: 91



Y Index: 129

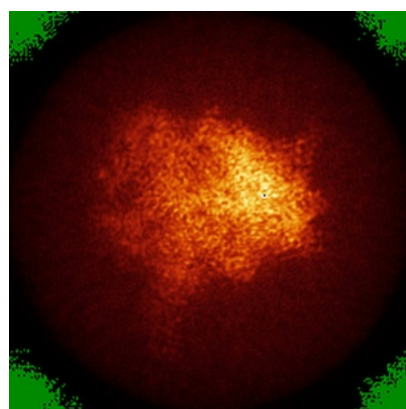


Z Index: 118

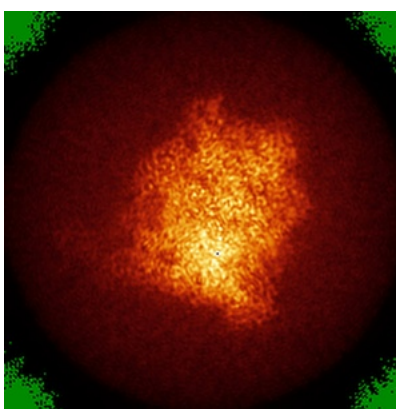
The images above show the largest variance slices of the map in three orthogonal directions.

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

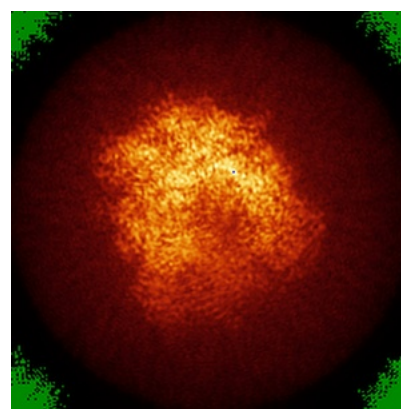
6.4.1 Primary map



X



Y

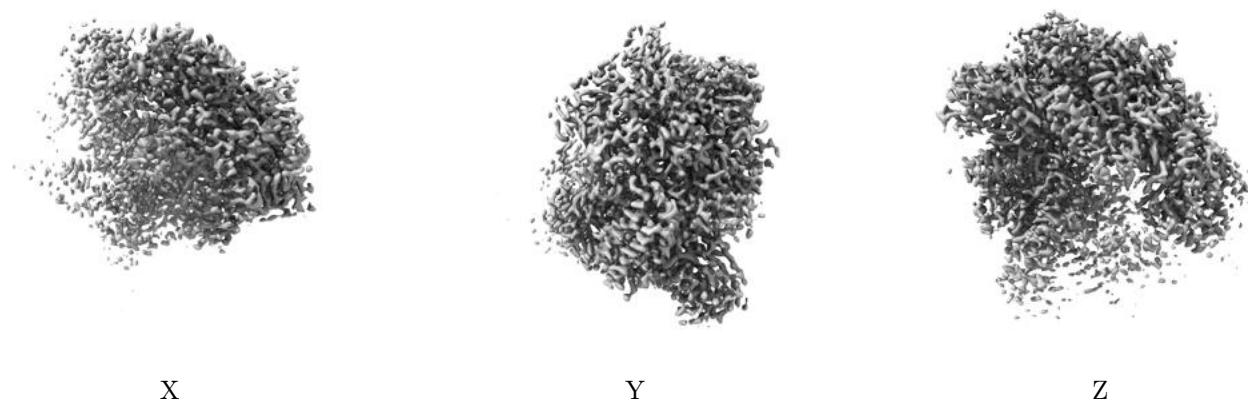


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

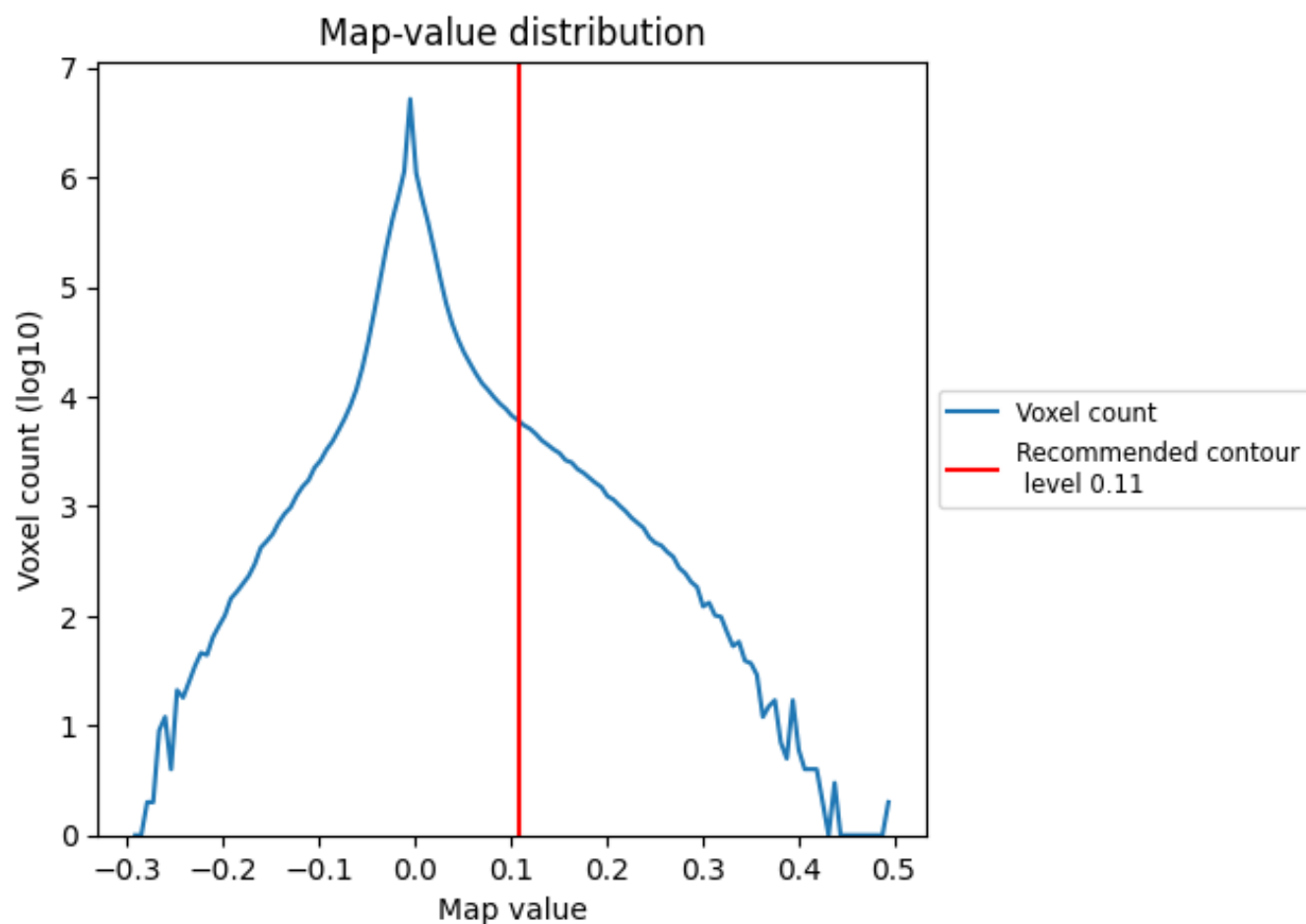
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

