



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 08:25 PM UTC

PDB ID : 8ZJJ / pdb_00008zjj
EMDB ID : EMD-60147
Title : Structure of DOCK5/ELMO1/Rac1 core (RhoG/DOCK5/ELMO1/Rac1 dataset, class 2)
Authors : Kukimoto-Niino, M.; Katsura, K.; Ishizuka-Katsura, Y.; Mishima-Tsumagari, C.; Yonemochi, M.; Inoue, M.; Nakagawa, R.; Kaushik, R.; Zhang, K.Y.J.; Shirouzu, M.
Deposited on : 2024-05-15
Resolution : 4.23 Å(reported)
Based on initial model : 7DPA

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

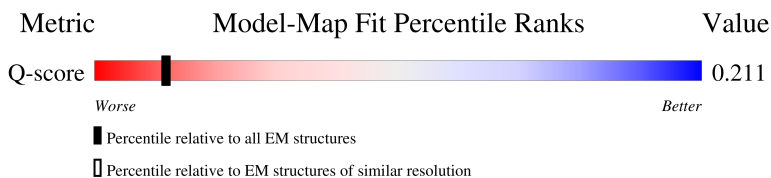
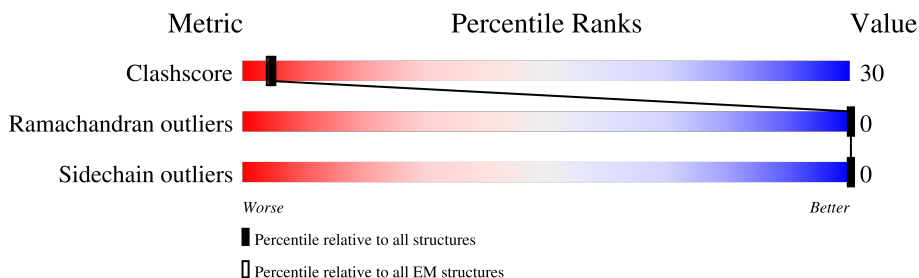
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.23 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.



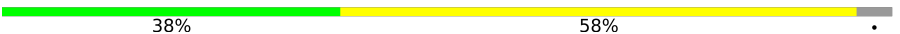
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4685 (3.74 - 4.73)

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	733	
1	D	733	
2	B	1648	
2	E	1648	

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Mol	Chain	Length	Quality of chain
3	C	184	 40% 57% .
3	F	184	 38% 58% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32858 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 Engulfment and cell motility protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	198	Total	C	N	O	S	0	0
			1608	1018	277	303	10		
1	D	198	Total	C	N	O	S	0	0
			1608	1018	277	303	10		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q92556
A	-4	GLY	-	expression tag	UNP Q92556
A	-3	SER	-	expression tag	UNP Q92556
A	-2	GLY	-	expression tag	UNP Q92556
A	-1	GLY	-	expression tag	UNP Q92556
A	0	SER	-	expression tag	UNP Q92556
D	-5	GLY	-	expression tag	UNP Q92556
D	-4	GLY	-	expression tag	UNP Q92556
D	-3	SER	-	expression tag	UNP Q92556
D	-2	GLY	-	expression tag	UNP Q92556
D	-1	GLY	-	expression tag	UNP Q92556
D	0	SER	-	expression tag	UNP Q92556

- Molecule 2 is a protein called Deducator of cytokinesis protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1642	Total	C	N	O	S	0	0
			13436	8618	2264	2484	70		
2	E	1642	Total	C	N	O	S	0	0
			13436	8618	2264	2484	70		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP Q9H7D0

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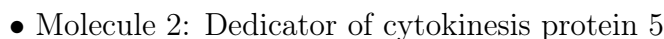
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP Q9H7D0
B	-3	SER	-	expression tag	UNP Q9H7D0
B	-2	GLY	-	expression tag	UNP Q9H7D0
B	-1	GLY	-	expression tag	UNP Q9H7D0
B	0	SER	-	expression tag	UNP Q9H7D0
B	1285	ARG	LYS	variant	UNP Q9H7D0
E	-5	GLY	-	expression tag	UNP Q9H7D0
E	-4	GLY	-	expression tag	UNP Q9H7D0
E	-3	SER	-	expression tag	UNP Q9H7D0
E	-2	GLY	-	expression tag	UNP Q9H7D0
E	-1	GLY	-	expression tag	UNP Q9H7D0
E	0	SER	-	expression tag	UNP Q9H7D0
E	1285	ARG	LYS	variant	UNP Q9H7D0

- Molecule 3 is a protein called Ras-related C3 botulinum toxin substrate 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	177	Total	C	N	O	S	0	0
			1385	890	228	259	8		
3	F	177	Total	C	N	O	S	0	0
			1385	890	228	259	8		

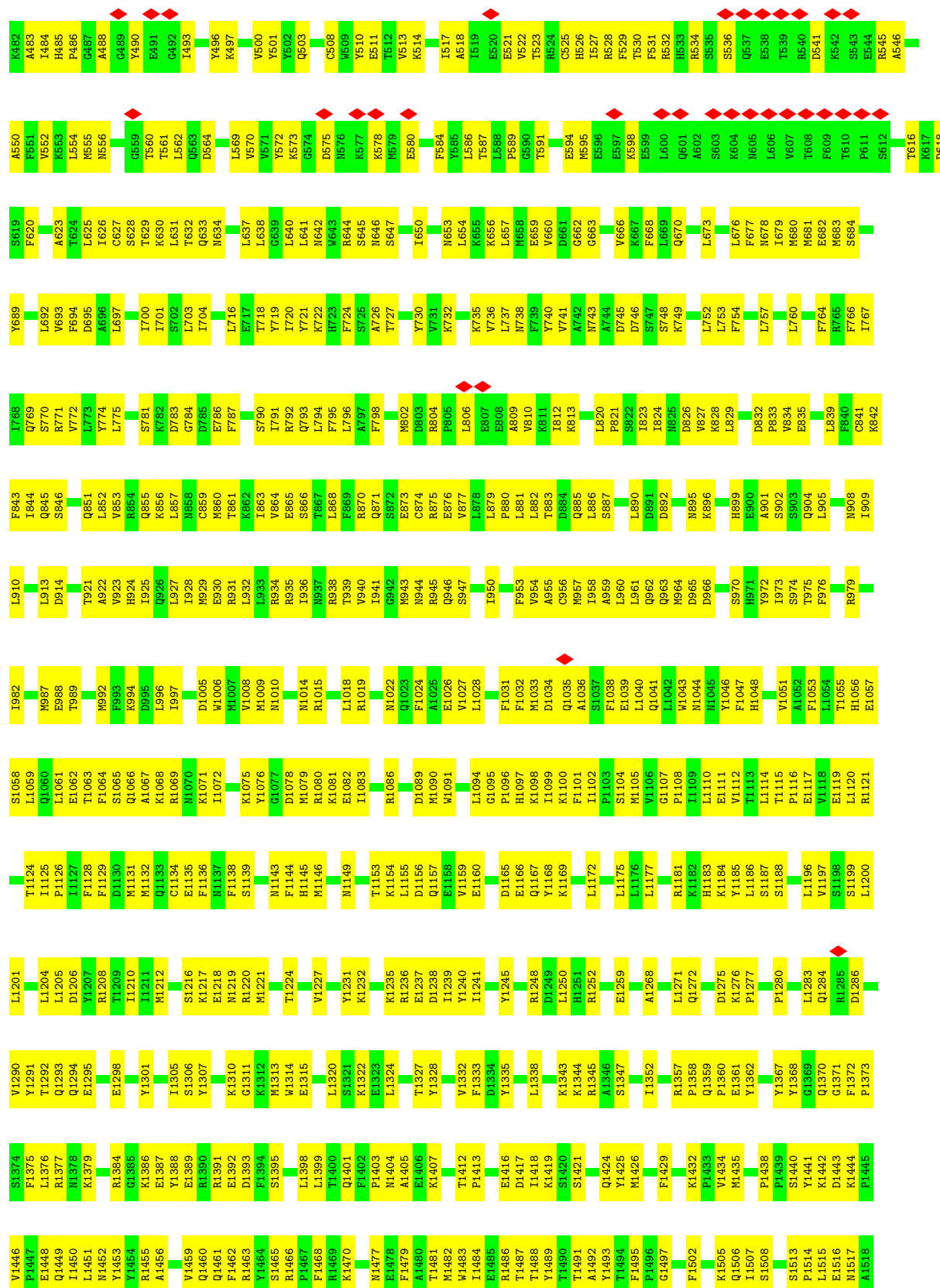
There are 16 discrepancies between the modelled and reference sequences:

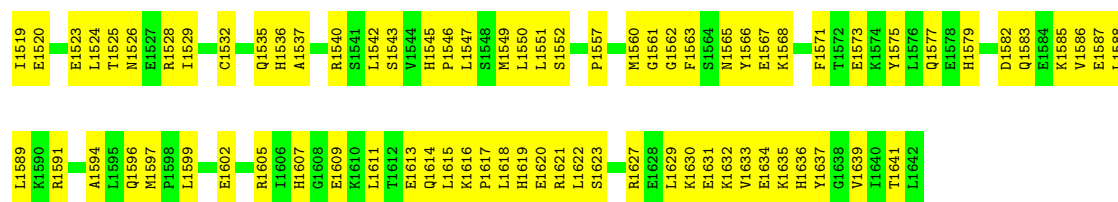
Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLY	-	expression tag	UNP P63000
C	-5	SER	-	expression tag	UNP P63000
C	-4	SER	-	expression tag	UNP P63000
C	-3	GLY	-	expression tag	UNP P63000
C	-2	SER	-	expression tag	UNP P63000
C	-1	SER	-	expression tag	UNP P63000
C	0	GLY	-	expression tag	UNP P63000
C	15	ALA	GLY	engineered mutation	UNP P63000
F	-6	GLY	-	expression tag	UNP P63000
F	-5	SER	-	expression tag	UNP P63000
F	-4	SER	-	expression tag	UNP P63000
F	-3	GLY	-	expression tag	UNP P63000
F	-2	SER	-	expression tag	UNP P63000
F	-1	SER	-	expression tag	UNP P63000
F	0	GLY	-	expression tag	UNP P63000
F	15	ALA	GLY	engineered mutation	UNP P63000



F1129	F1064	M992	L852	R771	D695	T626	P557	G489	L420	E340	E372	Q199
D1130	S1065	F993	V653	V772	A696	C627	D558	Y490	Y421	E341	K273	E200
M1131	Q1066	K994	R654	L773	L697	S628	G559	E491	D422	E491	L274	E201
M1132	A1067	D995	K855	Y774	L774	T629	G559	G492	R423	E491	N275	S203
Q1133	K1068	L996	K856	L775	I701	K630	T560	L493	R423	E491	N276	I204
E1135	R1069	I997	L857	L776	I702	K631	T561	Y496	T425	E491	L277	L205
F1136	N1070	D1005	N858	S781	S702	T632	Q633	K497	T425	E491	Q350	Q206
M1137	K1071	M929	C859	K782	L703	K634	D564	K497	A428	E491	V980	N207
F1138	E930	R860	D783	D783	L704	N635	L569	V500	R429	E491	F281	L208
S1139	R931	T861	D784	D785	K708	D636	V570	Y501	K430	E491	F281	D209
N1143	K1075	K862	D785	E786	L716	L637	V571	T602	G432	E491	L284	L210
F1144	G1076	V864	E787	E787	E717	L638	K573	Q503	F433	E491	S285	R211
H1145	D1078	S866	S866	S790	T718	G639	G574	C508	E435	E491	D288	Q213
M1146	R1079	T867	T867	T719	Y719	L640	D575	N509	L438	E491	L289	S214
N1149	K1081	L868	L868	R792	T720	N642	N576	Y510	P439	E491	L290	I215
T1153	E1082	R870	R870	Q793	Y721	K644	K577	E511	G440	E491	P292	F216
K1154	I1083	Q871	Q871	L794	K722	S645	K578	V513	D441	E491	V294	S217
L1155	R1086	D872	D872	L796	H723	S647	N579	K514	R443	E491	S295	T218
D1156	D1089	E873	E873	A797	S725	S647	E580	I517	D445	E491	L296	Y222
Q1157	M1090	R875	R875	F724	A726	N646	E580	A518	I446	E491	V297	L224
E1158	W1091	V877	V877	T727	T727	N650	F584	I519	L450	E491	Q299	Y225
V1159	L1094	L878	L878	Y730	Y730	N653	Y585	E520	L451	E491	R302	V226
E1160	G1095	L879	L879	V731	V731	L654	L586	E521	L451	E491	M306	N227
D1165	P1096	P880	P880	K735	K735	K656	L588	V522	D456	E491	E307	F231
E1166	H1097	L881	L881	V736	V736	L657	P589	T523	K460	E491	L308	A239
Q1167	K1098	R811	R811	L737	L737	N658	G590	R524	K461	E491	K309	E240
Y1168	T1099	K812	K812	R739	R739	D661	E594	H526	T462	E491	E310	L241
K1169	K1100	R813	R813	F739	F739	V660	N595	I527	K462	E491	G311	F242
F1170	F1101	Q885	Q885	Y740	Y740	D662	E596	R528	K463	E491	K312	M243
L1172	S1037	L886	L886	V741	V741	G663	E597	T530	K464	E491	K313	A244
L1175	F1038	S887	S887	A742	A742	V666	E599	F531	K465	E491	C316	L245
L1176	E1039	L890	L890	K743	K743	R667	E599	R532	N466	E491	G317	Y246
L1177	Q1040	D891	D891	A744	A744	F668	E599	R532	V466	E491	L318	P248
G1107	L1042	D892	D892	D745	D745	Q601	Q601	R534	E467	E491	R319	F253
P1108	W1043	N895	N895	S747	S747	Q602	A602	S536	E468	E491	P321	I254
K1182	N1044	K896	K896	S748	S748	S603	S603	Q537	T469	E491	F322	E256
H1183	N1045	H899	H899	K749	K749	K604	K604	E538	M470	E491	A325	N257
K1184	Y1046	A901	A901	L753	L753	F677	N605	T539	V471	E491	V326	Y258
Y1185	F1047	S902	S902	F754	F754	N678	L606	R540	H473	E491	M327	L259
S1187	H1048	S903	S903	L757	L757	L679	V607	D541	D474	E491	D328	I260
S1188	V1051	E835	E835	L760	L760	N680	T608	K542	E475	E491	I329	R261
L1196	F1053	L839	L839	K761	K761	M681	F609	S543	E476	E491	T330	W262
L1197	A1052	C841	C841	F764	F764	E682	N683	E544	E477	E491	D331	N257
S1198	T1055	R842	R842	R765	R765	S684	T610	F544	K478	E491	I332	I258
S1199	L1120	L910	L910	R766	R766	S689	S612	A546	L479	E491	I333	I261
L1200	H1057	L913	L913	I767	I767	L692	T616	A550	L480	E491	K336	R361
L1201	S1058	D914	D914	Q845	Q845	V693	K617	F552	A483	E491	D337	W262
L1204	Q1060	T921	T921	S846	S846	F694	D618	N555	I484	E491	V337	K269
L1205	L1061			S946	S946		S619	L554	H485	E491	D338	E270
D1206	E1062						F620	M555	P486	E491	K336	P268
Y1207	T1063			Q851	Q851		G623	T624	G487	E491	D339	K269
							L625		A488	E491		E270
										E491		I271

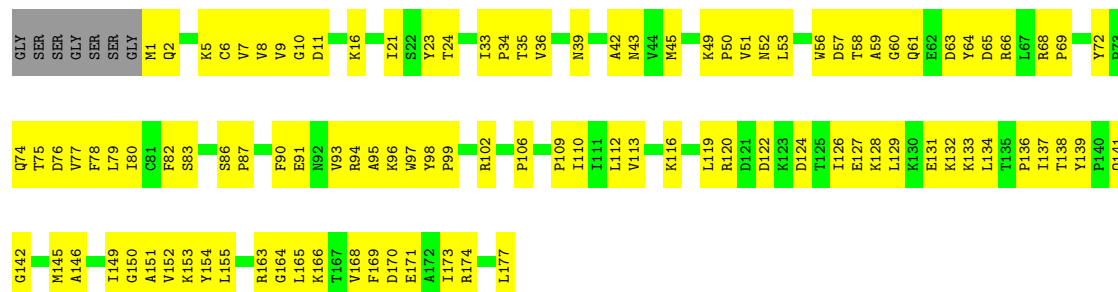






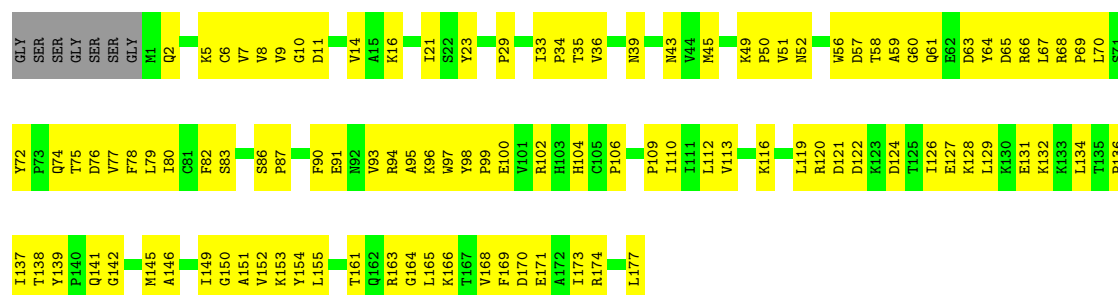
• Molecule 3: Ras-related C3 botulinum toxin substrate 1

Chain C: 40% 57%



• Molecule 3: Ras-related C3 botulinum toxin substrate 1

Chain F: 38% 58%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	128824	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	452.2, 452.2, 452.2	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.19	0/1641	0.44	0/2218
1	D	0.19	0/1641	0.44	0/2218
2	B	0.23	0/13722	0.45	0/18514
2	E	0.23	0/13722	0.44	0/18514
3	C	0.23	0/1415	0.43	0/1924
3	F	0.23	0/1415	0.43	0/1924
All	All	0.23	0/33556	0.44	0/45312

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
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	541	GLN	Peptide
1	D	541	GLN	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	1608	0	1617	115	0
1	D	1608	0	1617	115	0
2	B	13436	0	13516	795	0
2	E	13436	0	13516	802	0
3	C	1385	0	1407	89	0
3	F	1385	0	1407	94	0
All	All	32858	0	33080	1955	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 30.

