



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 07:52 PM UTC

PDB ID : 5M3M / pdb_00005m3m
EMDB ID : EMD-4148
Title : Free monomeric RNA polymerase I at 4.0A resolution
Authors : Neyer, S.; Kunz, M.; Geiss, C.; Hantsche, M.; Hodirnau, V.-V.; Seybert, A.;
Engel, C.; Scheffer, M.P.; Cramer, P.; Frangakis, A.S.
Deposited on : 2016-10-15
Resolution : 4.00 Å(reported)

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

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

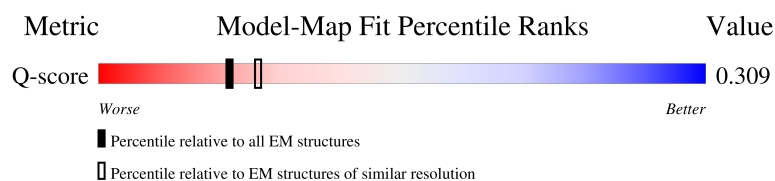
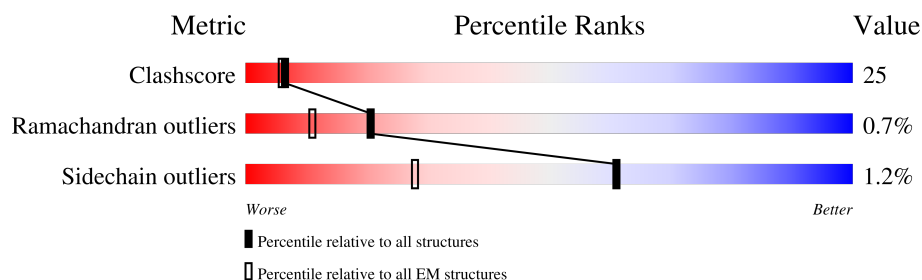
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	7587 (3.50 - 4.50)

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	1664	
2	B	1203	
3	C	335	
4	E	215	

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Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	125	
8	J	70	
9	K	142	
10	L	70	
11	M	415	
12	N	233	
13	D	137	
14	G	326	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	SO4	B	1301	-	-	X	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 33233 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 RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1462	Total	C	N	O	S	0	0
			11558	7304	2006	2187	61		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1166	Total	C	N	O	S	0	0
			9266	5864	1617	1734	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	305	Total	C	N	O	S	0	0
			2423	1539	416	460	8		

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	212	Total	C	N	O	S	0	0
			1735	1102	306	316	11		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	98	Total	C	N	O	S	0	0
			807	512	142	150	3		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	116	Total	C	N	O	S	0	0
			883	550	148	176	9		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 9 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	101	Total	C	N	O	S	0	0
			793	496	130	162	5		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 11 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	97	Total	C	N	O		0	0
			771	490	124	157			

- Molecule 12 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	131	Total	C	N	O	S	0	0
			1035	660	171	200	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	58	Total	C	N	O		0	0
			459	289	78	92			

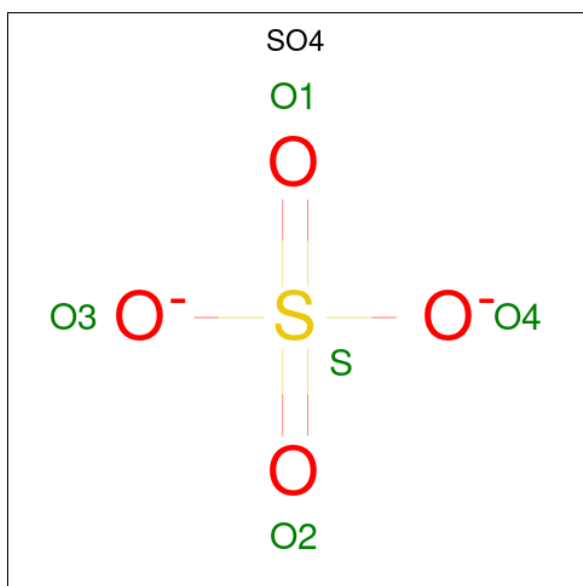
- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	192	Total	C	N	O	S	0	0
			1518	979	261	273	5		

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
15	A	2	Total	Zn	0
			2	2	
15	B	1	Total	Zn	0
			1	1	
15	I	2	Total	Zn	0
			2	2	
15	J	1	Total	Zn	0
			1	1	
15	L	1	Total	Zn	0
			1	1	

- Molecule 16 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

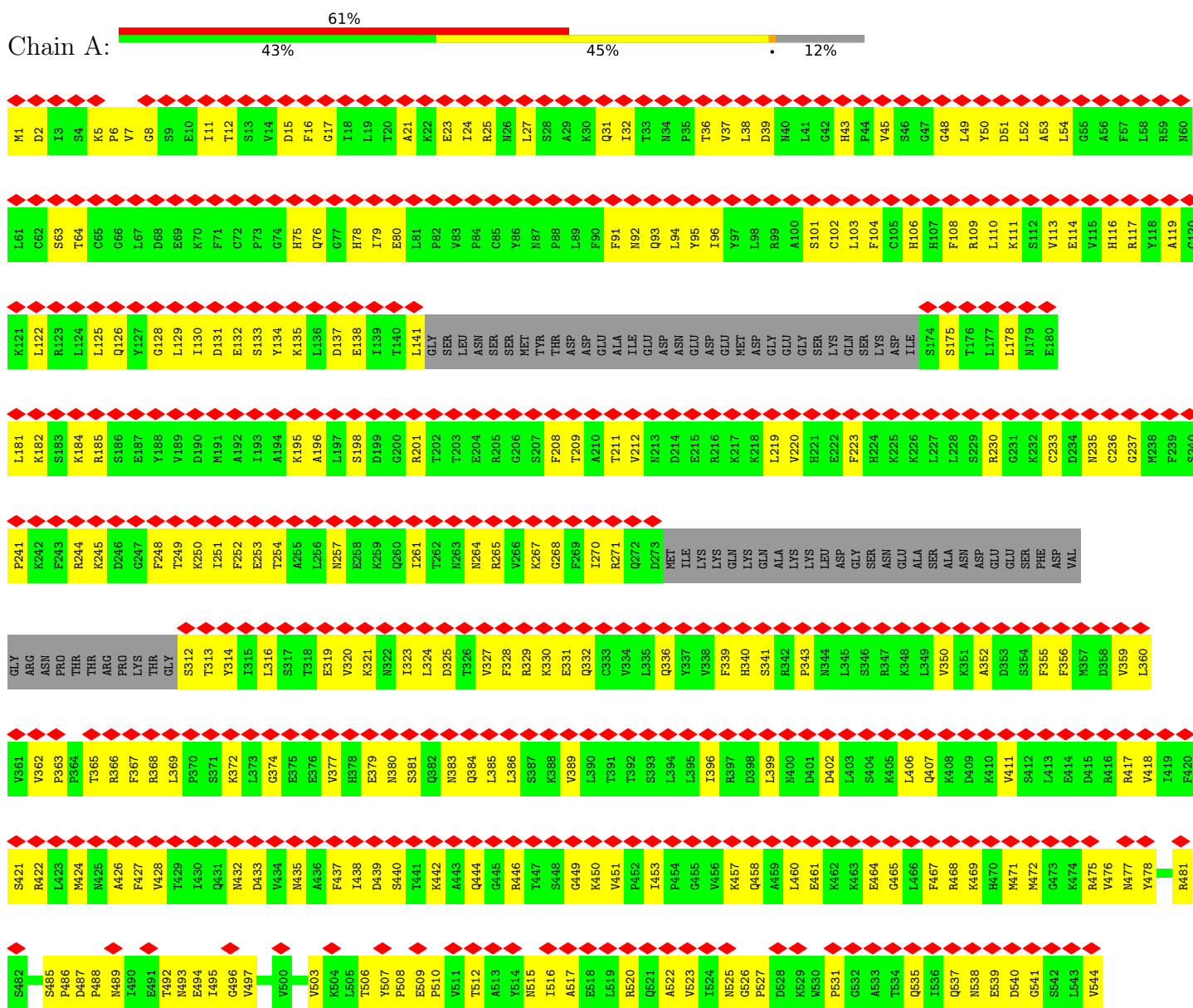


Mol	Chain	Residues	Atoms			AltConf
16	B	1	Total	O	S	0
			5	4	1	

3 Residue-property plots

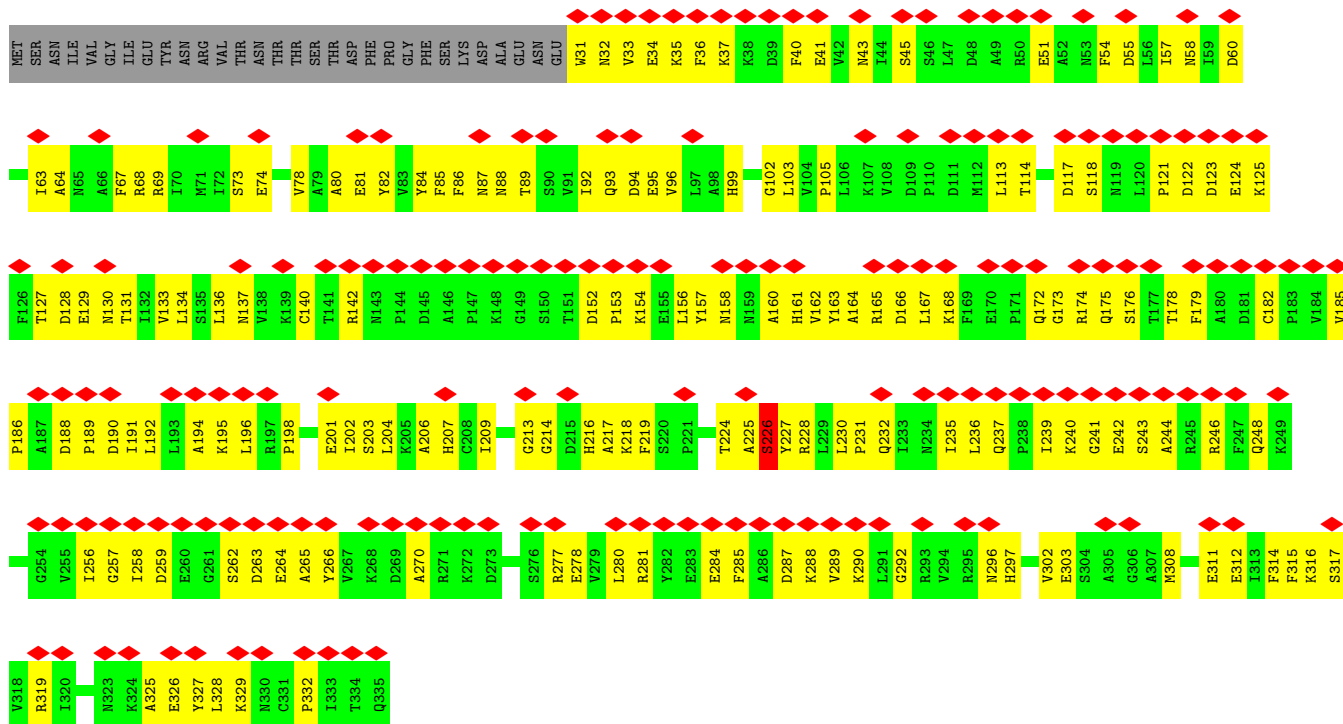
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 RPA190

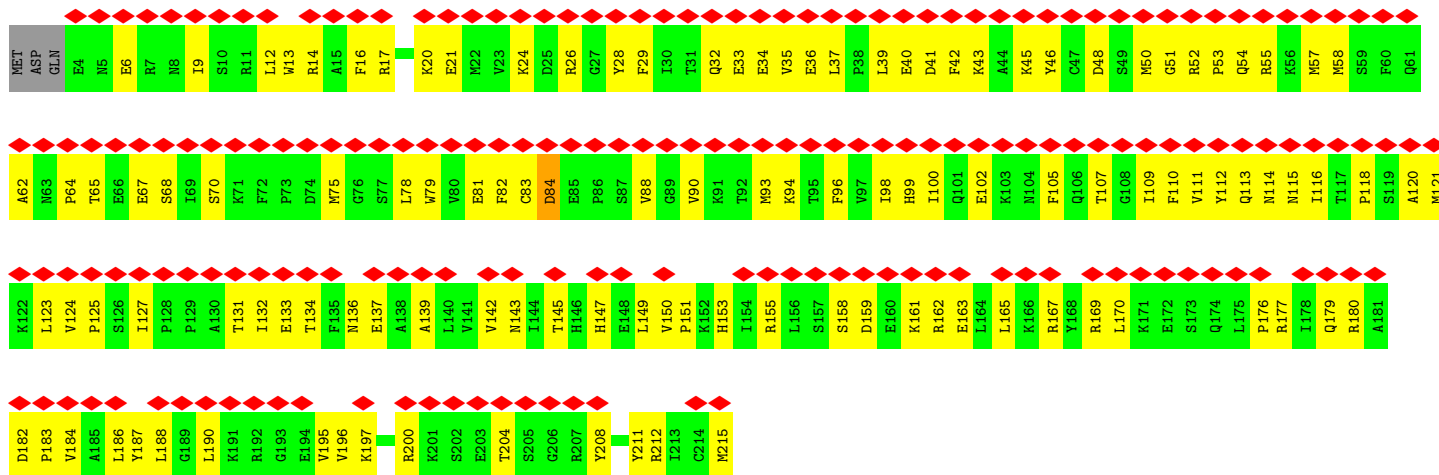
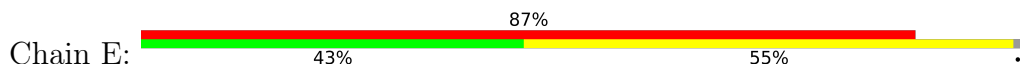


ILE	GLY	E1224	L1154	V1091	L1023	G954	R878	L810	T740	Q671	R606	S545
GLY	ASN	I1225	F1155	E1092	T1024	R955	L879	S811	P741	D672	V607	L546
ALA	ALA	V1226	K1156	S1093	K1025	R956	Q880	V812	P742			I547
VAL	VAL	M1227	S1157	A1094	E1028	M960	T882	R815	D743	S875	M610	G548
PRO	PRO	L1228	S1158	K1096	G1029	V961	L883	T824	M744	A676	E811	M549
ARG	ARG	A1229	D1159	K1097	V1030	S962	R884	R826	P745	T681	K612	S550
LEU	LEU	S1230	G1160	Y1097	H1031	K964	D885	A825	G746	S882	T613	V551
GLN	GLN	A1231	G1161	S1098			R886	F826	I747	D684	L614	E552
THR	THR	A1232	N1162	K1099	Y1034	P965	N887	T827	N748	S885	L616	Q553
ASP	ASP	I1233	E1163	K1100	D1035	L966	K888	C828	L749		H617	R554
VAL	VAL	K1234	K1164	T1101	N1036	P967	K889	G829	I750		Y618	K555
ALA	ALA	K1165	F1166	L1102		S968	G890	M830	S751		A619	K556
ASN	ASN	F1167	R1167	K1103	R1039	P969	T891	D831	K752		N620	A557
SER	SER			Y1104	D1040	Y972		D832	N753		T621	L557
SER	SER			R1105	D1041	E973	A894	L835	K756		G622	A558
ASN	ASN			K1106	D1042	T974		R834	N757		A623	N559
LYS	LYS			K1107	G1043	D975	K899	T836	Q694		Y624	Q560
ARG	ARG			H1108	T1044	A976		A837	Y697		N625	L561
GLU	GLU			H1109	V1045	M977	A902	E838	G998		A626	L562
GLU	GLU			K1110	V1046	A978	I903	G839	K762		D627	T563
ASP	ASP			K1111	F1048	G979	T904	R840	R701		F628	P564
ASN	ASN			P1112	Y981	G980	S905	K941	F702		D629	S565
ASP	ASP			H1113	M1049	Y982	Q906	W842	F703		G630	S566
GLN	GLN			H1114	K983	Y983	Y907	R843	D704		D631	N567
GLN	GLN			K1115	Y1050	G984	Y908	T944	G705		E632	V568
SER	SER			K1116	G1052	R985	S909	D945	H706		M633	S569
HIS	HIS			S1117	D1053	Y987	K910	L847	T707		N634	T570
LYS	LYS			V1118	A1054	S988	P913	K948	T772		M635	H571
THR	THR			K1119	I1055	K991	D914	T949	T708		H636	T572
LYS	LYS			Y1120	D1056	Q993	G915	S850	S710		N574	K575
ALA	ALA			D1121	T1058	E994	T916	V851	K711		N642	K576
VAL	VAL			L1124	K1059	Y995	K918	T853	I712		A643	V577
TYR	TYR			A1125	E1060	Y996	K919	G854	I713		A645	Y578
GLU	GLU			K1126	S1061	M1000	P921	R855	T714		E846	R579
PRO	PRO			Y1127	H1062	G1005	S924	E856	P717		A647	H580
ASP	ASP			N1128	M1063	L1006	L930	A858	I719		L648	I581
ASP	ASP			Y1129	T1064	I1007	G932	A859	F720		M649	K582
GLU	GLU			A1130	F1066	D1008	S936	E860	K721		N650	N583
GLU	GLU			K1131	E1067	T1009	N937	V861	F722		A651	R584
ILE	ILE			Y1132	L1070	D1008	G932	T862	P723		N652	D585
THR	THR			L1133	Y1074	A1010	S938	L864	L725		T653	V586
MET	MET			G1134	K1078	VAL	V938	D865	T726		D654	V587
ARG	ARG			S1135	K1079	THR	S941	K866	T727		S655	L588
ALA	ALA			V1136	Y1080	SER	Q942	D867	G728		Q856	M589
ALA	ALA			S1137	N1081	ARG	N944	T868	K729		Q730	N590
LYS	LYS			E1138	P1082	SER	C945	P869	I731		L658	R591
SER	SER			N1139	S1083		L946	A870	T732		T659	Q592
ASP	ASP			F1140	L1085	G1017	Q849	D871	T733		G663	T594
				Q1141	L1019	Y1018	Q950	D872	V735		L595	L596
				D1142	L1085	L1019	R953	P873	L736		P865	H596
				S1146	L1086	Y1086		E874	N738		V666	K597
				F1147	E1087	E1087		L876	V739		G667	A598
				L1148	H1088	H1088		K877			G668	S599
				D1149	L1089	L1089					L669	M600
				K1150	L1090	D1021					L670	M501
				S1152		C1022						K604
				K1153								V605

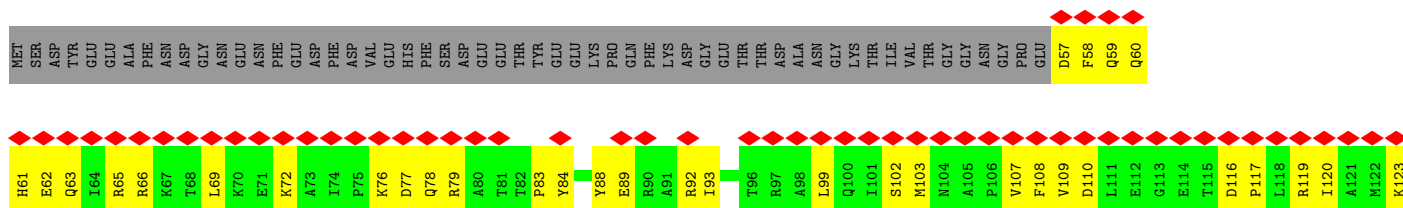


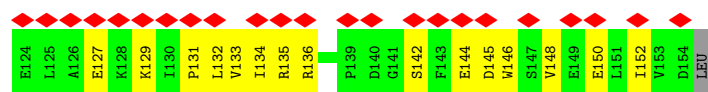


- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

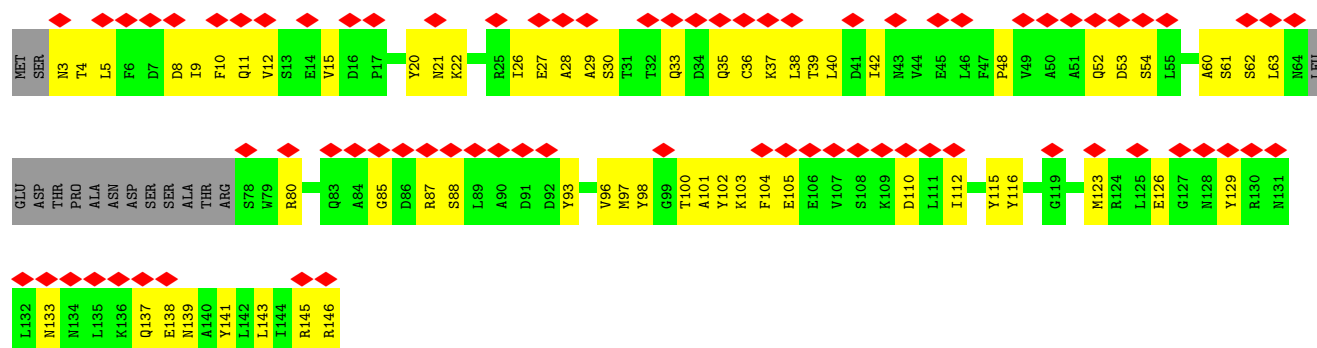


- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

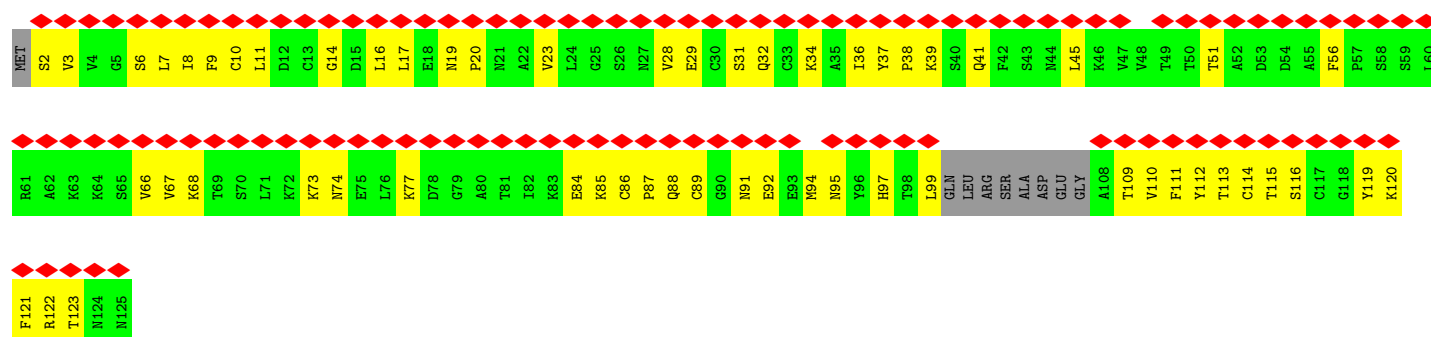




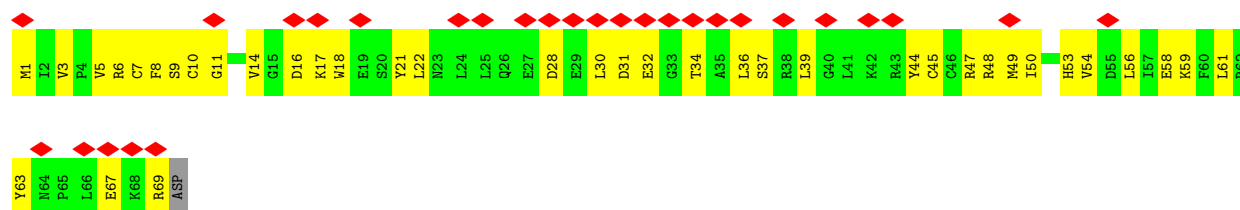
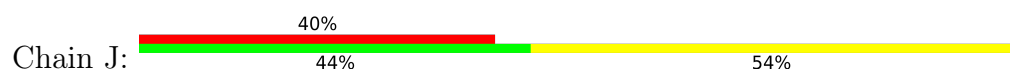
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 7: DNA-directed RNA polymerase I subunit RPA12

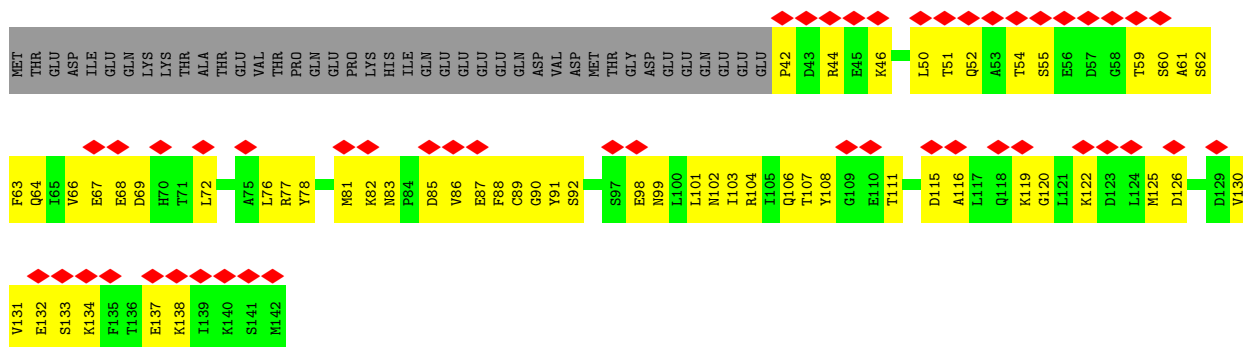


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



• Molecule 9: DNA-directed RNA polymerases I and III subunit RPAC2

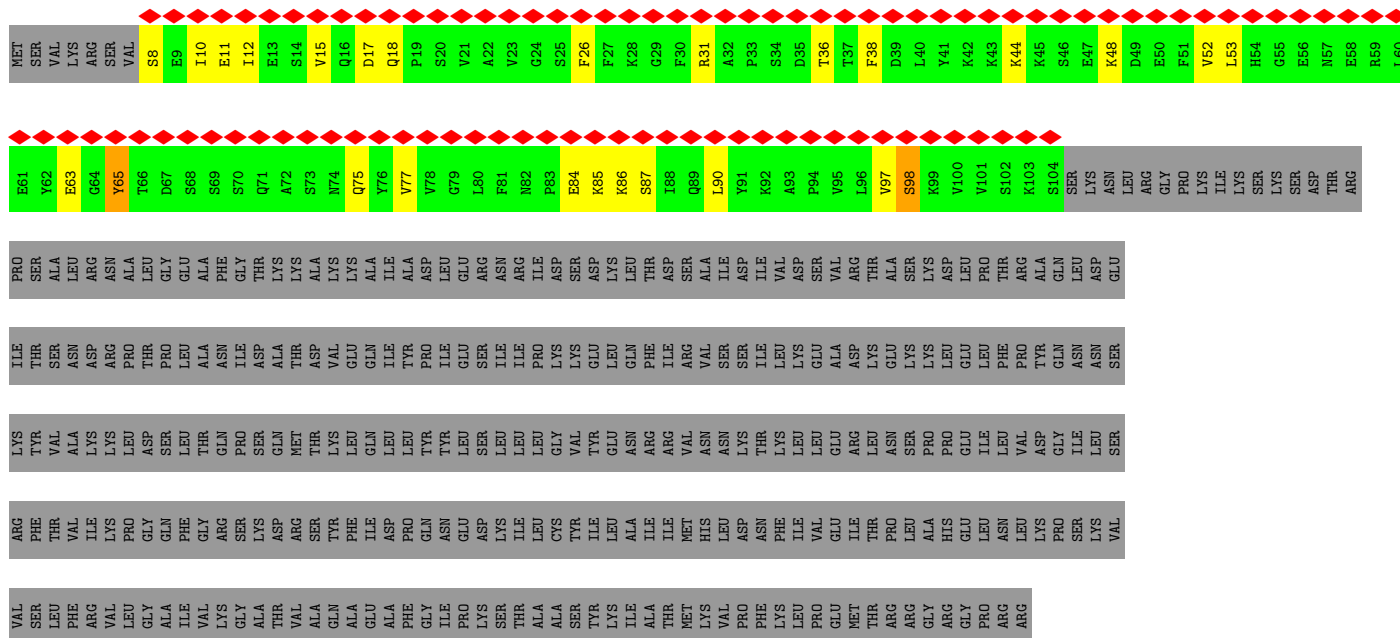




- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 11: DNA-directed RNA polymerase I subunit RPA49



- Molecule 12: DNA-directed RNA polymerase I subunit RPA34



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	94000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.094	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	241.49998, 241.49998, 241.49998	wwPDB
Map dimensions	230, 230, 230	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.36	0/11770	0.58	3/15895 (0.0%)
2	B	0.42	0/9471	0.59	0/12805
3	C	0.41	0/2475	0.57	0/3354
4	E	0.36	0/1771	0.59	2/2383 (0.1%)
5	F	0.31	0/821	0.53	0/1106
6	H	0.38	0/1070	0.56	0/1449
7	I	0.28	0/895	0.50	0/1205
8	J	0.44	0/578	0.60	0/775
9	K	0.44	0/804	0.60	0/1083
10	L	0.37	0/354	0.58	0/468
11	M	0.48	0/786	0.87	0/1057
12	N	0.46	0/1052	0.88	1/1418 (0.1%)
13	D	0.51	0/465	0.81	0/630
14	G	0.50	0/1555	0.84	3/2113 (0.1%)
All	All	0.40	0/33867	0.62	9/45741 (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	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1648	ASN	N-CA-C	7.34	122.65	112.45
1	A	1648	ASN	CA-C-N	6.91	134.13	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1648	ASN	C-N-CA	6.91	134.13	121.70
14	G	241	ARG	CD-NE-CZ	5.51	132.12	124.40
12	N	127	ASP	N-CA-C	-5.37	106.21	114.16
14	G	219	ASP	N-CA-C	5.28	116.80	109.31
14	G	241	ARG	NE-CZ-NH2	-5.24	114.49	119.20
4	E	84	ASP	CA-C-N	5.17	128.51	120.60
4	E	84	ASP	C-N-CA	5.17	128.51	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1649	VAL	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	11558	0	11642	688	0
2	B	9266	0	9151	568	0
3	C	2423	0	2412	160	0
4	E	1735	0	1764	103	0
5	F	807	0	827	45	0
6	H	1052	0	1021	48	0
7	I	883	0	879	61	0
8	J	569	0	585	37	0
9	K	793	0	790	62	0
10	L	352	0	374	20	0
11	M	771	0	755	11	0
12	N	1035	0	1069	28	0
13	D	459	0	462	8	0
14	G	1518	0	1528	34	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	B	5	0	0	8	0
All	All	33233	0	33259	1673	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 25.