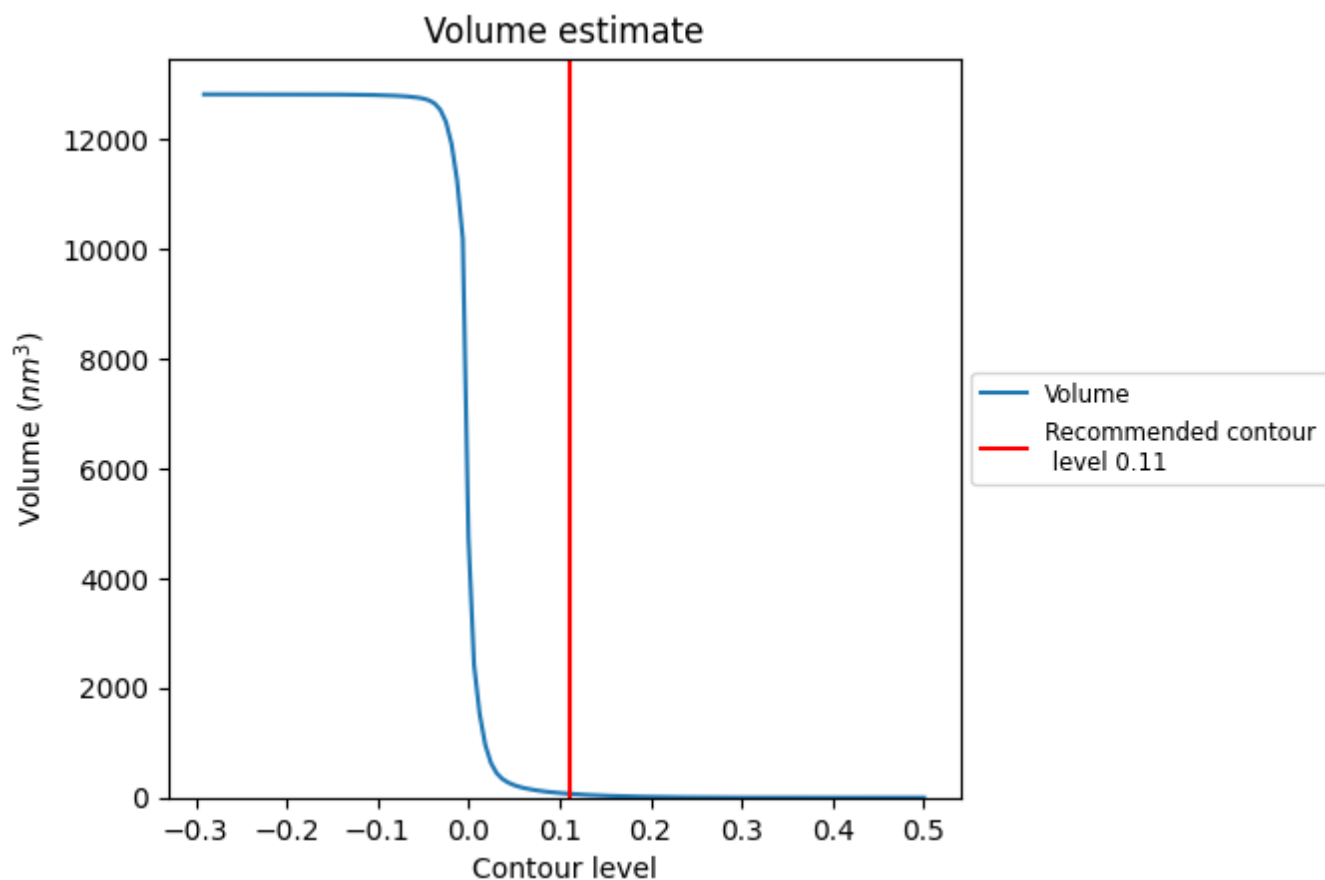
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