All (1955) 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:95:LEU:HA	2:B:98:TRP:HD1	1.38	0.89
2:E:144:LEU:HD13	2:E:147:LYS:HE2	1.55	0.89
2:B:1526:ASN:OD1	2:B:1596:GLN:NE2	2.07	0.88
2:E:1526:ASN:OD1	2:E:1596:GLN:NE2	2.07	0.87
2:B:144:LEU:HD13	2:B:147:LYS:HE2	1.55	0.87
2:E:95:LEU:HA	2:E:98:TRP:HD1	1.38	0.86
2:E:1621:ARG:HD3	3:F:67:LEU:HD22	1.57	0.86
1:A:719:ASN:O	2:B:1:MET:N	2.08	0.86
3:F:93:VAL:HA	3:F:97:TRP:HB2	1.57	0.86
3:C:93:VAL:HA	3:C:97:TRP:HB2	1.57	0.84
2:E:119:GLN:NE2	2:E:120:MET:SD	2.51	0.84
2:B:119:GLN:NE2	2:B:120:MET:SD	2.51	0.83
2:E:570:VAL:HG21	2:E:595:MET:HE2	1.59	0.83
2:B:14:VAL:HB	2:B:65:HIS:HB3	1.61	0.82
2:B:570:VAL:HG21	2:B:595:MET:HE2	1.59	0.82
2:E:828:LYS:HE2	2:E:833:PRO:HG3	1.61	0.82
2:E:1545:HIS:HD2	3:F:5:LYS:HE3	1.43	0.82
2:B:828:LYS:HE2	2:B:833:PRO:HG3	1.61	0.82
2:E:14:VAL:HB	2:E:65:HIS:HB3	1.61	0.81
2:E:1393:ASP:OD1	3:F:166:LYS:NZ	2.13	0.81
2:E:1543:SER:HG	2:E:1545:HIS:HD1	1.21	0.80
2:B:904:GLN:O	2:B:908:ASN:ND2	2.15	0.80
1:A:589:GLY:HA3	1:A:604:LEU:HB2	1.64	0.79
3:C:43:ASN:ND2	3:C:52:ASN:OD1	2.15	0.79
1:A:670:ASN:ND2	1:A:676:ASP:O	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:928:ILE:O	2:B:932:LEU:HB2	1.82	0.79
3:F:43:ASN:ND2	3:F:52:ASN:OD1	2.15	0.79
1:D:589:GLY:HA3	1:D:604:LEU:HB2	1.64	0.79
2:E:49:THR:OG1	2:E:52:ASN:OD1	2.01	0.79
2:E:1543:SER:OG	2:E:1545:HIS:ND1	2.16	0.79
2:B:4:TRP:HB3	2:B:39:GLU:HB3	1.65	0.79
2:B:166:ARG:NH1	2:B:167:ASP:OD1	2.16	0.79
1:D:670:ASN:ND2	1:D:676:ASP:O	2.15	0.79
2:E:166:ARG:NH1	2:E:167:ASP:OD1	2.16	0.79
2:E:928:ILE:O	2:E:932:LEU:HB2	1.83	0.79
2:E:904:GLN:O	2:E:908:ASN:ND2	2.15	0.78
1:A:724:TYR:HB3	2:B:4:TRP:HB2	1.66	0.78
2:E:4:TRP:HB3	2:E:39:GLU:HB3	1.65	0.78
1:A:563:ARG:HB3	1:A:573:LYS:HE3	1.65	0.78
2:B:49:THR:OG1	2:B:52:ASN:OD1	2.01	0.77
2:E:1594:ALA:HA	2:E:1597:MET:HE1	1.66	0.77
1:D:551:GLN:HA	1:D:554:ASN:HD22	1.48	0.77
2:B:1543:SER:HG	2:B:1545:HIS:HD1	1.31	0.77
1:D:667:ASP:OD2	1:D:679:SER:OG	2.03	0.77
3:F:39:ASN:H	3:F:57:ASP:HB3	1.50	0.77
3:F:98:TYR:HE1	3:F:149:ILE:HD13	1.50	0.77
2:E:98:TRP:HH2	2:E:155:GLY:HA3	1.50	0.76
1:D:563:ARG:HB3	1:D:573:LYS:HE3	1.66	0.76
2:B:1594:ALA:HA	2:B:1597:MET:HE1	1.66	0.76
1:D:700:ASP:HB2	2:E:32:GLY:HA2	1.66	0.76
1:A:551:GLN:HA	1:A:554:ASN:HD22	1.48	0.76
2:B:1536:HIS:O	2:B:1540:ARG:NH2	2.19	0.76
2:B:1543:SER:OG	2:B:1545:HIS:ND1	2.16	0.76
3:C:98:TYR:HE1	3:C:149:ILE:HD13	1.50	0.76
1:A:575:TRP:HZ3	1:A:588:TYR:HB2	1.51	0.75
2:E:1536:HIS:O	2:E:1540:ARG:NH2	2.19	0.75
2:B:921:THR:O	2:B:925:ILE:N	2.19	0.75
1:D:575:TRP:HZ3	1:D:588:TYR:HB2	1.51	0.75
1:A:667:ASP:OD2	1:A:679:SER:OG	2.03	0.75
3:C:39:ASN:H	3:C:57:ASP:HB3	1.50	0.75
2:E:641:LEU:O	2:E:644:ARG:NH1	2.20	0.75
2:B:98:TRP:HH2	2:B:155:GLY:HA3	1.50	0.75
2:B:197:LYS:HA	2:B:200:GLU:HG2	1.69	0.75
2:B:485:HIS:HB2	2:B:514:LYS:HB3	1.67	0.75
2:B:444:ASN:ND2	2:B:517:ILE:O	2.20	0.75
2:E:1277:PRO:HG3	2:E:1292:THR:HA	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:485:HIS:HB2	2:E:514:LYS:HB3	1.67	0.74
1:A:723:VAL:HG23	2:B:2:ALA:HB1	1.69	0.74
2:B:1579:HIS:HB3	2:B:1582:ASP:HB2	1.69	0.74
2:B:1314:TRP:HB2	2:B:1352:ILE:HD11	1.70	0.74
3:C:129:LEU:HA	3:C:132:LYS:HG2	1.70	0.74
2:B:1128:PHE:HA	2:B:1131:MET:HE3	1.68	0.74
3:C:7:VAL:HG23	3:C:75:THR:HG21	1.70	0.74
2:B:641:LEU:O	2:B:644:ARG:NH1	2.20	0.74
2:E:1067:ALA:O	2:E:1071:LYS:N	2.17	0.73
2:B:881:LEU:O	2:B:885:GLN:NE2	2.21	0.73
2:E:1579:HIS:HB3	2:E:1582:ASP:HB2	1.69	0.73
2:B:351:ILE:HG12	2:B:382:VAL:HG21	1.70	0.73
2:E:197:LYS:HA	2:E:200:GLU:HG2	1.69	0.73
2:E:444:ASN:ND2	2:E:517:ILE:O	2.20	0.73
2:E:881:LEU:O	2:E:885:GLN:NE2	2.21	0.73
2:E:1335:TYR:HA	2:E:1338:LEU:HD23	1.71	0.73
3:F:129:LEU:HA	3:F:132:LYS:HG2	1.70	0.73
2:B:1277:PRO:HG3	2:B:1292:THR:HA	1.68	0.73
2:B:771:ARG:NH2	2:B:781:SER:OG	2.22	0.72
2:E:351:ILE:HG12	2:E:382:VAL:HG21	1.70	0.72
2:E:1128:PHE:HA	2:E:1131:MET:HE3	1.68	0.72
3:F:7:VAL:HG23	3:F:75:THR:HG21	1.70	0.72
2:B:1080:ARG:HA	2:B:1083:ILE:HD12	1.72	0.72
1:A:717:PRO:HD2	2:B:1:MET:SD	2.29	0.72
2:B:1335:TYR:HA	2:B:1338:LEU:HD23	1.71	0.72
2:E:262:TRP:HA	2:E:268:PRO:HA	1.72	0.72
2:E:809:ALA:HB1	2:E:812:ILE:HB	1.71	0.72
1:D:535:GLU:O	1:D:539:LYS:HB3	1.89	0.72
1:A:535:GLU:O	1:A:539:LYS:HB3	1.89	0.72
2:E:1314:TRP:HB2	2:E:1352:ILE:HD11	1.70	0.72
2:B:809:ALA:HB1	2:B:812:ILE:HB	1.72	0.72
2:E:740:TYR:HA	2:E:749:LYS:HD3	1.70	0.72
2:B:740:TYR:HA	2:B:749:LYS:HD3	1.70	0.71
2:E:771:ARG:NH2	2:E:781:SER:OG	2.22	0.71
2:E:964:MET:O	2:E:1019:ARG:NH2	2.23	0.71
1:A:692:MET:HE1	2:B:122:TYR:CE2	2.25	0.71
2:E:1032:PHE:HB3	2:E:1043:TRP:HH2	1.55	0.71
1:A:723:VAL:HB	2:B:3:ARG:H	1.56	0.71
2:B:1032:PHE:HB3	2:B:1043:TRP:HH2	1.54	0.71
2:B:262:TRP:HA	2:B:268:PRO:HA	1.72	0.71
1:D:625:MET:HE1	1:D:637:VAL:HG23	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:576:TYR:HB2	1:D:598:GLU:HG2	1.73	0.70
2:E:12:TYR:HB2	2:E:67:LYS:HB2	1.73	0.70
2:E:241:LEU:HB2	2:E:260:ILE:HB	1.73	0.70
2:B:964:MET:O	2:B:1019:ARG:NH2	2.23	0.70
2:E:561:THR:HG21	2:E:631:LEU:HB3	1.74	0.70
2:B:241:LEU:HB2	2:B:260:ILE:HB	1.73	0.70
2:E:532:ARG:HA	2:E:546:ALA:HA	1.74	0.70
2:B:445:ASP:HB2	2:B:627:CYS:HB2	1.74	0.70
2:E:1080:ARG:HA	2:E:1083:ILE:HD12	1.72	0.70
2:B:441:ASP:O	2:B:629:THR:OG1	2.10	0.70
2:E:7:THR:HG22	2:E:9:ARG:H	1.55	0.70
2:B:12:TYR:HB2	2:B:67:LYS:HB2	1.73	0.70
2:B:532:ARG:HA	2:B:546:ALA:HA	1.73	0.70
2:B:7:THR:HG22	2:B:9:ARG:H	1.55	0.70
2:B:1169:LYS:HA	2:B:1172:LEU:HD12	1.74	0.70
1:A:576:TYR:HB2	1:A:598:GLU:HG2	1.73	0.70
2:B:1216:SER:OG	2:B:1401:GLN:NE2	2.25	0.70
2:E:1111:GLU:N	2:E:1111:GLU:OE1	2.25	0.70
2:E:1398:LEU:HD22	2:E:1426:MET:HE3	1.74	0.70
2:E:749:LYS:HG2	2:E:753:LEU:HD23	1.73	0.69
2:E:932:LEU:N	2:E:935:ARG:HH21	1.89	0.69
2:E:1272:GLN:OE1	2:E:1293:GLN:NE2	2.25	0.69
2:B:569:LEU:HB2	2:B:620:PHE:HB3	1.75	0.69
2:B:1516:GLU:HA	2:B:1519:ILE:HD12	1.73	0.69
1:A:561:CYS:SG	1:A:594:SER:OG	2.51	0.69
2:B:749:LYS:HG2	2:B:753:LEU:HD23	1.73	0.69
2:B:879:LEU:HD12	2:B:882:LEU:HB2	1.74	0.69
2:E:242:PHE:HB2	2:E:299:GLN:HB2	1.75	0.69
2:E:1516:GLU:HA	2:E:1519:ILE:HD12	1.73	0.69
2:E:1372:PHE:O	2:E:1377:ARG:NH2	2.23	0.69
2:B:932:LEU:N	2:B:935:ARG:HH21	1.89	0.69
1:A:688:THR:O	1:A:692:MET:HG2	1.93	0.69
2:E:1587:GLU:OE1	2:E:1591:ARG:NH2	2.25	0.69
1:A:625:MET:HE1	1:A:637:VAL:HG23	1.73	0.69
2:B:1398:LEU:HD22	2:B:1426:MET:HE3	1.74	0.69
2:E:445:ASP:HB2	2:E:627:CYS:HB2	1.74	0.69
2:E:921:THR:O	2:E:925:ILE:N	2.19	0.68
2:B:242:PHE:HB2	2:B:299:GLN:HB2	1.75	0.68
2:B:7:THR:O	2:B:10:GLN:NE2	2.26	0.68
2:B:101:ILE:HG21	2:B:159:LEU:HD21	1.76	0.68
2:B:1165:ASP:OD2	2:B:1168:TYR:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1272:GLN:OE1	2:B:1293:GLN:NE2	2.25	0.68
2:E:879:LEU:HD12	2:E:882:LEU:HB2	1.74	0.68
2:E:1216:SER:OG	2:E:1401:GLN:NE2	2.25	0.68
2:B:561:THR:HG21	2:B:631:LEU:HB3	1.74	0.68
1:D:561:CYS:SG	1:D:594:SER:OG	2.51	0.68
1:D:688:THR:O	1:D:692:MET:HG2	1.93	0.68
2:B:1587:GLU:OE1	2:B:1591:ARG:NH2	2.25	0.68
2:B:480:LEU:HD22	2:B:483:ALA:HB2	1.76	0.68
2:E:1115:THR:O	2:E:1121:ARG:NH2	2.27	0.68
2:E:569:LEU:HB2	2:E:620:PHE:HB3	1.75	0.68
2:B:23:GLN:HG2	2:B:58:ILE:HB	1.76	0.68
2:B:226:VAL:HB	2:B:279:ALA:HB3	1.76	0.68
1:D:701:LEU:HD11	2:E:16:ILE:HA	1.74	0.68
3:C:9:VAL:HG22	3:C:78:PHE:HZ	1.59	0.68
2:E:480:LEU:HD22	2:E:483:ALA:HB2	1.76	0.68
2:E:534:ARG:NE	2:E:541:ASP:OD1	2.27	0.67
2:E:441:ASP:O	2:E:629:THR:OG1	2.10	0.67
2:E:1169:LYS:HA	2:E:1172:LEU:HD12	1.74	0.67
2:B:95:LEU:HA	2:B:98:TRP:CD1	2.27	0.67
2:B:472:VAL:HG22	2:B:527:ILE:HG12	1.76	0.67
2:B:1111:GLU:N	2:B:1111:GLU:OE1	2.25	0.67
2:B:534:ARG:NE	2:B:541:ASP:OD1	2.27	0.67
2:B:1067:ALA:O	2:B:1071:LYS:N	2.17	0.67
2:B:1115:THR:O	2:B:1121:ARG:NH2	2.27	0.67
2:B:1372:PHE:O	2:B:1377:ARG:NH2	2.23	0.67
2:E:226:VAL:HB	2:E:279:ALA:HB3	1.76	0.67
2:E:1259:GLU:N	2:E:1259:GLU:OE1	2.27	0.67
2:E:297:VAL:HG22	2:E:326:VAL:HG22	1.76	0.67
2:B:297:VAL:HG22	2:B:326:VAL:HG22	1.76	0.67
2:B:1633:VAL:HA	2:B:1637:TYR:HB2	1.76	0.67
1:D:584:LYS:NZ	2:E:1403:PRO:HA	2.09	0.67
2:B:1149:ASN:OD1	2:B:1236:ARG:NH2	2.28	0.67
2:B:1315:GLU:OE1	2:B:1315:GLU:N	2.26	0.67
3:F:77:VAL:HG12	3:F:109:PRO:HG2	1.75	0.67
2:E:101:ILE:HG21	2:E:159:LEU:HD21	1.76	0.67
2:E:1149:ASN:OD1	2:E:1236:ARG:NH2	2.28	0.67
3:F:9:VAL:HG22	3:F:78:PHE:HZ	1.59	0.67
2:B:1117:GLU:OE2	2:B:1121:ARG:N	2.25	0.66
2:E:1315:GLU:OE1	2:E:1315:GLU:N	2.26	0.66
2:B:1523:GLU:HA	2:B:1526:ASN:ND2	2.11	0.66
2:B:1135:GLU:O	2:B:1139:SER:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:120:ARG:HH12	3:C:139:TYR:HB2	1.60	0.66