All (1673) 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)
2:B:656:LEU:O	12:N:153:VAL:HG11	1.62	0.97
3:C:225:ALA:O	3:C:226:SER:HB2	1.63	0.95
1:A:1501:ILE:HG22	1:A:1502:PRO:HD2	1.49	0.94
2:B:894:LYS:HG2	10:L:54:ARG:HH21	1.33	0.94
5:F:66:ARG:HA	5:F:69:LEU:HD12	1.50	0.93
1:A:15:ASP:HB2	2:B:1197:ARG:HB3	1.52	0.92
2:B:121:VAL:O	2:B:133:TYR:HE1	1.52	0.90
2:B:711:GLN:HG2	2:B:713:PRO:HD2	1.51	0.90
2:B:844:GLY:HA2	2:B:860:ALA:HB3	1.54	0.89
7:I:94:MET:HG2	7:I:114:CYS:HA	1.53	0.89
3:C:165:ARG:HB3	3:C:189:PRO:HB3	1.54	0.89
2:B:656:LEU:H	2:B:657:PRO:HD2	1.38	0.89
1:A:1258:ILE:O	1:A:1501:ILE:HG13	1.73	0.88
2:B:211:ARG:HH12	2:B:647:SER:HB2	1.37	0.88
2:B:894:LYS:CG	10:L:54:ARG:HH21	1.87	0.88
2:B:107:PRO:O	2:B:171:HIS:NE2	2.08	0.87
1:A:907:VAL:HG12	1:A:945:CYS:SG	2.15	0.86
2:B:657:PRO:O	2:B:659:ASP:N	2.09	0.86
2:B:894:LYS:HG2	10:L:54:ARG:NH2	1.89	0.86
1:A:846:ILE:HD13	1:A:906:GLN:HB3	1.54	0.86
2:B:1006:ASN:ND2	2:B:1010:ASN:O	2.08	0.85
1:A:109:ARG:NH1	1:A:230:ARG:O	2.09	0.85
1:A:908:VAL:HA	1:A:945:CYS:SG	2.16	0.84
1:A:842:TRP:CE2	1:A:910:LYS:NZ	2.45	0.84
2:B:745:GLN:HG2	2:B:800:TYR:HD2	1.43	0.84
1:A:666:VAL:HG23	1:A:667:ARG:HG3	1.59	0.83
5:F:103:MET:SD	14:G:112:PRO:CG	2.66	0.83
1:A:1504:ILE:CD1	1:A:1529:MET:HE3	2.08	0.83
1:A:1655:ASP:HB2	5:F:135:ARG:HB3	1.60	0.83
1:A:1006:LEU:CD1	2:B:716:MET:HE1	2.09	0.83
1:A:526:GLY:HA3	1:A:554:ARG:HH11	1.42	0.83
2:B:655:TYR:HE1	2:B:688:HIS:HE2	1.26	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:GLU:HG2	2:B:98:SER:HB3	1.61	0.83
1:A:862:THR:O	1:A:878:ARG:NH1	2.11	0.82
6:H:116:TYR:HB2	6:H:123:MET:HB3	1.60	0.82
1:A:1006:LEU:CD1	2:B:716:MET:SD	2.67	0.82
3:C:68:ARG:HD2	3:C:227:TYR:CD2	2.15	0.82
4:E:110:PHE:HB3	4:E:134:THR:HG22	1.61	0.82
1:A:440:SER:H	1:A:458:GLN:HE22	1.27	0.81
2:B:504:HIS:HB3	2:B:542:LEU:HD23	1.62	0.81
1:A:1263:LEU:HA	1:A:1498:ILE:HD11	1.60	0.81
1:A:943:ILE:HD11	2:B:958:MET:HB3	1.63	0.81
3:C:88:ASN:ND2	3:C:94:ASP:OD1	2.13	0.81
1:A:568:VAL:O	1:A:571:HIS:ND1	2.12	0.81
2:B:94:LYS:HB3	2:B:146:ASN:HA	1.63	0.81
2:B:209:GLN:NE2	2:B:215:MET:SD	2.53	0.81
10:L:48:CYS:HB3	10:L:52:GLY:H	1.44	0.81
2:B:501:ARG:NH2	2:B:546:ALA:O	2.13	0.81
1:A:594:THR:HG23	1:A:599:SER:HB2	1.63	0.81
5:F:62:GLU:OE2	14:G:90:LEU:CD1	2.28	0.81
1:A:943:ILE:HG23	1:A:986:PHE:HB2	1.63	0.80
1:A:1501:ILE:HB	1:A:1504:ILE:HB	1.61	0.80
1:A:719:ILE:HG12	6:H:97:MET:HG2	1.61	0.80
1:A:1262:LEU:HD22	1:A:1496:SER:O	1.81	0.80
1:A:101:SER:HA	1:A:108:PHE:HA	1.64	0.80
3:C:165:ARG:NH1	3:C:190:ASP:OD1	2.15	0.79
1:A:964:LYS:NZ	2:B:672:MET:O	2.15	0.79
1:A:936:SER:OG	1:A:938:VAL:HG23	1.81	0.79
1:A:945:CYS:O	1:A:946:LEU:CB	2.30	0.79
2:B:785:ASP:OD2	2:B:957:ARG:NH2	2.15	0.78
3:C:127:THR:H	3:C:130:ASN:HB2	1.47	0.78
2:B:201:LYS:HE2	2:B:487:VAL:HG22	1.66	0.78
1:A:546:LEU:HD22	1:A:554:ARG:HG2	1.64	0.78
1:A:1608:SER:O	1:A:1612:LYS:NZ	2.17	0.78
2:B:823:GLN:HG2	2:B:863:ASP:HA	1.65	0.77
14:G:22:LYS:HD3	14:G:128:GLN:HG2	1.65	0.77
7:I:99:LEU:HB2	7:I:109:THR:HB	1.64	0.77
9:K:88:PHE:HB3	9:K:106:GLN:HB2	1.66	0.77
5:F:103:MET:SD	14:G:112:PRO:HG2	2.25	0.77
1:A:1049:MET:HE1	1:A:1124:LEU:HB3	1.67	0.77
2:B:534:PRO:HG3	2:B:542:LEU:HB2	1.66	0.77
2:B:1103:VAL:HG12	2:B:1110:ILE:HG22	1.66	0.77
1:A:1302:TYR:HA	1:A:1305:GLU:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1006:LEU:HD13	2:B:716:MET:SD	2.24	0.76
2:B:13:THR:HG21	12:N:163:VAL:HG21	1.66	0.76
2:B:807:GLU:OE1	2:B:905:TYR:OH	2.01	0.76
3:C:258:ILE:HA	3:C:265:ALA:HA	1.66	0.76
2:B:612:LYS:NZ	2:B:624:LEU:O	2.18	0.76
2:B:1157:GLN:HB3	2:B:1168:VAL:HG13	1.66	0.76
8:J:9:SER:HB2	8:J:45:CYS:SG	2.26	0.76
1:A:1317:ILE:HA	1:A:1321:PHE:HB3	1.66	0.76
2:B:211:ARG:NH1	2:B:646:HIS:O	2.19	0.76
2:B:145:VAL:HB	2:B:150:GLU:HB3	1.66	0.76
2:B:168:ASN:HA	2:B:173:ASN:HD22	1.48	0.76
5:F:107:VAL:HG12	5:F:109:VAL:H	1.48	0.75
2:B:144:SER:HA	2:B:151:ASN:HA	1.68	0.75
3:C:284:GLU:O	3:C:288:LYS:NZ	2.19	0.75
1:A:1050:TYR:HB3	1:A:1054:ALA:HA	1.66	0.75
2:B:649:MET:HE3	2:B:666:PRO:HG2	1.69	0.75
1:A:620:ASN:OD1	1:A:667:ARG:NH2	2.19	0.75
1:A:363:PRO:O	1:A:368:ARG:NE	2.19	0.74
1:A:824:THR:HB	2:B:1023:ARG:HB2	1.69	0.74
2:B:657:PRO:C	2:B:659:ASP:H	1.94	0.74
1:A:339:PHE:O	1:A:1629:ASN:ND2	2.20	0.74
1:A:690:GLU:HB3	9:K:77:ARG:HH22	1.50	0.74
2:B:658:LEU:O	2:B:659:ASP:C	2.31	0.74
2:B:1104:CYS:HA	2:B:1173:THR:HG22	1.69	0.74
2:B:655:TYR:HE1	2:B:688:HIS:NE2	1.85	0.74
2:B:745:GLN:NE2	8:J:1:MET:SD	2.60	0.74
3:C:68:ARG:HD2	3:C:227:TYR:HD2	1.53	0.74
1:A:1319:ASN:O	1:A:1323:HIS:ND1	2.13	0.73
1:A:636:HIS:CG	2:B:1091:ARG:HH22	2.05	0.73
2:B:122:TYR:CZ	2:B:183:HIS:CD2	2.76	0.73
2:B:1090:ASP:HA	2:B:1094:ASN:HB2	1.69	0.73
1:A:1504:ILE:HD11	1:A:1529:MET:HE3	1.69	0.73
2:B:655:TYR:CE1	2:B:688:HIS:NE2	2.55	0.73
1:A:689:ARG:NH2	9:K:87:GLU:O	2.20	0.73
1:A:1006:LEU:CD1	2:B:716:MET:CE	2.66	0.73
1:A:1242:ILE:HG22	1:A:1536:ILE:HG22	1.69	0.73
2:B:58:GLY:O	2:B:62:ASN:ND2	2.21	0.73
2:B:20:GLU:HG2	2:B:24:ARG:HH12	1.53	0.73
9:K:87:GLU:H	9:K:107:THR:HA	1.54	0.73
3:C:172:GLN:H	3:C:175:GLN:HB2	1.53	0.73
1:A:945:CYS:O	1:A:946:LEU:CG	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:ASP:OD1	2:B:93:ASN:N	2.20	0.72
4:E:26:ARG:NH2	4:E:186:LEU:O	2.22	0.72
6:H:29:ALA:HA	6:H:37:LYS:HA	1.71	0.72
5:F:62:GLU:OE2	14:G:90:LEU:HD11	1.90	0.72
12:N:148:ILE:O	12:N:150:TYR:CD1	2.42	0.72
3:C:153:PRO:HA	3:C:156:LEU:HB2	1.72	0.72
1:A:1246:VAL:O	1:A:1517:ARG:NH2	2.23	0.72
2:B:795:GLU:OE1	3:C:217:ALA:N	2.19	0.72
1:A:487:ASP:OD1	1:A:489:ASN:ND2	2.23	0.72
3:C:43:ASN:HB2	3:C:55:ASP:HB2	1.72	0.72
2:B:1025:ASP:OD2	3:C:277:ARG:NH1	2.22	0.71
2:B:13:THR:HG21	12:N:163:VAL:CG2	2.20	0.71
7:I:97:HIS:HB2	7:I:111:PHE:HD2	1.55	0.71
2:B:239:VAL:HA	2:B:245:SER:HA	1.72	0.71
1:A:1274:GLU:OE2	1:A:1288:ARG:NH1	2.24	0.71
2:B:815:ARG:NH2	2:B:819:ASP:O	2.22	0.71
1:A:1006:LEU:HD12	2:B:716:MET:HE1	1.73	0.71
2:B:1127:CYS:SG	2:B:1171:ASN:ND2	2.64	0.71
1:A:842:TRP:CZ2	1:A:910:LYS:NZ	2.58	0.71
7:I:23:VAL:HG21	7:I:28:VAL:HG22	1.73	0.71
6:H:63:LEU:HB3	6:H:88:SER:HB2	1.71	0.71
11:M:38:PHE:HB3	11:M:53:LEU:HD11	1.73	0.71
2:B:122:TYR:CE2	2:B:183:HIS:HD2	2.09	0.70
2:B:186:GLU:HB3	2:B:189:GLU:HB2	1.73	0.70
6:H:102:TYR:CZ	6:H:115:TYR:HB3	2.25	0.70
1:A:757:ASN:OD1	1:A:767:ASN:N	2.20	0.70
7:I:97:HIS:HB2	7:I:111:PHE:CD2	2.27	0.70
1:A:103:LEU:HD12	1:A:241:PRO:HD2	1.72	0.70
2:B:874:TYR:CZ	2:B:876:SER:HB3	2.26	0.70
1:A:675:SER:OG	2:B:952:HIS:NE2	2.24	0.70
2:B:122:TYR:CE2	2:B:183:HIS:CD2	2.80	0.70
1:A:908:VAL:HG22	1:A:945:CYS:HB2	1.74	0.70
2:B:915:ASP:H	2:B:927:CYS:HB3	1.57	0.70
1:A:497:VAL:HB	1:A:607:VAL:HA	1.74	0.69
1:A:782:ASP:OD1	1:A:783:LYS:N	2.24	0.69
2:B:883:GLU:OE1	2:B:906:ARG:NH1	2.24	0.69
13:D:99:LEU:HB3	13:D:100:PRO:CD	2.22	0.69
6:H:3:ASN:N	6:H:61:SER:HG	1.90	0.69
2:B:645:GLY:O	2:B:648:ARG:NE	2.22	0.69
2:B:280:LEU:O	2:B:323:ARG:NH2	2.20	0.69
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:945:CYS:O	1:A:946:LEU:HB3	1.91	0.69
1:A:1504:ILE:HD13	1:A:1529:MET:HE3	1.75	0.69
2:B:161:LEU:HD12	2:B:162:PRO:HD2	1.74	0.69
2:B:884:GLU:H	2:B:904:LYS:HB3	1.58	0.69
1:A:130:ILE:O	1:A:133:SER:OG	2.09	0.69
1:A:1105:ARG:HH12	1:A:1138:GLU:HB3	1.56	0.69
1:A:1251:ALA:O	1:A:1255:CYS:N	2.22	0.69
2:B:122:TYR:CZ	2:B:183:HIS:HD2	2.11	0.69
1:A:956:ARG:HH21	1:A:979:GLY:HA3	1.58	0.69
2:B:504:HIS:CD2	2:B:506:GLY:H	2.11	0.69
2:B:699:ILE:N	16:B:1301:SO4:O3	2.26	0.69
2:B:609:ARG:HH21	2:B:626:ILE:HB	1.58	0.68
2:B:714:ARG:HE	2:B:957:ARG:HB3	1.58	0.68
2:B:1015:SER:HB2	2:B:1022:LEU:HD21	1.73	0.68
1:A:1573:TYR:HB3	7:I:122:ARG:HH12	1.57	0.68
2:B:700:LEU:N	16:B:1301:SO4:O4	2.27	0.68
2:B:234:ILE:HG12	2:B:381:LEU:HD13	1.76	0.68
2:B:143:TRP:O	2:B:152:LEU:N	2.25	0.68
2:B:457:ILE:HG22	2:B:461:MET:HG2	1.75	0.68
2:B:921:HIS:NE2	2:B:965:GLU:OE1	2.26	0.68
7:I:97:HIS:H	7:I:111:PHE:HB2	1.58	0.68
2:B:505:ARG:HB3	2:B:509:PHE:HD2	1.58	0.68
2:B:658:LEU:HD13	2:B:658:LEU:N	2.07	0.68
3:C:160:ALA:O	3:C:196:LEU:N	2.27	0.68
9:K:86:VAL:HA	9:K:107:THR:HG22	1.75	0.68
5:F:79:ARG:NH1	5:F:145:ASP:O	2.27	0.68
1:A:1006:LEU:HD11	2:B:716:MET:SD	2.31	0.68
1:A:1263:LEU:HB3	1:A:1496:SER:HB2	1.74	0.68
2:B:894:LYS:CG	10:L:54:ARG:NH2	2.53	0.68
2:B:1201:GLU:HG2	2:B:1203:LYS:HG2	1.76	0.68
5:F:65:ARG:O	5:F:69:LEU:HG	1.94	0.68
1:A:1501:ILE:CG2	1:A:1502:PRO:HD2	2.24	0.68
1:A:1573:TYR:O	7:I:122:ARG:NH1	2.27	0.68
7:I:3:VAL:HG22	7:I:8:ILE:HG12	1.75	0.68
1:A:6:PRO:O	13:D:15:THR:OG1	2.07	0.68
1:A:1275:THR:OG1	1:A:1289:SER:OG	2.12	0.68
1:A:1040:ASP:OD1	1:A:1041:ALA:N	2.26	0.67
6:H:8:ASP:OD1	6:H:9:ILE:N	2.26	0.67
1:A:1573:TYR:HA	7:I:122:ARG:HH22	1.60	0.67
3:C:314:PHE:O	3:C:317:SER:OG	2.09	0.67
1:A:486:PRO:O	1:A:615:ARG:NH2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:752:VAL:HG22	2:B:979:GLN:HB2	1.75	0.67
4:E:37:LEU:HD11	4:E:41:ASP:HB2	1.76	0.67
1:A:475:ARG:HA	2:B:1070:ARG:HA	1.77	0.67
1:A:830:MET:SD	2:B:963:PHE:HB3	2.33	0.67
3:C:230:LEU:HD12	3:C:231:PRO:HD2	1.77	0.67
4:E:55:ARG:HB3	4:E:82:PHE:HB2	1.77	0.67
1:A:874:GLU:OE2	1:A:878:ARG:NE	2.24	0.67
1:A:366:ARG:HA	1:A:369:LEU:HG	1.76	0.67
1:A:509:GLU:N	1:A:577:VAL:O	2.28	0.67
1:A:1288:ARG:NE	1:A:1480:THR:O	2.27	0.67
3:C:88:ASN:O	10:L:60:ARG:NH1	2.28	0.67
3:C:240:LYS:HB3	3:C:264:GLU:HG2	1.77	0.67
4:E:26:ARG:HH21	4:E:187:TYR:C	2.03	0.67
1:A:209:THR:H	1:A:212:VAL:HB	1.58	0.67
1:A:1262:LEU:CD2	1:A:1496:SER:O	2.43	0.67
1:A:1447:GLN:HE21	1:A:1459:LYS:HA	1.60	0.67
2:B:564:ILE:O	2:B:567:SER:OG	2.12	0.67
1:A:79:ILE:N	1:A:360:LEU:O	2.29	0.66
1:A:54:LEU:HD22	1:A:76:GLN:HA	1.76	0.66
1:A:1490:GLU:HA	7:I:56:PHE:HZ	1.59	0.66
2:B:760:TYR:HB3	2:B:762:MET:HE3	1.77	0.66
3:C:73:SER:O	3:C:214:GLY:N	2.27	0.66
7:I:20:PRO:HB3	7:I:39:LYS:HG3	1.78	0.66
1:A:537:GLN:HE21	1:A:541:GLY:HA2	1.59	0.66
1:A:584:ARG:HD2	5:F:116:ASP:HB2	1.76	0.66
2:B:862:PHE:HA	2:B:869:THR:HA	1.77	0.66
1:A:588:LEU:HB3	1:A:636:HIS:HB2	1.76	0.66
1:A:1053:ASP:OD2	1:A:1580:ARG:NH2	2.21	0.66
1:A:826:PHE:CE1	1:A:924:SER:OG	2.45	0.66
1:A:862:THR:HA	7:I:67:VAL:HG12	1.78	0.66
5:F:99:LEU:O	5:F:102:SER:OG	2.14	0.66
1:A:131:ASP:HA	1:A:134:TYR:HD2	1.60	0.66
1:A:747:ILE:HG22	1:A:774:GLY:HA2	1.78	0.66
1:A:826:PHE:CZ	1:A:924:SER:HB3	2.30	0.66
3:C:329:LYS:HE3	9:K:122:LYS:HB2	1.77	0.66
1:A:321:LYS:HB2	1:A:356:PHE:HE2	1.60	0.66
1:A:16:PHE:HB3	1:A:1626:VAL:HG22	1.77	0.65
2:B:264:TRP:CD1	2:B:265:ARG:HG2	2.30	0.65
2:B:379:ARG:HE	2:B:580:GLY:HA2	1.60	0.65
1:A:17:GLY:O	2:B:1195:ARG:N	2.24	0.65
1:A:690:GLU:HG3	9:K:81:MET:HE2	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1315:ASN:OD1	1:A:1319:ASN:ND2	2.28	0.65
1:A:1059:LYS:NZ	1:A:1176:ARG:O	2.26	0.65
1:A:1105:ARG:NH1	1:A:1138:GLU:OE1	2.29	0.65
2:B:121:VAL:O	2:B:133:TYR:CE1	2.43	0.65
1:A:1138:GLU:O	1:A:1142:ASP:N	2.25	0.65
2:B:94:LYS:N	2:B:146:ASN:OD1	2.24	0.65
2:B:335:ARG:NH2	2:B:344:GLN:O	2.28	0.65
2:B:449:VAL:HA	2:B:452:ARG:HH21	1.60	0.65
2:B:94:LYS:O	2:B:146:ASN:N	2.26	0.65
2:B:1071:VAL:HG21	2:B:1091:ARG:HD2	1.78	0.65
3:C:128:ASP:O	3:C:175:GLN:NE2	2.30	0.65
1:A:694:GLN:NE2	9:K:91:TYR:O	2.29	0.65
2:B:434:ARG:NH2	2:B:436:MET:SD	2.69	0.65
3:C:257:GLY:O	3:C:266:TYR:N	2.24	0.65
5:F:84:TYR:HA	5:F:152:ILE:HB	1.78	0.65
1:A:1242:ILE:HA	1:A:1536:ILE:HA	1.79	0.65
2:B:841:ASP:OD1	2:B:842:GLU:N	2.29	0.65
1:A:1461:ASN:OD1	1:A:1462:PHE:N	2.28	0.65
1:A:1615:TYR:CD2	1:A:1616:GLU:HG3	2.32	0.65
1:A:873:PRO:O	1:A:877:LYS:N	2.26	0.65
2:B:1187:SER:O	2:B:1190:SER:OG	2.15	0.65
7:I:91:ASN:OD1	7:I:92:GLU:N	2.30	0.65
1:A:383:ASN:HA	1:A:386:LEU:HD12	1.79	0.65
1:A:492:THR:O	1:A:620:ASN:ND2	2.28	0.64
13:D:99:LEU:HB3	13:D:100:PRO:HD3	1.78	0.64
2:B:662:ASP:OD1	2:B:663:ILE:N	2.30	0.64
6:H:3:ASN:OD1	6:H:4:THR:N	2.30	0.64
9:K:88:PHE:O	9:K:106:GLN:N	2.28	0.64
2:B:13:THR:CG2	12:N:163:VAL:CG2	2.75	0.64
2:B:705:PRO:HA	2:B:981:SER:HB2	1.77	0.64
4:E:176:PRO:HB2	4:E:212:ARG:HD3	1.79	0.64
1:A:316:LEU:HD22	1:A:427:PHE:HE2	1.61	0.64
1:A:704:ASP:HB3	1:A:706:HIS:ND1	2.11	0.64
2:B:946:ASP:OD1	8:J:9:SER:OG	2.16	0.64
4:E:20:LYS:NZ	4:E:34:GLU:O	2.30	0.64
1:A:713:VAL:HG12	1:A:737:LEU:HD21	1.79	0.64
2:B:1016:GLY:O	3:C:69:ARG:NH2	2.31	0.64
1:A:550:SER:N	1:A:553:GLN:OE1	2.20	0.64
1:A:1654:PHE:HB2	5:F:89:GLU:HG2	1.79	0.64
3:C:225:ALA:HA	3:C:302:VAL:HA	1.79	0.64
1:A:718:THR:OG1	1:A:730:GLN:NE2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:656:LEU:H	2:B:657:PRO:CD	2.11	0.64
2:B:718:GLN:HE22	2:B:1034:GLN:HE22	1.43	0.64
3:C:95:GLU:OE1	3:C:95:GLU:N	2.29	0.64
1:A:117:ARG:HH21	1:A:137:ASP:CG	2.07	0.63
1:A:943:ILE:HD11	2:B:958:MET:CB	2.28	0.63
3:C:32:ASN:OD1	3:C:33:VAL:N	2.30	0.63
1:A:1186:GLY:O	1:A:1190:SER:N	2.31	0.63
2:B:894:LYS:O	2:B:895:PHE:CG	2.50	0.63
3:C:163:TYR:N	3:C:166:ASP:OD2	2.26	0.63
2:B:353:VAL:HG13	2:B:357:ILE:HD12	1.79	0.63
8:J:44:TYR:HA	8:J:47:ARG:HD3	1.78	0.63
1:A:1000:MET:HG2	2:B:520:LEU:HB3	1.80	0.63
2:B:938:PHE:HZ	3:C:227:TYR:CE2	2.16	0.63
7:I:28:VAL:O	7:I:37:TYR:N	2.30	0.63
1:A:1501:ILE:HG22	1:A:1502:PRO:CD	2.27	0.63
1:A:1635:ASP:OD1	1:A:1636:SER:N	2.32	0.63
1:A:1185:VAL:O	1:A:1189:ALA:N	2.28	0.63
4:E:62:ALA:HB3	4:E:78:LEU:HB3	1.79	0.63
2:B:211:ARG:NH1	2:B:401:GLU:OE1	2.32	0.63
7:I:114:CYS:N	7:I:119:TYR:O	2.27	0.63
1:A:1101:THR:HG22	1:A:1120:TYR:HB3	1.80	0.62
2:B:676:VAL:N	2:B:680:GLU:OE1	2.31	0.62
2:B:1038:HIS:NE2	2:B:1042:ASP:OD2	2.27	0.62
3:C:216:HIS:ND1	3:C:218:LYS:HG2	2.14	0.62
6:H:3:ASN:N	6:H:61:SER:OG	2.33	0.62
1:A:399:LEU:HD21	1:A:422:ARG:HB3	1.80	0.62
1:A:943:ILE:HD11	2:B:958:MET:CG	2.30	0.62
2:B:286:ARG:HD3	7:I:9:PHE:CD1	2.35	0.62
2:B:576:THR:HG21	12:N:95:ILE:CG2	2.29	0.62
2:B:629:VAL:HG22	2:B:671:TYR:HE2	1.65	0.62
3:C:278:GLU:OE2	3:C:281:ARG:NH1	2.30	0.62
1:A:949:GLN:HA	1:A:981:TYR:HA	1.80	0.62
1:A:949:GLN:HB2	1:A:981:TYR:HD1	1.64	0.62
1:A:245:LYS:HA	1:A:251:ILE:HA	1.81	0.62
1:A:93:GLN:HA	1:A:96:ILE:HD12	1.81	0.62
1:A:535:GLN:HG2	1:A:545:SER:HA	1.82	0.62
2:B:51:ALA:HA	2:B:54:GLU:HB2	1.81	0.62
2:B:480:GLN:O	2:B:484:TYR:OH	2.10	0.62
2:B:757:TYR:CE2	2:B:762:MET:HB2	2.34	0.62
1:A:325:ASP:HB3	1:A:329:ARG:HH12	1.65	0.62
1:A:560:GLN:O	1:A:575:LYS:NZ	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:122:ASP:HA	3:C:125:LYS:HB3	1.81	0.62
4:E:155:ARG:HA	4:E:196:VAL:HG12	1.82	0.62
5:F:103:MET:SD	14:G:112:PRO:HG3	2.39	0.62
1:A:54:LEU:O	1:A:75:HIS:N	2.31	0.62
1:A:908:VAL:HG22	1:A:945:CYS:CB	2.30	0.62
1:A:1497:ILE:HG23	1:A:1500:GLN:HB3	1.82	0.62
4:E:41:ASP:O	4:E:45:LYS:N	2.33	0.62
6:H:21:ASN:OD1	6:H:22:LYS:N	2.33	0.62
9:K:54:THR:HA	9:K:61:ALA:HA	1.81	0.62
7:I:113:THR:OG1	7:I:120:LYS:NZ	2.28	0.61
1:A:834:ARG:HH12	2:B:1007:TYR:HE2	1.45	0.61
1:A:1299:ASN:HA	1:A:1302:TYR:CE2	2.36	0.61
2:B:96:SER:HB2	2:B:144:SER:HB3	1.80	0.61
1:A:196:ALA:HA	1:A:201:ARG:HH21	1.64	0.61
1:A:584:ARG:HG2	1:A:644:ARG:HH22	1.65	0.61
1:A:841:LYS:O	1:A:844:THR:OG1	2.18	0.61
1:A:527:PRO:HG2	1:A:547:ILE:HA	1.81	0.61