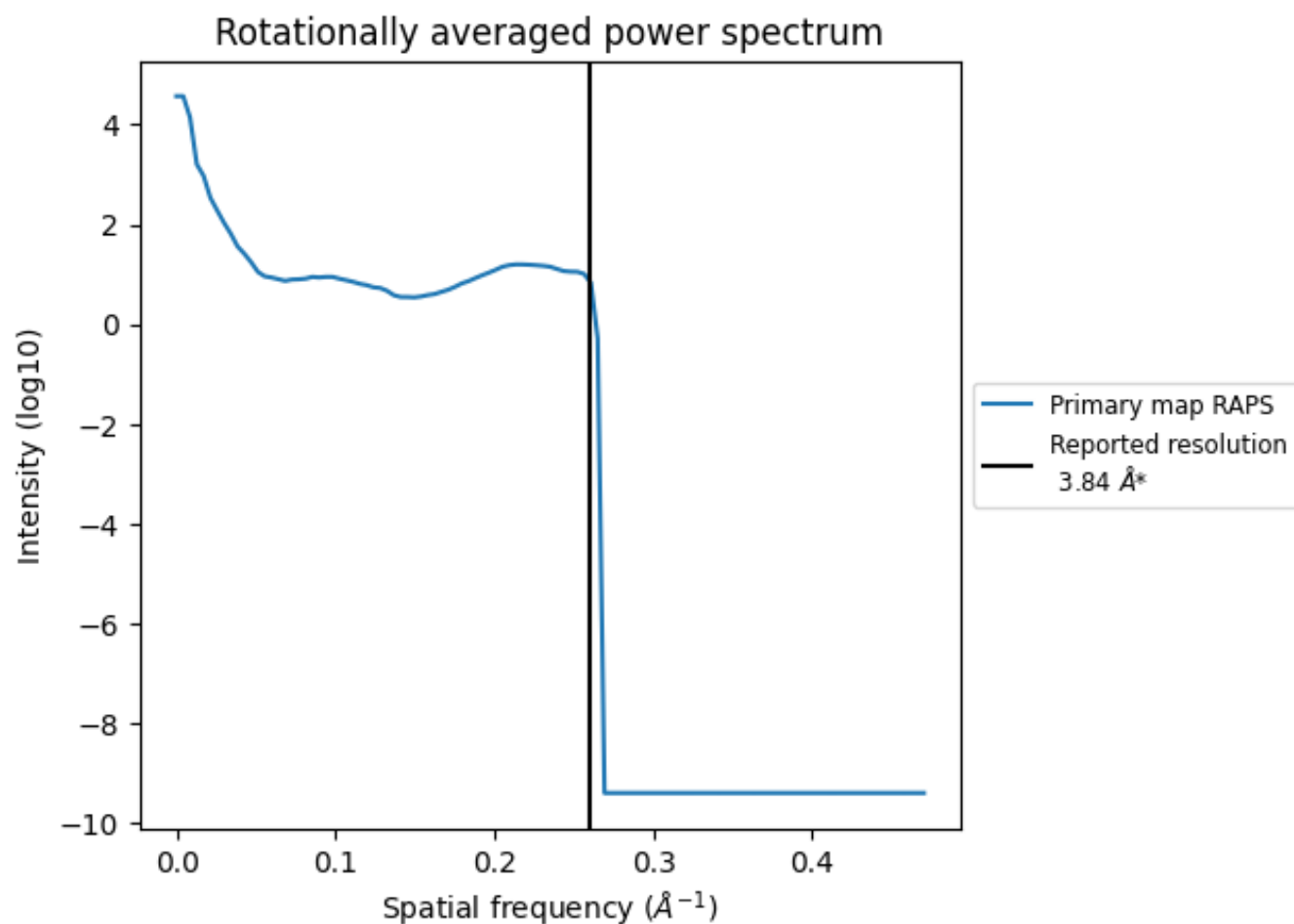
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 69 nm³; this corresponds to an approximate mass of 63 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 0.260 Å⁻¹

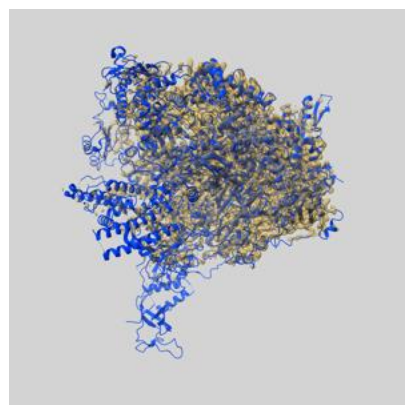
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

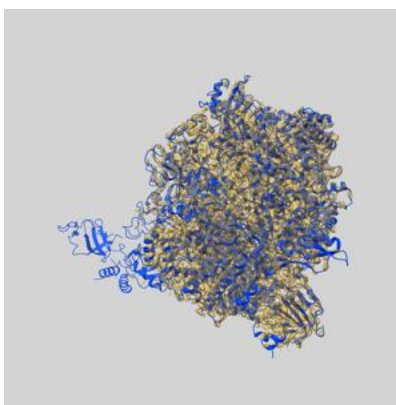
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11840 and PDB model 7AOC. Per-residue inclusion information can be found in section [3](#) on page [7](#).