3:C:77:VAL:HG12	3:C:109:PRO:HG2	1.75	0.66
2:E:1633:VAL:HA	2:E:1637:TYR:HB2	1.77	0.66
3:F:120:ARG:HH12	3:F:139:TYR:HB2	1.61	0.66
2:E:1135:GLU:O	2:E:1139:SER:N	2.29	0.66
2:E:1165:ASP:OD2	2:E:1168:TYR:N	2.26	0.66
2:E:1523:GLU:HA	2:E:1526:ASN:ND2	2.11	0.66
2:B:278:GLN:HB2	2:B:425:THR:HG23	1.79	0.65
2:E:23:GLN:HG2	2:E:58:ILE:HB	1.76	0.65
2:B:958:ILE:HA	2:B:961:LEU:HD12	1.78	0.65
2:B:879:LEU:HD23	2:B:931:ARG:HH22	1.62	0.65
2:E:545:ARG:NH1	2:E:546:ALA:HB3	2.12	0.65
2:E:730:TYR:HB2	2:E:767:ILE:HG23	1.78	0.65
2:B:1143:ASN:OD1	2:B:1145:HIS:ND1	2.30	0.65
1:D:723:VAL:HG23	2:E:2:ALA:HB1	1.79	0.65
2:E:472:VAL:HG22	2:E:527:ILE:HG12	1.76	0.65
2:E:958:ILE:HA	2:E:961:LEU:HD12	1.78	0.65
2:E:1143:ASN:OD1	2:E:1145:HIS:ND1	2.30	0.65
2:B:545:ARG:NH1	2:B:546:ALA:HB3	2.12	0.65
2:E:1276:LYS:NZ	2:E:1277:PRO:O	2.30	0.65
2:E:1536:HIS:HA	2:E:1542:LEU:HD13	1.79	0.65
2:B:1117:GLU:OE1	2:B:1119:GLU:N	2.30	0.64
2:B:1275:ASP:O	2:B:1292:THR:OG1	2.11	0.64
2:E:318:LEU:HB3	2:E:500:VAL:HG21	1.80	0.64
1:A:550:GLN:O	1:A:554:ASN:ND2	2.30	0.64
2:B:59:PHE:HD2	2:B:64:ILE:HG12	1.63	0.64
2:E:1117:GLU:OE1	2:E:1119:GLU:N	2.31	0.64
2:E:1416:GLU:HA	2:E:1419:LYS:HG2	1.79	0.64
2:E:1552:SER:HB3	3:F:39:ASN:HD22	1.63	0.64
2:E:37:ILE:HG21	2:E:45:TYR:HB3	1.79	0.64
3:C:11:ASP:O	3:C:16:LYS:NZ	2.28	0.64
1:D:550:GLN:O	1:D:554:ASN:ND2	2.30	0.64
2:E:278:GLN:HB2	2:E:425:THR:HG23	1.79	0.64
2:E:569:LEU:N	2:E:620:PHE:O	2.31	0.64
2:B:1536:HIS:HA	2:B:1542:LEU:HD13	1.79	0.64
1:D:727:ASN:O	2:E:46:ARG:NH2	2.31	0.64
2:E:7:THR:O	2:E:10:GLN:NE2	2.26	0.64
2:B:556:ASN:N	2:B:560:THR:O	2.29	0.64
2:B:1015:ARG:HA	2:B:1018:LEU:HD12	1.80	0.64
1:A:622:CYS:HB2	1:A:625:MET:HG2	1.78	0.64
2:E:95:LEU:HA	2:E:98:TRP:CD1	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1259:GLU:OE1	2:B:1259:GLU:N	2.27	0.64
2:E:1545:HIS:CD2	3:F:5:LYS:HE3	2.28	0.64
2:B:318:LEU:HB3	2:B:500:VAL:HG21	1.80	0.63
2:B:730:TYR:HB2	2:B:767:ILE:HG23	1.78	0.63
2:B:1059:LEU:O	2:B:1063:THR:OG1	2.16	0.63
3:F:23:TYR:HB2	3:F:165:LEU:HD21	1.80	0.63
2:B:569:LEU:N	2:B:620:PHE:O	2.31	0.63
2:B:1024:PHE:HA	2:B:1027:VAL:HG22	1.80	0.63
2:B:1177:LEU:HD22	2:B:1181:ARG:HH22	1.64	0.63
1:D:622:CYS:HB2	1:D:625:MET:HG2	1.78	0.63
2:B:37:ILE:HG21	2:B:45:TYR:HB3	1.79	0.63
2:B:1276:LYS:NZ	2:B:1277:PRO:O	2.30	0.63
3:F:116:LYS:HB3	3:F:119:LEU:HB2	1.81	0.63
2:B:1416:GLU:HA	2:B:1419:LYS:HG2	1.79	0.63
2:B:37:ILE:HA	2:B:47:GLY:HA3	1.81	0.63
2:B:1248:ARG:HH11	2:B:1252:ARG:NH1	1.96	0.63
2:E:59:PHE:HD2	2:E:64:ILE:HG12	1.63	0.63
2:B:327:MET:HG2	2:B:346:ILE:HG23	1.81	0.63
2:B:1057:GLU:HA	2:B:1061:LEU:HD23	1.81	0.63
2:E:1248:ARG:HH11	2:E:1252:ARG:NH1	1.96	0.63
3:C:116:LYS:HB3	3:C:119:LEU:HB2	1.81	0.63
3:C:119:LEU:HA	3:C:122:ASP:HB2	1.80	0.63
2:E:228:PHE:HB3	2:E:277:LEU:HB3	1.80	0.63
2:E:989:THR:HG21	2:E:1024:PHE:HE2	1.64	0.63
2:E:1024:PHE:HA	2:E:1027:VAL:HG22	1.80	0.63
3:F:93:VAL:HG13	3:F:94:ARG:HD2	1.81	0.63
2:B:1284:GLN:HG2	2:B:1286:ASP:H	1.64	0.63
1:D:622:CYS:HB3	1:D:624:HIS:CD2	2.34	0.63
2:E:37:ILE:HA	2:E:47:GLY:HA3	1.81	0.63
2:E:228:PHE:HZ	2:E:231:PHE:HB2	1.64	0.63
2:E:349:GLN:HB2	2:E:392:VAL:HG13	1.81	0.63
2:E:1015:ARG:HA	2:E:1018:LEU:HD12	1.80	0.63
3:C:23:TYR:HB2	3:C:165:LEU:HD21	1.81	0.62
2:E:470:MET:HE1	2:E:513:VAL:HG21	1.81	0.62
2:E:879:LEU:HD23	2:E:931:ARG:HH22	1.62	0.62
2:E:1284:GLN:HG2	2:E:1286:ASP:H	1.64	0.62
2:B:228:PHE:HZ	2:B:231:PHE:HB2	1.64	0.62
2:B:228:PHE:HB3	2:B:277:LEU:HB3	1.80	0.62
1:D:551:GLN:OE1	1:D:552:ARG:NH2	2.32	0.62
2:E:851:GLN:O	2:E:856:LYS:NZ	2.32	0.62
2:B:1575:TYR:O	2:B:1579:HIS:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:853:VAL:O	2:E:857:LEU:HG	2.00	0.62
2:B:989:THR:HG21	2:B:1024:PHE:HE2	1.64	0.62
2:E:463:PRO:HD2	2:E:503:GLN:HB3	1.81	0.62
2:E:1034:ASP:OD1	2:E:1097:HIS:NE2	2.28	0.62
2:B:474:ASP:O	2:B:526:HIS:NE2	2.33	0.62
2:B:1248:ARG:HH11	2:B:1252:ARG:HH12	1.46	0.62
1:A:622:CYS:HB3	1:A:624:HIS:CD2	2.34	0.62
2:B:569:LEU:HD12	2:B:620:PHE:HD2	1.65	0.62
2:B:1588:LEU:HD23	2:B:1591:ARG:HE	1.64	0.62
2:E:327:MET:HG2	2:E:346:ILE:HG23	1.81	0.62
2:B:1120:LEU:O	2:B:1124:THR:OG1	2.09	0.62
3:C:170:ASP:HB3	3:C:174:ARG:HH21	1.64	0.62
2:E:940:VAL:HG13	2:E:992:MET:HE1	1.82	0.62
2:E:1120:LEU:O	2:E:1124:THR:OG1	2.09	0.62
2:B:87:LEU:HD23	2:B:91:LEU:HD23	1.81	0.62
3:C:93:VAL:HG13	3:C:94:ARG:HD2	1.81	0.62
2:E:87:LEU:HD23	2:E:91:LEU:HD23	1.81	0.62
2:B:101:ILE:O	2:B:105:LEU:HG	2.00	0.62
2:E:569:LEU:HD12	2:E:620:PHE:HD2	1.65	0.62
2:E:1177:LEU:HD22	2:E:1181:ARG:HH22	1.64	0.62
2:E:1513:SER:O	2:E:1517:ASN:ND2	2.33	0.62
1:A:551:GLN:OE1	1:A:552:ARG:NH2	2.32	0.62
2:B:463:PRO:HD2	2:B:503:GLN:HB3	1.81	0.62
2:B:470:MET:HE1	2:B:513:VAL:HG21	1.81	0.62
2:B:851:GLN:O	2:B:856:LYS:NZ	2.32	0.62
2:B:940:VAL:HG13	2:B:992:MET:HE1	1.82	0.62
2:B:1602:GLU:HA	2:B:1605:ARG:HG2	1.82	0.62
1:D:562:PHE:N	1:D:575:TRP:O	2.33	0.62
2:E:296:LEU:HB2	2:E:329:ILE:HD13	1.81	0.62
2:E:809:ALA:HB3	2:E:813:LYS:HZ2	1.64	0.62
3:F:119:LEU:HA	3:F:122:ASP:HB2	1.80	0.62
1:A:562:PHE:N	1:A:575:TRP:O	2.33	0.61
2:B:853:VAL:O	2:B:857:LEU:HG	1.99	0.61
2:B:1513:SER:O	2:B:1517:ASN:ND2	2.33	0.61
2:E:556:ASN:N	2:E:560:THR:O	2.29	0.61
2:E:883:THR:OG1	2:E:931:ARG:NH1	2.33	0.61
1:A:673:LEU:HB3	1:A:675:LYS:HZ3	1.62	0.61
2:B:589:PRO:HB3	2:B:594:GLU:HB3	1.80	0.61
1:D:584:LYS:HZ3	2:E:1403:PRO:HA	1.63	0.61
1:D:723:VAL:HB	2:E:3:ARG:H	1.65	0.61
2:B:296:LEU:HB2	2:B:329:ILE:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349:GLN:HB2	2:B:392:VAL:HG13	1.81	0.61
2:B:1043:TRP:H	2:B:1043:TRP:HE3	1.48	0.61
3:C:126:ILE:HG23	3:C:136:PRO:HG2	1.82	0.61
2:E:1043:TRP:H	2:E:1043:TRP:HE3	1.48	0.61
2:E:1057:GLU:HA	2:E:1061:LEU:HD23	1.81	0.61
3:F:170:ASP:HB3	3:F:174:ARG:HH21	1.64	0.61
2:B:883:THR:OG1	2:B:931:ARG:NH1	2.33	0.61
2:B:1520:GLU:HA	2:B:1523:GLU:OE2	2.01	0.61
2:E:474:ASP:O	2:E:526:HIS:NE2	2.33	0.61
2:E:1032:PHE:HB3	2:E:1043:TRP:CH2	2.36	0.61
2:E:1078:ASP:OD1	2:E:1081:LYS:N	2.34	0.61
2:B:883:THR:HG21	2:B:931:ARG:HB3	1.83	0.61
2:E:1275:ASP:O	2:E:1292:THR:OG1	2.11	0.61
2:E:1520:GLU:HA	2:E:1523:GLU:OE2	2.01	0.61
2:E:1468:PHE:CE2	2:E:1470:LYS:HB2	2.36	0.61
3:F:126:ILE:HG23	3:F:136:PRO:HG2	1.82	0.61
2:B:1066:GLN:HA	2:B:1069:ARG:NH1	2.16	0.61
1:D:548:ILE:O	1:D:552:ARG:HG2	2.01	0.61
2:E:101:ILE:O	2:E:105:LEU:HG	2.00	0.61
2:E:589:PRO:HB3	2:E:594:GLU:HB3	1.80	0.61
2:E:1066:GLN:HA	2:E:1069:ARG:NH1	2.16	0.61
2:E:1231:TYR:O	2:E:1235:LYS:N	2.34	0.61
2:E:1477:ASN:HB3	2:E:1568:LYS:NZ	2.16	0.61
2:E:1602:GLU:HA	2:E:1605:ARG:HG2	1.81	0.61
1:A:722:PHE:HA	2:B:2:ALA:HA	1.82	0.60
1:D:580:SER:HB2	1:D:585:VAL:HG22	1.83	0.60
2:E:25:VAL:HG12	2:E:55:LYS:HE2	1.83	0.60
2:E:834:VAL:HB	2:E:873:GLU:HG2	1.83	0.60
2:E:1630:LYS:O	2:E:1634:GLU:HG2	2.01	0.60
2:B:3:ARG:HH22	2:B:42:GLU:H	1.50	0.60
2:B:1328:TYR:HA	2:B:1332:VAL:HG12	1.83	0.60
2:E:3:ARG:HH22	2:E:42:GLU:H	1.50	0.60
2:E:91:LEU:HD11	2:E:128:ARG:HG3	1.82	0.60
2:B:46:ARG:HB3	2:B:58:ILE:HG13	1.84	0.60
2:B:1630:LYS:O	2:B:1634:GLU:HG2	2.01	0.60
1:D:573:LYS:N	1:D:593:GLU:OE2	2.35	0.60
2:E:929:MET:HE3	2:E:973:ILE:HG13	1.84	0.60
2:B:826:ASP:HA	2:B:829:LEU:HB2	1.83	0.60
2:B:1477:ASN:HB3	2:B:1568:LYS:NZ	2.16	0.60
2:E:155:GLY:HA2	2:E:158:MET:SD	2.40	0.60
2:E:826:ASP:HA	2:E:829:LEU:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:902:SER:HA	2:E:905:LEU:HD12	1.84	0.60
2:E:1248:ARG:HH11	2:E:1252:ARG:HH12	1.46	0.60
2:E:1446:VAL:HB	2:E:1450:ILE:HD11	1.84	0.60
2:E:1563:PHE:HA	2:E:1566:TYR:CD2	2.37	0.60
1:A:670:ASN:HA	1:A:673:LEU:HB2	1.83	0.60
2:B:465:ASN:OD1	2:B:503:GLN:N	2.34	0.60
2:B:1563:PHE:HA	2:B:1566:TYR:CD2	2.37	0.60
2:E:85:LEU:O	2:E:88:VAL:HG22	2.02	0.60
2:E:1588:LEU:HD23	2:E:1591:ARG:HE	1.65	0.60
2:B:155:GLY:HA2	2:B:158:MET:SD	2.40	0.60
2:B:929:MET:HE3	2:B:973:ILE:HG13	1.84	0.60
3:F:8:VAL:O	3:F:58:THR:OG1	2.19	0.60
2:B:1446:VAL:HB	2:B:1450:ILE:HD11	1.84	0.60
3:C:146:ALA:O	3:C:150:GLY:N	2.34	0.60
2:E:19:TYR:O	2:E:28:SER:HA	2.02	0.60
3:F:169:PHE:O	3:F:173:ILE:HG12	2.02	0.60
1:A:580:SER:HB2	1:A:585:VAL:HG22	1.83	0.60
2:B:25:VAL:HG12	2:B:55:LYS:HE2	1.83	0.60
2:B:91:LEU:HD11	2:B:128:ARG:HG3	1.82	0.60
2:B:792:ARG:HA	2:B:795:PHE:HD2	1.67	0.60
2:B:1468:PHE:CE2	2:B:1470:LYS:HB2	2.36	0.60
3:C:8:VAL:O	3:C:58:THR:OG1	2.19	0.60
2:E:244:ALA:HB2	2:E:257:ASN:HA	1.84	0.60
2:E:883:THR:HG21	2:E:931:ARG:HB3	1.83	0.60
2:B:834:VAL:HB	2:B:873:GLU:HG2	1.84	0.59
2:B:1392:GLU:HB2	3:C:166:LYS:NZ	2.17	0.59