1:A:1559:ARG:HA	1:A:1562:ILE:HD12	1.82	0.61
3:C:81:GLU:HG3	3:C:82:TYR:CD2	2.36	0.61
3:C:236:LEU:N	3:C:288:LYS:O	2.28	0.61
4:E:165:LEU:O	4:E:169:ARG:N	2.33	0.61
6:H:11:GLN:NE2	6:H:52:GLN:OE1	2.34	0.61
7:I:91:ASN:HD22	7:I:116:SER:H	1.46	0.61
8:J:5:VAL:HG12	8:J:6:ARG:HG3	1.82	0.61
1:A:669:LEU:HG	1:A:810:LEU:HD11	1.83	0.61
1:A:1651:THR:HB	5:F:92:ARG:NH1	2.15	0.61
2:B:265:ARG:O	2:B:267:ASN:ND2	2.33	0.61
1:A:264:ASN:O	1:A:268:GLY:N	2.33	0.61
1:A:1243:TRP:NE1	1:A:1533:GLU:O	2.31	0.61
4:E:183:PRO:O	4:E:187:TYR:N	2.33	0.61
2:B:1161:ASP:OD1	2:B:1165:ASN:N	2.34	0.61
1:A:1056:ASP:OD1	1:A:1057:ILE:N	2.34	0.61
1:A:1624:LYS:HA	1:A:1627:LEU:HD12	1.81	0.61
2:B:609:ARG:NH2	2:B:626:ILE:HB	2.15	0.61
2:B:714:ARG:HH21	2:B:957:ARG:HA	1.66	0.61
2:B:110:ASN:N	2:B:118:GLU:HG2	2.15	0.60
2:B:369:ASP:OD1	2:B:372:ARG:NH1	2.33	0.60
2:B:655:TYR:CD2	2:B:657:PRO:HD2	2.35	0.60
8:J:31:ASP:OD1	8:J:34:THR:N	2.33	0.60
2:B:626:ILE:N	2:B:668:GLU:OE1	2.34	0.60
7:I:6:SER:HA	7:I:45:LEU:HD22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:GLU:HG3	1:A:975:ASP:H	1.67	0.60
1:A:1272:VAL:HG11	1:A:1485:MET:HG2	1.82	0.60
2:B:168:ASN:OD1	2:B:169:ARG:N	2.35	0.60
2:B:552:SER:OG	2:B:648:ARG:N	2.34	0.60
5:F:108:PHE:HE2	5:F:131:PRO:HG3	1.65	0.60
1:A:244:ARG:HH22	1:A:312:SER:HB3	1.65	0.60
1:A:385:LEU:HD13	1:A:437:PHE:HA	1.83	0.60
1:A:538:ASN:HA	1:A:575:LYS:HG2	1.83	0.60
1:A:943:ILE:HD11	2:B:958:MET:SD	2.40	0.60
1:A:945:CYS:O	1:A:946:LEU:HD23	2.01	0.60
1:A:539:GLU:HB3	1:A:570:THR:HB	1.83	0.60
6:H:105:GLU:O	6:H:112:ILE:HG23	2.00	0.60
1:A:643:ALA:HB1	2:B:1087:LEU:HD23	1.83	0.60
3:C:87:ASN:H	3:C:203:SER:HB3	1.66	0.60
4:E:155:ARG:HD3	4:E:190:LEU:HD22	1.83	0.60
1:A:36:THR:HG22	1:A:45:VAL:HG21	1.84	0.60
2:B:184:LYS:HD2	2:B:735:HIS:NE2	2.17	0.60
2:B:249:VAL:HG11	2:B:261:ARG:HH21	1.67	0.60
3:C:134:LEU:O	3:C:206:ALA:N	2.31	0.60
5:F:72:LYS:HB3	5:F:142:SER:HA	1.84	0.60
1:A:37:VAL:HG12	1:A:38:LEU:HG	1.83	0.60
1:A:1497:ILE:CG2	1:A:1500:GLN:HB3	2.31	0.60
1:A:244:ARG:O	1:A:252:PHE:N	2.32	0.60
1:A:1263:LEU:HB3	1:A:1496:SER:CB	2.32	0.60
1:A:509:GLU:HB2	1:A:577:VAL:HB	1.83	0.60
1:A:615:ARG:HH12	2:B:929:ARG:HH21	1.50	0.60
2:B:698:SER:H	2:B:701:ALA:HB3	1.66	0.60
1:A:36:THR:HB	1:A:45:VAL:HG11	1.84	0.59
1:A:1049:MET:HB3	4:E:208:TYR:HE1	1.67	0.59
2:B:444:ARG:O	2:B:448:ARG:N	2.28	0.59
2:B:588:ILE:HG12	2:B:642:LEU:HD12	1.82	0.59
2:B:796:ARG:NH2	8:J:9:SER:O	2.35	0.59
3:C:164:ALA:HB2	3:C:191:ILE:HB	1.82	0.59
3:C:277:ARG:HB3	3:C:280:LEU:HD12	1.84	0.59
4:E:114:ASN:OD1	4:E:115:ASN:N	2.35	0.59
7:I:8:ILE:HG22	7:I:17:LEU:HD12	1.84	0.59
8:J:69:ARG:NH2	10:L:33:GLU:OE2	2.35	0.59
9:K:50:LEU:O	9:K:54:THR:HG23	2.03	0.59
9:K:87:GLU:N	9:K:106:GLN:O	2.34	0.59
1:A:497:VAL:HG21	1:A:605:VAL:HG13	1.84	0.59
1:A:1603:MET:HG2	1:A:1612:LYS:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:521:LEU:HB3	2:B:523:GLU:OE1	2.02	0.59
2:B:609:ARG:HG3	2:B:655:TYR:OH	2.01	0.59
1:A:621:THR:O	1:A:625:ASN:N	2.35	0.59
1:A:1646:LEU:HD22	14:G:109:PRO:HB3	1.84	0.59
1:A:1648:ASN:HB3	1:A:1649:VAL:HG23	1.83	0.59
2:B:261:ARG:NH1	2:B:268:GLU:OE2	2.35	0.59
2:B:50:ASN:HB3	2:B:54:GLU:OE1	2.02	0.59
2:B:745:GLN:HB3	2:B:800:TYR:HB3	1.83	0.59
12:N:89:ILE:HG12	12:N:139:VAL:HG22	1.85	0.59
2:B:150:GLU:HB2	2:B:441:LYS:HE2	1.85	0.59
2:B:887:LEU:HB2	10:L:56:LEU:HB2	1.84	0.59
2:B:1128:CYS:H	2:B:1170:GLY:HA3	1.68	0.59
9:K:116:ALA:HA	9:K:119:LYS:HB3	1.85	0.59
1:A:417:ARG:O	1:A:421:SER:N	2.35	0.59
1:A:1578:SER:HB3	1:A:1581:HIS:CD2	2.38	0.59
1:A:1640:ARG:NE	1:A:1646:LEU:O	2.34	0.59
2:B:912:GLN:N	2:B:915:ASP:OD2	2.26	0.59
6:H:93:TYR:HA	6:H:145:ARG:HB3	1.84	0.59
2:B:839:LYS:HG3	2:B:857:PRO:HD2	1.85	0.59
2:B:884:GLU:O	2:B:904:LYS:N	2.30	0.59
1:A:641:GLU:O	1:A:645:ALA:N	2.30	0.59
1:A:1640:ARG:O	1:A:1645:LYS:N	2.35	0.59
2:B:944:GLN:N	2:B:944:GLN:OE1	2.36	0.59
2:B:1128:CYS:HB3	2:B:1131:CYS:HB2	1.84	0.59
3:C:68:ARG:HD2	3:C:227:TYR:CE2	2.37	0.59
3:C:87:ASN:O	3:C:203:SER:N	2.33	0.59
4:E:177:ARG:HG3	4:E:215:MET:HG3	1.84	0.59
1:A:1053:ASP:OD1	1:A:1054:ALA:N	2.34	0.58
2:B:15:ASP:OD1	2:B:16:PHE:N	2.35	0.58
2:B:1013:MET:HB2	2:B:1022:LEU:HD12	1.84	0.58
4:E:12:LEU:HD11	4:E:58:MET:HE1	1.84	0.58
2:B:996:PHE:O	2:B:999:GLN:N	2.36	0.58
9:K:122:LYS:NZ	9:K:126:ASP:OD2	2.31	0.58
1:A:267:LYS:HG2	1:A:270:ILE:HD12	1.85	0.58
2:B:698:SER:O	2:B:702:ASN:ND2	2.36	0.58
2:B:1128:CYS:O	2:B:1132:SER:N	2.36	0.58
11:M:10:ILE:HB	12:N:70:LEU:HB3	1.86	0.58
1:A:481:ARG:HE	1:A:632:GLU:HB2	1.68	0.58
1:A:945:CYS:C	1:A:946:LEU:HG	2.27	0.58
1:A:468:ARG:HA	1:A:472:MET:HB2	1.84	0.58
1:A:1486:VAL:HG23	7:I:51:THR:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1656:VAL:HG11	14:G:107:ILE:HB	1.84	0.58
2:B:523:GLU:OE1	2:B:523:GLU:N	2.34	0.58
3:C:242:GLU:HG3	3:C:246:ARG:NE	2.18	0.58
12:N:69:SER:OG	12:N:70:LEU:N	2.37	0.58
1:A:596:HIS:CD2	1:A:598:ALA:HB3	2.38	0.58
1:A:1443:GLN:O	1:A:1447:GLN:N	2.27	0.58
3:C:32:ASN:H	3:C:35:LYS:HD2	1.67	0.58
14:G:30:GLU:HA	14:G:32:ASN:N	2.18	0.58
1:A:579:ARG:HH22	1:A:585:ASP:CG	2.11	0.58
1:A:659:THR:OG1	1:A:664:SER:N	2.33	0.58
1:A:846:ILE:HD13	1:A:906:GLN:CB	2.29	0.58
1:A:1298:ASP:HB2	1:A:1301:GLU:CD	2.29	0.58
6:H:103:LYS:HD2	6:H:115:TYR:CD2	2.38	0.58
10:L:27:LEU:HA	10:L:39:SER:HB2	1.85	0.58
1:A:590:ASN:OD1	1:A:591:ARG:N	2.37	0.58
2:B:13:THR:CG2	12:N:163:VAL:HG22	2.33	0.58
2:B:164:MET:HB2	2:B:194:PHE:HE1	1.68	0.58
2:B:576:THR:CG2	12:N:95:ILE:HG22	2.34	0.58
4:E:83:CYS:N	4:E:111:VAL:O	2.36	0.58
1:A:320:VAL:HA	1:A:323:ILE:HD12	1.85	0.58
1:A:435:ASN:ND2	1:A:442:LYS:O	2.37	0.58
1:A:1101:THR:HA	1:A:1104:TYR:HD2	1.68	0.58
1:A:1154:LEU:O	1:A:1158:SER:N	2.37	0.58
1:A:1497:ILE:HG22	1:A:1497:ILE:O	2.04	0.58
2:B:236:ILE:HG21	2:B:377:MET:HE1	1.86	0.58
2:B:796:ARG:NH2	8:J:8:PHE:O	2.36	0.58
2:B:832:TRP:HH2	2:B:837:LEU:HG	1.68	0.58
4:E:147:HIS:HB3	4:E:150:VAL:HG23	1.85	0.58
1:A:659:THR:O	1:A:663:GLY:N	2.33	0.57
1:A:956:ARG:NH2	1:A:979:GLY:HA3	2.19	0.57
1:A:1287:ALA:HA	1:A:1478:ALA:HB2	1.86	0.57
2:B:658:LEU:O	2:B:660:LYS:HG3	2.03	0.57
1:A:341:SER:N	1:A:1628:ASP:O	2.35	0.57
3:C:325:ALA:HA	3:C:328:LEU:HB3	1.86	0.57
1:A:236:CYS:HB2	1:A:271:ARG:HD2	1.86	0.57
1:A:1315:ASN:HA	1:A:1318:SER:HB2	1.85	0.57
2:B:894:LYS:HG3	10:L:54:ARG:HH21	1.69	0.57
2:B:1105:ARG:HB3	2:B:1172:GLU:HB3	1.87	0.57
1:A:522:ALA:O	1:A:526:GLY:N	2.38	0.57
1:A:697:TYR:CE1	9:K:104:ARG:HG3	2.39	0.57
2:B:42:VAL:HG21	2:B:190:ILE:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:757:TYR:CZ	2:B:762:MET:HB2	2.40	0.57
6:H:103:LYS:HB3	6:H:115:TYR:HB2	1.86	0.57
8:J:3:VAL:HG21	8:J:18:TRP:CG	2.39	0.57
2:B:972:GLY:O	2:B:976:GLY:N	2.38	0.57
1:A:2:ASP:HB3	1:A:5:LYS:HD3	1.87	0.57
1:A:689:ARG:HH11	9:K:81:MET:HE1	1.68	0.57
1:A:826:PHE:HZ	1:A:924:SER:HB3	1.68	0.57
6:H:38:LEU:HD11	6:H:123:MET:HG3	1.86	0.57
14:G:56:ASN:HB3	14:G:59:GLN:HB3	1.87	0.57
1:A:208:PHE:HA	1:A:212:VAL:HG11	1.87	0.57
1:A:975:ASP:OD2	1:A:977:MET:HB3	2.04	0.57
4:E:17:ARG:NH1	4:E:35:VAL:O	2.38	0.57
12:N:148:ILE:O	12:N:150:TYR:N	2.38	0.57
2:B:489:GLU:HG3	2:B:495:ARG:HE	1.70	0.56
4:E:110:PHE:N	4:E:133:GLU:O	2.28	0.56
1:A:1254:PHE:O	1:A:1257:SER:OG	2.18	0.56
2:B:656:LEU:O	12:N:153:VAL:CG1	2.46	0.56
2:B:745:GLN:HG2	2:B:800:TYR:CD2	2.33	0.56
1:A:7:VAL:HG11	2:B:1176:VAL:HA	1.86	0.56
1:A:11:ILE:HD11	2:B:1176:VAL:HG21	1.86	0.56
2:B:320:LEU:HD13	2:B:326:VAL:HA	1.86	0.56
3:C:232:GLN:HB3	3:C:292:GLY:C	2.30	0.56
3:C:257:GLY:HA3	3:C:266:TYR:CZ	2.40	0.56
1:A:836:THR:HG23	1:A:839:GLY:H	1.71	0.56
2:B:832:TRP:CH2	2:B:837:LEU:HG	2.41	0.56
6:H:85:GLY:O	6:H:87:ARG:NH1	2.38	0.56
7:I:29:GLU:HB2	7:I:36:ILE:HG13	1.87	0.56
7:I:89:CYS:SG	7:I:116:SER:OG	2.59	0.56
1:A:592:GLN:NE2	2:B:1075:GLU:OE2	2.39	0.56
1:A:966:LEU:HB3	1:A:969:PHE:HD2	1.70	0.56
1:A:1082:PRO:HA	1:A:1085:LEU:HD12	1.87	0.56
2:B:852:VAL:HG13	2:B:856:ASP:HB2	1.88	0.56
2:B:893:ASN:ND2	2:B:895:PHE:CD2	2.69	0.56
3:C:236:LEU:HD11	3:C:290:LYS:HG3	1.86	0.56
1:A:95:TYR:CG	1:A:245:LYS:HD3	2.40	0.56
1:A:365:THR:O	1:A:369:LEU:N	2.38	0.56
1:A:744:MET:HE3	1:A:1078:LYS:HB2	1.88	0.56
1:A:846:ILE:CD1	1:A:906:GLN:HB3	2.31	0.56
1:A:1454:HIS:HB2	1:A:1457:ILE:HD12	1.88	0.56
1:A:683:LYS:HD2	6:H:20:TYR:CE2	2.41	0.56
1:A:828:CYS:SG	1:A:829:GLY:N	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:259:ASP:N	3:C:264:GLU:O	2.39	0.56
1:A:1649:VAL:HG12	1:A:1650:GLY:N	2.21	0.56
2:B:815:ARG:HE	2:B:821:ILE:HA	1.71	0.56
2:B:815:ARG:NE	2:B:821:ILE:HA	2.21	0.56
3:C:121:PRO:O	3:C:125:LYS:N	2.33	0.56
4:E:96:PHE:HE2	4:E:132:ILE:HG23	1.70	0.56
1:A:804:GLU:H	1:A:804:GLU:CD	2.14	0.56
2:B:462:GLN:O	2:B:466:SER:N	2.29	0.56
2:B:569:GLY:HA3	12:N:90:MET:HE1	1.87	0.56
2:B:750:PRO:HB3	2:B:1032:TYR:CG	2.41	0.56
2:B:787:MET:SD	2:B:917:PHE:HB2	2.46	0.56
7:I:10:CYS:HB2	7:I:17:LEU:HD21	1.88	0.56
1:A:372:LYS:HB3	1:A:377:VAL:HA	1.88	0.55
1:A:606:ARG:NH2	9:K:98:GLU:OE2	2.39	0.55
1:A:1242:ILE:HD11	1:A:1517:ARG:NE	2.20	0.55
2:B:654:ARG:NH2	2:B:659:ASP:OD2	2.37	0.55
2:B:659:ASP:O	2:B:660:LYS:HG3	2.06	0.55
2:B:987:ASN:OD1	2:B:990:ASP:N	2.35	0.55
2:B:492:ASN:OD1	2:B:495:ARG:N	2.29	0.55
2:B:677:THR:H	2:B:680:GLU:CD	2.14	0.55
8:J:32:GLU:N	8:J:32:GLU:OE1	2.38	0.55
2:B:492:ASN:HD21	2:B:723:LYS:HA	1.71	0.55
3:C:117:ASP:OD1	3:C:118:SER:N	2.39	0.55
1:A:885:ASP:OD1	1:A:887:ASN:N	2.39	0.55
2:B:218:ILE:HG23	2:B:231:HIS:HD2	1.71	0.55
6:H:5:LEU:H	6:H:60:ALA:HA	1.70	0.55
7:I:66:VAL:HG23	7:I:67:VAL:HG13	1.89	0.55
9:K:68:GLU:H	9:K:99:ASN:HB3	1.70	0.55
1:A:316:LEU:HD22	1:A:427:PHE:CE2	2.41	0.55
2:B:700:LEU:N	16:B:1301:SO4:S	2.73	0.55
2:B:783:MET:HA	2:B:950:ASN:HD22	1.71	0.55
3:C:87:ASN:ND2	3:C:201:GLU:OE2	2.39	0.55
2:B:387:GLY:O	2:B:634:ARG:NH1	2.40	0.55
2:B:599:GLU:H	2:B:599:GLU:CD	2.15	0.55
14:G:35:SER:HG	14:G:132:VAL:H	1.55	0.55
1:A:885:ASP:OD2	1:A:888:LYS:HG3	2.07	0.55
2:B:23:SER:O	2:B:27:ASN:N	2.32	0.55
2:B:190:ILE:HD11	2:B:496:PHE:HE2	1.72	0.55
2:B:362:LEU:HD12	2:B:370:LYS:HG2	1.89	0.55
3:C:179:PHE:HA	3:C:182:CYS:SG	2.47	0.55
9:K:77:ARG:HD2	9:K:91:TYR:HE1	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:15:VAL:HG22	11:M:90:LEU:HB2	1.88	0.55
1:A:908:VAL:CA	1:A:945:CYS:SG	2.92	0.55
1:A:1449:ALA:O	1:A:1452:SER:OG	2.13	0.55
1:A:1648:ASN:H	1:A:1649:VAL:HB	1.71	0.55
2:B:1077:ASP:HA	2:B:1080:ILE:HD12	1.89	0.55
9:K:50:LEU:HD21	9:K:64:GLN:HB2	1.88	0.55
1:A:829:GLY:N	1:A:832:ASP:OD2	2.40	0.55
8:J:31:ASP:CG	8:J:34:THR:H	2.14	0.55
9:K:63:PHE:HB2	9:K:103:ILE:HB	1.89	0.55
1:A:503:VAL:HA	1:A:580:HIS:CE1	2.42	0.55
1:A:652:ASN:CG	1:A:653:THR:H	2.15	0.55
2:B:177:PRO:HA	2:B:180:LEU:HD12	1.89	0.55
2:B:529:CYS:SG	2:B:532:HIS:N	2.73	0.55
3:C:89:THR:OG1	3:C:201:GLU:N	2.29	0.55
2:B:675:ALA:O	2:B:689:VAL:HA	2.06	0.54
2:B:718:GLN:OE1	2:B:922:GLY:N	2.40	0.54
14:G:229:LEU:HD12	14:G:230:ARG:H	1.72	0.54
1:A:1549:VAL:O	1:A:1553:TYR:N	2.34	0.54
1:A:1606:SER:O	1:A:1612:LYS:NZ	2.34	0.54
2:B:504:HIS:CB	2:B:542:LEU:HD23	2.36	0.54
2:B:609:ARG:HE	2:B:626:ILE:HD12	1.72	0.54
1:A:1651:THR:O	1:A:1654:PHE:N	2.39	0.54
2:B:132:SER:OG	2:B:196:VAL:HA	2.07	0.54
2:B:584:CYS:N	2:B:596:VAL:O	2.41	0.54
2:B:743:ARG:NH2	8:J:1:MET:SD	2.80	0.54
9:K:134:LYS:O	9:K:138:LYS:HG2	2.07	0.54
1:A:689:ARG:NH1	9:K:81:MET:HE1	2.22	0.54
1:A:883:LEU:HD22	1:A:972:TYR:HE1	1.72	0.54
1:A:1105:ARG:NH2	1:A:1142:ASP:OD1	2.40	0.54
2:B:700:LEU:N	16:B:1301:SO4:O1	2.27	0.54
1:A:113:VAL:HA	1:A:182:LYS:HD3	1.90	0.54
1:A:657:TYR:O	1:A:666:VAL:HG22	2.08	0.54
1:A:771:PHE:HE1	1:A:776:LEU:HD13	1.72	0.54
2:B:54:GLU:OE2	2:B:168:ASN:ND2	2.39	0.54
2:B:505:ARG:HB3	2:B:509:PHE:CD2	2.41	0.54
1:A:1204:THR:HG22	1:A:1205:PHE:H	1.73	0.54
1:A:1310:LYS:O	1:A:1314:GLN:N	2.28	0.54
4:E:143:ASN:OD1	4:E:145:THR:N	2.41	0.54
1:A:535:GLN:HB2	1:A:578:TYR:HD2	1.73	0.54
1:A:1289:SER:HA	1:A:1475:GLU:HA	1.89	0.54
2:B:656:LEU:HB3	2:B:657:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:117:PRO:HA	5:F:120:ILE:HD12	1.90	0.54
1:A:472:MET:HB3	2:B:1073:GLU:HG2	1.90	0.54
2:B:57:ASP:OD1	2:B:59:GLY:N	2.39	0.54
3:C:311:GLU:OE1	3:C:311:GLU:N	2.30	0.54
10:L:46:VAL:HG13	10:L:56:LEU:HD12	1.90	0.54
11:M:12:ILE:HD12	12:N:67:LEU:HB2	1.90	0.54
1:A:916:THR:O	1:A:919:LYS:NZ	2.40	0.54
1:A:1111:GLU:O	1:A:1116:GLN:NE2	2.41	0.54
1:A:1294:MET:HE3	1:A:1470:CYS:HB3	1.89	0.54
1:A:1533:GLU:OE2	4:E:14:ARG:NH2	2.39	0.54
3:C:152:ASP:OD2	3:C:154:LYS:HB2	2.08	0.54
3:C:248:GLN:HG3	3:C:256:ILE:HB	1.89	0.54
4:E:83:CYS:HB2	4:E:110:PHE:CZ	2.42	0.54
1:A:368:ARG:O	1:A:383:ASN:ND2	2.38	0.54
1:A:583:ASN:OD1	1:A:606:ARG:HA	2.08	0.54
2:B:21:ARG:NH2	8:J:53:HIS:O	2.41	0.54
2:B:840:LEU:HA	2:B:846:PRO:HA	1.90	0.54
6:H:103:LYS:HD2	6:H:115:TYR:HD2	1.73	0.54
7:I:31:SER:O	7:I:34:LYS:NZ	2.32	0.54
2:B:379:ARG:HE	2:B:580:GLY:CA	2.21	0.53
6:H:112:ILE:HD12	6:H:129:TYR:HB3	1.90	0.53
1:A:27:LEU:HA	2:B:1129:ARG:HG2	1.91	0.53
1:A:467:PHE:O	1:A:471:MET:HB2	2.08	0.53
2:B:274:VAL:HA	2:B:277:LEU:HD12	1.90	0.53
6:H:36:CYS:HA	6:H:126:GLU:O	2.08	0.53
7:I:74:ASN:O	7:I:77:LYS:HG2	2.09	0.53
1:A:53:ALA:HA	1:A:63:SER:HB2	1.89	0.53
1:A:327:VAL:O	1:A:331:GLU:N	2.35	0.53
1:A:494:GLU:HG2	1:A:604:LYS:HB2	1.90	0.53
1:A:1200:MET:HG2	1:A:1573:TYR:CD1	2.43	0.53
1:A:1559:ARG:NH2	4:E:200:ARG:HD3	2.24	0.53
3:C:213:GLY:HA2	3:C:219:PHE:HB2	1.89	0.53
1:A:32:ILE:HG21	1:A:49:LEU:HD23	1.90	0.53
2:B:1134:ARG:HD3	2:B:1167:PHE:HE1	1.72	0.53
14:G:20:HIS:O	14:G:20:HIS:ND1	2.38	0.53
1:A:1524:VAL:HG21	1:A:1545:ASP:HB2	1.91	0.53
2:B:894:LYS:C	2:B:896:GLN:H	2.16	0.53
2:B:1107:CYS:O	2:B:1197:ARG:NH1	2.42	0.53
3:C:43:ASN:O	3:C:55:ASP:N	2.39	0.53
1:A:39:ASP:OD1	1:A:43:HIS:N	2.41	0.53
1:A:211:THR:HG23	4:E:177:ARG:NH1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:GLY:HA2	1:A:731:ILE:HD12	1.91	0.53
1:A:1031:HIS:CE1	1:A:1039:ARG:HB2	2.43	0.53
1:A:1542:THR:HG22	4:E:149:LEU:HD11	1.90	0.53
2:B:171:HIS:O	2:B:175:MET:HE3	2.08	0.53
2:B:560:ARG:O	2:B:563:SER:OG	2.19	0.53
1:A:752:LYS:HG2	1:A:768:GLU:HA	1.89	0.53
2:B:560:ARG:NH1	2:B:618:PRO:HB2	2.23	0.53
7:I:91:ASN:HD21	7:I:115:THR:HB	1.74	0.53
1:A:477:ASN:HB3	2:B:1048:SER:O	2.09	0.53
1:A:783:LYS:HG3	1:A:787:GLY:HA3	1.89	0.53
1:A:1153:LYS:HA	1:A:1156:LYS:NZ	2.23	0.53
1:A:1530:TRP:CG	4:E:142:VAL:HG21	2.44	0.53
4:E:180:ARG:N	4:E:215:MET:OXT	2.41	0.53
5:F:83:PRO:O	5:F:152:ILE:N	2.31	0.53
14:G:132:VAL:HG22	14:G:232:THR:HG22	1.90	0.53
2:B:134:ARG:HG2	2:B:162:PRO:HA	1.91	0.53
4:E:64:PRO:HG3	4:E:75:MET:HG2	1.91	0.53
1:A:17:GLY:N	2:B:1195:ARG:O	2.40	0.53
1:A:1260:LYS:HE3	1:A:1500:GLN:HB2	1.90	0.53
1:A:1657:LEU:HD11	5:F:135:ARG:CB	2.39	0.53
2:B:983:PRO:HB2	2:B:984:TRP:CE3	2.44	0.53
1:A:244:ARG:N	1:A:252:PHE:O	2.33	0.52
2:B:798:PHE:HA	8:J:8:PHE:CZ	2.44	0.52
4:E:6:GLU:HA	4:E:9:ILE:HD12	1.92	0.52
4:E:48:ASP:OD1	4:E:52:ARG:N	2.24	0.52
4:E:90:VAL:HG13	4:E:123:LEU:HD11	1.89	0.52
6:H:30:SER:HB3	6:H:33:GLN:O	2.09	0.52
1:A:648:LEU:O	1:A:652:ASN:ND2	2.42	0.52