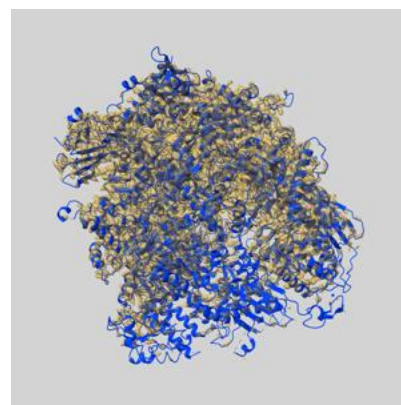
9.1 Map-model overlay [i](#)



X



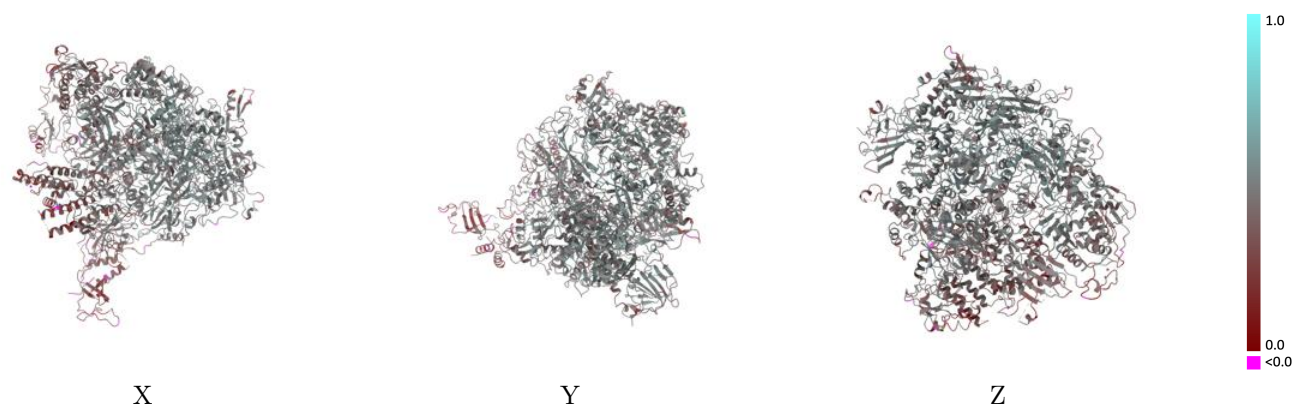
Y



Z

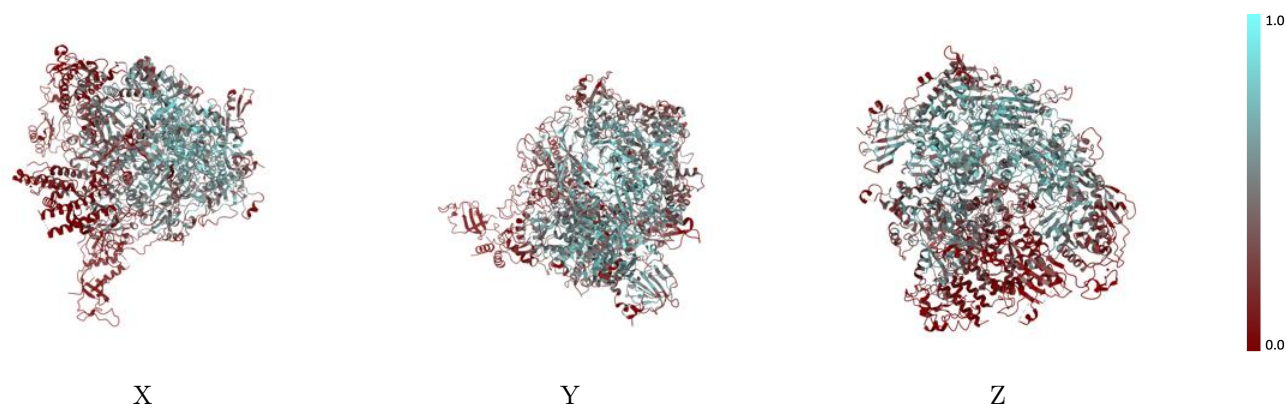
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