1:D:670:ASN:HA	1:D:673:LEU:HB2	1.83	0.59
1:A:548:ILE:O	1:A:552:ARG:HG2	2.01	0.59
2:B:1231:TYR:O	2:B:1235:LYS:N	2.34	0.59
2:B:1462:PHE:O	2:B:1489:TYR:N	2.35	0.59
2:B:85:LEU:O	2:B:88:VAL:HG22	2.02	0.59
2:B:244:ALA:HB2	2:B:257:ASN:HA	1.84	0.59
2:B:843:PHE:O	2:B:846:SER:OG	2.20	0.59
2:E:208:LEU:HD23	2:E:211:ARG:HH21	1.67	0.59
2:E:281:PHE:HD1	2:E:428:ALA:HB3	1.66	0.59
1:A:573:LYS:N	1:A:593:GLU:OE2	2.35	0.59
2:B:19:TYR:O	2:B:28:SER:HA	2.02	0.59
2:E:1059:LEU:O	2:E:1063:THR:OG1	2.16	0.59
2:E:1117:GLU:OE2	2:E:1121:ARG:N	2.25	0.59
3:F:11:ASP:O	3:F:16:LYS:NZ	2.28	0.59
2:B:522:VAL:HA	2:B:525:CYS:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:94:THR:HG22	2:E:98:TRP:NE1	2.17	0.59
2:B:208:LEU:HD23	2:B:211:ARG:HH21	1.67	0.59
2:B:281:PHE:HD1	2:B:428:ALA:HB3	1.66	0.59
2:B:855:GLN:OE1	2:B:855:GLN:N	2.35	0.59
2:B:1032:PHE:HB3	2:B:1043:TRP:CH2	2.36	0.59
2:B:1399:LEU:HD11	2:B:1407:LYS:HD2	1.85	0.59
3:F:146:ALA:O	3:F:150:GLY:N	2.34	0.59
1:A:607:LYS:NZ	1:A:608:LEU:O	2.35	0.59
2:B:545:ARG:NH2	2:B:580:GLU:OE1	2.36	0.59
2:B:1523:GLU:O	2:B:1526:ASN:N	2.36	0.59
1:D:590:ASP:H	1:D:604:LEU:HD22	1.68	0.59
2:E:529:PHE:O	2:E:550:ALA:N	2.27	0.59
1:A:679:SER:HB3	1:A:681:LEU:HG	1.85	0.59
2:B:1044:ASN:HA	2:B:1105:MET:HE2	1.85	0.59
1:D:530:SER:HA	1:D:533:ILE:HD12	1.84	0.59
2:E:467:GLU:O	2:E:531:PHE:HA	2.03	0.59
2:E:843:PHE:O	2:E:846:SER:OG	2.20	0.59
2:E:1520:GLU:HA	2:E:1523:GLU:CD	2.28	0.59
2:E:1523:GLU:O	2:E:1526:ASN:N	2.36	0.59
2:B:254:ILE:HD12	2:B:294:VAL:HG13	1.84	0.59
2:B:1078:ASP:OD1	2:B:1081:LYS:N	2.34	0.59
2:E:46:ARG:HB3	2:E:58:ILE:HG13	1.84	0.59
2:E:254:ILE:HD12	2:E:294:VAL:HG13	1.84	0.59
2:E:1044:ASN:HA	2:E:1105:MET:HE2	1.85	0.59
2:B:473:HIS:ND1	2:B:477:GLY:O	2.32	0.59
2:B:1440:SER:H	2:B:1442:LYS:HZ3	1.51	0.59
2:E:972:TYR:HA	2:E:975:THR:OG1	2.03	0.59
1:A:530:SER:HA	1:A:533:ILE:HD12	1.84	0.58
2:B:1034:ASP:OD1	2:B:1097:HIS:NE2	2.28	0.58
2:E:522:VAL:HA	2:E:525:CYS:HB2	1.85	0.58
2:E:545:ARG:NH2	2:E:580:GLU:OE1	2.36	0.58
2:E:792:ARG:HA	2:E:795:PHE:HD2	1.67	0.58
2:E:1399:LEU:HD11	2:E:1407:LYS:HD2	1.85	0.58
2:B:94:THR:HG22	2:B:98:TRP:NE1	2.17	0.58
2:B:181:ILE:HD11	2:B:956:CYS:HA	1.85	0.58
2:B:242:PHE:HD2	2:B:257:ASN:HB3	1.67	0.58
2:B:730:TYR:OH	2:B:771:ARG:NH1	2.36	0.58
1:D:607:LYS:NZ	1:D:608:LEU:O	2.35	0.58
1:D:679:SER:HB3	1:D:681:LEU:HG	1.85	0.58
2:B:902:SER:HA	2:B:905:LEU:HD12	1.84	0.58
2:B:1520:GLU:HA	2:B:1523:GLU:CD	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:169:PHE:O	3:C:173:ILE:HG12	2.02	0.58
2:E:1328:TYR:HA	2:E:1332:VAL:HG12	1.83	0.58
1:A:590:ASP:H	1:A:604:LEU:HD22	1.68	0.58
2:B:1117:GLU:CD	2:B:1120:LEU:HG	2.29	0.58
2:B:1404:ASN:OD1	2:B:1424:GLN:HB2	2.04	0.58
1:D:717:PRO:HD2	2:E:1:MET:SD	2.44	0.58
2:E:181:ILE:HD11	2:E:956:CYS:HA	1.85	0.58
2:B:979:ARG:NH1	2:B:1031:PHE:O	2.36	0.58
3:C:45:MET:HA	3:C:50:PRO:HA	1.85	0.58
2:E:842:LYS:O	2:E:845:GLN:NE2	2.37	0.58
2:B:972:TYR:HA	2:B:975:THR:OG1	2.03	0.58
2:E:1072:ILE:O	2:E:1076:TYR:N	2.35	0.58
2:B:470:MET:HA	2:B:529:PHE:HA	1.86	0.58
2:E:450:LEU:HB3	2:E:620:PHE:HZ	1.69	0.58
2:E:529:PHE:HB2	2:E:550:ALA:HB3	1.86	0.58
2:E:1117:GLU:CD	2:E:1120:LEU:HG	2.29	0.58
2:E:200:GLU:HA	2:E:203:SER:HB2	1.86	0.58
2:E:518:ALA:HB3	2:E:521:GLU:HG2	1.85	0.58
2:B:143:GLU:HG3	2:B:147:LYS:NZ	2.19	0.58
2:B:1525:THR:HA	2:B:1528:ARG:HH11	1.68	0.58
2:B:1618:LEU:O	2:B:1622:LEU:HG	2.04	0.58
2:E:855:GLN:OE1	2:E:855:GLN:N	2.34	0.58
2:E:1238:ASP:HA	2:E:1241:ILE:HD12	1.86	0.58
2:E:1404:ASN:OD1	2:E:1424:GLN:HB2	2.03	0.58
2:B:25:VAL:HG23	2:B:57:GLY:HA2	1.86	0.58
2:B:192:LYS:O	2:B:195:GLU:HG2	2.03	0.58
2:B:467:GLU:O	2:B:531:PHE:HA	2.03	0.58
2:E:192:LYS:O	2:E:195:GLU:HG2	2.03	0.58
2:B:529:PHE:O	2:B:550:ALA:N	2.27	0.57
3:C:49:LYS:NZ	3:C:50:PRO:O	2.31	0.57
2:E:1618:LEU:O	2:E:1622:LEU:HG	2.04	0.57
2:B:166:ARG:NH2	2:B:168:ASP:HB2	2.19	0.57
2:B:879:LEU:O	2:B:882:LEU:N	2.38	0.57
2:B:1238:ASP:HA	2:B:1241:ILE:HD12	1.86	0.57
2:E:979:ARG:NH1	2:E:1031:PHE:O	2.36	0.57
2:E:1371:GLY:C	2:E:1424:GLN:HE21	2.12	0.57
2:E:1525:THR:HA	2:E:1528:ARG:HH11	1.68	0.57
3:F:45:MET:HA	3:F:50:PRO:HA	1.86	0.57
2:B:1483:TRP:CE2	2:B:1514:PRO:HD3	2.39	0.57
1:D:673:LEU:HB3	1:D:675:LYS:HZ3	1.70	0.57
2:E:166:ARG:NH2	2:E:168:ASP:HB2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:302:ARG:NH2	2:E:375:GLU:OE1	2.37	0.57
2:B:529:PHE:N	2:B:550:ALA:O	2.37	0.57
2:E:242:PHE:HD2	2:E:257:ASN:HB3	1.67	0.57
2:E:1483:TRP:CE2	2:E:1514:PRO:HD3	2.39	0.57
1:A:673:LEU:HB3	1:A:675:LYS:NZ	2.20	0.57
2:B:154:HIS:NE2	2:B:201:GLU:OE2	2.27	0.57
2:B:302:ARG:NH2	2:B:375:GLU:OE1	2.37	0.57
2:E:46:ARG:HA	2:E:57:GLY:O	2.05	0.57
2:B:842:LYS:O	2:B:845:GLN:NE2	2.37	0.57
2:B:930:GLU:O	2:B:935:ARG:NH2	2.38	0.57
2:B:1063:THR:HA	2:B:1069:ARG:HD3	1.87	0.57
2:B:1284:GLN:HE21	2:B:1286:ASP:HB2	1.70	0.57
2:B:1371:GLY:C	2:B:1424:GLN:HE21	2.12	0.57
2:B:1586:VAL:HA	2:B:1589:LEU:HD12	1.87	0.57
2:B:518:ALA:HB3	2:B:521:GLU:HG2	1.85	0.57
2:E:529:PHE:N	2:E:550:ALA:O	2.37	0.57
2:E:1135:GLU:OE1	2:E:1139:SER:OG	2.22	0.57
2:B:529:PHE:HB2	2:B:550:ALA:HB3	1.86	0.57
2:B:890:LEU:HD22	2:B:935:ARG:HG3	1.86	0.57
2:E:143:GLU:HG3	2:E:147:LYS:NZ	2.19	0.57
2:E:474:ASP:OD1	2:E:478:LYS:N	2.38	0.57
2:E:554:LEU:O	2:E:562:LEU:N	2.37	0.57
2:E:876:GLU:OE1	2:E:876:GLU:N	2.37	0.57
2:E:890:LEU:HD22	2:E:935:ARG:HG3	1.86	0.57
2:E:997:ILE:HD13	2:E:1053:PHE:HB2	1.86	0.57
2:E:1362:TYR:CE1	2:E:1384:ARG:HG3	2.40	0.57
2:E:1506:GLN:NE2	2:E:1507:ILE:O	2.38	0.57
2:B:1091:TRP:HA	2:B:1094:LEU:HD23	1.87	0.57
2:E:1126:PRO:HD3	2:E:1175:LEU:HD13	1.86	0.57
2:E:1462:PHE:O	2:E:1489:TYR:N	2.35	0.57
2:B:102:TRP:CH2	2:B:118:GLN:HG3	2.40	0.57
2:B:757:LEU:HA	2:B:760:LEU:HG	1.86	0.57
2:B:1126:PRO:HD3	2:B:1175:LEU:HD13	1.87	0.57
2:B:1362:TYR:CE1	2:B:1384:ARG:HG3	2.40	0.57
1:D:673:LEU:HB3	1:D:675:LYS:NZ	2.20	0.57
2:E:757:LEU:HA	2:E:760:LEU:HG	1.86	0.57
2:E:793:GLN:HA	2:E:796:LEU:HG	1.87	0.57
2:E:1196:LEU:O	2:E:1199:SER:OG	2.22	0.57
2:E:1563:PHE:O	2:E:1567:GLU:HG2	2.05	0.57
2:B:793:GLN:HA	2:B:796:LEU:HG	1.87	0.56
2:B:994:LYS:NZ	2:B:1048:HIS:HB3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:25:VAL:HG23	2:E:57:GLY:HA2	1.86	0.56
2:E:465:ASN:OD1	2:E:503:GLN:N	2.34	0.56
2:E:1284:GLN:HE21	2:E:1286:ASP:HB2	1.70	0.56
2:E:1391:ARG:NH2	3:F:29:PRO:HD3	2.19	0.56
3:F:94:ARG:NH1	3:F:145:MET:HG2	2.20	0.56
2:B:193:ARG:NH1	2:B:196:GLU:OE2	2.36	0.56
2:B:474:ASP:OD1	2:B:478:LYS:N	2.38	0.56
2:B:1506:GLN:NE2	2:B:1507:ILE:O	2.38	0.56
2:E:1586:VAL:HA	2:E:1589:LEU:HD12	1.86	0.56
2:B:450:LEU:HB3	2:B:620:PHE:HZ	1.69	0.56
2:B:876:GLU:N	2:B:876:GLU:OE1	2.37	0.56
2:B:925:ILE:HA	2:B:928:ILE:HD12	1.87	0.56
2:B:962:GLN:O	2:B:1019:ARG:NH1	2.39	0.56
2:B:970:SER:O	2:B:974:SER:OG	2.24	0.56
2:B:997:ILE:HD13	2:B:1053:PHE:HB2	1.86	0.56
2:B:1219:ASN:OD1	2:B:1401:GLN:NE2	2.39	0.56
2:E:102:TRP:CH2	2:E:118:GLN:HG3	2.40	0.56
2:E:239:ALA:HB3	2:E:262:TRP:HB3	1.88	0.56
2:E:470:MET:HA	2:E:529:PHE:HA	1.86	0.56
2:E:730:TYR:OH	2:E:771:ARG:NH1	2.36	0.56
2:E:930:GLU:O	2:E:935:ARG:NH2	2.38	0.56
2:E:1470:LYS:HB3	2:E:1483:TRP:CD1	2.40	0.56
1:A:652:LEU:HB3	1:A:654:PHE:CE2	2.41	0.56
2:B:200:GLU:HA	2:B:203:SER:HB2	1.86	0.56
2:E:879:LEU:O	2:E:882:LEU:N	2.37	0.56
2:E:994:LYS:NZ	2:E:1048:HIS:HB3	2.20	0.56
2:E:1063:THR:HA	2:E:1069:ARG:HD3	1.87	0.56
2:B:680:MET:HE3	2:B:693:VAL:HG21	1.87	0.56
2:B:1099:ILE:HD13	2:B:1138:PHE:HB2	1.88	0.56
2:E:10:GLN:NE2	2:E:37:ILE:O	2.38	0.56
2:E:1205:LEU:HD13	2:E:1208:ARG:HD3	1.88	0.56
2:B:46:ARG:HA	2:B:57:GLY:O	2.05	0.56
2:E:473:HIS:ND1	2:E:477:GLY:O	2.32	0.56
2:E:914:ASP:HB2	2:E:963:GLN:NE2	2.21	0.56
2:E:925:ILE:HA	2:E:928:ILE:HD12	1.87	0.56
2:E:1245:TYR:HD2	2:E:1248:ARG:HH21	1.54	0.56
2:E:1532:CYS:O	2:E:1535:GLN:NE2	2.39	0.56
2:E:94:THR:O	2:E:97:GLU:HG3	2.06	0.56
2:E:1615:LEU:O	2:E:1619:HIS:N	2.30	0.56
1:A:692:MET:HE1	2:B:122:TYR:HE2	1.70	0.56
2:B:94:THR:O	2:B:97:GLU:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1205:LEU:HD13	2:B:1208:ARG:HD3	1.88	0.56
2:B:1563:PHE:O	2:B:1567:GLU:HG2	2.05	0.56
2:E:193:ARG:NH1	2:E:196:GLU:OE2	2.36	0.56
2:E:195:GLU:HA	2:E:198:ILE:HG12	1.87	0.56
2:E:1219:ASN:OD1	2:E:1401:GLN:NE2	2.39	0.56
1:A:570:ARG:O	1:A:570:ARG:HG2	2.06	0.56
2:B:165:VAL:O	2:B:171:ASN:ND2	2.27	0.56
2:B:195:GLU:HA	2:B:198:ILE:HG12	1.88	0.56
1:D:652:LEU:HB3	1:D:654:PHE:CE2	2.41	0.56
2:E:473:HIS:HB2	2:E:526:HIS:CE1	2.41	0.56
2:E:680:MET:HE3	2:E:693:VAL:HG21	1.88	0.56