2:B:72:VAL:HG22	2:B:96:SER:HA	1.91	0.52
2:B:238:SER:O	2:B:246:GLN:N	2.31	0.52
2:B:29:PRO:HB2	2:B:177:PRO:HG2	1.92	0.52
2:B:832:TRP:HZ3	2:B:836:TRP:HB2	1.74	0.52
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.43	0.52
1:A:195:LYS:O	1:A:198:SER:OG	2.20	0.52
1:A:488:PRO:HD3	1:A:618:TYR:HE2	1.75	0.52
2:B:773:VAL:HG22	2:B:947:ILE:HB	1.92	0.52
2:B:936:MET:HE1	2:B:948:ILE:HD11	1.90	0.52
1:A:16:PHE:CE2	1:A:1625:ALA:HB1	2.45	0.52
1:A:1656:VAL:C	1:A:1657:LEU:HD12	2.35	0.52
2:B:758:ASP:C	2:B:761:GLY:H	2.17	0.52
1:A:1301:GLU:O	1:A:1305:GLU:N	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:516:THR:HG22	2:B:519:LYS:HE2	1.91	0.52
2:B:757:TYR:O	2:B:761:GLY:N	2.43	0.52
2:B:832:TRP:CZ3	2:B:834:LYS:HA	2.44	0.52
2:B:1014:TYR:HE2	3:C:228:ARG:HA	1.75	0.52
3:C:84:TYR:HE2	3:C:207:HIS:HE2	1.57	0.52
3:C:121:PRO:HD2	3:C:124:GLU:OE1	2.10	0.52
1:A:945:CYS:O	1:A:946:LEU:HG	2.09	0.52
1:A:1023:LEU:HD21	1:A:1226:VAL:HG11	1.92	0.52
3:C:165:ARG:NH1	3:C:190:ASP:HA	2.25	0.52
7:I:87:PRO:HG2	7:I:119:TYR:CE2	2.43	0.52
1:A:50:TYR:OH	1:A:383:ASN:ND2	2.43	0.52
9:K:59:THR:O	9:K:106:GLN:HA	2.10	0.52
1:A:861:VAL:HA	7:I:68:LYS:HD3	1.92	0.52
1:A:943:ILE:HG22	1:A:943:ILE:O	2.09	0.52
1:A:1582:LEU:O	1:A:1586:ALA:N	2.35	0.52
2:B:1106:GLU:HB2	2:B:1172:GLU:HB2	1.90	0.52
9:K:51:THR:O	9:K:54:THR:OG1	2.18	0.52
13:D:48:GLU:OE2	13:D:90:LYS:NZ	2.43	0.52
1:A:945:CYS:O	1:A:946:LEU:CD2	2.57	0.52
2:B:23:SER:HA	2:B:26:ILE:HB	1.92	0.52
1:A:879:LEU:O	1:A:883:LEU:N	2.30	0.51
1:A:1034:TYR:CE1	5:F:136:ARG:HD3	2.44	0.51
2:B:143:TRP:HB3	2:B:152:LEU:HB2	1.92	0.51
11:M:75:GLN:HB2	12:N:60:SER:HA	1.91	0.51
1:A:236:CYS:HB3	1:A:271:ARG:HH11	1.73	0.51
1:A:1114:TYR:HE1	1:A:1115:LYS:HE3	1.75	0.51
2:B:745:GLN:HB3	2:B:800:TYR:O	2.09	0.51
3:C:153:PRO:O	3:C:157:TYR:N	2.43	0.51
3:C:188:ASP:HB2	3:C:191:ILE:HG13	1.93	0.51
4:E:107:THR:HG23	4:E:131:THR:HG23	1.92	0.51
1:A:1238:MET:HB2	1:A:1521:THR:OG1	2.10	0.51
1:A:1243:TRP:HD1	1:A:1535:PHE:C	2.19	0.51
1:A:1264:SER:HB2	7:I:56:PHE:HD1	1.75	0.51
1:A:1310:LYS:HA	1:A:1313:LEU:HB3	1.92	0.51
2:B:404:LEU:HD12	2:B:407:PHE:CE2	2.46	0.51
2:B:576:THR:HG23	12:N:95:ILE:HG22	1.92	0.51
2:B:602:LYS:HB2	2:B:628:TYR:CZ	2.46	0.51
4:E:17:ARG:HG2	4:E:21:GLU:OE2	2.11	0.51
7:I:86:CYS:HB3	7:I:91:ASN:H	1.76	0.51
2:B:397:THR:HA	2:B:400:GLN:OE1	2.10	0.51
2:B:788:ILE:HB	2:B:948:ILE:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:GLU:OE2	1:A:384:GLN:NE2	2.26	0.51
1:A:509:GLU:OE2	1:A:579:ARG:NE	2.43	0.51
1:A:1050:TYR:CE2	1:A:1580:ARG:HD3	2.46	0.51
1:A:1100:LYS:HG2	1:A:1104:TYR:HE2	1.76	0.51
2:B:74:PHE:HE2	2:B:343:ASP:HB3	1.74	0.51
2:B:335:ARG:NH2	2:B:342:PRO:O	2.44	0.51
3:C:173:GLY:O	3:C:176:SER:OG	2.19	0.51
2:B:527:PHE:O	2:B:546:ALA:N	2.29	0.51
6:H:129:TYR:O	6:H:133:ASN:N	2.43	0.51
7:I:23:VAL:HB	7:I:39:LYS:HZ1	1.76	0.51
14:G:30:GLU:HA	14:G:32:ASN:H	1.74	0.51
1:A:1193:VAL:O	1:A:1196:PRO:HD2	2.10	0.51
1:A:1647:ASN:HB3	1:A:1650:GLY:H	1.75	0.51
2:B:167:SER:OG	2:B:170:CYS:N	2.43	0.51
2:B:589:ASP:OD1	2:B:643:PHE:HA	2.11	0.51
2:B:938:PHE:CZ	3:C:227:TYR:CE2	2.98	0.51
3:C:87:ASN:OD1	3:C:88:ASN:N	2.44	0.51
3:C:236:LEU:HD12	3:C:287:ASP:O	2.11	0.51
1:A:129:LEU:HB3	1:A:132:GLU:CD	2.36	0.51
1:A:135:LYS:HA	1:A:138:GLU:CD	2.36	0.51
1:A:352:ALA:HA	1:A:355:PHE:HD2	1.75	0.51
1:A:949:GLN:HG3	1:A:950:GLN:O	2.11	0.51
1:A:1303:SER:HA	1:A:1308:VAL:H	1.75	0.51
2:B:341:SER:OG	2:B:343:ASP:OD1	2.12	0.51
2:B:573:ALA:HB2	2:B:594:GLY:HA2	1.92	0.51
2:B:584:CYS:HB3	2:B:596:VAL:HG23	1.93	0.51
2:B:1118:PRO:HD3	2:B:1124:SER:HB2	1.92	0.51
3:C:161:HIS:HB2	3:C:163:TYR:CE1	2.45	0.51
4:E:113:GLN:HA	4:E:137:GLU:CD	2.36	0.51
7:I:84:GLU:N	7:I:92:GLU:O	2.40	0.51
1:A:1609:SER:O	1:A:1612:LYS:N	2.44	0.51
2:B:136:LYS:HA	2:B:160:GLY:HA2	1.92	0.51
2:B:145:VAL:N	2:B:150:GLU:O	2.41	0.51
6:H:35:GLN:HE22	6:H:110:ASP:HB3	1.75	0.51
1:A:126:GLN:HB3	1:A:343:PRO:HG3	1.92	0.51
1:A:806:ALA:HA	1:A:809:VAL:HB	1.92	0.51
2:B:346:ASP:HA	2:B:349:VAL:HB	1.93	0.51
5:F:127:GLU:HB3	5:F:129:LYS:HG2	1.93	0.51
1:A:21:ALA:HA	1:A:24:ILE:HB	1.91	0.50
1:A:208:PHE:CE2	1:A:1607:THR:HG23	2.47	0.50
1:A:321:LYS:HB2	1:A:356:PHE:CE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:174:ARG:O	3:C:178:THR:N	2.38	0.50
1:A:368:ARG:HA	1:A:380:ASN:ND2	2.27	0.50
1:A:723:TYR:CD1	1:A:724:PRO:HD2	2.47	0.50
2:B:322:ASN:HB3	2:B:325:GLN:HG3	1.93	0.50
2:B:937:PRO:HB2	2:B:1013:MET:HE2	1.94	0.50
3:C:167:LEU:C	3:C:168:LYS:HD2	2.36	0.50
9:K:54:THR:HG22	9:K:62:SER:H	1.77	0.50
1:A:119:ALA:HA	1:A:122:LEU:HD12	1.93	0.50
1:A:381:SER:HB2	1:A:453:ILE:HG23	1.93	0.50
1:A:826:PHE:CZ	1:A:924:SER:CB	2.95	0.50
1:A:962:SER:HB3	2:B:670:VAL:HG12	1.92	0.50
2:B:72:VAL:HG11	2:B:94:LYS:HG3	1.94	0.50
3:C:45:SER:H	3:C:54:PHE:HA	1.76	0.50
3:C:332:PRO:HD3	9:K:42:PRO:HB2	1.94	0.50
4:E:28:TYR:HE1	4:E:64:PRO:HG3	1.76	0.50
4:E:145:THR:HG21	4:E:187:TYR:CE2	2.47	0.50
1:A:49:LEU:HB3	1:A:368:ARG:HH12	1.75	0.50
1:A:91:PHE:CE2	1:A:245:LYS:HD2	2.46	0.50
1:A:526:GLY:HA3	1:A:554:ARG:NH1	2.20	0.50
1:A:551:VAL:HG22	1:A:554:ARG:HH21	1.76	0.50
1:A:1516:LYS:HG3	1:A:1518:VAL:HG23	1.94	0.50
2:B:326:VAL:O	2:B:330:LEU:HG	2.11	0.50
2:B:559:SER:O	2:B:562:PRO:HD2	2.12	0.50
2:B:1131:CYS:HB2	2:B:1170:GLY:HA2	1.92	0.50
3:C:142:ARG:NH2	8:J:67:GLU:OE2	2.44	0.50
1:A:324:LEU:HA	1:A:327:VAL:HB	1.93	0.50
1:A:591:ARG:HB2	1:A:633:MET:HE3	1.94	0.50
2:B:20:GLU:HG2	2:B:24:ARG:NH1	2.23	0.50
2:B:517:VAL:HG23	2:B:518:ARG:HG3	1.92	0.50
1:A:248:PHE:CE2	1:A:444:GLN:HG2	2.46	0.50
1:A:487:ASP:O	1:A:617:HIS:HA	2.12	0.50
1:A:496:GLY:HA3	1:A:615:ARG:HB2	1.94	0.50
1:A:551:VAL:HA	1:A:554:ARG:HH21	1.76	0.50
1:A:1025:LYS:HE3	1:A:1611:MET:HG3	1.93	0.50
1:A:1188:ILE:O	1:A:1192:SER:OG	2.25	0.50
2:B:76:GLY:H	2:B:92:GLY:HA3	1.76	0.50
2:B:1127:CYS:HG	2:B:1159:TRP:CD1	2.29	0.50
3:C:87:ASN:N	3:C:203:SER:HB3	2.26	0.50
6:H:102:TYR:CE1	6:H:115:TYR:HB3	2.47	0.50
1:A:538:ASN:HB2	1:A:540:ASP:OD1	2.10	0.50
1:A:651:ALA:O	1:A:656:GLN:NE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1138:GLU:HA	1:A:1141:GLN:HB3	1.92	0.50
1:A:1530:TRP:CD2	4:E:142:VAL:HG21	2.47	0.50
2:B:150:GLU:HG2	2:B:441:LYS:HG2	1.93	0.50
2:B:655:TYR:CD1	2:B:688:HIS:CD2	3.00	0.50
2:B:657:PRO:C	2:B:659:ASP:N	2.59	0.50
2:B:923:GLN:HE22	2:B:957:ARG:HD2	1.77	0.50
3:C:133:VAL:HG22	3:C:207:HIS:ND1	2.26	0.50
4:E:113:GLN:HG2	4:E:137:GLU:OE2	2.12	0.50
1:A:1288:ARG:O	1:A:1476:LEU:N	2.40	0.50
2:B:352:GLU:OE2	2:B:356:ARG:NE	2.42	0.50
3:C:93:GLN:H	3:C:93:GLN:CD	2.20	0.50
1:A:488:PRO:HD2	2:B:781:TYR:CE1	2.47	0.50
1:A:618:TYR:CZ	2:B:783:MET:HB2	2.46	0.50
1:A:721:LYS:HB3	6:H:96:VAL:HB	1.93	0.50
1:A:937:ASN:O	1:A:941:SER:HB3	2.12	0.50
2:B:368:GLN:HG3	2:B:372:ARG:NH1	2.27	0.50
2:B:393:ASN:HD22	2:B:396:ALA:HB2	1.77	0.50
4:E:46:TYR:O	4:E:53:PRO:HA	2.12	0.50
14:G:47:VAL:HB	14:G:65:HIS:CD2	2.47	0.50
1:A:887:ASN:O	1:A:891:ILE:HG12	2.12	0.49
1:A:1074:TYR:O	1:A:1078:LYS:HG2	2.12	0.49
1:A:1224:GLU:O	1:A:1228:THR:OG1	2.27	0.49
2:B:74:PHE:HA	2:B:93:ASN:O	2.12	0.49
2:B:211:ARG:NH1	2:B:647:SER:HB2	2.18	0.49
6:H:28:ALA:N	6:H:38:LEU:O	2.40	0.49
2:B:25:PHE:CD1	8:J:59:LYS:HD2	2.48	0.49
2:B:443:LYS:HA	2:B:446:MET:HB3	1.94	0.49
2:B:966:SER:OG	2:B:1029:GLY:HA3	2.12	0.49
3:C:99:HIS:CE1	3:C:103:LEU:HD11	2.47	0.49
6:H:101:ALA:HB2	6:H:116:TYR:CZ	2.47	0.49
1:A:102:CYS:HB2	1:A:109:ARG:HG2	1.92	0.49
1:A:672:ASP:HA	1:A:675:SER:HB2	1.93	0.49
1:A:713:VAL:O	1:A:738:ASN:ND2	2.38	0.49
2:B:752:VAL:HA	2:B:979:GLN:O	2.12	0.49
8:J:8:PHE:HB2	8:J:48:ARG:HH22	1.77	0.49
9:K:91:TYR:CD2	9:K:101:LEU:HD11	2.46	0.49
1:A:717:PRO:HG2	1:A:720:PHE:CD1	2.47	0.49
1:A:1299:ASN:HA	1:A:1302:TYR:CZ	2.48	0.49
1:A:1300:ASN:O	1:A:1304:GLU:N	2.35	0.49
1:A:1462:PHE:HD1	1:A:1470:CYS:HB2	1.77	0.49
1:A:1568:ASN:HA	1:A:1571:SER:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:54:GLN:O	4:E:58:MET:HG3	2.13	0.49
11:M:65:TYR:CE1	11:M:97:VAL:HB	2.48	0.49
1:A:363:PRO:HD2	1:A:368:ARG:HD3	1.94	0.49
1:A:833:LEU:O	1:A:944:MET:HE3	2.13	0.49
1:A:1545:ASP:O	1:A:1548:ALA:N	2.44	0.49
2:B:753:LYS:O	2:B:981:SER:N	2.38	0.49
2:B:854:GLU:HG3	2:B:874:TYR:O	2.13	0.49
3:C:51:GLU:HA	3:C:303:GLU:HA	1.94	0.49
1:A:1643:VAL:HB	1:A:1645:LYS:HG2	1.95	0.49
2:B:827:PHE:CD1	2:B:869:THR:HG21	2.48	0.49
2:B:828:GLY:HA3	2:B:862:PHE:CD1	2.48	0.49
4:E:48:ASP:OD1	4:E:51:GLY:N	2.45	0.49
1:A:250:LYS:HD3	1:A:428:VAL:HG22	1.94	0.49
1:A:631:ASP:OD1	1:A:631:ASP:N	2.43	0.49
1:A:945:CYS:C	1:A:946:LEU:CG	2.85	0.49
1:A:1066:PHE:O	1:A:1070:LEU:N	2.43	0.49
1:A:1263:LEU:HG	1:A:1267:ILE:HD11	1.95	0.49
3:C:41:GLU:HB3	3:C:57:ILE:HB	1.95	0.49
1:A:942:GLN:HA	1:A:946:LEU:O	2.12	0.49
1:A:1129:PRO:HA	1:A:1135:SER:HB3	1.94	0.49
2:B:417:ILE:O	2:B:421:LEU:HG	2.11	0.49
2:B:658:LEU:O	2:B:659:ASP:O	2.30	0.49
3:C:86:PHE:HB2	3:C:203:SER:OG	2.13	0.49
6:H:62:SER:OG	6:H:63:LEU:N	2.42	0.49
1:A:219:LEU:O	1:A:223:PHE:N	2.27	0.49
1:A:636:HIS:CB	2:B:1091:ARG:HH22	2.26	0.49
2:B:371:PHE:O	2:B:375:LEU:HG	2.13	0.49
3:C:125:LYS:O	3:C:130:ASN:ND2	2.45	0.49
4:E:82:PHE:HA	4:E:111:VAL:HB	1.95	0.49
1:A:690:GLU:OE1	1:A:690:GLU:N	2.31	0.49
1:A:756:LYS:O	1:A:759:TYR:HD2	1.95	0.49
1:A:1194:GLY:O	1:A:1197:SER:OG	2.23	0.49
2:B:851:TYR:HB2	2:B:881:TYR:CE2	2.48	0.49
4:E:78:LEU:HD12	4:E:107:THR:O	2.12	0.49
2:B:311:ARG:HE	7:I:16:LEU:HD21	1.78	0.48
3:C:241:GLY:N	3:C:263:ASP:OD2	2.46	0.48
7:I:95:ASN:O	7:I:113:THR:N	2.45	0.48
8:J:58:GLU:O	8:J:61:LEU:N	2.44	0.48
1:A:614:LEU:O	1:A:615:ARG:HD2	2.13	0.48
2:B:576:THR:CG2	12:N:95:ILE:CG2	2.91	0.48
4:E:96:PHE:CZ	4:E:110:PHE:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:110:PHE:O	4:E:134:THR:HA	2.12	0.48
7:I:114:CYS:HB3	7:I:119:TYR:N	2.28	0.48
1:A:117:ARG:HB3	1:A:185:ARG:CZ	2.43	0.48
1:A:831:ASP:HB2	1:A:917:MET:CE	2.43	0.48
2:B:985:ILE:O	12:N:160:VAL:HG21	2.12	0.48
4:E:46:TYR:CE1	4:E:58:MET:HA	2.48	0.48
4:E:177:ARG:NE	4:E:179:GLN:HE22	2.11	0.48
7:I:2:SER:HB2	7:I:11:LEU:HD21	1.95	0.48
12:N:111:VAL:HG13	12:N:122:ALA:HB2	1.96	0.48
1:A:659:THR:OG1	1:A:663:GLY:N	2.46	0.48
1:A:1127:TYR:HB3	1:A:1132:TYR:HD2	1.77	0.48
2:B:527:PHE:CE1	2:B:666:PRO:HG3	2.48	0.48
2:B:568:LEU:HD13	2:B:604:ILE:HG23	1.95	0.48
2:B:613:VAL:O	2:B:660:LYS:NZ	2.22	0.48
2:B:1104:CYS:N	2:B:1109:SER:O	2.37	0.48
3:C:64:ALA:O	3:C:67:PHE:N	2.45	0.48
11:M:11:GLU:N	11:M:86:LYS:O	2.36	0.48
1:A:94:LEU:HD12	1:A:355:PHE:HB3	1.95	0.48
1:A:827:THR:HG21	2:B:1026:ILE:HA	1.95	0.48
1:A:1603:MET:SD	1:A:1612:LYS:HA	2.54	0.48
2:B:103:SER:OG	2:B:138:LEU:HB2	2.13	0.48
2:B:168:ASN:OD1	2:B:169:ARG:HG2	2.13	0.48
2:B:176:SER:O	2:B:180:LEU:HG	2.13	0.48
2:B:655:TYR:HD1	2:B:688:HIS:CD2	2.32	0.48
2:B:801:GLY:O	2:B:802:THR:OG1	2.23	0.48
3:C:60:ASP:OD2	3:C:63:ILE:N	2.45	0.48
3:C:237:GLN:HE21	3:C:288:LYS:HG2	1.78	0.48
4:E:98:ILE:O	4:E:102:GLU:N	2.42	0.48
1:A:950:GLN:HE21	1:A:982:VAL:HG21	1.78	0.48
1:A:1189:ALA:HA	1:A:1581:HIS:ND1	2.29	0.48
1:A:1654:PHE:CD2	5:F:92:ARG:HD3	2.49	0.48
2:B:212:ASN:OD1	2:B:238:SER:HA	2.14	0.48
2:B:341:SER:N	2:B:344:GLN:OE1	2.47	0.48
3:C:315:PHE:HB3	3:C:319:ARG:HH12	1.79	0.48
1:A:464:GLU:O	1:A:468:ARG:HD3	2.14	0.48
1:A:884:ARG:NH2	2:B:633:THR:O	2.43	0.48
1:A:1636:SER:O	1:A:1640:ARG:HG2	2.13	0.48
2:B:21:ARG:HA	2:B:24:ARG:HH11	1.78	0.48
2:B:388:GLU:O	2:B:634:ARG:HA	2.13	0.48
2:B:587:GLN:HG2	2:B:592:ILE:HG12	1.94	0.48
3:C:248:GLN:NE2	3:C:256:ILE:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:26:ILE:HD12	6:H:42:ILE:HD12	1.96	0.48
9:K:50:LEU:HB2	9:K:62:SER:HB2	1.95	0.48
1:A:855:ARG:NH1	1:A:868:THR:O	2.45	0.48
1:A:968:SER:HA	2:B:674:ILE:O	2.13	0.48
1:A:1648:ASN:N	1:A:1649:VAL:HB	2.28	0.48
2:B:156:ARG:NE	2:B:455:GLU:OE2	2.36	0.48
3:C:185:VAL:HG12	3:C:186:PRO:O	2.14	0.48
8:J:5:VAL:O	8:J:14:VAL:N	2.44	0.48
1:A:257:ASN:O	1:A:261:ILE:HD12	2.14	0.48
1:A:368:ARG:HA	1:A:380:ASN:HD22	1.78	0.48
1:A:830:MET:HG2	2:B:1027:TYR:CE1	2.49	0.48
1:A:1172:LEU:O	1:A:1176:ARG:N	2.34	0.48
2:B:449:VAL:HG22	2:B:452:ARG:HH21	1.79	0.48
1:A:1052:GLY:HA2	4:E:208:TYR:CE1	2.49	0.48
1:A:1336:GLN:NE2	1:A:1483:LEU:HD21	2.29	0.48
2:B:18:THR:O	2:B:22:GLU:HG2	2.12	0.48
2:B:173:ASN:OD1	2:B:174:LYS:HG3	2.14	0.48
2:B:641:TYR:HB3	2:B:643:PHE:CE2	2.49	0.48
3:C:235:ILE:HA	3:C:289:VAL:HG22	1.95	0.48
1:A:717:PRO:HG2	1:A:720:PHE:CE1	2.49	0.47
1:A:1256:LYS:O	1:A:1259:SER:HB2	2.13	0.47
1:A:1258:ILE:O	1:A:1501:ILE:CG1	2.53	0.47
1:A:1638:SER:O	1:A:1642:VAL:HG23	2.14	0.47
2:B:827:PHE:HE2	2:B:842:GLU:HA	1.79	0.47
2:B:939:SER:OG	2:B:942:GLY:N	2.47	0.47
3:C:34:GLU:OE1	3:C:37:LYS:HD3	2.14	0.47
3:C:154:LYS:HZ3	3:C:161:HIS:H	1.62	0.47
1:A:220:VAL:HA	1:A:223:PHE:HB3	1.95	0.47
1:A:457:LYS:HG3	1:A:1619:CYS:SG	2.54	0.47
1:A:711:LYS:HZ3	9:K:60:SER:HB2	1.79	0.47
1:A:1183:GLU:HA	5:F:88:TYR:OH	2.14	0.47
1:A:1501:ILE:HB	1:A:1504:ILE:CB	2.38	0.47
2:B:13:THR:HG23	12:N:163:VAL:HG22	1.96	0.47
2:B:135:GLY:O	2:B:161:LEU:N	2.36	0.47
2:B:832:TRP:CZ3	2:B:836:TRP:HB2	2.49	0.47
2:B:1019:GLY:O	3:C:227:TYR:OH	2.32	0.47
8:J:36:LEU:HD21	8:J:50:ILE:HG21	1.95	0.47
1:A:253:GLU:N	1:A:313:THR:O	2.38	0.47
1:A:516:ILE:O	1:A:520:ARG:HG3	2.14	0.47
1:A:848:LYS:O	1:A:851:VAL:HG23	2.14	0.47
1:A:1451:ILE:HG12	1:A:1457:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:40:PHE:CE2	9:K:131:VAL:HG22	2.50	0.47
3:C:86:PHE:HB3	10:L:62:LYS:HE3	1.95	0.47
4:E:99:HIS:HA	4:E:102:GLU:CD	2.39	0.47
5:F:110:ASP:O	5:F:123:LYS:NZ	2.33	0.47
9:K:54:THR:HG22	9:K:61:ALA:HA	1.96	0.47
1:A:671:GLN:HB2	2:B:783:MET:HE3	1.95	0.47
1:A:977:MET:HB2	1:A:983:LYS:NZ	2.29	0.47
1:A:1034:TYR:CZ	5:F:136:ARG:HB3	2.49	0.47
1:A:1317:ILE:O	1:A:1322:ILE:HG12	2.14	0.47
1:A:1326:GLU:OE2	1:A:1457:ILE:HG13	2.14	0.47
2:B:641:TYR:HB3	2:B:643:PHE:HE2	1.80	0.47
2:B:800:TYR:HE2	3:C:96:VAL:HG22	1.79	0.47
2:B:824:HIS:NE2	2:B:864:ASP:OD2	2.46	0.47
3:C:113:LEU:HD11	3:C:131:THR:N	2.29	0.47
2:B:284:SER:HB2	7:I:14:GLY:HA3	1.95	0.47
2:B:421:LEU:HA	2:B:424:ILE:HD12	1.97	0.47
4:E:13:TRP:CD1	4:E:39:LEU:HA	2.49	0.47
6:H:93:TYR:CD2	6:H:143:LEU:HD23	2.49	0.47
6:H:100:THR:OG1	6:H:139:ASN:OD1	2.22	0.47
10:L:29:TYR:HD1	10:L:58:LYS:HA	1.79	0.47
10:L:41:SER:N	10:L:44:ASP:OD2	2.25	0.47
1:A:523:VAL:HG21	1:A:561:LEU:HD11	1.97	0.47
1:A:1256:LYS:HD3	1:A:1305:GLU:O	2.14	0.47
2:B:335:ARG:HG3	2:B:340:ALA:HB3	1.96	0.47
2:B:449:VAL:HG22	2:B:452:ARG:NH2	2.30	0.47
2:B:611:TRP:C	2:B:620:LEU:HD21	2.40	0.47
3:C:154:LYS:HZ3	3:C:161:HIS:N	2.12	0.47
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.97	0.47
1:A:49:LEU:HD22	1:A:386:LEU:HD13	1.94	0.47
1:A:114:GLU:OE1	1:A:117:ARG:HD3	2.14	0.47
1:A:380:ASN:HB3	1:A:383:ASN:ND2	2.29	0.47
1:A:437:PHE:HD2	1:A:438:ILE:HG13	1.79	0.47
1:A:517:ALA:HA	1:A:520:ARG:HD3	1.96	0.47
1:A:885:ASP:CG	1:A:888:LYS:H	2.22	0.47
1:A:1049:MET:HB3	4:E:208:TYR:CE1	2.47	0.47
1:A:1482:LYS:HB3	2:B:308:LEU:HD21	1.96	0.47
1:A:1545:ASP:O	1:A:1547:ALA:N	2.48	0.47
2:B:382:TYR:O	2:B:386:ALA:N	2.29	0.47