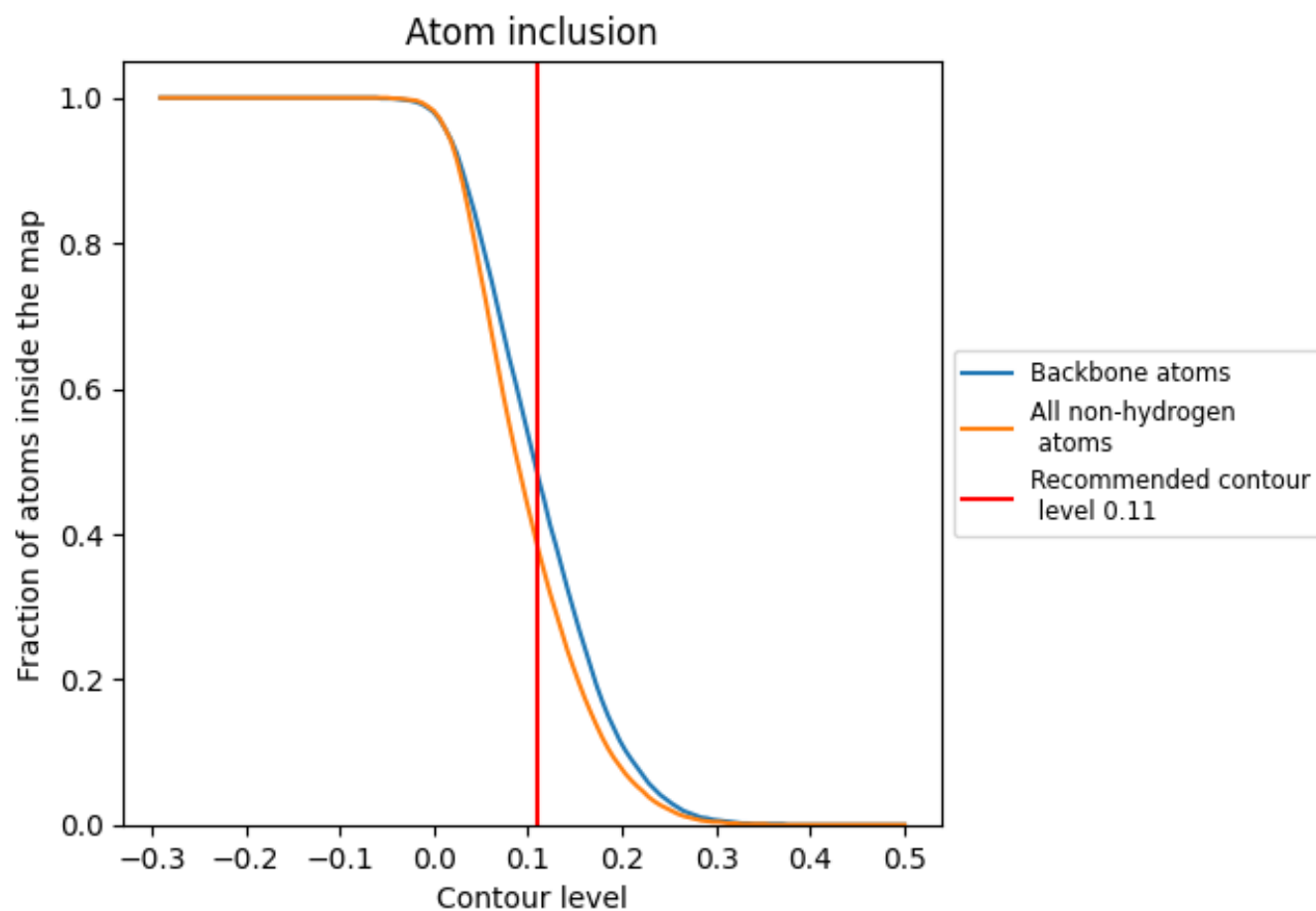
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 38% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3830	0.4490
A	0.3510	0.4410
B	0.4770	0.4760
C	0.4280	0.4710
D	0.0000	0.2440
E	0.2120	0.4140
F	0.4690	0.4850
G	0.0660	0.3150
H	0.4210	0.4760
I	0.0280	0.3530
J	0.5830	0.5020
K	0.5320	0.4940
L	0.4420	0.4940