2:E:1099:ILE:HD13	2:E:1138:PHE:HB2	1.88	0.56
2:B:10:GLN:NE2	2:B:37:ILE:O	2.37	0.55
2:B:508:CYS:HB3	2:B:510:TYR:HE2	1.72	0.55
2:B:1466:ARG:H	2:B:1484:ILE:HG23	1.72	0.55
2:E:45:TYR:HD2	2:E:64:ILE:HG13	1.71	0.55
2:E:166:ARG:O	2:E:171:ASN:HA	2.05	0.55
2:E:1091:TRP:HA	2:E:1094:LEU:HD23	1.87	0.55
1:A:700:ASP:HB2	2:B:32:GLY:HA2	1.87	0.55
2:B:226:VAL:O	2:B:279:ALA:N	2.33	0.55
2:B:228:PHE:HA	2:B:401:VAL:HG12	1.88	0.55
2:B:319:ARG:NH1	2:B:497:LYS:O	2.40	0.55
2:E:319:ARG:NH1	2:E:497:LYS:O	2.40	0.55
2:E:922:ALA:HA	2:E:925:ILE:HD12	1.88	0.55
2:E:1477:ASN:HB3	2:E:1568:LYS:HZ1	1.70	0.55
1:A:537:LYS:HG3	1:A:694:ILE:HG21	1.89	0.55
2:E:228:PHE:HA	2:E:401:VAL:HG12	1.88	0.55
2:B:25:VAL:HG21	2:B:56:LYS:HG3	1.89	0.55
2:B:239:ALA:HB3	2:B:262:TRP:HB3	1.88	0.55
2:B:1206:ASP:O	2:B:1210:ILE:HG12	2.07	0.55
2:B:1360:PRO:HA	2:B:1387:GLU:HA	1.88	0.55
2:B:1450:ILE:HG13	2:B:1451:LEU:HD22	1.88	0.55
2:B:1532:CYS:O	2:B:1535:GLN:NE2	2.39	0.55
2:E:246:TYR:HA	2:E:253:PHE:HA	1.88	0.55
2:E:962:GLN:O	2:E:1019:ARG:NH1	2.39	0.55
1:A:699:LEU:HD12	2:B:128:ARG:HE	1.71	0.55
2:B:473:HIS:HB2	2:B:526:HIS:CE1	2.42	0.55
2:B:914:ASP:HB2	2:B:963:GLN:NE2	2.21	0.55
3:C:94:ARG:NH1	3:C:145:MET:HG2	2.20	0.55
2:B:922:ALA:HA	2:B:925:ILE:HD12	1.88	0.55
3:C:153:LYS:NZ	3:C:154:TYR:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:154:HIS:HB2	2:E:197:LYS:HD3	1.88	0.55
2:E:225:TYR:N	2:E:404:LYS:O	2.32	0.55
2:E:970:SER:O	2:E:974:SER:OG	2.24	0.55
2:B:154:HIS:HB2	2:B:197:LYS:HD3	1.88	0.55
2:B:1440:SER:H	2:B:1442:LYS:NZ	2.04	0.55
1:D:532:PRO:HG3	1:D:708:ASP:HA	1.89	0.55
2:E:131:ILE:HD11	2:E:144:LEU:HG	1.89	0.55
2:E:1441:TYR:CE2	2:E:1450:ILE:HD12	2.42	0.55
2:E:1466:ARG:H	2:E:1484:ILE:HG23	1.71	0.55
3:F:174:ARG:HA	3:F:177:LEU:HB2	1.89	0.55
2:B:1245:TYR:HD2	2:B:1248:ARG:HH21	1.54	0.55
2:B:166:ARG:O	2:B:171:ASN:HA	2.06	0.55
2:B:1440:SER:N	2:B:1442:LYS:HZ3	2.04	0.55
2:B:1594:ALA:HA	2:B:1597:MET:CE	2.36	0.55
3:C:174:ARG:HA	3:C:177:LEU:HB2	1.89	0.55
2:E:1440:SER:H	2:E:1442:LYS:NZ	2.04	0.55
2:E:1575:TYR:O	2:E:1579:HIS:N	2.31	0.55
2:B:259:LEU:HD23	2:B:490:TYR:CG	2.42	0.55
2:B:865:GLU:N	2:B:865:GLU:OE1	2.40	0.55
2:B:973:ILE:HD13	2:B:976:PHE:CZ	2.42	0.55
2:B:1477:ASN:HB3	2:B:1568:LYS:HZ1	1.71	0.55
2:E:1062:GLU:OE2	2:E:1080:ARG:NH1	2.40	0.55
2:E:1183:HIS:CG	2:E:1184:LYS:H	2.25	0.55
2:E:1360:PRO:HA	2:E:1387:GLU:HA	1.88	0.55
2:E:1435:MET:SD	2:E:1455:ARG:HD3	2.47	0.55
2:B:45:TYR:HD2	2:B:64:ILE:HG13	1.71	0.54
2:B:809:ALA:HB3	2:B:813:LYS:HZ2	1.72	0.54
2:B:1040:LEU:HD12	2:B:1097:HIS:CE1	2.42	0.54
2:B:1441:TYR:CE2	2:B:1450:ILE:HD12	2.42	0.54
2:B:1470:LYS:HB3	2:B:1483:TRP:CD1	2.40	0.54
2:E:1177:LEU:O	2:E:1181:ARG:HG2	2.07	0.54
3:F:153:LYS:NZ	3:F:154:TYR:O	2.40	0.54
1:A:719:ASN:ND2	1:A:721:ASP:OD1	2.40	0.54
2:B:791:ILE:HG22	2:B:795:PHE:CE2	2.43	0.54
2:B:1248:ARG:NH1	2:B:1252:ARG:HH12	2.05	0.54
1:D:576:TYR:CD1	1:D:591:LEU:HG	2.42	0.54
2:E:259:LEU:HD23	2:E:490:TYR:CG	2.42	0.54
2:E:1450:ILE:HG13	2:E:1451:LEU:HD22	1.88	0.54
3:F:39:ASN:OD1	3:F:56:TRP:HA	2.07	0.54
1:A:532:PRO:HG3	1:A:708:ASP:HA	1.89	0.54
1:A:627:GLU:HG2	1:A:631:LEU:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1062:GLU:OE2	2:B:1080:ARG:NH1	2.40	0.54
2:B:1121:ARG:O	2:B:1125:ILE:HD12	2.08	0.54
2:B:1183:HIS:CG	2:B:1184:LYS:H	2.25	0.54
2:B:1470:LYS:H	2:B:1481:THR:HB	1.72	0.54
2:E:526:HIS:CE1	2:E:586:LEU:HD21	2.43	0.54
2:E:1248:ARG:NH1	2:E:1252:ARG:HH12	2.05	0.54
3:F:61:GLN:O	3:F:68:ARG:NH2	2.41	0.54
1:A:716:GLU:HG3	2:B:44:TRP:CZ2	2.43	0.54
2:B:1177:LEU:O	2:B:1181:ARG:HG2	2.07	0.54
2:E:115:ARG:HA	2:E:118:GLN:OE1	2.07	0.54
2:E:116:GLN:HG3	2:E:120:MET:HE1	1.89	0.54
2:E:973:ILE:HD13	2:E:976:PHE:CZ	2.42	0.54
2:E:294:VAL:H	2:E:330:THR:HG1	1.53	0.54
2:E:1434:VAL:HB	2:E:1461:GLN:HB2	1.89	0.54
3:F:5:LYS:HB3	3:F:75:THR:HG23	1.90	0.54
1:A:726:CYS:HA	2:B:46:ARG:HH22	1.72	0.54
2:B:167:ASP:OD1	2:B:167:ASP:N	2.40	0.54
2:B:892:ASP:OD1	2:B:895:ASN:ND2	2.41	0.54
2:B:1072:ILE:O	2:B:1076:TYR:N	2.35	0.54
2:B:1435:MET:SD	2:B:1455:ARG:HD3	2.47	0.54
2:E:471:SER:HB2	2:E:479:LEU:HD13	1.90	0.54
2:E:865:GLU:OE1	2:E:865:GLU:N	2.40	0.54
2:E:1470:LYS:H	2:E:1481:THR:HB	1.72	0.54
2:B:760:LEU:HD22	2:B:764:PHE:HE2	1.73	0.54
2:B:1062:GLU:O	2:B:1068:LYS:HB3	2.08	0.54
2:E:166:ARG:HH22	2:E:168:ASP:HB2	1.73	0.54
2:E:791:ILE:HG22	2:E:795:PHE:CE2	2.43	0.54
2:E:870:ARG:HH12	2:E:874:CYS:N	2.06	0.54
2:E:892:ASP:OD1	2:E:895:ASN:ND2	2.41	0.54
2:B:59:PHE:CZ	2:B:63:TYR:HB3	2.42	0.54
2:B:870:ARG:HH12	2:B:874:CYS:N	2.06	0.54
2:B:1557:PRO:HB2	2:B:1560:MET:O	2.07	0.54
2:E:167:ASP:OD1	2:E:167:ASP:N	2.40	0.54
2:E:896:LYS:HA	2:E:899:HIS:CE1	2.43	0.54
2:E:1121:ARG:O	2:E:1125:ILE:HD12	2.08	0.54
2:E:1206:ASP:O	2:E:1210:ILE:HG12	2.07	0.54
2:E:654:LEU:HB3	2:E:692:LEU:HB3	1.89	0.54
1:A:579:LEU:HA	1:A:586:LEU:HD13	1.90	0.54
2:B:131:ILE:HD11	2:B:144:LEU:HG	1.89	0.54
2:B:1434:VAL:HB	2:B:1461:GLN:HB2	1.89	0.54
1:D:570:ARG:O	1:D:570:ARG:HG2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:25:VAL:HG21	2:E:56:LYS:HG3	1.89	0.54
2:E:1040:LEU:HD12	2:E:1097:HIS:CE1	2.42	0.54
2:E:1292:THR:HG23	2:E:1295:GLU:H	1.73	0.54
1:A:576:TYR:CD1	1:A:591:LEU:HG	2.42	0.53
2:B:896:LYS:HA	2:B:899:HIS:CE1	2.43	0.53
2:B:1135:GLU:OE1	2:B:1139:SER:OG	2.22	0.53
3:C:39:ASN:OD1	3:C:56:TRP:HA	2.07	0.53
3:C:61:GLN:O	3:C:68:ARG:NH2	2.41	0.53
3:C:87:PRO:HA	3:C:90:PHE:CD2	2.43	0.53
2:E:973:ILE:HA	2:E:976:PHE:CE1	2.43	0.53
2:E:1015:ARG:HH21	2:E:1076:TYR:HE1	1.56	0.53
2:E:1495:PHE:HE1	2:E:1502:PHE:HD2	1.55	0.53
2:E:1557:PRO:HB2	2:E:1560:MET:O	2.08	0.53
2:B:654:LEU:HB3	2:B:692:LEU:HB3	1.89	0.53
2:B:1095:GLY:H	2:B:1098:LYS:HE3	1.73	0.53
2:B:1292:THR:HG23	2:B:1295:GLU:H	1.73	0.53
1:D:537:LYS:HG3	1:D:694:ILE:HG21	1.89	0.53
2:B:115:ARG:HA	2:B:118:GLN:OE1	2.07	0.53
2:B:973:ILE:HA	2:B:976:PHE:CE1	2.43	0.53
2:B:1495:PHE:HE1	2:B:1502:PHE:HD2	1.55	0.53
1:D:579:LEU:HA	1:D:586:LEU:HD13	1.90	0.53
2:E:224:LEU:HD13	2:E:333:ILE:HG12	1.90	0.53
2:E:760:LEU:HD22	2:E:764:PHE:HE2	1.73	0.53
2:E:866:SER:C	2:E:868:LEU:H	2.16	0.53
2:E:1097:HIS:HA	2:E:1100:LYS:HE2	1.91	0.53
1:A:723:VAL:HB	2:B:3:ARG:N	2.23	0.53
2:B:116:GLN:HG3	2:B:120:MET:HE1	1.89	0.53
2:B:224:LEU:HD13	2:B:333:ILE:HG12	1.90	0.53
2:B:225:TYR:N	2:B:404:LYS:O	2.32	0.53
2:B:246:TYR:HA	2:B:253:PHE:HA	1.88	0.53
2:B:471:SER:HB2	2:B:479:LEU:HD13	1.90	0.53
1:D:627:GLU:HG2	1:D:631:LEU:HB2	1.90	0.53
1:D:711:PRO:HD2	2:E:17:TYR:CE1	2.42	0.53
1:D:719:ASN:ND2	1:D:721:ASP:OD1	2.40	0.53
2:E:59:PHE:CZ	2:E:63:TYR:HB3	2.42	0.53
2:E:1562:GLY:HA3	3:F:36:VAL:HB	1.89	0.53
2:B:9:ARG:HD3	2:B:68:GLU:HG2	1.91	0.53
2:B:965:ASP:OD1	2:B:966:ASP:N	2.42	0.53
2:B:1562:GLY:HA3	3:C:36:VAL:HB	1.91	0.53
3:C:7:VAL:HA	3:C:56:TRP:HB2	1.90	0.53
1:D:711:PRO:HD2	2:E:17:TYR:HE1	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:166:ARG:HG2	2:E:173:LEU:HB2	1.91	0.53
2:E:508:CYS:HB3	2:E:510:TYR:HE2	1.72	0.53
2:E:1418:ILE:HG21	2:E:1425:TYR:HB2	1.91	0.53
2:B:526:HIS:CE1	2:B:586:LEU:HD21	2.43	0.53
2:B:1059:LEU:HD12	2:B:1116:PRO:HB2	1.90	0.53
1:D:536:LEU:HA	1:D:539:LYS:HE3	1.91	0.53
2:E:422:ASP:OD1	2:E:425:THR:OG1	2.22	0.53
2:B:820:LEU:O	2:B:823:ILE:HG12	2.09	0.53
2:B:1615:LEU:O	2:B:1619:HIS:N	2.30	0.53
1:D:588:TYR:N	1:D:603:SER:OG	2.42	0.53
2:B:554:LEU:O	2:B:562:LEU:N	2.37	0.53
2:B:730:TYR:CE1	2:B:771:ARG:HD3	2.44	0.53
1:D:550:GLN:CD	1:D:554:ASN:HD21	2.17	0.53
1:D:670:ASN:O	1:D:674:GLY:N	2.42	0.53
2:E:1015:ARG:HE	2:E:1076:TYR:HD1	1.57	0.53
2:B:866:SER:C	2:B:868:LEU:H	2.16	0.53
2:B:1597:MET:HE3	2:B:1633:VAL:HG21	1.91	0.53
3:C:5:LYS:HB3	3:C:75:THR:HG23	1.90	0.53
1:D:548:ILE:HD13	2:E:106:TYR:CE1	2.44	0.53
2:E:6:PRO:HA	2:E:38:LEU:O	2.09	0.53
2:E:1062:GLU:O	2:E:1068:LYS:HB3	2.08	0.53
2:E:1063:THR:HA	2:E:1069:ARG:HH11	1.73	0.53
2:E:1588:LEU:O	2:E:1591:ARG:HG2	2.08	0.53
1:A:550:GLN:CD	1:A:554:ASN:HD21	2.17	0.53
2:B:166:ARG:HG2	2:B:173:LEU:HB2	1.91	0.53
2:B:1097:HIS:HA	2:B:1100:LYS:HE2	1.91	0.53
2:B:1418:ILE:HG21	2:B:1425:TYR:HB2	1.91	0.53
2:E:1183:HIS:HB3	2:E:1187:SER:OG	2.09	0.53
1:A:552:ARG:NH1	1:A:664:ILE:HG12	2.24	0.52
2:B:1588:LEU:O	2:B:1591:ARG:HG2	2.08	0.52
2:B:4:TRP:CZ3	2:B:46:ARG:HG2	2.44	0.52
2:B:552:VAL:HB	2:B:569:LEU:HD21	1.91	0.52
2:B:879:LEU:HA	2:B:882:LEU:HD12	1.91	0.52
2:B:1561:GLY:O	2:B:1565:ASN:ND2	2.39	0.52
2:E:59:PHE:CE2	2:E:63:TYR:HB3	2.44	0.52
2:E:857:LEU:HA	2:E:860:MET:SD	2.49	0.52
3:F:7:VAL:HA	3:F:56:TRP:HB2	1.90	0.52
3:F:59:ALA:O	3:F:68:ARG:NH1	2.30	0.52