2:B:745:GLN:CB	2:B:800:TYR:HB3	2.45	0.47
2:B:810:ASP:HB2	2:B:900:THR:HG23	1.95	0.47
2:B:861:TYR:CE2	2:B:870:LYS:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:943:ILE:O	2:B:945:PRO:HD3	2.15	0.47
2:B:1105:ARG:N	2:B:1172:GLU:O	2.47	0.47
2:B:1152:PHE:HZ	14:G:235:ASN:OD1	1.97	0.47
3:C:162:VAL:N	3:C:194:ALA:O	2.47	0.47
3:C:232:GLN:O	3:C:292:GLY:N	2.47	0.47
3:C:284:GLU:HG3	3:C:285:PHE:N	2.29	0.47
9:K:72:LEU:O	9:K:76:LEU:N	2.34	0.47
1:A:476:VAL:N	2:B:1069:ILE:O	2.41	0.47
1:A:852:ASP:OD2	1:A:855:ARG:NH2	2.47	0.47
2:B:172:LEU:HA	2:B:175:MET:SD	2.55	0.47
2:B:286:ARG:HD3	7:I:9:PHE:CG	2.49	0.47
2:B:472:SER:OG	2:B:474:SER:O	2.33	0.47
2:B:1053:ASN:OD1	2:B:1055:LEU:N	2.47	0.47
3:C:60:ASP:HB2	9:K:78:TYR:CZ	2.50	0.47
7:I:38:PRO:HD2	7:I:41:GLN:OE1	2.15	0.47
14:G:137:ILE:HG13	14:G:227:GLY:O	2.13	0.47
1:A:51:ASP:OD1	1:A:52:LEU:N	2.48	0.47
1:A:838:GLU:HA	1:A:841:LYS:HB3	1.97	0.47
2:B:146:ASN:HB2	2:B:149:GLU:HB3	1.96	0.47
2:B:648:ARG:O	2:B:650:LEU:HG	2.15	0.47
2:B:894:LYS:O	2:B:895:PHE:CD2	2.68	0.47
1:A:24:ILE:HG21	1:A:359:VAL:HG21	1.97	0.47
1:A:512:THR:OG1	1:A:515:ASN:OD1	2.20	0.47
2:B:103:SER:O	2:B:137:LEU:HD12	2.15	0.47
2:B:228:SER:O	2:B:254:ASN:N	2.33	0.47
2:B:399:HIS:O	2:B:400:GLN:HG3	2.15	0.47
2:B:921:HIS:NE2	2:B:962:MET:HA	2.29	0.47
3:C:231:PRO:HG2	3:C:270:ALA:HB1	1.96	0.47
6:H:10:PHE:HB3	6:H:28:ALA:HB1	1.96	0.47
7:I:2:SER:O	7:I:8:ILE:HA	2.15	0.47
13:D:46:GLU:OE1	13:D:47:LYS:HE2	2.15	0.47
1:A:175:SER:HA	1:A:178:LEU:HD12	1.97	0.46
1:A:781:LEU:HB3	1:A:786:TYR:HE2	1.79	0.46
1:A:1094:ALA:O	1:A:1098:SER:N	2.36	0.46
2:B:1119:ARG:NH2	2:B:1160:GLU:OE2	2.48	0.46
2:B:1152:PHE:CE2	14:G:129:VAL:HG21	2.51	0.46
3:C:78:VAL:HA	3:C:209:ILE:O	2.16	0.46
3:C:161:HIS:CD2	3:C:195:LYS:HG2	2.50	0.46
3:C:262:SER:O	3:C:264:GLU:HG3	2.15	0.46
4:E:118:PRO:O	4:E:121:MET:HB2	2.14	0.46
9:K:91:TYR:HD2	9:K:101:LEU:HD11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:GLN:HE22	1:A:350:VAL:N	2.13	0.46
1:A:440:SER:H	1:A:458:GLN:NE2	2.03	0.46
1:A:672:ASP:O	1:A:676:ALA:N	2.46	0.46
1:A:681:THR:HG21	1:A:781:LEU:HG	1.97	0.46
1:A:1034:TYR:CE2	5:F:136:ARG:HB3	2.51	0.46
1:A:1539:ASP:HA	4:E:147:HIS:CD2	2.50	0.46
2:B:726:MET:HE2	2:B:742:TYR:HB3	1.97	0.46
2:B:822:THR:HG22	2:B:823:GLN:HG3	1.97	0.46
2:B:894:LYS:C	2:B:896:GLN:N	2.72	0.46
2:B:929:ARG:HG2	2:B:931:TRP:HE3	1.80	0.46
3:C:136:LEU:HB3	3:C:204:LEU:HD11	1.98	0.46
3:C:137:ASN:HA	3:C:202:ILE:O	2.14	0.46
4:E:40:GLU:H	4:E:40:GLU:CD	2.22	0.46
9:K:66:VAL:HG12	9:K:67:GLU:N	2.31	0.46
1:A:641:GLU:OE1	1:A:644:ARG:HD3	2.15	0.46
1:A:781:LEU:HB3	1:A:786:TYR:CE2	2.50	0.46
5:F:57:ASP:O	5:F:61:HIS:N	2.34	0.46
8:J:18:TRP:CH2	8:J:22:LEU:HD21	2.51	0.46
1:A:91:PHE:HE2	1:A:245:LYS:HD2	1.80	0.46
1:A:261:ILE:O	1:A:265:ARG:HG2	2.15	0.46
1:A:267:LYS:HA	1:A:270:ILE:HD12	1.97	0.46
1:A:487:ASP:HA	2:B:781:TYR:HE1	1.80	0.46
1:A:943:ILE:HG12	1:A:986:PHE:CD2	2.51	0.46
1:A:1113:HIS:HA	1:A:1116:GLN:HG2	1.97	0.46
2:B:677:THR:OG1	2:B:680:GLU:HG3	2.15	0.46
2:B:693:PRO:O	2:B:696:ILE:HG12	2.15	0.46
2:B:1152:PHE:HZ	14:G:235:ASN:CG	2.22	0.46
3:C:308:MET:SD	3:C:316:LYS:NZ	2.86	0.46
4:E:90:VAL:O	4:E:94:LYS:N	2.35	0.46
4:E:163:GLU:O	4:E:167:ARG:N	2.44	0.46
4:E:197:LYS:HA	4:E:211:TYR:CE1	2.50	0.46
8:J:34:THR:HA	8:J:37:SER:HB2	1.96	0.46
1:A:108:PHE:CE2	1:A:331:GLU:HG3	2.50	0.46
1:A:842:TRP:CD2	1:A:910:LYS:NZ	2.74	0.46
1:A:842:TRP:CE3	1:A:910:LYS:HG2	2.50	0.46
1:A:1272:VAL:HG22	1:A:1292:ILE:HG23	1.98	0.46
2:B:65:VAL:HA	2:B:68:ILE:HD12	1.97	0.46
2:B:190:ILE:HD11	2:B:496:PHE:CE2	2.51	0.46
2:B:202:LEU:O	2:B:486:VAL:HG12	2.15	0.46
2:B:377:MET:O	2:B:381:LEU:N	2.35	0.46
3:C:131:THR:O	3:C:175:GLN:NE2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:91:ASN:HD22	7:I:116:SER:N	2.13	0.46
1:A:64:THR:HB	1:A:75:HIS:CD2	2.51	0.46
1:A:141:LEU:HD21	1:A:184:LYS:HZ2	1.79	0.46
1:A:572:THR:HA	14:G:52:MET:HE1	1.97	0.46
1:A:1311:GLU:O	1:A:1315:ASN:N	2.29	0.46
1:A:1311:GLU:OE1	1:A:1311:GLU:N	2.38	0.46
1:A:1322:ILE:O	1:A:1325:LEU:N	2.46	0.46
2:B:246:GLN:NE2	2:B:247:THR:H	2.14	0.46
2:B:489:GLU:HB3	2:B:491:ILE:HG12	1.98	0.46
3:C:162:VAL:O	3:C:192:LEU:HD12	2.15	0.46
4:E:48:ASP:CG	4:E:50:MET:HB3	2.41	0.46
13:D:33:THR:HG23	13:D:96:PHE:HD1	1.80	0.46
1:A:544:VAL:HG13	1:A:549:MET:HE1	1.97	0.46
1:A:551:VAL:HG22	1:A:554:ARG:NH2	2.31	0.46
1:A:694:GLN:O	1:A:698:GLY:N	2.39	0.46
1:A:1100:LYS:HG2	1:A:1104:TYR:CE2	2.51	0.46
2:B:102:VAL:HA	2:B:139:LEU:HD23	1.97	0.46
2:B:322:ASN:OD1	2:B:323:ARG:N	2.49	0.46
2:B:749:THR:O	2:B:770:ASN:ND2	2.48	0.46
2:B:859:CYS:SG	2:B:860:ALA:N	2.88	0.46
2:B:1110:ILE:O	2:B:1113:THR:OG1	2.19	0.46
3:C:57:ILE:HG22	3:C:58:ASN:ND2	2.30	0.46
4:E:93:MET:HG2	4:E:120:ALA:HB1	1.98	0.46
1:A:719:ILE:HG12	6:H:97:MET:CG	2.40	0.46
1:A:756:LYS:HB2	1:A:759:TYR:CE2	2.50	0.46
1:A:831:ASP:N	1:A:831:ASP:OD1	2.49	0.46
1:A:1034:TYR:OH	1:A:1653:SER:O	2.33	0.46
1:A:1229:ALA:CB	1:A:1597:ALA:HB2	2.46	0.46
1:A:1312:GLU:O	1:A:1316:VAL:N	2.26	0.46
1:A:1570:PHE:O	1:A:1574:ALA:N	2.49	0.46
2:B:321:GLN:HB3	7:I:32:GLN:NE2	2.31	0.46
2:B:889:GLY:HA3	10:L:54:ARG:HB3	1.96	0.46
8:J:16:ASP:OD1	8:J:17:LYS:N	2.48	0.46
1:A:478:TYR:CE1	2:B:1048:SER:HB2	2.51	0.46
1:A:880:GLN:HE22	2:B:633:THR:H	1.63	0.46
1:A:1657:LEU:HD11	5:F:135:ARG:HB2	1.98	0.46
2:B:445:TYR:HA	2:B:448:ARG:NH1	2.31	0.46
2:B:712:SER:N	2:B:713:PRO:HD2	2.30	0.46
4:E:136:ASN:HB3	4:E:139:ALA:HB3	1.98	0.46
1:A:131:ASP:HA	1:A:134:TYR:CD2	2.47	0.46
1:A:907:VAL:HG12	1:A:945:CYS:HG	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:PRO:HG2	2:B:178:TYR:HD1	1.80	0.46
2:B:699:ILE:N	16:B:1301:SO4:S	2.88	0.46
1:A:314:TYR:CE2	1:A:316:LEU:HA	2.50	0.45
1:A:435:ASN:O	1:A:439:ASP:N	2.48	0.45
1:A:985:ARG:HG3	1:A:988:SER:H	1.81	0.45
1:A:1039:ARG:HD2	1:A:1043:GLY:O	2.17	0.45
2:B:322:ASN:HB3	2:B:325:GLN:CG	2.46	0.45
2:B:501:ARG:HH22	2:B:549:CYS:HB3	1.82	0.45
2:B:576:THR:HG21	12:N:95:ILE:HG22	1.98	0.45
5:F:109:VAL:HG22	5:F:110:ASP:H	1.82	0.45
11:M:65:TYR:HE1	11:M:97:VAL:HB	1.81	0.45
1:A:125:LEU:C	1:A:128:GLY:H	2.24	0.45
1:A:741:PRO:HA	1:A:742:PRO:HD3	1.86	0.45
1:A:943:ILE:CD1	2:B:958:MET:HB3	2.42	0.45
2:B:658:LEU:HD13	2:B:658:LEU:H	1.79	0.45
2:B:814:ASN:OD1	2:B:815:ARG:N	2.50	0.45
3:C:31:TRP:CH2	3:C:33:VAL:HA	2.52	0.45
3:C:325:ALA:O	3:C:329:LYS:N	2.25	0.45
8:J:17:LYS:HD3	8:J:39:LEU:HB3	1.97	0.45
11:M:26:PHE:CE1	11:M:98:SER:HB2	2.51	0.45
1:A:324:LEU:O	1:A:328:PHE:N	2.27	0.45
1:A:367:PHE:CD1	2:B:1184:TYR:HD1	2.34	0.45
1:A:1263:LEU:C	1:A:1265:GLU:N	2.74	0.45
1:A:1550:LEU:HA	1:A:1554:GLY:O	2.16	0.45
2:B:301:PHE:O	2:B:305:ARG:HG2	2.16	0.45
2:B:756:LEU:HD23	2:B:759:ASP:OD2	2.15	0.45
2:B:857:PRO:HB3	2:B:871:ILE:HD11	1.99	0.45
5:F:77:ASP:OD1	5:F:78:GLN:N	2.50	0.45
1:A:588:LEU:HD11	1:A:600:MET:HG2	1.99	0.45
1:A:826:PHE:HA	2:B:1023:ARG:HH22	1.82	0.45
1:A:1302:TYR:O	1:A:1306:TYR:N	2.48	0.45
2:B:307:GLU:OE1	7:I:7:LEU:HD11	2.17	0.45
2:B:1099:THR:OG1	2:B:1180:PHE:HB2	2.16	0.45
2:B:1105:ARG:NH1	2:B:1172:GLU:OE1	2.49	0.45
9:K:77:ARG:HD2	9:K:91:TYR:CE1	2.52	0.45
9:K:92:SER:O	9:K:101:LEU:HD12	2.17	0.45
1:A:460:LEU:HB3	1:A:1618:THR:HG21	1.97	0.45
1:A:1504:ILE:HD13	1:A:1529:MET:CE	2.45	0.45
2:B:286:ARG:O	2:B:290:ASP:N	2.26	0.45
2:B:649:MET:O	2:B:666:PRO:HD3	2.17	0.45
2:B:921:HIS:CD2	2:B:962:MET:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1053:ASN:OD1	2:B:1054:SER:N	2.49	0.45
4:E:29:PHE:HB2	4:E:65:THR:HG22	1.97	0.45
5:F:57:ASP:HA	5:F:60:GLN:HB3	1.98	0.45
1:A:697:TYR:HE2	9:K:91:TYR:C	2.24	0.45
1:A:706:HIS:CD2	1:A:808:LYS:HD3	2.51	0.45
1:A:904:THR:C	1:A:906:GLN:H	2.25	0.45
1:A:1061:SER:OG	1:A:1062:HIS:N	2.49	0.45
2:B:468:GLY:HA2	2:B:485:THR:HG23	1.98	0.45
3:C:152:ASP:O	3:C:156:LEU:HG	2.16	0.45
3:C:154:LYS:HE2	3:C:161:HIS:CE1	2.51	0.45
6:H:80:ARG:HG3	9:K:108:TYR:CZ	2.52	0.45
1:A:23:GLU:O	1:A:27:LEU:HG	2.17	0.45
1:A:1294:MET:HE2	1:A:1472:PHE:HE2	1.82	0.45
2:B:31:ASP:OD1	2:B:32:LYS:N	2.43	0.45
2:B:263:SER:HA	2:B:268:GLU:HA	1.98	0.45
2:B:527:PHE:CZ	2:B:666:PRO:HG3	2.51	0.45
2:B:968:ALA:HA	2:B:971:ALA:HB3	1.99	0.45
4:E:79:TRP:HB2	4:E:105:PHE:CE1	2.51	0.45
8:J:7:CYS:HA	8:J:49:MET:HG3	1.98	0.45
1:A:418:VAL:O	1:A:422:ARG:HG2	2.17	0.45
1:A:855:ARG:NH1	1:A:866:LYS:O	2.50	0.45
1:A:1024:THR:HG22	1:A:1190:SER:HB3	1.99	0.45
1:A:1124:LEU:HD23	1:A:1135:SER:OG	2.17	0.45
2:B:96:SER:N	2:B:144:SER:O	2.44	0.45
2:B:427:GLN:HG2	2:B:449:VAL:HG13	1.99	0.45
2:B:443:LYS:O	2:B:446:MET:HB3	2.17	0.45
2:B:772:VAL:O	2:B:946:ASP:HB2	2.17	0.45
2:B:1182:LEU:HA	2:B:1185:LEU:HB3	1.98	0.45
3:C:239:ILE:HD11	3:C:288:LYS:HB2	1.99	0.45
5:F:108:PHE:CE2	5:F:131:PRO:HG3	2.49	0.45
6:H:40:LEU:HD23	6:H:42:ILE:HD11	1.98	0.45
1:A:15:ASP:N	2:B:1197:ARG:O	2.30	0.45
1:A:316:LEU:HB2	1:A:319:GLU:HG3	1.98	0.45
1:A:475:ARG:NH2	2:B:1070:ARG:HH22	2.15	0.45
1:A:831:ASP:HB2	1:A:917:MET:HE1	1.99	0.45
1:A:1654:PHE:HE1	5:F:134:ILE:HG12	1.81	0.45
2:B:128:GLN:NE2	2:B:735:HIS:O	2.50	0.45
2:B:336:VAL:C	2:B:339:GLN:H	2.25	0.45
2:B:537:SER:N	2:B:538:PRO:HD2	2.32	0.45
3:C:240:LYS:HB3	3:C:264:GLU:CG	2.46	0.45
1:A:92:ASN:O	1:A:96:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:MET:O	1:A:428:VAL:HG23	2.17	0.45
1:A:1056:ASP:OD2	1:A:1058:THR:OG1	2.28	0.45
1:A:1580:ARG:NH2	4:E:204:THR:HG21	2.31	0.45
2:B:46:ILE:HD12	2:B:46:ILE:H	1.82	0.45
2:B:750:PRO:HB3	2:B:1032:TYR:CD1	2.52	0.45
7:I:2:SER:HA	7:I:9:PHE:H	1.82	0.45
1:A:208:PHE:HE2	1:A:1607:THR:HG23	1.80	0.44
1:A:1187:ILE:HG13	2:B:1080:ILE:HG22	1.99	0.44
2:B:30:LYS:HG2	2:B:178:TYR:CG	2.52	0.44
2:B:555:GLN:HB2	2:B:646:HIS:CE1	2.51	0.44
2:B:827:PHE:HD1	2:B:869:THR:HG21	1.82	0.44
3:C:58:ASN:HA	3:C:296:ASN:HB3	1.99	0.44
8:J:18:TRP:CE2	8:J:22:LEU:HD11	2.52	0.44
9:K:66:VAL:O	9:K:68:GLU:HG2	2.17	0.44
14:G:17:ILE:C	14:G:19:LYS:H	2.25	0.44
1:A:106:HIS:HB2	1:A:330:LYS:HE3	1.99	0.44
1:A:753:ASN:ND2	1:A:766:GLU:O	2.50	0.44
1:A:907:VAL:C	1:A:945:CYS:SG	3.00	0.44
1:A:1040:ASP:HB3	1:A:1042:ASP:OD1	2.17	0.44
4:E:46:TYR:HA	4:E:57:MET:HE3	1.97	0.44
5:F:66:ARG:HA	5:F:69:LEU:CD1	2.34	0.44
5:F:144:GLU:OE1	5:F:146:TRP:NE1	2.40	0.44
6:H:98:TYR:HD1	6:H:141:TYR:CD1	2.35	0.44
1:A:920:PHE:CD1	1:A:921:PRO:HA	2.52	0.44
2:B:106:LYS:HE2	2:B:168:ASN:O	2.17	0.44
2:B:371:PHE:CE2	2:B:375:LEU:HD11	2.53	0.44
2:B:372:ARG:HH21	2:B:574:SER:HA	1.83	0.44
2:B:692:THR:H	2:B:695:ASN:ND2	2.16	0.44
2:B:709:PHE:CE2	2:B:992:PRO:HG2	2.52	0.44
2:B:938:PHE:CZ	2:B:1014:TYR:HB2	2.51	0.44
3:C:36:PHE:CE1	3:C:40:PHE:HB2	2.52	0.44
3:C:319:ARG:NH2	9:K:132:GLU:OE2	2.51	0.44
4:E:88:VAL:HB	4:E:116:ILE:HA	1.99	0.44
9:K:116:ALA:O	9:K:120:GLY:N	2.36	0.44
1:A:12:THR:HG21	2:B:1201:GLU:CD	2.43	0.44
1:A:659:THR:HG23	1:A:664:SER:O	2.17	0.44
1:A:1527:GLN:H	1:A:1527:GLN:CD	2.24	0.44
2:B:218:ILE:HA	2:B:231:HIS:O	2.17	0.44
2:B:286:ARG:HD2	2:B:286:ARG:HA	1.75	0.44
2:B:854:GLU:OE1	2:B:877:SER:HA	2.17	0.44
2:B:999:GLN:O	2:B:1003:ALA:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ASP:OD2	1:A:43:HIS:HB2	2.17	0.44
1:A:79:ILE:HB	1:A:360:LEU:HB2	1.99	0.44
1:A:771:PHE:CD1	1:A:776:LEU:HA	2.52	0.44
1:A:1000:MET:HG3	2:B:520:LEU:HD23	1.98	0.44
1:A:1158:SER:OG	1:A:1159:ASP:N	2.50	0.44
2:B:968:ALA:HB2	2:B:996:PHE:CE1	2.52	0.44
3:C:326:GLU:HB2	9:K:125:MET:HE3	1.99	0.44
4:E:17:ARG:HH12	4:E:36:GLU:HA	1.82	0.44
4:E:112:TYR:CD2	4:E:116:ILE:HD11	2.52	0.44
6:H:48:PRO:O	6:H:146:ARG:NH2	2.50	0.44
1:A:21:ALA:HA	1:A:24:ILE:HD12	2.00	0.44
1:A:1233:ILE:HD11	1:A:1236:PRO:HA	1.99	0.44
2:B:228:SER:O	2:B:254:ASN:ND2	2.50	0.44
2:B:442:ASP:HB3	2:B:445:TYR:HB3	1.99	0.44
2:B:705:PRO:HB2	2:B:706:PHE:HD2	1.82	0.44
3:C:114:THR:OG1	3:C:129:GLU:O	2.35	0.44
3:C:332:PRO:HG2	9:K:44:ARG:HA	1.99	0.44
8:J:28:ASP:HB3	8:J:30:LEU:HG	2.00	0.44
1:A:237:GLY:HA3	1:A:267:LYS:HE2	1.99	0.44
1:A:507:TYR:O	1:A:578:TYR:HA	2.18	0.44
1:A:1316:VAL:HG13	1:A:1320:GLN:HE21	1.82	0.44
2:B:683:ASN:O	2:B:685:VAL:HG23	2.17	0.44
2:B:1152:PHE:CZ	14:G:235:ASN:OD1	2.71	0.44
2:B:1159:TRP:CE2	2:B:1167:PHE:HB2	2.53	0.44
9:K:50:LEU:HB2	9:K:62:SER:CB	2.47	0.44
9:K:133:SER:O	9:K:137:GLU:HG3	2.17	0.44
10:L:33:GLU:HB3	10:L:53:HIS:CD2	2.52	0.44
1:A:552:GLU:HA	1:A:555:LYS:HB2	1.98	0.44
1:A:842:TRP:CE3	1:A:910:LYS:CG	3.00	0.44
1:A:842:TRP:O	1:A:845:ASP:N	2.51	0.44
2:B:104:ILE:O	2:B:169:ARG:NE	2.51	0.44
2:B:275:MET:SD	2:B:330:LEU:HD21	2.58	0.44
2:B:428:VAL:O	2:B:431:ASP:HB2	2.17	0.44
3:C:68:ARG:CD	3:C:227:TYR:CE2	3.00	0.44
3:C:123:ASP:N	3:C:123:ASP:OD1	2.49	0.44
9:K:83:ASN:OD1	9:K:85:ASP:N	2.51	0.44
1:A:336:GLN:O	1:A:340:HIS:ND1	2.50	0.44
2:B:35:PHE:CE1	2:B:761:GLY:HA3	2.53	0.44
2:B:861:TYR:CE1	2:B:872:LYS:HE2	2.53	0.44
2:B:908:ARG:HD2	3:C:95:GLU:HG3	1.99	0.44
3:C:57:ILE:HG13	3:C:297:HIS:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:18:TRP:CZ2	8:J:22:LEU:HD21	2.53	0.44
9:K:69:ASP:N	9:K:69:ASP:OD1	2.51	0.44
1:A:95:TYR:CD2	1:A:245:LYS:HD3	2.53	0.43
1:A:132:GLU:CD	1:A:132:GLU:H	2.24	0.43
1:A:960:MET:HG2	2:B:523:GLU:OE2	2.18	0.43
1:A:1200:MET:HE2	1:A:1573:TYR:HB2	2.00	0.43
3:C:73:SER:OG	3:C:74:GLU:HG3	2.18	0.43
3:C:95:GLU:O	3:C:99:HIS:N	2.36	0.43
3:C:140:CYS:HA	3:C:158:ASN:O	2.18	0.43
4:E:54:GLN:HB2	4:E:57:MET:HE2	1.99	0.43
4:E:177:ARG:CZ	4:E:179:GLN:HE22	2.31	0.43
1:A:117:ARG:NH2	1:A:137:ASP:OD2	2.49	0.43
1:A:461:GLU:C	1:A:465:GLY:HA2	2.43	0.43
1:A:525:ASN:ND2	1:A:531:PRO:O	2.45	0.43
1:A:996:TYR:CZ	2:B:520:LEU:HD21	2.53	0.43
1:A:1537:ASP:OD1	1:A:1538:VAL:N	2.51	0.43
2:B:676:VAL:HB	2:B:680:GLU:OE2	2.18	0.43
2:B:1056:THR:O	2:B:1058:GLN:HG3	2.18	0.43
2:B:1102:SER:OG	2:B:1175:THR:HG22	2.17	0.43
3:C:243:SER:N	3:C:246:ARG:HH21	2.15	0.43
4:E:20:LYS:NZ	4:E:34:GLU:HG2	2.33	0.43
6:H:12:VAL:HG11	6:H:15:VAL:HG23	1.99	0.43
8:J:17:LYS:O	8:J:21:TYR:N	2.40	0.43
14:G:163:PRO:HG2	14:G:166:TRP:CD1	2.52	0.43
1:A:31:GLN:HB2	1:A:78:HIS:CE1	2.53	0.43
1:A:32:ILE:HD12	1:A:48:GLY:O	2.18	0.43
1:A:352:ALA:HA	1:A:355:PHE:CD2	2.52	0.43
1:A:440:SER:N	1:A:458:GLN:HE22	2.06	0.43
4:E:67:GLU:HA	4:E:70:SER:OG	2.18	0.43
7:I:19:ASN:O	7:I:23:VAL:HG23	2.18	0.43
11:M:8:SER:O	12:N:71:PRO:HA	2.19	0.43
1:A:389:VAL:HG22	1:A:433:ASP:HB3	2.00	0.43
1:A:711:LYS:NZ	9:K:60:SER:HB2	2.33	0.43
1:A:1641:ILE:C	1:A:1644:GLY:H	2.25	0.43
2:B:840:LEU:HD13	2:B:860:ALA:HB2	2.01	0.43
3:C:216:HIS:CD2	10:L:70:ARG:HE	2.36	0.43
1:A:27:LEU:O	2:B:1129:ARG:HD2	2.18	0.43
1:A:506:THR:HA	1:A:579:ARG:O	2.19	0.43
1:A:1500:GLN:C	1:A:1501:ILE:HD13	2.44	0.43
2:B:208:VAL:O	2:B:401:GLU:N	2.41	0.43
6:H:26:ILE:O	6:H:40:LEU:N	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:ILE:O	1:A:735:VAL:HB	2.17	0.43
1:A:1195:GLU:HB3	1:A:1196:PRO:HD3	2.00	0.43
2:B:222:PHE:HB2	2:B:231:HIS:HA	1.99	0.43
2:B:361:HIS:CE1	2:B:362:LEU:HG	2.54	0.43
2:B:464:PHE:O	2:B:468:GLY:N	2.50	0.43
2:B:587:GLN:HE21	2:B:592:ILE:HG12	1.84	0.43
2:B:698:SER:HB2	16:B:1301:SO4:O3	2.18	0.43
3:C:240:LYS:HA	3:C:244:ALA:HB2	1.99	0.43
4:E:42:PHE:O	4:E:46:TYR:N	2.50	0.43