2:B:72:GLU:O	2:B:76:GLN:NE2	2.42	0.52
2:B:1063:THR:HA	2:B:1069:ARG:HH11	1.73	0.52
2:E:4:TRP:CZ3	2:E:46:ARG:HG2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:226:VAL:O	2:E:279:ALA:N	2.33	0.52
2:E:1632:LYS:O	2:E:1636:HIS:N	2.42	0.52
3:F:102:ARG:HD3	3:F:149:ILE:HD11	1.91	0.52
1:A:667:ASP:HB3	1:A:677:MET:SD	2.49	0.52
2:B:1632:LYS:O	2:B:1636:HIS:N	2.42	0.52
3:C:102:ARG:HD3	3:C:149:ILE:HD11	1.91	0.52
2:E:154:HIS:NE2	2:E:201:GLU:OE2	2.27	0.52
2:E:647:SER:HA	2:E:650:ILE:HG13	1.92	0.52
2:E:1059:LEU:HD12	2:E:1116:PRO:HB2	1.90	0.52
3:F:87:PRO:HA	3:F:90:PHE:CD2	2.44	0.52
3:F:120:ARG:NH2	3:F:139:TYR:H	2.07	0.52
2:B:59:PHE:CE2	2:B:63:TYR:HB3	2.44	0.52
2:B:325:ALA:HB1	2:B:346:ILE:HG22	1.92	0.52
2:B:1358:PRO:HB2	2:B:1387:GLU:HB2	1.92	0.52
1:D:545:LEU:O	1:D:549:LYS:HG3	2.09	0.52
1:D:552:ARG:NH1	1:D:664:ILE:HG12	2.24	0.52
2:E:450:LEU:O	2:E:510:TYR:N	2.43	0.52
2:E:552:VAL:HB	2:E:569:LEU:HD21	1.91	0.52
2:E:1062:GLU:O	2:E:1069:ARG:N	2.43	0.52
3:F:132:LYS:HD2	3:F:134:LEU:HD12	1.92	0.52
1:A:578:ARG:HH22	1:A:601:HIS:H	1.58	0.52
2:B:30:GLN:N	2:B:33:ASP:OD2	2.43	0.52
2:B:736:VAL:HG12	2:B:740:TYR:CE2	2.45	0.52
3:C:132:LYS:HD2	3:C:134:LEU:HD12	1.92	0.52
2:E:188:GLU:OE2	2:E:192:LYS:HE3	2.09	0.52
2:E:1095:GLY:H	2:E:1098:LYS:HE3	1.73	0.52
2:E:1440:SER:H	2:E:1442:LYS:HZ3	1.57	0.52
1:A:588:TYR:N	1:A:603:SER:OG	2.42	0.52
1:A:643:SER:HA	1:A:652:LEU:O	2.09	0.52
2:B:1062:GLU:O	2:B:1069:ARG:N	2.43	0.52
2:B:1217:LYS:HG2	2:B:1220:ARG:HH21	1.74	0.52
2:E:429:ARG:NH1	2:E:445:ASP:OD1	2.43	0.52
2:E:965:ASP:OD1	2:E:966:ASP:N	2.42	0.52
2:E:1259:GLU:HG3	2:E:1497:GLY:O	2.10	0.52
2:B:246:TYR:CZ	2:B:383:LEU:HD21	2.45	0.52
1:D:640:LEU:O	1:D:655:ILE:HA	2.10	0.52
2:E:1358:PRO:HB2	2:E:1387:GLU:HB2	1.92	0.52
2:E:1597:MET:HE3	2:E:1633:VAL:HG21	1.91	0.52
2:B:6:PRO:HA	2:B:38:LEU:O	2.09	0.52
2:B:64:ILE:HG22	2:B:66:LEU:HD22	1.91	0.52
2:B:1015:ARG:HH21	2:B:1076:TYR:HE1	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1183:HIS:HB3	2:B:1187:SER:OG	2.09	0.52
2:B:1259:GLU:HG3	2:B:1497:GLY:O	2.10	0.52
2:E:730:TYR:CE1	2:E:771:ARG:HD3	2.44	0.52
2:E:875:ARG:HG2	2:E:924:HIS:CE1	2.45	0.52
1:A:536:LEU:HA	1:A:539:LYS:HE3	1.91	0.52
1:A:657:PRO:HB2	1:A:661:GLU:OE2	2.10	0.52
1:A:670:ASN:O	1:A:674:GLY:N	2.42	0.52
2:B:91:LEU:O	2:B:95:LEU:HG	2.10	0.52
2:B:188:GLU:OE2	2:B:192:LYS:HE3	2.09	0.52
2:B:430:LYS:NZ	2:B:433:PHE:O	2.43	0.52
2:B:806:LEU:HG	2:B:810:VAL:HG22	1.92	0.52
2:B:1196:LEU:O	2:B:1199:SER:OG	2.22	0.52
1:D:667:ASP:HB3	1:D:677:MET:SD	2.49	0.52
2:E:30:GLN:N	2:E:33:ASP:OD2	2.43	0.52
2:E:736:VAL:HG12	2:E:740:TYR:CE2	2.45	0.52
2:E:754:PHE:HA	2:E:757:LEU:HD12	1.91	0.52
2:B:166:ARG:HH22	2:B:168:ASP:HB2	1.73	0.51
2:B:736:VAL:HG12	2:B:740:TYR:HE2	1.75	0.51
2:B:1015:ARG:HE	2:B:1076:TYR:HD1	1.57	0.51
2:E:9:ARG:HD3	2:E:68:GLU:HG2	1.91	0.51
2:E:325:ALA:HB1	2:E:346:ILE:HG22	1.92	0.51
2:E:1594:ALA:HA	2:E:1597:MET:CE	2.37	0.51
2:B:133:SER:HB2	2:B:135:THR:HG23	1.93	0.51
2:B:787:PHE:O	2:B:791:ILE:HG12	2.10	0.51
2:B:940:VAL:HG23	2:B:950:ILE:HD11	1.92	0.51
2:E:98:TRP:O	2:E:102:TRP:HB2	2.11	0.51
2:B:857:LEU:HA	2:B:860:MET:SD	2.49	0.51
2:B:875:ARG:HG2	2:B:924:HIS:CE1	2.45	0.51
2:B:1104:SER:OG	2:B:1105:MET:HG2	2.10	0.51
1:D:643:SER:HA	1:D:652:LEU:O	2.09	0.51
2:E:569:LEU:HD23	2:E:591:THR:HG22	1.93	0.51
2:E:736:VAL:HG12	2:E:740:TYR:HE2	1.75	0.51
2:E:1440:SER:N	2:E:1442:LYS:HZ3	2.09	0.51
2:E:1631:GLU:O	2:E:1635:LYS:HG3	2.11	0.51
2:B:429:ARG:NH1	2:B:445:ASP:OD1	2.43	0.51
2:B:647:SER:HA	2:B:650:ILE:HG13	1.92	0.51
2:B:1217:LYS:O	2:B:1221:MET:HG3	2.11	0.51
1:D:578:ARG:HH22	1:D:601:HIS:H	1.58	0.51
2:E:787:PHE:O	2:E:791:ILE:HG12	2.10	0.51
2:E:820:LEU:O	2:E:823:ILE:HG12	2.09	0.51
2:E:879:LEU:HA	2:E:882:LEU:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1217:LYS:HG2	2:E:1220:ARG:HH21	1.74	0.51
2:E:1217:LYS:O	2:E:1221:MET:HG3	2.11	0.51
1:A:640:LEU:O	1:A:655:ILE:HA	2.10	0.51
2:B:754:PHE:HA	2:B:757:LEU:HD12	1.91	0.51
2:E:875:ARG:HG2	2:E:924:HIS:NE2	2.26	0.51
2:E:1104:SER:OG	2:E:1105:MET:HG2	2.10	0.51
2:E:1395:SER:O	2:E:1399:LEU:HG	2.11	0.51
2:B:443:ARG:NE	2:B:445:ASP:OD2	2.44	0.51
2:B:1395:SER:O	2:B:1399:LEU:HG	2.11	0.51
2:E:64:ILE:HG22	2:E:66:LEU:HD22	1.91	0.51
2:E:72:GLU:O	2:E:76:GLN:NE2	2.42	0.51
2:E:246:TYR:CZ	2:E:383:LEU:HD21	2.45	0.51
3:F:138:THR:H	3:F:141:GLN:NE2	2.09	0.51
2:B:857:LEU:O	2:B:860:MET:HG2	2.11	0.51
2:B:1231:TYR:CZ	2:B:1239:ILE:HD12	2.46	0.51
2:B:1492:ALA:HB2	2:B:1505:LYS:HE3	1.92	0.51
3:C:91:GLU:O	3:C:95:ALA:HB3	2.11	0.51
3:C:120:ARG:NH2	3:C:139:TYR:H	2.07	0.51
2:E:204:ILE:HG13	2:E:211:ARG:HB3	1.91	0.51
2:E:1231:TYR:CZ	2:E:1239:ILE:HD12	2.46	0.51
1:A:727:ASN:O	2:B:46:ARG:NH2	2.44	0.51
1:D:550:GLN:NE2	1:D:554:ASN:HD21	2.09	0.51
1:D:724:TYR:HB3	2:E:4:TRP:HB2	1.91	0.51
2:B:204:ILE:HG13	2:B:211:ARG:HB3	1.91	0.51
3:C:138:THR:H	3:C:141:GLN:NE2	2.09	0.51
2:E:909:ILE:HG13	2:E:910:LEU:HD12	1.92	0.51
2:E:1492:ALA:HB2	2:E:1505:LYS:HE3	1.92	0.51
2:B:638:LEU:O	2:B:642:ASN:N	2.44	0.51
2:B:1277:PRO:HA	2:B:1293:GLN:HG3	1.93	0.51
3:C:98:TYR:CE1	3:C:149:ILE:HD13	2.40	0.51
2:E:443:ARG:NE	2:E:445:ASP:OD2	2.44	0.51
2:E:638:LEU:O	2:E:642:ASN:N	2.44	0.51
2:E:795:PHE:HA	2:E:798:PHE:CD2	2.46	0.51
2:E:823:ILE:HD12	2:E:827:VAL:HG21	1.93	0.51
2:E:1448:GLU:OE1	2:E:1452:ASN:ND2	2.44	0.51
1:A:545:LEU:O	1:A:549:LYS:HG3	2.09	0.50
1:A:726:CYS:C	2:B:46:ARG:HH22	2.20	0.50
2:B:1099:ILE:C	2:B:1101:PHE:H	2.19	0.50
2:B:1536:HIS:ND1	2:B:1547:LEU:HD11	2.27	0.50
1:D:657:PRO:HB2	1:D:661:GLU:OE2	2.10	0.50
1:D:706:ILE:HG23	2:E:17:TYR:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:91:LEU:O	2:E:95:LEU:HG	2.10	0.50
2:E:133:SER:HB2	2:E:135:THR:HG23	1.92	0.50
2:E:950:ILE:O	2:E:954:VAL:HG23	2.11	0.50
2:B:795:PHE:HA	2:B:798:PHE:CD2	2.46	0.50
2:E:1208:ARG:HB2	2:E:1212:MET:HE1	1.92	0.50
2:E:1536:HIS:ND1	2:E:1547:LEU:HD11	2.27	0.50
2:E:1607:HIS:O	2:E:1611:LEU:N	2.44	0.50
3:F:91:GLU:O	3:F:95:ALA:HB3	2.11	0.50
2:E:806:LEU:HG	2:E:810:VAL:HG22	1.92	0.50
2:E:1032:PHE:HA	2:E:1036:ALA:HB3	1.94	0.50
2:E:1062:GLU:O	2:E:1069:ARG:HD3	2.12	0.50
2:B:823:ILE:HD12	2:B:827:VAL:HG21	1.93	0.50
2:B:1343:LYS:HE2	2:E:1343:LYS:HE2	1.93	0.50
2:B:1607:HIS:O	2:B:1611:LEU:N	2.44	0.50
2:B:1631:GLU:O	2:B:1635:LYS:HG3	2.11	0.50
2:E:852:LEU:HB3	2:E:855:GLN:HB2	1.93	0.50
2:E:1136:PHE:HA	2:E:1139:SER:OG	2.12	0.50
2:B:36:HIS:N	2:B:48:TYR:O	2.45	0.50
2:B:584:PHE:O	2:B:587:THR:OG1	2.25	0.50
2:B:1208:ARG:HB2	2:B:1212:MET:HE1	1.92	0.50
2:B:1449:GLN:OE1	2:B:1449:GLN:N	2.34	0.50
2:B:1452:ASN:HA	2:B:1455:ARG:HG2	1.93	0.50
2:E:36:HIS:N	2:E:48:TYR:O	2.45	0.50
2:E:940:VAL:HG23	2:E:950:ILE:HD11	1.92	0.50
2:E:973:ILE:HD13	2:E:976:PHE:HZ	1.76	0.50
2:E:987:MET:SD	2:E:988:GLU:HG3	2.52	0.50
2:E:1368:TYR:O	2:E:1425:TYR:N	2.40	0.50
2:B:569:LEU:HD23	2:B:591:THR:HG22	1.93	0.50
2:B:659:GLU:OE1	2:B:659:GLU:N	2.43	0.50
2:B:1136:PHE:HA	2:B:1139:SER:OG	2.12	0.50
2:B:1418:ILE:HA	2:B:1421:SER:HB3	1.94	0.50
2:E:1277:PRO:HA	2:E:1293:GLN:HG3	1.93	0.50
2:B:98:TRP:O	2:B:102:TRP:HB2	2.10	0.50
2:B:852:LEU:HB3	2:B:855:GLN:HB2	1.93	0.50
2:B:875:ARG:HG2	2:B:924:HIS:NE2	2.26	0.50
2:B:1032:PHE:HA	2:B:1036:ALA:HB3	1.93	0.50
2:E:430:LYS:NZ	2:E:433:PHE:O	2.43	0.50
2:E:1099:ILE:C	2:E:1101:PHE:H	2.19	0.50
2:E:1460:GLN:NE2	2:E:1491:THR:O	2.29	0.50
2:B:114:PHE:O	2:B:118:GLN:NE2	2.44	0.50
2:B:319:ARG:O	2:B:500:VAL:N	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:760:LEU:HD22	2:B:764:PHE:CE2	2.47	0.50
2:B:950:ILE:O	2:B:954:VAL:HG23	2.11	0.50
3:C:59:ALA:O	3:C:68:ARG:NH1	2.30	0.50
2:E:114:PHE:O	2:E:118:GLN:NE2	2.45	0.50
2:E:584:PHE:O	2:E:587:THR:OG1	2.25	0.50
2:E:1418:ILE:HA	2:E:1421:SER:HB3	1.94	0.50
2:B:909:ILE:HG13	2:B:910:LEU:HD12	1.92	0.50
2:B:973:ILE:HD13	2:B:976:PHE:HZ	1.76	0.50
2:B:1145:HIS:O	2:B:1149:ASN:ND2	2.45	0.50
2:B:1448:GLU:OE1	2:B:1452:ASN:ND2	2.44	0.50
2:E:637:LEU:HD11	2:E:660:VAL:HG11	1.94	0.50
2:E:994:LYS:HZ2	2:E:1048:HIS:HB3	1.75	0.50
1:A:564:LYS:HG3	1:A:575:TRP:CD1	2.47	0.49
2:B:422:ASP:OD1	2:B:425:THR:OG1	2.22	0.49
2:B:1460:GLN:NE2	2:B:1491:THR:O	2.29	0.49
2:E:98:TRP:CH2	2:E:155:GLY:HA3	2.40	0.49
2:E:225:TYR:CE2	2:E:227:ASN:HB2	2.47	0.49
2:E:570:VAL:CG2	2:E:595:MET:HE2	2.39	0.49
2:E:857:LEU:O	2:E:860:MET:HG2	2.11	0.49
3:F:5:LYS:N	3:F:76:ASP:OD2	2.39	0.49
1:A:550:GLN:NE2	1:A:554:ASN:HD21	2.09	0.49
2:B:859:CYS:O	2:B:863:ILE:HG12	2.12	0.49
1:D:536:LEU:HG	2:E:18:ASN:OD1	2.12	0.49
2:E:19:TYR:HB2	2:E:59:PHE:HE1	1.77	0.49