4:E:55:ARG:HD2	4:E:82:PHE:HB3	1.99	0.43
4:E:79:TRP:HE1	4:E:81:GLU:HB2	1.83	0.43
1:A:507:TYR:CD1	1:A:508:PRO:HD2	2.54	0.43
1:A:1162:ASN:ND2	1:A:1164:LYS:HB2	2.34	0.43
2:B:181:VAL:HG13	8:J:63:TYR:HE1	1.83	0.43
2:B:315:LYS:HE3	2:B:315:LYS:HB3	1.83	0.43
2:B:343:ASP:OD1	2:B:344:GLN:HG3	2.18	0.43
2:B:650:LEU:HD22	2:B:663:ILE:HG22	2.00	0.43
4:E:40:GLU:HA	4:E:43:LYS:CE	2.49	0.43
5:F:146:TRP:HA	5:F:150:GLU:OE2	2.18	0.43
9:K:63:PHE:O	9:K:102:ASN:HA	2.19	0.43
1:A:265:ARG:C	1:A:268:GLY:H	2.27	0.43
1:A:589:MET:SD	1:A:635:MET:HA	2.59	0.43
1:A:975:ASP:OD1	1:A:977:MET:N	2.48	0.43
1:A:1303:SER:O	1:A:1307:ASP:HA	2.18	0.43
1:A:1501:ILE:CG2	1:A:1502:PRO:CD	2.94	0.43
2:B:1073:GLU:HB3	2:B:1076:ARG:HH21	1.83	0.43
2:B:1128:CYS:SG	2:B:1130:ARG:HB3	2.59	0.43
4:E:78:LEU:HD21	4:E:109:ILE:HD12	2.00	0.43
1:A:446:ARG:NH2	1:A:450:LYS:HB3	2.33	0.43
1:A:449:GLY:C	1:A:451:VAL:H	2.27	0.43
2:B:718:GLN:O	2:B:721:MET:N	2.52	0.43
2:B:1134:ARG:HD3	2:B:1167:PHE:CE1	2.52	0.43
3:C:60:ASP:HB3	3:C:63:ILE:CD1	2.49	0.43
1:A:12:THR:O	1:A:1634:LEU:HD12	2.18	0.43
1:A:735:VAL:O	1:A:739:VAL:HG22	2.19	0.43
1:A:1108:HIS:O	1:A:1111:GLU:HG2	2.18	0.43
1:A:1148:LEU:HB3	1:A:1163:GLU:OE2	2.18	0.43
1:A:1148:LEU:HD22	1:A:1163:GLU:HG3	2.01	0.43
1:A:1263:LEU:CB	1:A:1496:SER:CB	2.97	0.43
2:B:57:ASP:HB2	2:B:63:LEU:HD11	2.01	0.43
2:B:552:SER:O	2:B:647:SER:N	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:910:THR:HB	2:B:911:PRO:HD2	2.00	0.43
3:C:123:ASP:OD1	3:C:124:GLU:N	2.49	0.43
3:C:311:GLU:HG2	3:C:312:GLU:N	2.33	0.43
12:N:81:THR:HG22	12:N:86:ASP:HB3	2.01	0.43
1:A:53:ALA:O	1:A:64:THR:OG1	2.26	0.42
1:A:510:PRO:HA	1:A:576:LYS:HG2	2.01	0.42
1:A:522:ALA:HA	1:A:525:ASN:HB2	2.01	0.42
1:A:805:VAL:O	1:A:809:VAL:HG23	2.19	0.42
1:A:1463:ASP:HB2	1:A:1469:TRP:CD1	2.54	0.42
1:A:1510:PRO:HG3	1:A:1520:VAL:HG23	2.01	0.42
1:A:1511:GLU:OE1	7:I:73:LYS:HD2	2.20	0.42
2:B:345:SER:O	2:B:349:VAL:HG23	2.19	0.42
2:B:501:ARG:NH2	2:B:549:CYS:HB3	2.34	0.42
2:B:700:LEU:HD13	16:B:1301:SO4:O1	2.19	0.42
4:E:159:ASP:HA	4:E:162:ARG:HG2	2.00	0.42
8:J:7:CYS:HB3	8:J:10:CYS:HB2	1.99	0.42
1:A:731:ILE:O	1:A:735:VAL:HG23	2.19	0.42
1:A:950:GLN:HE21	1:A:982:VAL:CG2	2.32	0.42
1:A:1657:LEU:HB2	5:F:133:VAL:O	2.20	0.42
2:B:156:ARG:CZ	2:B:450:LEU:HD13	2.49	0.42
2:B:282:HIS:N	2:B:323:ARG:HD2	2.34	0.42
2:B:698:SER:OG	16:B:1301:SO4:O4	2.23	0.42
3:C:37:LYS:HG3	9:K:130:VAL:HG13	2.00	0.42
3:C:60:ASP:HB3	3:C:63:ILE:HD12	2.01	0.42
3:C:137:ASN:OD1	3:C:203:SER:HA	2.19	0.42
3:C:213:GLY:HA2	3:C:216:HIS:O	2.19	0.42
4:E:68:SER:HB3	4:E:75:MET:SD	2.59	0.42
5:F:57:ASP:OD1	5:F:58:PHE:N	2.47	0.42
14:G:160:ASN:OD1	14:G:160:ASN:N	2.52	0.42
1:A:875:LEU:O	1:A:879:LEU:HG	2.19	0.42
1:A:908:VAL:CG1	1:A:941:SER:HB2	2.49	0.42
1:A:1442:VAL:O	1:A:1446:ARG:N	2.29	0.42
1:A:1559:ARG:HG3	1:A:1586:ALA:HB1	2.01	0.42
2:B:407:PHE:O	2:B:411:MET:HG3	2.19	0.42
2:B:789:ILE:HD12	2:B:927:CYS:SG	2.58	0.42
4:E:182:ASP:OD2	4:E:184:VAL:HB	2.19	0.42
7:I:20:PRO:O	7:I:39:LYS:NZ	2.52	0.42
7:I:84:GLU:HG2	7:I:94:MET:HB2	2.01	0.42
9:K:55:SER:N	9:K:60:SER:O	2.37	0.42
12:N:78:THR:HB	12:N:79:THR:H	1.56	0.42
1:A:254:THR:HA	1:A:312:SER:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:THR:HB	2:B:1023:ARG:HH11	1.83	0.42
1:A:946:LEU:HA	1:A:984:GLY:O	2.19	0.42
1:A:1573:TYR:HA	7:I:122:ARG:NH2	2.31	0.42
2:B:107:PRO:HG2	2:B:133:TYR:CE2	2.54	0.42
4:E:16:PHE:CZ	4:E:20:LYS:HE3	2.55	0.42
5:F:76:LYS:HG3	5:F:79:ARG:CZ	2.50	0.42
8:J:45:CYS:O	8:J:48:ARG:HG2	2.20	0.42
12:N:94:ASP:HB3	12:N:99:LEU:HG	2.00	0.42
1:A:54:LEU:HA	1:A:75:HIS:HB2	2.00	0.42
1:A:586:VAL:HB	1:A:648:LEU:HD21	2.01	0.42
1:A:648:LEU:HD23	1:A:648:LEU:HA	1.86	0.42
1:A:826:PHE:CG	1:A:827:THR:N	2.88	0.42
1:A:993:GLN:H	1:A:993:GLN:CD	2.27	0.42
1:A:1005:GLY:HA2	1:A:1008:ASP:HB2	2.02	0.42
1:A:1458:THR:HG21	1:A:1475:GLU:CD	2.45	0.42
2:B:314:LYS:O	2:B:315:LYS:HB3	2.19	0.42
2:B:528:LEU:HA	2:B:528:LEU:HD23	1.76	0.42
2:B:534:PRO:HB2	2:B:538:PRO:HG2	2.01	0.42
2:B:893:ASN:O	2:B:895:PHE:HD2	2.02	0.42
2:B:894:LYS:O	2:B:896:GLN:N	2.53	0.42
2:B:936:MET:HA	2:B:937:PRO:HD2	1.87	0.42
3:C:31:TRP:HA	3:C:35:LYS:NZ	2.35	0.42
3:C:31:TRP:CE3	9:K:82:LYS:HD2	2.53	0.42
4:E:98:ILE:O	4:E:102:GLU:HG3	2.19	0.42
1:A:465:GLY:O	1:A:469:LYS:N	2.32	0.42
1:A:471:MET:HE1	2:B:1185:LEU:HD22	2.01	0.42
1:A:618:TYR:CE1	2:B:783:MET:HB2	2.55	0.42
1:A:844:THR:O	1:A:848:LYS:HG3	2.19	0.42
1:A:967:PRO:HB3	2:B:674:ILE:HD12	2.02	0.42
1:A:1204:THR:HG22	1:A:1205:PHE:N	2.34	0.42
2:B:143:TRP:CD1	2:B:152:LEU:HD12	2.54	0.42
2:B:327:LEU:HD23	2:B:330:LEU:HD12	2.01	0.42
2:B:1105:ARG:H	2:B:1173:THR:HA	1.84	0.42
3:C:128:ASP:OD1	3:C:129:GLU:N	2.52	0.42
1:A:316:LEU:HG	1:A:319:GLU:CD	2.44	0.42
1:A:652:ASN:OD1	1:A:652:ASN:N	2.53	0.42
2:B:343:ASP:OD1	2:B:344:GLN:N	2.53	0.42
2:B:675:ALA:HB2	2:B:686:HIS:CG	2.54	0.42
4:E:55:ARG:HG3	4:E:84:ASP:HA	2.01	0.42
9:K:134:LYS:HA	9:K:137:GLU:OE1	2.20	0.42
1:A:372:LYS:HD2	1:A:374:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:LYS:HG3	9:K:106:GLN:NE2	2.35	0.42
1:A:1055:ILE:HD11	1:A:1174:TYR:CE1	2.54	0.42
4:E:53:PRO:HG2	4:E:55:ARG:HH12	1.85	0.42
5:F:59:GLN:O	5:F:63:GLN:HG3	2.19	0.42
8:J:54:VAL:HG12	8:J:56:LEU:H	1.84	0.42
1:A:253:GLU:O	1:A:312:SER:N	2.53	0.42
1:A:428:VAL:O	1:A:432:ASN:N	2.51	0.42
1:A:589:MET:HE3	1:A:633:MET:HE2	2.02	0.42
1:A:733:THR:O	1:A:737:LEU:N	2.47	0.42
1:A:836:THR:CG2	1:A:839:GLY:H	2.33	0.42
1:A:908:VAL:HG11	1:A:941:SER:HB2	2.02	0.42
1:A:1456:PHE:CD1	1:A:1476:LEU:HD23	2.54	0.42
2:B:527:PHE:HE2	2:B:669:GLN:OE1	2.02	0.42
2:B:1031:VAL:HG12	2:B:1032:TYR:O	2.19	0.42
4:E:151:PRO:HG2	4:E:153:HIS:CE1	2.54	0.42
6:H:10:PHE:O	6:H:54:SER:HA	2.20	0.42
6:H:104:PHE:CE2	6:H:137:GLN:HB2	2.54	0.42
1:A:579:ARG:NH1	1:A:582:LYS:HG2	2.34	0.42
1:A:636:HIS:HB3	2:B:1091:ARG:HH22	1.85	0.42
1:A:1112:PRO:HG2	1:A:1115:LYS:HG2	2.01	0.42
1:A:1162:ASN:HB3	1:A:1165:LYS:HD3	2.01	0.42
1:A:1215:VAL:HG22	1:A:1216:THR:N	2.35	0.42
2:B:240:ARG:HH11	2:B:360:VAL:HG21	1.85	0.42
4:E:24:LYS:HE2	4:E:32:GLN:HE22	1.85	0.42
9:K:111:THR:HB	9:K:115:ASP:OD2	2.19	0.42
1:A:572:THR:HA	14:G:52:MET:CE	2.49	0.41
1:A:744:MET:HG3	1:A:745:PRO:HD2	2.01	0.41
1:A:1588:MET:O	1:A:1591:ARG:NH1	2.49	0.41
2:B:361:HIS:NE2	2:B:362:LEU:HG	2.34	0.41
2:B:714:ARG:HH21	2:B:957:ARG:HG2	1.85	0.41
2:B:939:SER:OG	2:B:943:ILE:N	2.51	0.41
3:C:92:ILE:HG12	8:J:1:MET:HE2	2.00	0.41
4:E:26:ARG:HE	4:E:188:LEU:HA	1.85	0.41
5:F:132:LEU:O	5:F:148:VAL:HG23	2.19	0.41
1:A:116:HIS:HB3	1:A:185:ARG:NH1	2.35	0.41
1:A:749:LEU:O	1:A:770:LEU:HD12	2.21	0.41
1:A:812:VAL:HG22	1:A:815:ARG:HH21	1.84	0.41
1:A:1240:LEU:O	1:A:1519:LEU:N	2.37	0.41
1:A:1293:HIS:ND1	1:A:1471:GLU:OE1	2.53	0.41
2:B:74:PHE:CE2	2:B:343:ASP:HB3	2.55	0.41
2:B:395:ASP:CG	2:B:505:ARG:HH22	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:556:SER:HB3	2:B:621:PRO:HG3	2.02	0.41
3:C:105:PRO:HG3	8:J:6:ARG:NH2	2.34	0.41
3:C:165:ARG:HB3	3:C:189:PRO:CB	2.37	0.41
7:I:112:TYR:N	7:I:121:PHE:O	2.54	0.41
12:N:148:ILE:HD13	12:N:150:TYR:OH	2.20	0.41
1:A:734:THR:O	1:A:737:LEU:HB3	2.20	0.41
1:A:751:SER:OG	1:A:752:LYS:N	2.53	0.41
1:A:793:ILE:O	1:A:797:LEU:HG	2.20	0.41
2:B:349:VAL:O	2:B:352:GLU:HB3	2.19	0.41
2:B:372:ARG:NH2	2:B:574:SER:HA	2.36	0.41
2:B:470:LEU:N	2:B:481:VAL:O	2.28	0.41
2:B:828:GLY:N	2:B:869:THR:OG1	2.36	0.41
2:B:894:LYS:HB3	10:L:45:ALA:HB1	2.02	0.41
2:B:1107:CYS:HB2	2:B:1195:ARG:NH2	2.35	0.41
3:C:80:ALA:HB3	3:C:102:GLY:HA2	2.02	0.41
4:E:13:TRP:NE1	4:E:39:LEU:HA	2.35	0.41
1:A:1:MET:HA	2:B:1098:TYR:CE2	2.55	0.41
1:A:126:GLN:HB3	1:A:343:PRO:CD	2.51	0.41
1:A:476:VAL:HG22	2:B:1069:ILE:O	2.20	0.41
1:A:596:HIS:NE2	1:A:598:ALA:HB3	2.34	0.41
1:A:747:ILE:HG13	1:A:748:ASN:N	2.36	0.41
1:A:1020:GLN:NE2	1:A:1191:GLN:HA	2.35	0.41
1:A:1268:ASP:H	1:A:1296:PHE:HA	1.85	0.41
1:A:1483:LEU:HA	1:A:1483:LEU:HD23	1.86	0.41
1:A:1600:ARG:HB2	1:A:1616:GLU:OE2	2.20	0.41
2:B:325:GLN:HA	2:B:328:GLN:OE1	2.20	0.41
2:B:712:SER:O	2:B:715:ASN:N	2.53	0.41
2:B:743:ARG:HG2	2:B:744:LEU:O	2.21	0.41
3:C:262:SER:C	3:C:264:GLU:H	2.28	0.41
7:I:6:SER:C	7:I:7:LEU:HD12	2.46	0.41
1:A:248:PHE:O	1:A:249:THR:OG1	2.32	0.41
1:A:707:THR:HG23	1:A:709:ARG:C	2.45	0.41
2:B:1189:LEU:HD12	2:B:1196:LEU:HD11	2.03	0.41
4:E:24:LYS:HE2	4:E:32:GLN:NE2	2.36	0.41
5:F:77:ASP:OD1	5:F:78:GLN:HG3	2.21	0.41
5:F:116:ASP:OD2	5:F:119:ARG:HG2	2.20	0.41
7:I:23:VAL:HB	7:I:39:LYS:NZ	2.34	0.41
7:I:88:GLN:OE1	7:I:119:TYR:HB2	2.21	0.41
8:J:7:CYS:O	8:J:11:GLY:N	2.48	0.41
14:G:29:ASP:OD1	14:G:30:GLU:N	2.52	0.41
14:G:106:LYS:HE3	14:G:106:LYS:HB2	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:GLN:O	1:A:411:VAL:HG23	2.21	0.41
1:A:485:SER:HB2	1:A:615:ARG:NE	2.36	0.41
1:A:618:TYR:OH	2:B:783:MET:HB2	2.21	0.41
1:A:1031:HIS:HA	1:A:1184:ALA:HA	2.03	0.41
1:A:1154:LEU:HA	1:A:1157:SER:OG	2.20	0.41
1:A:1245:ASP:OD1	1:A:1246:VAL:N	2.53	0.41
1:A:1643:VAL:HG12	1:A:1643:VAL:O	2.20	0.41
2:B:253:LEU:HD22	2:B:257:GLN:HB2	2.01	0.41
2:B:323:ARG:O	2:B:327:LEU:HG	2.20	0.41
3:C:140:CYS:O	3:C:198:PRO:HA	2.20	0.41
3:C:230:LEU:HD22	3:C:297:HIS:ND1	2.35	0.41
4:E:147:HIS:HB3	4:E:150:VAL:CG2	2.50	0.41
7:I:110:VAL:O	7:I:123:THR:N	2.37	0.41
9:K:89:CYS:SG	9:K:90:GLY:N	2.94	0.41
13:D:82:LEU:O	13:D:86:ILE:HG23	2.20	0.41
1:A:440:SER:OG	1:A:458:GLN:NE2	2.54	0.41
1:A:1006:LEU:O	1:A:1007:ILE:C	2.63	0.41
2:B:555:GLN:HB2	2:B:646:HIS:HE1	1.85	0.41
2:B:584:CYS:HB2	2:B:598:HIS:HA	2.02	0.41
2:B:915:ASP:H	2:B:927:CYS:CB	2.29	0.41
3:C:327:TYR:HE2	9:K:46:LYS:HE2	1.85	0.41
5:F:89:GLU:O	5:F:93:ILE:HG12	2.20	0.41
1:A:487:ASP:CG	1:A:489:ASN:HD22	2.25	0.41
1:A:693:GLN:HE22	9:K:88:PHE:HA	1.85	0.41
1:A:1268:ASP:HA	1:A:1297:PHE:CZ	2.56	0.41
1:A:1300:ASN:OD1	1:A:1301:GLU:N	2.53	0.41
2:B:307:GLU:HG3	7:I:7:LEU:HD21	2.02	0.41
2:B:457:ILE:O	2:B:460:LYS:N	2.54	0.41
2:B:699:ILE:O	2:B:703:LEU:HG	2.20	0.41
3:C:85:PHE:HB2	10:L:65:VAL:HB	2.02	0.41
3:C:216:HIS:HB3	3:C:219:PHE:CD2	2.56	0.41
4:E:33:GLU:OE1	4:E:33:GLU:N	2.40	0.41
4:E:165:LEU:HD22	4:E:170:LEU:O	2.21	0.41
6:H:12:VAL:N	6:H:53:ASP:O	2.49	0.41
1:A:76:GLN:HB2	1:A:362:VAL:O	2.20	0.41
1:A:233:CYS:SG	1:A:235:ASN:HB2	2.61	0.41
1:A:399:LEU:HD11	1:A:422:ARG:HD2	2.03	0.41
1:A:717:PRO:HB3	1:A:726:TRP:CE2	2.55	0.41
1:A:736:LEU:HD23	1:A:736:LEU:HA	1.81	0.41
1:A:800:VAL:O	1:A:1079:LYS:HD2	2.21	0.41
1:A:826:PHE:HB3	2:B:777:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:ARG:O	1:A:882:ILE:N	2.33	0.41
2:B:225:ARG:HB2	2:B:229:TYR:CD2	2.56	0.41
2:B:252:TYR:CE1	2:B:256:GLY:HA2	2.56	0.41
2:B:285:ASP:O	2:B:289:PHE:N	2.40	0.41
2:B:556:SER:OG	2:B:623:ASP:OD2	2.32	0.41
2:B:790:ASN:HD21	2:B:944:GLN:HB3	1.85	0.41
2:B:1079:LEU:HD12	2:B:1088:LEU:HD13	2.03	0.41
3:C:84:TYR:O	3:C:204:LEU:HA	2.21	0.41
4:E:109:ILE:HG12	4:E:133:GLU:HB2	2.03	0.41
4:E:158:SER:O	4:E:161:LYS:HB3	2.21	0.41
6:H:15:VAL:HG13	6:H:26:ILE:HG12	2.03	0.41
7:I:85:LYS:HA	7:I:91:ASN:O	2.21	0.41
9:K:133:SER:OG	9:K:137:GLU:OE2	2.35	0.41
1:A:487:ASP:OD2	1:A:489:ASN:HB2	2.21	0.41
1:A:991:LYS:HB2	1:A:994:GLU:CD	2.46	0.41
2:B:581:PRO:HB3	2:B:637:TYR:CE1	2.56	0.41
2:B:706:PHE:HE2	2:B:752:VAL:HG11	1.85	0.41
2:B:707:SER:O	2:B:710:ASN:N	2.43	0.41
3:C:262:SER:C	3:C:264:GLU:N	2.79	0.41
4:E:127:ILE:HD11	4:E:132:ILE:HD11	2.02	0.41
7:I:120:LYS:HE3	7:I:120:LYS:HB3	1.90	0.41
10:L:48:CYS:HB3	10:L:52:GLY:N	2.24	0.41
1:A:244:ARG:HH21	1:A:252:PHE:HD2	1.68	0.40
1:A:706:HIS:CG	1:A:808:LYS:HE2	2.55	0.40
1:A:1317:ILE:HA	1:A:1321:PHE:CB	2.44	0.40
1:A:1648:ASN:O	1:A:1652:GLY:HA3	2.19	0.40
2:B:161:LEU:O	2:B:163:VAL:HG23	2.20	0.40
2:B:885:VAL:HG22	2:B:903:ILE:HG23	2.02	0.40
2:B:1084:THR:HB	2:B:1087:LEU:HD12	2.03	0.40
3:C:165:ARG:HH12	3:C:190:ASP:HA	1.85	0.40
1:A:8:GLY:CA	14:G:115:PHE:CZ	3.05	0.40
1:A:102:CYS:SG	1:A:104:PHE:HD2	2.45	0.40
1:A:141:LEU:HD13	1:A:181:LEU:HD13	2.03	0.40
1:A:396:ILE:HG12	1:A:426:ALA:HB1	2.03	0.40
1:A:402:ASP:O	1:A:406:LEU:HG	2.21	0.40
1:A:803:PRO:O	1:A:807:ALA:N	2.30	0.40
1:A:808:LYS:NZ	1:A:815:ARG:HH22	2.19	0.40
1:A:1459:LYS:HB2	1:A:1473:LYS:HB3	2.02	0.40
2:B:228:SER:C	2:B:254:ASN:HD22	2.29	0.40
2:B:359:LEU:HD22	2:B:361:HIS:HE1	1.85	0.40
2:B:445:TYR:O	2:B:449:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:538:PRO:HB2	2:B:542:LEU:HD12	2.03	0.40
2:B:886:ASN:HB2	2:B:902:SER:OG	2.22	0.40
6:H:137:GLN:C	6:H:138:GLU:HG3	2.46	0.40
7:I:8:ILE:O	7:I:16:LEU:HD12	2.21	0.40
12:N:70:LEU:HA	12:N:71:PRO:HD3	1.84	0.40
1:A:885:ASP:HB3	1:A:888:LYS:HB2	2.02	0.40
2:B:306:LEU:O	2:B:309:LEU:HB3	2.21	0.40
2:B:492:ASN:OD1	2:B:494:TYR:N	2.54	0.40
2:B:1152:PHE:CZ	14:G:129:VAL:HG21	2.56	0.40
3:C:224:THR:HG23	3:C:225:ALA:N	2.36	0.40
4:E:48:ASP:OD2	4:E:50:MET:HB3	2.21	0.40
4:E:195:VAL:HG13	4:E:212:ARG:O	2.21	0.40
11:M:11:GLU:O	11:M:87:SER:HA	2.22	0.40
14:G:35:SER:OG	14:G:132:VAL:N	2.46	0.40
14:G:50:ALA:HA	14:G:113:PHE:CD2	2.56	0.40
1:A:25:ARG:NH2	1:A:80:GLU:OE1	2.52	0.40
1:A:557:LEU:O	1:A:561:LEU:HG	2.20	0.40
1:A:854:GLY:HA3	1:A:974:THR:O	2.22	0.40
1:A:930:LEU:C	1:A:932:GLY:H	2.29	0.40
1:A:1246:VAL:HG12	1:A:1247:SER:O	2.21	0.40
1:A:1316:VAL:HG13	1:A:1320:GLN:NE2	2.36	0.40
2:B:330:LEU:HD23	2:B:330:LEU:HA	1.87	0.40
2:B:331:GLY:O	2:B:335:ARG:HB2	2.20	0.40
3:C:319:ARG:CZ	3:C:319:ARG:HB2	2.52	0.40
6:H:27:GLU:HA	6:H:39:THR:HA	2.04	0.40
14:G:73:TYR:CZ	14:G:238:THR:HG21	2.57	0.40
1:A:52:LEU:C	1:A:63:SER:H	2.29	0.40
1:A:110:LEU:HD12	1:A:111:LYS:H	1.86	0.40
1:A:493:ASN:HA	1:A:653:THR:HG21	2.02	0.40
1:A:495:ILE:HD12	1:A:615:ARG:O	2.21	0.40
1:A:1148:LEU:HD21	1:A:1166:PHE:CD2	2.56	0.40
1:A:1250:GLN:O	1:A:1254:PHE:N	2.39	0.40
1:A:1615:TYR:CE2	1:A:1616:GLU:HG3	2.57	0.40
2:B:61:LEU:H	2:B:61:LEU:HG	1.70	0.40
2:B:562:PRO:HA	2:B:565:LEU:HD12	2.04	0.40
2:B:588:ILE:O	2:B:591:LYS:N	2.54	0.40
3:C:88:ASN:OD1	3:C:202:ILE:HG12	2.20	0.40
3:C:204:LEU:C	3:C:204:LEU:HD12	2.46	0.40
4:E:143:ASN:CG	4:E:145:THR:HG1	2.24	0.40
9:K:52:GLN:H	9:K:52:GLN:CD	2.28	0.40
13:D:37:LEU:HD23	13:D:37:LEU:HA	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:62:MET:HE2	14:G:84:TYR:HE1	1.86	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	1448/1664 (87%)	1364 (94%)	75 (5%)	9 (1%)	21	57
2	B	1158/1203 (96%)	1110 (96%)	41 (4%)	7 (1%)	21	57
3	C	303/335 (90%)	283 (93%)	19 (6%)	1 (0%)	36	70
4	E	210/215 (98%)	202 (96%)	8 (4%)	0	100	100
5	F	96/155 (62%)	94 (98%)	2 (2%)	0	100	100
6	H	127/146 (87%)	124 (98%)	3 (2%)	0	100	100
7	I	112/125 (90%)	108 (96%)	4 (4%)	0	100	100
8	J	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
9	K	99/142 (70%)	95 (96%)	4 (4%)	0	100	100
10	L	42/70 (60%)	38 (90%)	4 (10%)	0	100	100
11	M	95/415 (23%)	86 (90%)	7 (7%)	2 (2%)	5	32
12	N	125/233 (54%)	108 (86%)	13 (10%)	4 (3%)	3	25
13	D	54/137 (39%)	50 (93%)	2 (4%)	2 (4%)	2	22
14	G	186/326 (57%)	171 (92%)	13 (7%)	2 (1%)	11	44
All	All	4122/5236 (79%)	3894 (94%)	201 (5%)	27 (1%)	20	54