2:E:451:ILE:HD11	2:E:623:ALA:HB2	1.94	0.49
2:E:1617:PRO:HG3	3:F:70:LEU:HD22	1.94	0.49
2:B:987:MET:SD	2:B:988:GLU:HG3	2.52	0.49
2:E:1145:HIS:O	2:E:1149:ASN:ND2	2.45	0.49
2:E:1452:ASN:HA	2:E:1455:ARG:HG2	1.93	0.49
2:B:19:TYR:HB2	2:B:59:PHE:HE1	1.77	0.49
2:B:184:PHE:HA	2:B:1009:MET:HE3	1.94	0.49
2:B:225:TYR:CE2	2:B:227:ASN:HB2	2.47	0.49
2:B:844:ILE:HG21	2:B:881:LEU:HD21	1.94	0.49
2:B:1038:PHE:O	2:B:1039:GLU:HG2	2.13	0.49
2:E:760:LEU:HD22	2:E:764:PHE:CE2	2.47	0.49
2:B:572:TYR:OH	2:B:589:PRO:O	2.17	0.49
2:E:1129:PHE:HA	2:E:1132:MET:HG3	1.94	0.49
2:B:319:ARG:NH2	2:B:511:GLU:OE2	2.39	0.49
2:B:638:LEU:HA	2:B:641:LEU:HB2	1.95	0.49
2:B:1529:ILE:HB	2:B:1599:LEU:HD21	1.93	0.49
2:B:1537:ALA:HA	2:B:1540:ARG:HH22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5:LYS:N	3:C:76:ASP:OD2	2.39	0.49
1:D:564:LYS:HG3	1:D:575:TRP:CD1	2.47	0.49
1:D:688:THR:O	1:D:691:SER:OG	2.27	0.49
2:E:184:PHE:HA	2:E:1009:MET:HE3	1.94	0.49
2:E:859:CYS:O	2:E:863:ILE:HG12	2.12	0.49
2:B:331:ASP:HB3	2:B:336:LYS:HD2	1.95	0.49
2:B:450:LEU:O	2:B:510:TYR:N	2.43	0.49
2:B:1062:GLU:O	2:B:1069:ARG:HD3	2.12	0.49
2:B:1468:PHE:HB3	2:B:1483:TRP:O	2.13	0.49
2:E:94:THR:O	2:E:98:TRP:CD1	2.65	0.49
2:B:188:GLU:O	2:B:192:LYS:HG2	2.13	0.49
2:B:254:ILE:O	2:B:431:MET:N	2.39	0.49
2:B:1393:ASP:OD1	3:C:166:LYS:NZ	2.45	0.49
2:B:1467:PRO:HG3	3:C:33:ILE:HG12	1.95	0.49
2:E:165:VAL:O	2:E:171:ASN:ND2	2.27	0.49
2:E:1537:ALA:HA	2:E:1540:ARG:HH22	1.77	0.49
3:F:82:PHE:HE1	3:F:112:LEU:HG	1.78	0.49
2:B:738:ASN:HA	2:B:741:VAL:HG12	1.94	0.49
2:B:1479:PHE:HA	2:B:1482:MET:HG2	1.95	0.49
2:E:201:GLU:O	2:E:205:LEU:HB3	2.13	0.49
2:E:554:LEU:HA	2:E:562:LEU:HB2	1.94	0.49
2:E:719:TYR:O	2:E:724:PHE:N	2.46	0.49
1:A:569:ARG:HG2	1:A:569:ARG:O	2.13	0.49
2:B:94:THR:O	2:B:98:TRP:CD1	2.65	0.49
2:B:319:ARG:NH2	2:B:496:TYR:OH	2.46	0.49
2:B:328:ASP:OD1	2:B:328:ASP:N	2.44	0.49
2:B:1028:LEU:O	2:B:1032:PHE:HB2	2.13	0.49
2:B:1607:HIS:NE2	2:B:1619:HIS:HB2	2.28	0.49
2:E:923:VAL:O	2:E:927:LEU:HG	2.13	0.49
2:E:1573:GLU:O	2:E:1577:GLN:NE2	2.45	0.49
2:B:10:GLN:HG3	2:B:37:ILE:HB	1.95	0.48
2:B:1102:ILE:HD11	2:B:1134:CYS:HB2	1.95	0.48
2:B:1307:TYR:O	2:B:1311:GLY:N	2.44	0.48
2:E:89:GLN:O	2:E:92:THR:OG1	2.28	0.48
2:E:1028:LEU:O	2:E:1032:PHE:HB2	2.13	0.48
2:E:1038:PHE:O	2:E:1039:GLU:HG2	2.13	0.48
2:E:1449:GLN:OE1	2:E:1449:GLN:N	2.34	0.48
2:B:1010:ASN:O	2:B:1014:ASN:ND2	2.46	0.48
2:B:1438:PRO:HB2	2:B:1441:TYR:HB2	1.95	0.48
2:B:1452:ASN:HA	2:B:1455:ARG:CG	2.43	0.48
1:D:687:ASP:OD1	1:D:688:THR:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:738:ASN:HA	2:E:741:VAL:HG12	1.94	0.48
2:B:201:GLU:O	2:B:205:LEU:HB3	2.13	0.48
2:B:700:ILE:O	2:B:703:LEU:HG	2.14	0.48
2:B:961:LEU:HA	2:B:964:MET:HE2	1.95	0.48
2:B:1159:VAL:O	2:B:1208:ARG:NH1	2.47	0.48
2:B:1443:ASP:OD1	2:B:1444:LYS:HD3	2.13	0.48
2:E:188:GLU:O	2:E:192:LYS:HG2	2.13	0.48
2:E:1010:ASN:O	2:E:1014:ASN:ND2	2.46	0.48
2:E:1438:PRO:HB2	2:E:1441:TYR:HB2	1.95	0.48
2:E:1585:LYS:HA	2:E:1588:LEU:HD12	1.94	0.48
2:B:451:ILE:HD11	2:B:623:ALA:HB2	1.94	0.48
2:B:1573:GLU:O	2:B:1577:GLN:NE2	2.46	0.48
3:C:61:GLN:HG3	3:C:63:ASP:OD1	2.14	0.48
2:E:844:ILE:HG21	2:E:881:LEU:HD21	1.94	0.48
2:E:904:GLN:OE1	2:E:908:ASN:ND2	2.25	0.48
2:E:1102:ILE:HD11	2:E:1134:CYS:HB2	1.95	0.48
2:E:1529:ILE:HB	2:E:1599:LEU:HD21	1.93	0.48
2:B:1623:SER:HB3	2:B:1627:ARG:HH12	1.79	0.48
3:C:82:PHE:HE1	3:C:112:LEU:HG	1.78	0.48
3:C:124:ASP:O	3:C:127:GLU:HG2	2.14	0.48
2:E:226:VAL:HG22	2:E:403:LEU:HD22	1.95	0.48
2:E:319:ARG:NH2	2:E:496:TYR:OH	2.46	0.48
2:E:319:ARG:O	2:E:500:VAL:N	2.34	0.48
2:E:328:ASP:N	2:E:328:ASP:OD1	2.44	0.48
2:E:1328:TYR:HB3	2:E:1338:LEU:HD22	1.95	0.48
2:E:1443:ASP:OD1	2:E:1444:LYS:HD3	2.13	0.48
3:F:49:LYS:HZ2	3:F:51:VAL:HG12	1.78	0.48
2:B:554:LEU:HA	2:B:562:LEU:HB2	1.94	0.48
2:B:637:LEU:HD11	2:B:660:VAL:HG11	1.94	0.48
2:B:745:ASP:OD1	2:B:745:ASP:N	2.47	0.48
2:B:1125:ILE:N	2:B:1126:PRO:HD2	2.29	0.48
2:B:1129:PHE:HA	2:B:1132:MET:HG3	1.95	0.48
2:E:638:LEU:HA	2:E:641:LEU:HB2	1.95	0.48
2:E:1561:GLY:O	2:E:1565:ASN:ND2	2.39	0.48
3:F:61:GLN:HG3	3:F:63:ASP:OD1	2.14	0.48
2:B:471:SER:N	2:B:528:ARG:O	2.47	0.48
2:B:719:TYR:O	2:B:724:PHE:N	2.46	0.48
1:D:569:ARG:HG2	1:D:569:ARG:O	2.13	0.48
2:E:1201:LEU:O	2:E:1205:LEU:HD23	2.14	0.48
2:E:1324:LEU:O	2:E:1327:THR:OG1	2.27	0.48
2:E:1372:PHE:CZ	2:E:1424:GLN:HB3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1536:HIS:CD2	2:E:1542:LEU:HB3	2.49	0.48
2:B:35:VAL:HG23	2:B:37:ILE:HG13	1.96	0.48
2:B:129:SER:HA	2:B:132:LEU:HD12	1.95	0.48
2:B:923:VAL:O	2:B:927:LEU:HG	2.13	0.48
2:B:1056:HIS:ND1	2:B:1057:GLU:OE2	2.46	0.48
2:B:1328:TYR:HB3	2:B:1338:LEU:HD22	1.95	0.48
2:E:961:LEU:HA	2:E:964:MET:HE2	1.95	0.48
2:E:1452:ASN:HA	2:E:1455:ARG:CG	2.43	0.48
2:B:127:TRP:O	2:B:131:ILE:HG12	2.14	0.48
2:B:226:VAL:HG22	2:B:403:LEU:HD22	1.95	0.48
2:B:1372:PHE:CZ	2:B:1424:GLN:HB3	2.49	0.48
2:B:1536:HIS:CD2	2:B:1542:LEU:HB3	2.49	0.48
3:C:94:ARG:CZ	3:C:145:MET:HG2	2.43	0.48
1:D:575:TRP:CZ3	1:D:588:TYR:HB2	2.40	0.48
2:E:700:ILE:O	2:E:703:LEU:HG	2.14	0.48
2:E:1168:TYR:CE1	2:E:1172:LEU:HD11	2.49	0.48
2:E:1479:PHE:HA	2:E:1482:MET:HG2	1.95	0.48
1:A:646:TYR:CE1	1:A:652:LEU:HG	2.49	0.48
1:A:687:ASP:OD1	1:A:688:THR:N	2.46	0.48
1:A:701:LEU:HD23	2:B:31:ILE:HG23	1.96	0.48
2:B:575:ASP:HB3	2:B:578:LYS:HB2	1.96	0.48
2:B:727:THR:O	2:B:774:TYR:HB2	2.14	0.48
2:B:809:ALA:HB3	2:B:813:LYS:NZ	2.29	0.48
2:B:1149:ASN:HA	2:B:1236:ARG:HH22	1.79	0.48
2:B:1231:TYR:CE2	2:B:1239:ILE:HD12	2.49	0.48
1:D:701:LEU:HD23	2:E:31:ILE:HG23	1.96	0.48
2:E:157:ARG:HE	2:E:198:ILE:HG22	1.79	0.48
2:E:716:LEU:O	2:E:720:ILE:HG13	2.14	0.48
2:E:1157:GLN:O	2:E:1160:GLU:HG3	2.14	0.48
2:E:1159:VAL:O	2:E:1208:ARG:NH1	2.47	0.48
2:B:653:ASN:O	2:B:657:LEU:HG	2.14	0.47
2:B:1417:ASP:N	2:B:1417:ASP:OD1	2.47	0.47
2:B:1585:LYS:HA	2:B:1588:LEU:HD12	1.94	0.47
2:E:10:GLN:HG3	2:E:37:ILE:HB	1.95	0.47
2:E:473:HIS:CE1	2:E:479:LEU:HB2	2.49	0.47
2:E:1268:ALA:HA	2:E:1271:LEU:HD13	1.96	0.47
3:F:63:ASP:OD1	3:F:64:TYR:N	2.47	0.47
1:A:688:THR:O	1:A:691:SER:OG	2.27	0.47
2:B:676:LEU:HB3	2:B:693:VAL:HG13	1.97	0.47
2:B:1201:LEU:O	2:B:1205:LEU:HD23	2.14	0.47
2:E:129:SER:HA	2:E:132:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:783:ASP:HB3	2:E:786:GLU:HB2	1.94	0.47
3:F:94:ARG:CZ	3:F:145:MET:HG2	2.43	0.47
3:F:124:ASP:O	3:F:127:GLU:HG2	2.14	0.47
1:A:707:PRO:HG2	1:A:711:PRO:HD3	1.96	0.47
2:B:940:VAL:C	2:B:992:MET:HE1	2.39	0.47
2:B:1028:LEU:HA	2:B:1032:PHE:HD1	1.80	0.47
2:B:1051:VAL:O	2:B:1055:THR:OG1	2.30	0.47
3:C:153:LYS:HG2	3:C:171:GLU:HG2	1.96	0.47
2:E:254:ILE:O	2:E:431:MET:N	2.39	0.47
2:E:331:ASP:HB3	2:E:336:LYS:HD2	1.95	0.47
2:E:1621:ARG:HH22	3:F:70:LEU:HD13	1.79	0.47
2:E:1623:SER:HB3	2:E:1627:ARG:HH12	1.78	0.47
3:F:82:PHE:CD2	3:F:90:PHE:HE1	2.33	0.47
2:B:157:ARG:HE	2:B:198:ILE:HG22	1.79	0.47
2:B:1452:ASN:OD1	2:B:1453:TYR:N	2.48	0.47
2:E:745:ASP:OD1	2:E:745:ASP:N	2.47	0.47
2:E:992:MET:O	2:E:996:LEU:HD23	2.15	0.47
2:E:1056:HIS:ND1	2:E:1057:GLU:OE2	2.46	0.47
2:B:484:ILE:O	2:B:493:ILE:N	2.31	0.47
1:D:646:TYR:CE1	1:D:652:LEU:HG	2.49	0.47
1:D:692:MET:HE1	2:E:122:TYR:CE2	2.50	0.47
2:E:127:TRP:O	2:E:131:ILE:HG12	2.14	0.47
2:E:170:GLY:O	2:E:172:ILE:HG23	2.15	0.47
2:E:471:SER:N	2:E:528:ARG:O	2.47	0.47
2:E:1125:ILE:N	2:E:1126:PRO:HD2	2.29	0.47
2:E:1216:SER:OG	2:E:1219:ASN:OD1	2.33	0.47
2:E:1290:VAL:HG23	2:E:1291:TYR:H	1.80	0.47
2:E:1623:SER:HB3	2:E:1627:ARG:NH1	2.29	0.47
3:F:9:VAL:HG22	3:F:78:PHE:CZ	2.46	0.47
1:A:588:TYR:CE1	1:A:608:LEU:HB2	2.50	0.47
2:B:1168:TYR:CE1	2:B:1172:LEU:HD11	2.49	0.47
2:B:1449:GLN:HA	2:B:1452:ASN:ND2	2.30	0.47
3:C:83:SER:HB3	3:C:86:SER:HB3	1.97	0.47
2:E:676:LEU:HB3	2:E:693:VAL:HG13	1.97	0.47
2:E:874:CYS:SG	2:E:875:ARG:N	2.88	0.47
1:A:584:LYS:O	1:A:607:LYS:NZ	2.46	0.47
2:B:327:MET:HE3	2:B:327:MET:HB3	1.70	0.47
2:B:783:ASP:HB3	2:B:786:GLU:HB2	1.94	0.47
2:B:790:SER:HA	2:B:793:GLN:CD	2.39	0.47
2:B:976:PHE:HB2	2:B:982:ILE:HD12	1.96	0.47
2:E:3:ARG:HH22	2:E:42:GLU:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:145:LYS:O	2:E:149:THR:OG1	2.25	0.47
2:E:450:LEU:HD13	2:E:468:VAL:HB	1.97	0.47
2:E:469:THR:O	2:E:530:THR:OG1	2.31	0.47
2:E:941:ILE:O	2:E:944:ASN:HB2	2.15	0.47
2:E:1231:TYR:CE2	2:E:1239:ILE:HD12	2.49	0.47
2:E:1417:ASP:N	2:E:1417:ASP:OD1	2.47	0.47
2:E:1449:GLN:HA	2:E:1452:ASN:ND2	2.30	0.47
2:E:1605:ARG:O	2:E:1609:GLU:HG3	2.14	0.47
3:F:10:GLY:O	3:F:60:GLY:HA3	2.15	0.47