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	946	LEU

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Mol	Chain	Res	Type
2	B	657	PRO
2	B	658	LEU
2	B	659	ASP
3	C	226	SER
12	N	149	ASP
13	D	99	LEU
2	B	891	GLU
13	D	98	GLY
1	A	652	ASN
1	A	1649	VAL
2	B	892	SER
11	M	85	LYS
14	G	99	ASP
2	B	656	LEU
11	M	36	THR
12	N	115	SER
14	G	100	THR
1	A	905	SER
1	A	1264	SER
2	B	655	TYR
1	A	1050	TYR
1	A	1061	SER
12	N	70	LEU
1	A	1225	ILE
12	N	39	PRO
1	A	1569	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	1292/1465 (88%)	1286 (100%)	6 (0%)	81	82
2	B	1022/1053 (97%)	1020 (100%)	2 (0%)	87	87
3	C	269/296 (91%)	268 (100%)	1 (0%)	84	84
4	E	194/197 (98%)	194 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	88/137 (64%)	88 (100%)	0	100	100
6	H	115/128 (90%)	115 (100%)	0	100	100
7	I	103/110 (94%)	103 (100%)	0	100	100
8	J	64/65 (98%)	64 (100%)	0	100	100
9	K	91/130 (70%)	91 (100%)	0	100	100
10	L	39/57 (68%)	39 (100%)	0	100	100
11	M	88/371 (24%)	77 (88%)	11 (12%)	4	20
12	N	124/220 (56%)	117 (94%)	7 (6%)	19	43
13	D	55/116 (47%)	50 (91%)	5 (9%)	9	30
14	G	170/291 (58%)	157 (92%)	13 (8%)	12	36
All	All	3714/4636 (80%)	3669 (99%)	45 (1%)	61	73

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

Mol	Chain	Res	Type
1	A	938	VAL
1	A	942	GLN
1	A	944	MET
1	A	1261	VAL
1	A	1499	ARG
1	A	1504	ILE
2	B	655	TYR
2	B	658	LEU
3	C	226	SER
11	M	17	ASP
11	M	18	GLN
11	M	31	ARG
11	M	44	LYS
11	M	48	LYS
11	M	52	VAL
11	M	63	GLU
11	M	65	TYR
11	M	77	VAL
11	M	84	GLU
11	M	98	SER
12	N	51	GLN
12	N	81	THR
12	N	89	ILE

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Mol	Chain	Res	Type
12	N	124	THR
12	N	135	LYS
12	N	141	GLU
12	N	145	ILE
13	D	15	THR
13	D	29	GLN
13	D	38	GLN
13	D	80	THR
13	D	99	LEU
14	G	21	LYS
14	G	24	VAL
14	G	35	SER
14	G	39	VAL
14	G	139	ILE
14	G	147	LEU
14	G	167	THR
14	G	169	VAL
14	G	223	GLU
14	G	230	ARG
14	G	239	THR
14	G	241	ARG
14	G	243	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	60	ASN
1	A	213	ASN
1	A	263	ASN
1	A	378	HIS
1	A	458	GLN
1	A	470	HIS
1	A	489	ASN
1	A	521	GLN
1	A	537	GLN
1	A	694	GLN
1	A	730	GLN
1	A	880	GLN
1	A	942	GLN
1	A	950	GLN
1	A	1031	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1108	HIS
1	A	1116	GLN
1	A	1315	ASN
1	A	1319	ASN
1	A	1447	GLN
1	A	1453	HIS
2	B	43	GLN
2	B	45	HIS
2	B	243	GLN
2	B	246	GLN
2	B	248	ASN
2	B	254	ASN
2	B	267	ASN
2	B	469	ASN
2	B	504	HIS
2	B	547	HIS
2	B	587	GLN
2	B	686	HIS
2	B	702	ASN
2	B	893	ASN
2	B	1008	HIS
2	B	1034	GLN
2	B	1089	GLN
2	B	1115	GLN
2	B	1171	ASN
3	C	43	ASN
3	C	58	ASN
3	C	99	HIS
3	C	172	GLN
3	C	296	ASN
3	C	297	HIS
3	C	335	GLN
4	E	32	GLN
4	E	146	HIS
4	E	179	GLN
6	H	11	GLN
6	H	35	GLN
6	H	52	GLN
7	I	21	ASN
7	I	32	GLN
8	J	26	GLN
9	K	70	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	M	18	GLN
11	M	82	ASN
12	N	61	ASN
12	N	132	GLN
13	D	23	HIS
14	G	23	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	SO4	B	1301	-	4,4,4	0.22	0	6,6,6	0.36	0

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.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1301	SO4	8	0

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.

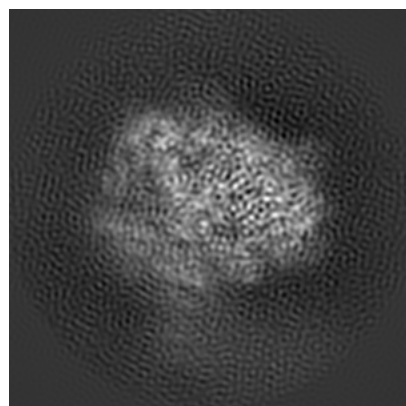
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4148. These allow visual inspection of the internal detail of the map and identification of artifacts.

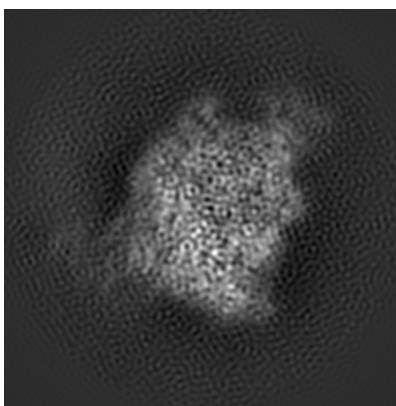
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

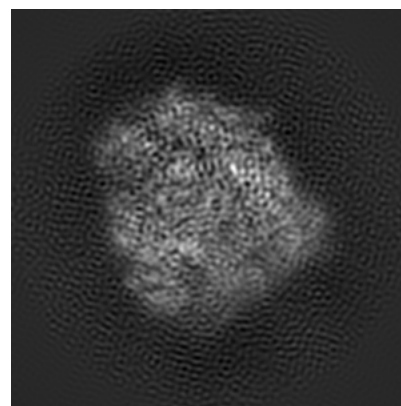
6.1.1 Primary map



X

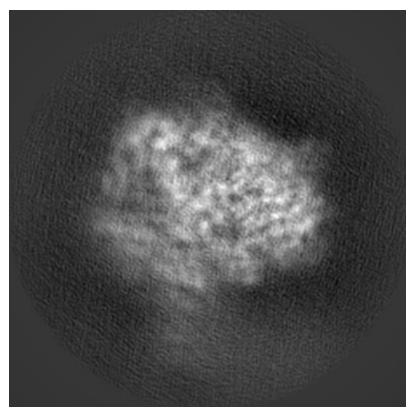


Y

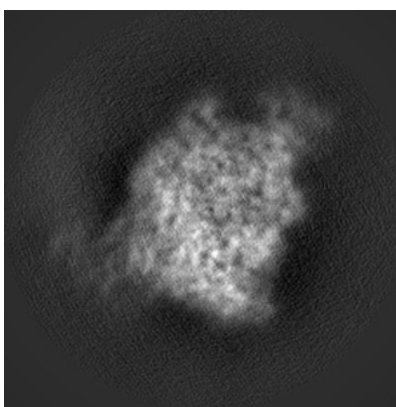


Z

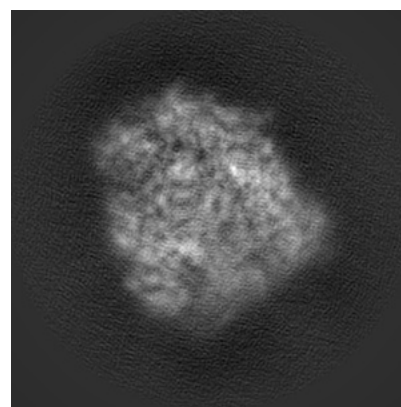
6.1.2 Raw map



X



Y

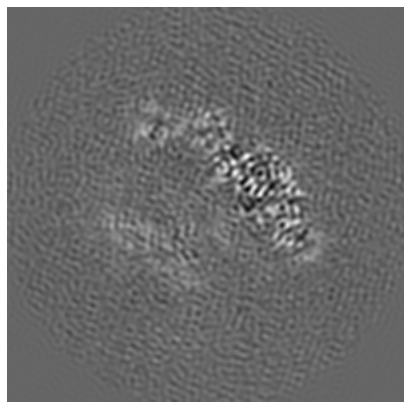


Z

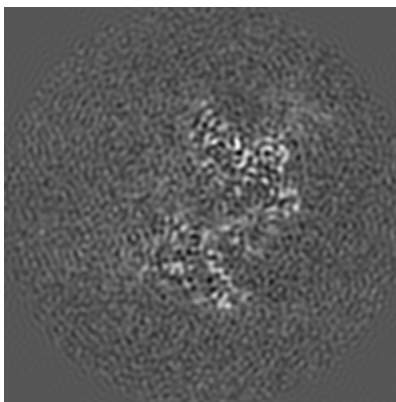
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

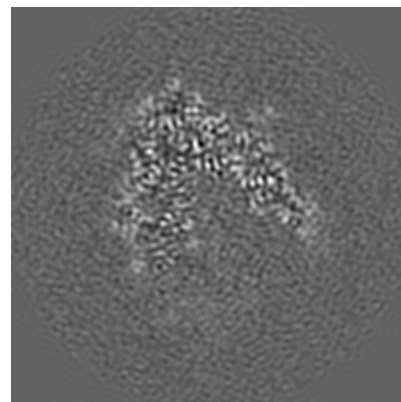
6.2.1 Primary map



X Index: 115

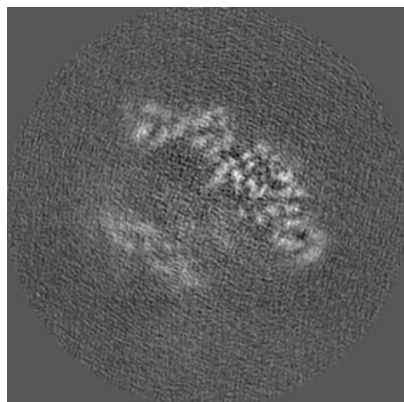


Y Index: 115

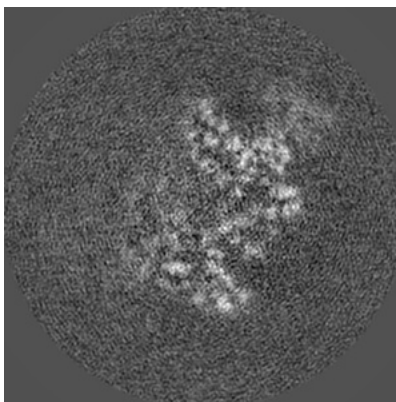


Z Index: 115

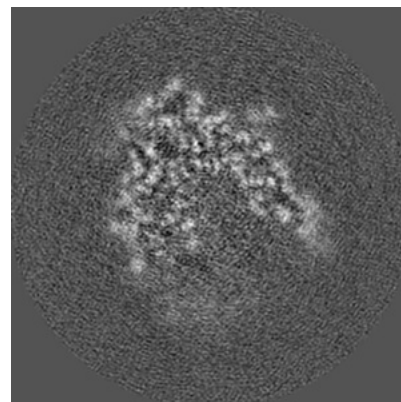
6.2.2 Raw map



X Index: 115



Y Index: 115

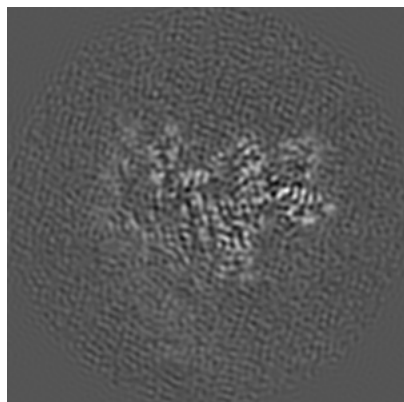


Z Index: 115

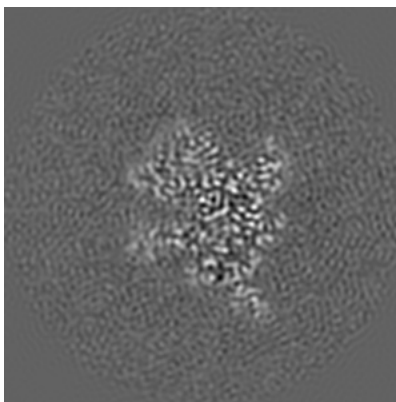
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

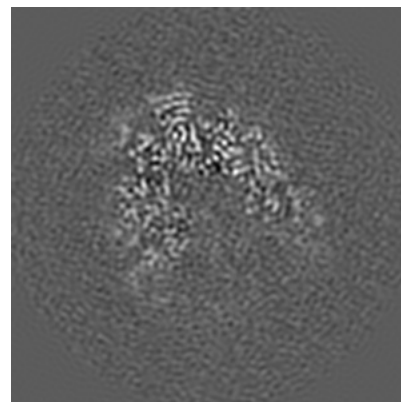
6.3.1 Primary map



X Index: 95

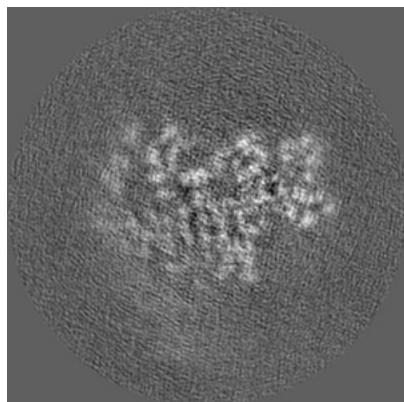


Y Index: 137

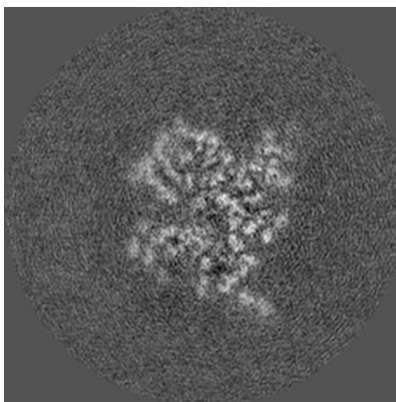


Z Index: 120

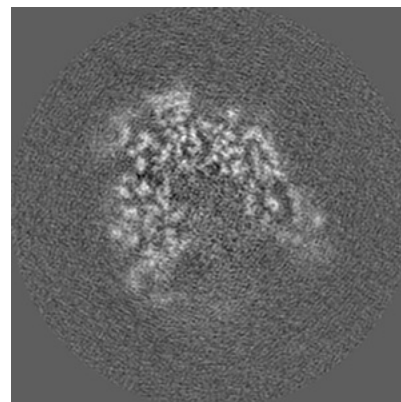
6.3.2 Raw map



X Index: 96



Y Index: 134

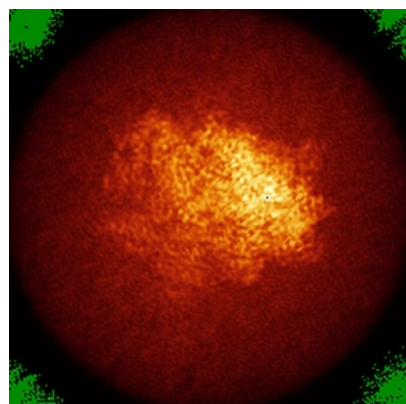


Z Index: 120

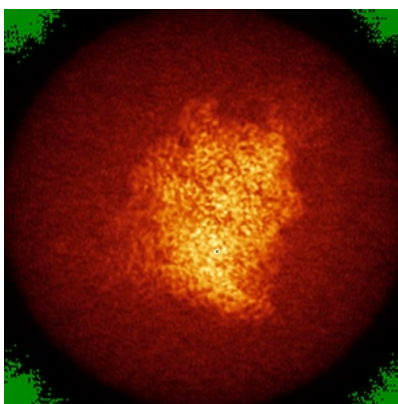
The images above show the largest variance slices of the map in three orthogonal directions.

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

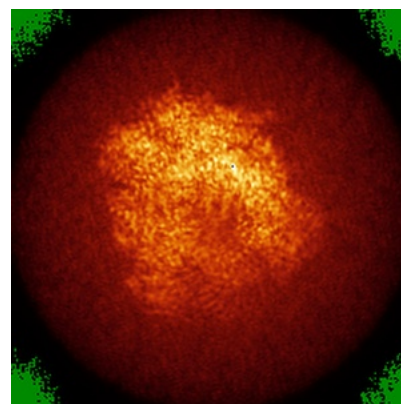
6.4.1 Primary map



X

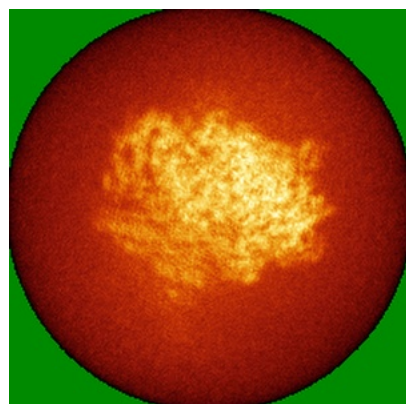


Y

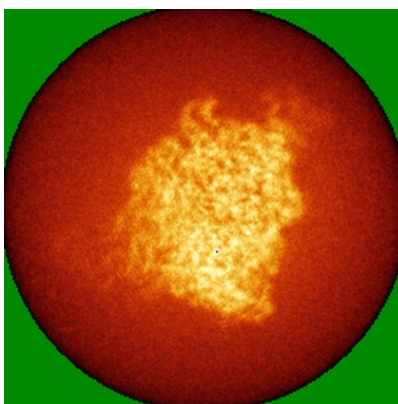


Z

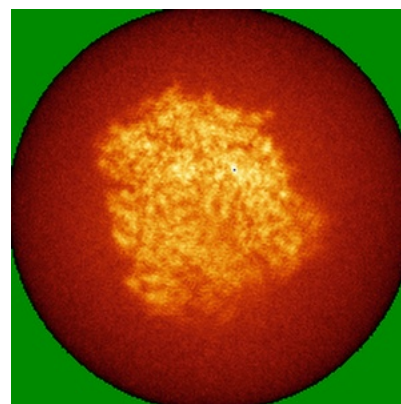
6.4.2 Raw map



X



Y

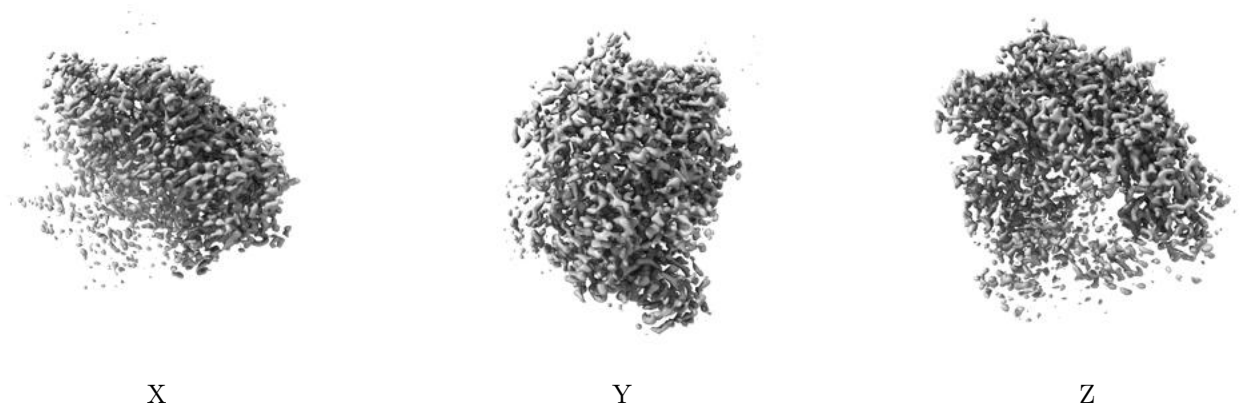


Z

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

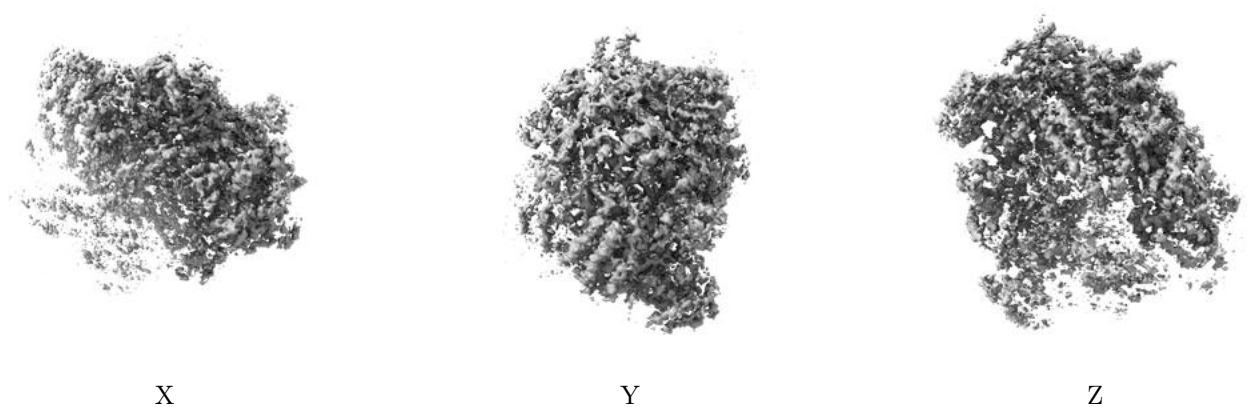
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

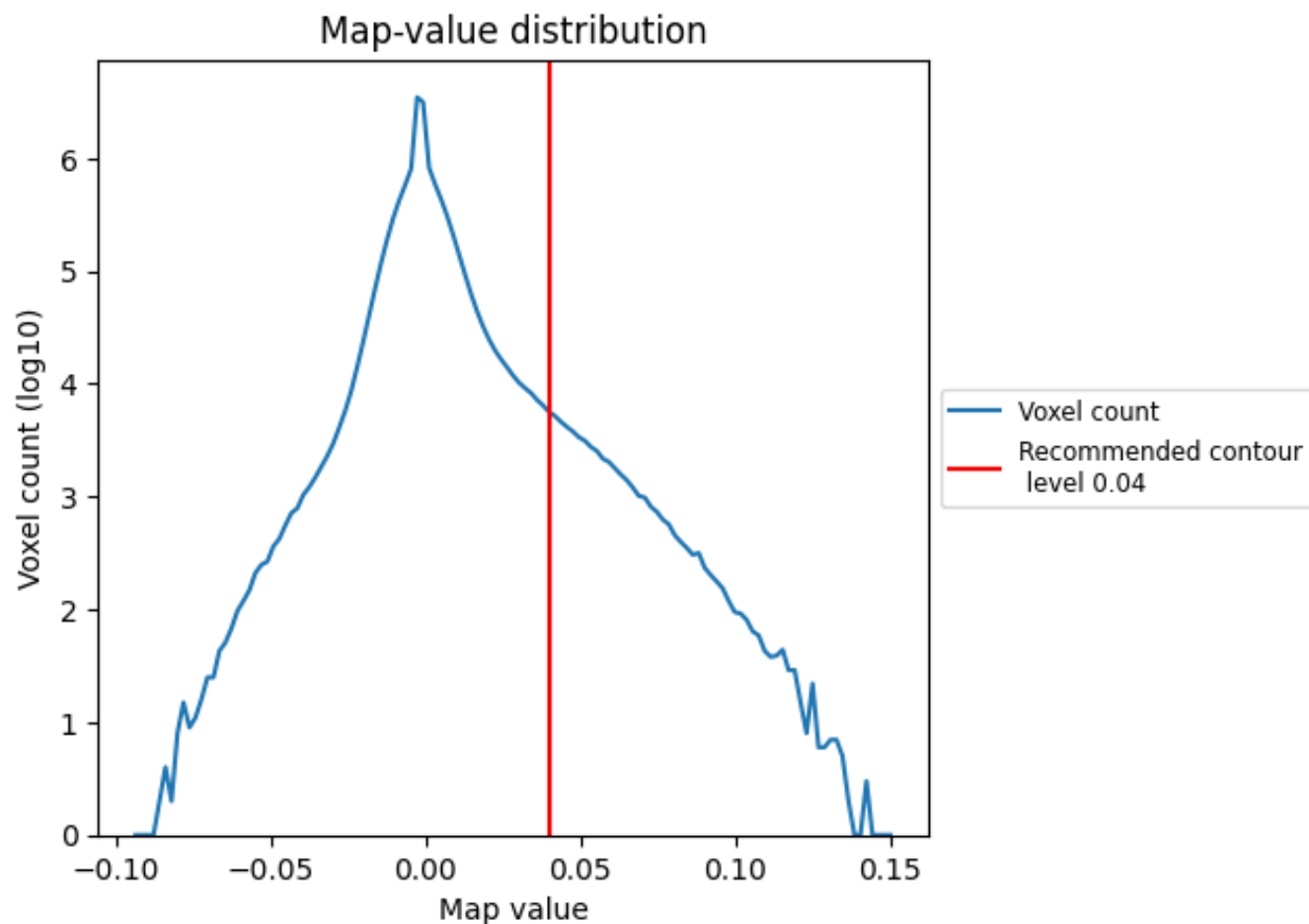
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

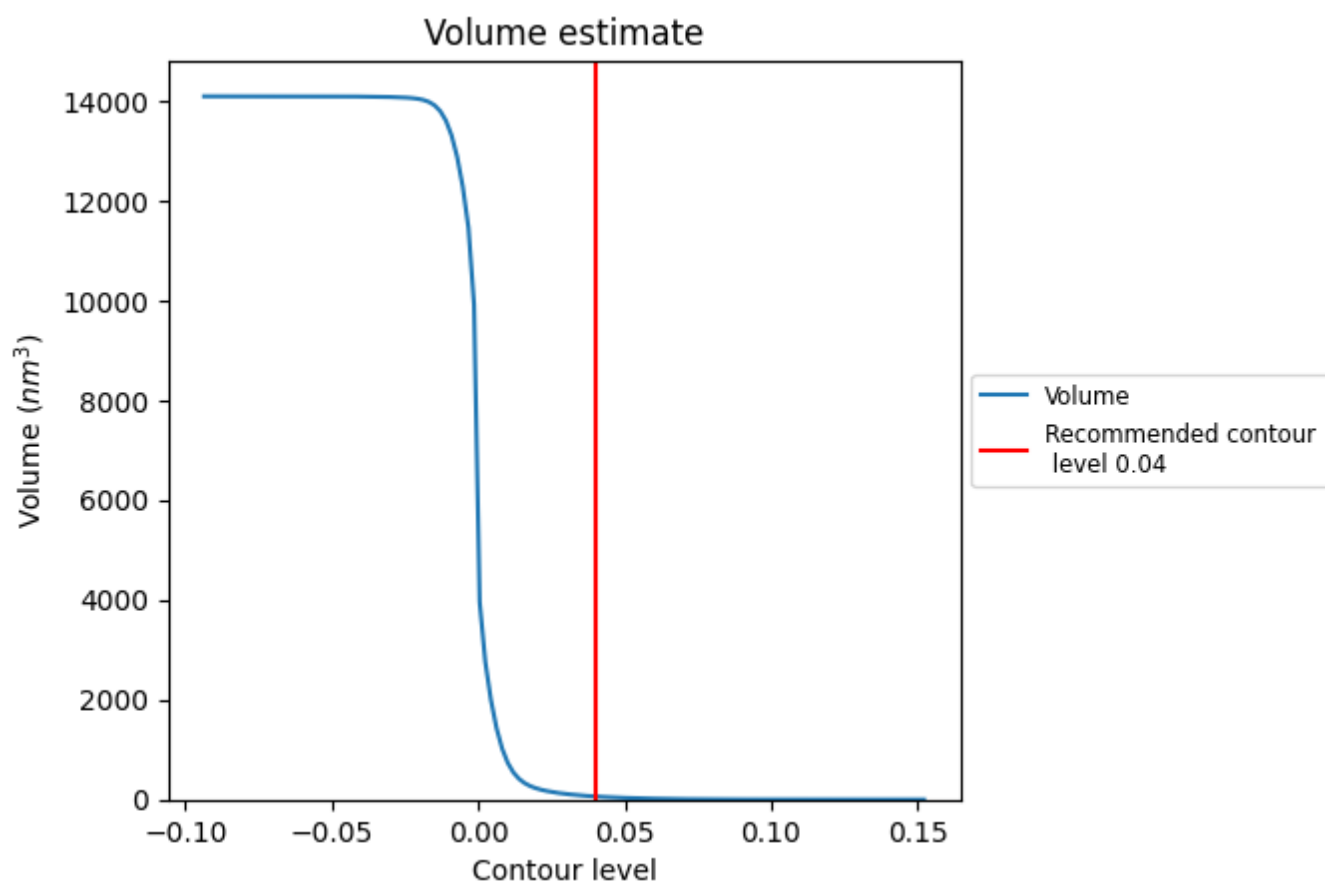
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

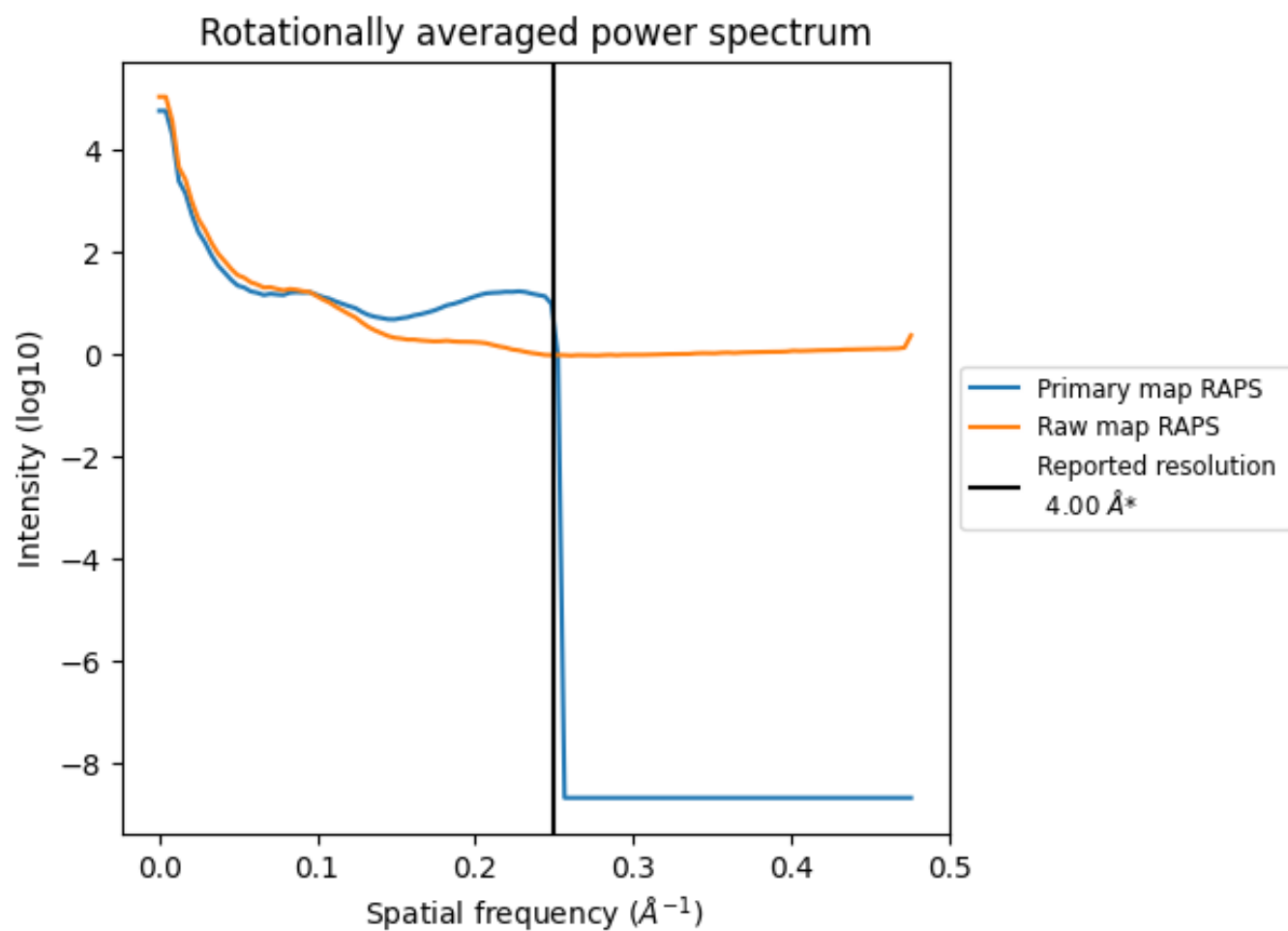
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 62 nm^3 ; this corresponds to an approximate mass of 56 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 ⓘ

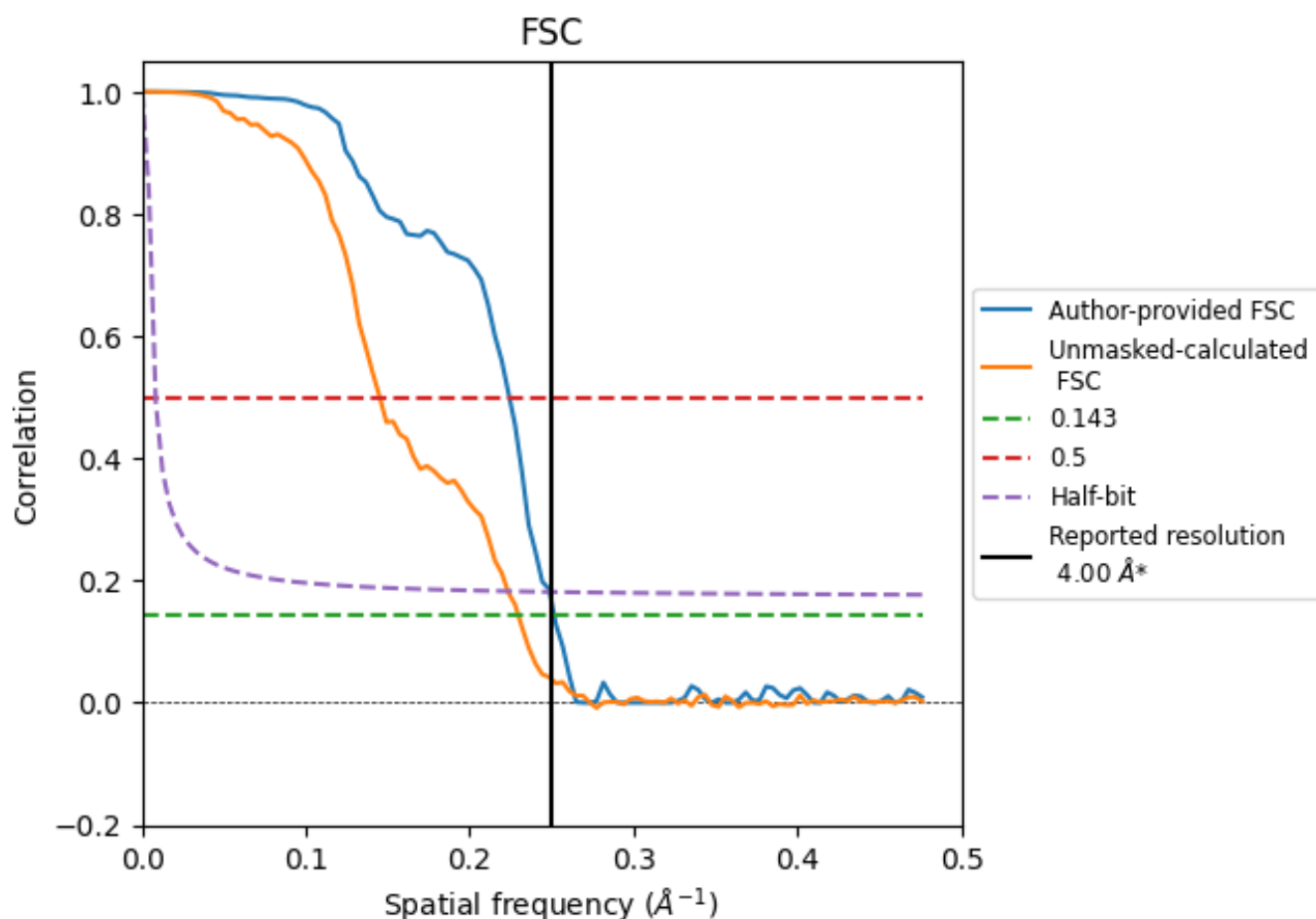


*Reported resolution corresponds to spatial frequency of 0.250 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.250 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

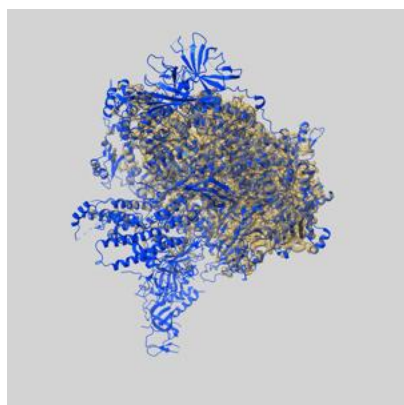
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.98	4.46	4.02
Unmasked-calculated*	4.35	6.89	4.48

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

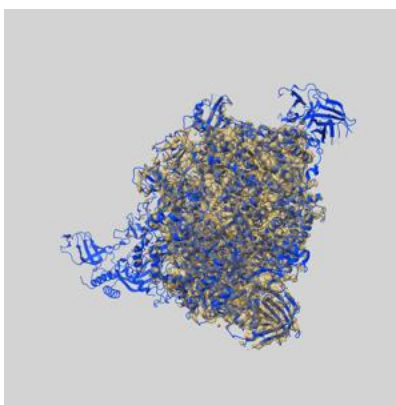
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4148 and PDB model 5M3M. Per-residue inclusion information can be found in section [3](#) on page [7](#).

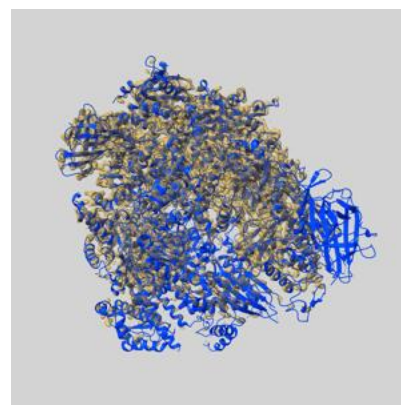
9.1 Map-model overlay [i](#)



X



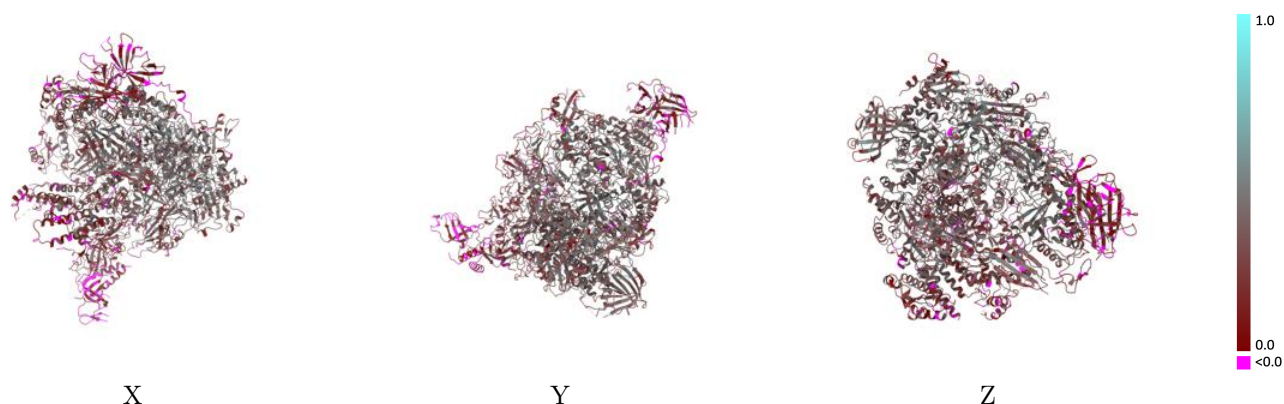
Y



Z

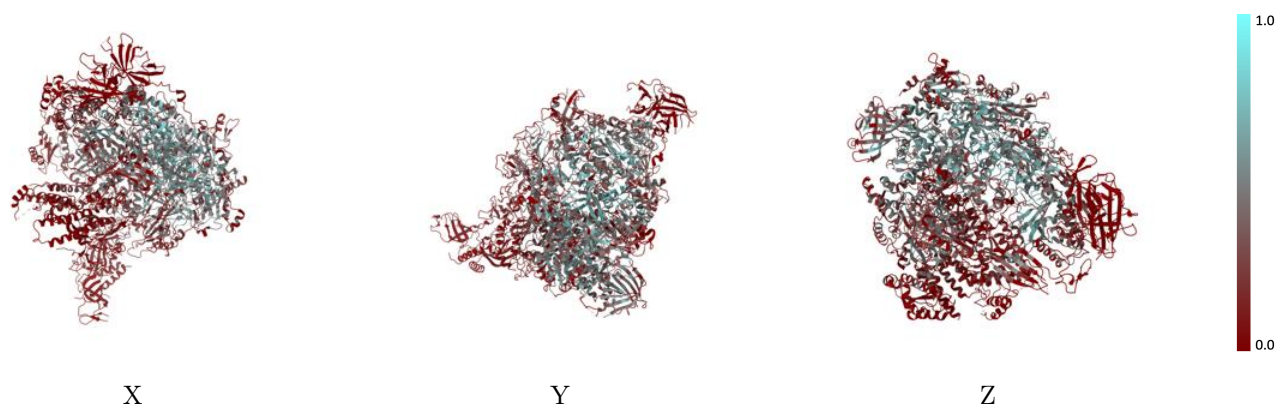
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



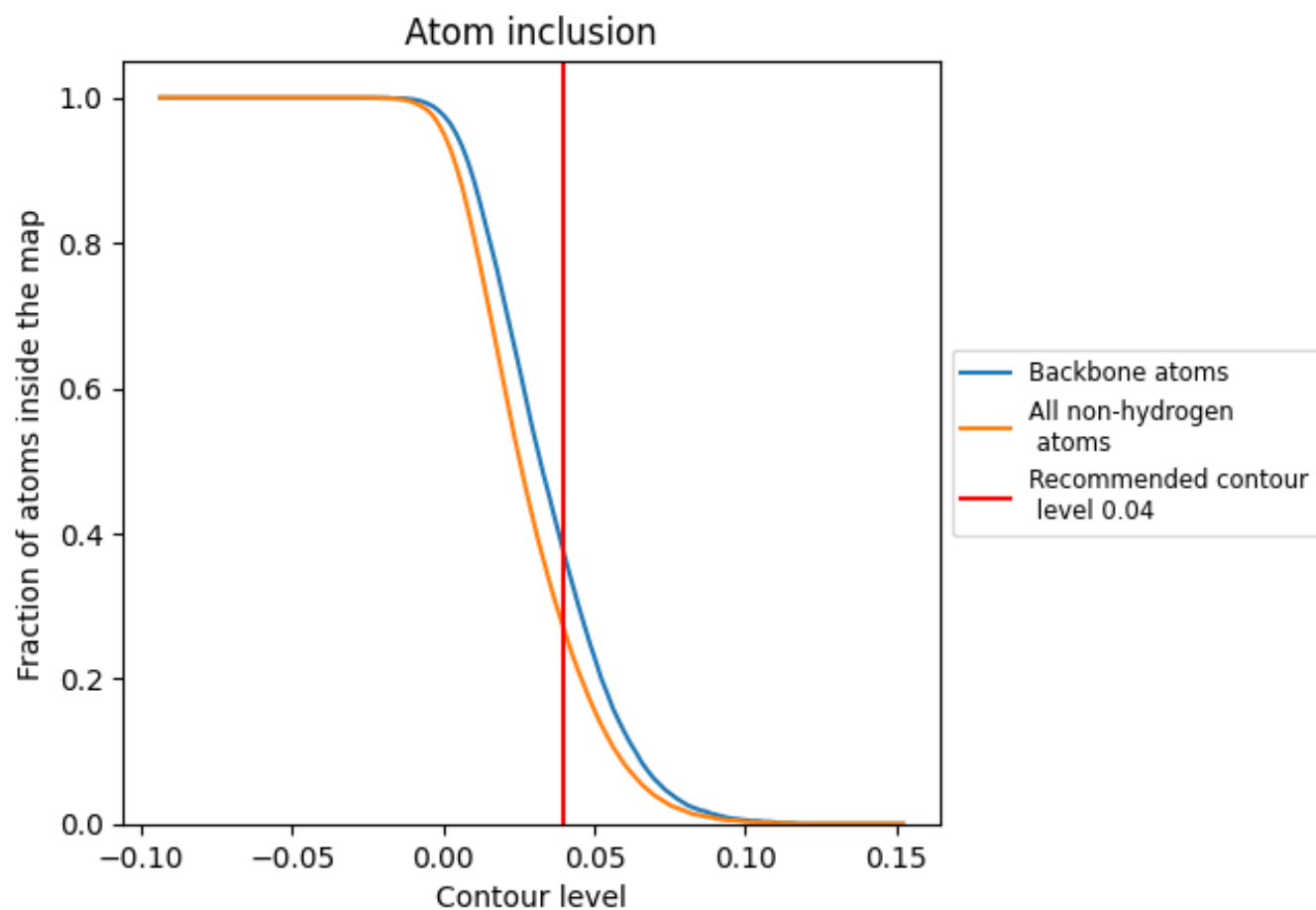
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 37% of all backbone atoms, 27% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2670	0.3090
A	0.2530	0.3180
B	0.3860	0.3650
C	0.3500	0.3600
D	0.0040	0.0810
E	0.1450	0.2700
F	0.1920	0.2950
G	0.0080	0.1250
H	0.3410	0.3680
I	0.0630	0.2470
J	0.4730	0.3920
K	0.3930	0.3660
L	0.3350	0.3610
M	0.0030	0.1250
N	0.0000	0.0710

1.0

0.0

<0.0