2:B:1065:SER:OG	2:B:1068:LYS:HE3	2.15	0.47
2:B:1216:SER:OG	2:B:1219:ASN:OD1	2.33	0.47
2:B:1361:GLU:OE1	2:B:1389:GLU:N	2.47	0.47
2:B:1623:SER:HB3	2:B:1627:ARG:NH1	2.29	0.47
3:C:63:ASP:OD1	3:C:64:TYR:N	2.47	0.47
2:E:575:ASP:HB3	2:E:578:LYS:HB2	1.96	0.47
2:E:1391:ARG:HD2	2:E:1429:PHE:HA	1.97	0.47
3:F:6:CYS:C	3:F:56:TRP:HD1	2.23	0.47
2:B:921:THR:OG1	2:B:924:HIS:HB3	2.14	0.47
1:D:585:VAL:HG12	1:D:607:LYS:HD2	1.97	0.47
2:E:653:ASN:O	2:E:657:LEU:HG	2.14	0.47
2:E:727:THR:O	2:E:774:TYR:HB2	2.14	0.47
2:E:790:SER:HA	2:E:793:GLN:CD	2.39	0.47
2:E:921:THR:OG1	2:E:924:HIS:HB3	2.14	0.47
2:E:934:ARG:NH1	2:E:938:ARG:HG2	2.30	0.47
2:E:1237:GLU:O	2:E:1240:TYR:HB3	2.15	0.47
2:E:1452:ASN:OD1	2:E:1453:TYR:N	2.48	0.47
2:E:1607:HIS:NE2	2:E:1619:HIS:HB2	2.28	0.47
2:B:355:THR:HG21	2:B:372:VAL:HG22	1.96	0.47
2:B:646:ASN:ND2	2:B:653:ASN:HD21	2.13	0.47
2:B:716:LEU:O	2:B:720:ILE:HG13	2.14	0.47
2:B:874:CYS:SG	2:B:875:ARG:N	2.88	0.47
2:B:1237:GLU:O	2:B:1240:TYR:HB3	2.15	0.47
2:B:1605:ARG:O	2:B:1609:GLU:HG3	2.14	0.47
3:C:6:CYS:C	3:C:56:TRP:HD1	2.23	0.47
2:E:1361:GLU:OE1	2:E:1389:GLU:N	2.47	0.47
1:A:680:ASP:OD1	1:A:681:LEU:N	2.48	0.46
1:A:727:ASN:N	2:B:46:ARG:HH22	2.13	0.46
2:E:677:PHE:O	2:E:681:MET:HG2	2.15	0.46
2:E:1149:ASN:HA	2:E:1236:ARG:HH22	1.79	0.46
2:E:1583:GLN:O	2:E:1586:VAL:HG12	2.16	0.46
3:F:98:TYR:CE1	3:F:149:ILE:HD13	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:153:LYS:HG2	3:F:171:GLU:HG2	1.96	0.46
3:F:164:GLY:O	3:F:168:VAL:N	2.36	0.46
1:A:585:VAL:HG12	1:A:607:LYS:HD2	1.97	0.46
2:B:3:ARG:HH22	2:B:42:GLU:HB2	1.79	0.46
2:B:65:HIS:HD2	2:B:67:LYS:HD2	1.80	0.46
2:B:450:LEU:HD13	2:B:468:VAL:HB	1.97	0.46
2:B:1166:GLU:O	2:B:1169:LYS:HG2	2.15	0.46
2:B:1344:LYS:O	2:B:1347:SER:OG	2.25	0.46
3:C:82:PHE:CD2	3:C:90:PHE:HE1	2.33	0.46
2:E:163:LEU:HD23	2:E:1005:ASP:HB3	1.96	0.46
2:E:694:PHE:HZ	2:E:737:LEU:HD13	1.81	0.46
2:E:861:THR:HA	2:E:864:VAL:HG22	1.97	0.46
2:E:1468:PHE:HB3	2:E:1483:TRP:O	2.13	0.46
2:B:202:LYS:H	2:B:202:LYS:HG2	1.49	0.46
2:B:288:ASP:HA	2:B:291:ARG:HE	1.80	0.46
2:B:288:ASP:HA	2:B:291:ARG:NE	2.31	0.46
2:B:346:ILE:HB	2:B:399:LEU:HD21	1.98	0.46
2:B:473:HIS:CE1	2:B:479:LEU:HB2	2.49	0.46
2:B:1166:GLU:H	2:B:1166:GLU:CD	2.23	0.46
3:C:95:ALA:O	3:C:99:PRO:HG2	2.16	0.46
2:E:65:HIS:HD2	2:E:67:LYS:HD2	1.80	0.46
2:E:259:LEU:HD22	2:E:486:PRO:HB2	1.98	0.46
3:F:95:ALA:O	3:F:99:PRO:HG2	2.15	0.46
2:B:992:MET:O	2:B:996:LEU:HD23	2.15	0.46
2:B:1294:GLN:HG3	2:B:1298:GLU:OE2	2.16	0.46
2:B:1372:PHE:N	2:B:1424:GLN:HG2	2.31	0.46
2:B:1566:TYR:OH	3:C:36:VAL:HG21	2.16	0.46
1:D:700:ASP:CG	2:E:14:VAL:HG13	2.40	0.46
2:E:1047:PHE:HB2	2:E:1105:MET:CE	2.46	0.46
2:B:170:GLY:O	2:B:172:ILE:HG23	2.15	0.46
2:B:945:ARG:HH11	2:B:946:GLN:H	1.63	0.46
2:B:1322:LYS:HG2	2:B:1345:ARG:NH1	2.31	0.46
3:C:113:VAL:HA	3:C:155:LEU:O	2.15	0.46
1:D:575:TRP:HB2	1:D:589:GLY:O	2.16	0.46
2:E:59:PHE:CD2	2:E:64:ILE:HG12	2.48	0.46
2:E:88:VAL:O	2:E:91:LEU:HG	2.15	0.46
2:E:140:GLU:O	2:E:144:LEU:HD23	2.16	0.46
2:E:940:VAL:C	2:E:992:MET:HE1	2.39	0.46
2:E:1166:GLU:O	2:E:1169:LYS:HG2	2.15	0.46
2:E:1561:GLY:C	2:E:1565:ASN:HD22	2.22	0.46
2:B:429:ARG:HE	2:B:429:ARG:HB2	1.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1047:PHE:HB2	2:B:1105:MET:CE	2.46	0.46
2:B:1583:GLN:O	2:B:1586:VAL:HG12	2.15	0.46
2:E:35:VAL:HG23	2:E:37:ILE:HG13	1.96	0.46
2:E:288:ASP:HA	2:E:291:ARG:HE	1.80	0.46
2:E:680:MET:O	2:E:684:SER:HB3	2.16	0.46
2:E:700:ILE:O	2:E:704:ILE:HG13	2.15	0.46
3:F:164:GLY:O	3:F:168:VAL:HG23	2.16	0.46
1:A:575:TRP:HB2	1:A:589:GLY:O	2.16	0.46
1:A:697:ARG:HA	1:A:697:ARG:NH1	2.31	0.46
2:B:259:LEU:HD22	2:B:486:PRO:HB2	1.98	0.46
2:B:941:ILE:O	2:B:944:ASN:HB2	2.15	0.46
2:B:1635:LYS:HD2	2:B:1636:HIS:N	2.31	0.46
1:D:707:PRO:HG2	1:D:711:PRO:HD3	1.96	0.46
2:E:346:ILE:HB	2:E:399:LEU:HD21	1.98	0.46
2:E:484:ILE:O	2:E:493:ILE:N	2.31	0.46
2:E:745:ASP:H	2:E:804:ARG:HH12	1.62	0.46
2:E:809:ALA:HB3	2:E:813:LYS:NZ	2.29	0.46
2:E:945:ARG:HH11	2:E:946:GLN:H	1.63	0.46
2:E:1635:LYS:HD2	2:E:1636:HIS:N	2.31	0.46
3:F:90:PHE:HA	3:F:93:VAL:HG12	1.97	0.46
2:B:29:LEU:HD12	2:B:59:PHE:CD1	2.51	0.46
2:B:560:THR:HG21	2:B:634:ASN:O	2.16	0.46
2:B:901:ALA:O	2:B:905:LEU:HG	2.16	0.46
2:B:934:ARG:NH1	2:B:938:ARG:HG2	2.30	0.46
2:B:1157:GLN:O	2:B:1160:GLU:HG3	2.14	0.46
2:B:1205:LEU:HA	2:B:1208:ARG:HD3	1.97	0.46
2:B:1391:ARG:HD2	2:B:1429:PHE:HA	1.97	0.46
3:C:90:PHE:CE2	3:C:137:ILE:HB	2.51	0.46
2:E:355:THR:HG21	2:E:372:VAL:HG22	1.96	0.46
2:E:879:LEU:O	2:E:880:PRO:C	2.59	0.46
2:E:1165:ASP:O	2:E:1168:TYR:HB3	2.16	0.46
2:E:1359:GLN:HG3	2:E:1456:ALA:HB2	1.98	0.46
3:F:6:CYS:SG	3:F:79:LEU:HD23	2.56	0.46
3:F:90:PHE:CE2	3:F:137:ILE:HB	2.51	0.46
1:A:530:SER:O	1:A:534:LEU:N	2.37	0.46
2:B:113:LEU:O	2:B:116:GLN:HG2	2.15	0.46
2:B:700:ILE:O	2:B:704:ILE:HG13	2.15	0.46
3:C:7:VAL:HG13	3:C:56:TRP:HB2	1.98	0.46
3:C:164:GLY:O	3:C:168:VAL:HG23	2.16	0.46
1:D:588:TYR:CE1	1:D:608:LEU:HB2	2.50	0.46
2:E:832:ASP:OD2	2:E:835:GLU:N	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1028:LEU:HA	2:E:1032:PHE:HD1	1.80	0.46
2:E:1166:GLU:CD	2:E:1166:GLU:H	2.23	0.46
2:E:1167:GLN:CD	2:E:1167:GLN:H	2.24	0.46
2:E:1294:GLN:HG3	2:E:1298:GLU:OE2	2.16	0.46
2:E:1546:PRO:O	2:E:1549:MET:HB2	2.16	0.46
3:F:2:GLN:HE21	3:F:51:VAL:CG1	2.29	0.46
3:F:5:LYS:HD2	3:F:74:GLN:O	2.16	0.46
3:F:102:ARG:NH2	3:F:106:PRO:O	2.47	0.46
1:A:560:THR:O	1:A:576:TYR:HA	2.15	0.46
1:A:574:PHE:HB2	1:A:593:GLU:HA	1.98	0.46
2:B:34:THR:O	2:B:50:LEU:HB2	2.15	0.46
2:B:98:TRP:CH2	2:B:155:GLY:HA3	2.40	0.46
2:B:570:VAL:CG2	2:B:595:MET:HE2	2.39	0.46
2:B:1324:LEU:O	2:B:1327:THR:OG1	2.27	0.46
3:C:90:PHE:HA	3:C:93:VAL:HG12	1.97	0.46
1:D:560:THR:O	1:D:576:TYR:HA	2.15	0.46
1:D:697:ARG:NH1	1:D:697:ARG:HA	2.31	0.46
2:E:113:LEU:O	2:E:116:GLN:HG2	2.15	0.46
2:E:288:ASP:HA	2:E:291:ARG:NE	2.31	0.46
2:E:560:THR:HG21	2:E:634:ASN:O	2.16	0.46
2:E:746:ASP:CG	2:E:748:SER:HG	2.24	0.46
2:E:1143:ASN:HD21	2:E:1145:HIS:CE1	2.34	0.46
2:E:1514:PRO:HA	2:E:1517:ASN:HD22	1.81	0.46
2:B:721:TYR:HA	2:B:769:GLN:NE2	2.31	0.45
2:B:1224:THR:HA	2:B:1227:VAL:HG12	1.98	0.45
2:B:1290:VAL:HG23	2:B:1291:TYR:H	1.80	0.45
3:C:102:ARG:NH2	3:C:106:PRO:O	2.47	0.45
2:E:29:LEU:HD12	2:E:59:PHE:CD1	2.51	0.45
2:E:646:ASN:ND2	2:E:653:ASN:HD21	2.13	0.45
3:F:7:VAL:HG13	3:F:56:TRP:HB2	1.98	0.45
3:F:113:VAL:HA	3:F:155:LEU:O	2.15	0.45
1:A:643:SER:OG	1:A:653:ASN:ND2	2.45	0.45
2:B:140:GLU:O	2:B:144:LEU:HD23	2.16	0.45
2:B:166:ARG:HB3	2:B:171:ASN:HA	1.98	0.45
2:B:187:HIS:NE2	2:B:1008:VAL:HB	2.31	0.45
2:B:469:THR:O	2:B:530:THR:OG1	2.31	0.45
2:B:677:PHE:O	2:B:681:MET:HG2	2.15	0.45
2:B:861:THR:HA	2:B:864:VAL:HG22	1.97	0.45
2:B:1061:LEU:HA	2:B:1064:PHE:CZ	2.51	0.45
2:B:1268:ALA:HA	2:B:1271:LEU:HD13	1.96	0.45
2:E:166:ARG:HB3	2:E:171:ASN:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:523:THR:HA	2:E:555:MET:SD	2.57	0.45
2:E:670:GLN:HA	2:E:673:LEU:HD12	1.97	0.45
2:E:976:PHE:HB2	2:E:982:ILE:HD12	1.96	0.45
2:E:1307:TYR:O	2:E:1311:GLY:N	2.44	0.45
3:F:83:SER:HB3	3:F:86:SER:HB3	1.97	0.45
2:B:163:LEU:HD23	2:B:1005:ASP:HB3	1.97	0.45
2:B:832:ASP:OD2	2:B:835:GLU:N	2.26	0.45
2:B:876:GLU:HA	2:B:924:HIS:HE2	1.81	0.45
2:B:1107:GLY:HA2	2:B:1110:LEU:HD13	1.99	0.45
2:B:1165:ASP:O	2:B:1168:TYR:HB3	2.16	0.45
2:B:1276:LYS:HA	2:B:1276:LYS:HD2	1.84	0.45
2:B:1561:GLY:C	2:B:1565:ASN:HD22	2.22	0.45
2:E:471:SER:O	2:E:528:ARG:N	2.26	0.45
2:E:936:ILE:O	2:E:940:VAL:HG12	2.17	0.45
2:B:680:MET:O	2:B:684:SER:HB3	2.16	0.45
2:B:732:LYS:HA	2:B:735:LYS:HD3	1.98	0.45
2:B:745:ASP:H	2:B:804:ARG:HH12	1.62	0.45
2:B:821:PRO:O	2:B:824:ILE:HG12	2.16	0.45
2:B:1143:ASN:HD21	2:B:1145:HIS:CE1	2.33	0.45
2:B:1546:PRO:O	2:B:1549:MET:HB2	2.16	0.45
3:C:5:LYS:HD2	3:C:74:GLN:O	2.16	0.45
3:C:10:GLY:O	3:C:60:GLY:HA3	2.15	0.45
1:D:574:PHE:HB2	1:D:593:GLU:HA	1.98	0.45
1:D:607:LYS:HE3	1:D:609:PRO:HA	1.99	0.45
2:E:721:TYR:HA	2:E:769:GLN:NE2	2.31	0.45
2:E:961:LEU:HA	2:E:964:MET:CE	2.46	0.45
2:E:1322:LYS:HG2	2:E:1345:ARG:NH1	2.31	0.45
3:F:80:ILE:HG23	3:F:112:LEU:HD12	1.98	0.45
2:B:59:PHE:CD2	2:B:64:ILE:HG12	2.48	0.45
2:B:883:THR:HA	2:B:886:LEU:HG	1.99	0.45
2:E:34:THR:O	2:E:50:LEU:HB2	2.15	0.45
2:E:732:LYS:HA	2:E:735:LYS:HD3	1.98	0.45
2:E:1065:SER:OG	2:E:1068:LYS:HB2	2.16	0.45
2:E:1079:MET:HA	2:E:1082:GLU:OE2	2.17	0.45
2:E:1623:SER:HB3	2:E:1627:ARG:NH2	2.32	0.45
3:F:65:ASP:HA	3:F:68:ARG:HG2	1.99	0.45
1:A:607:LYS:HE3	1:A:609:PRO:HA	1.99	0.45
2:B:333:ILE:O	2:B:405:LEU:HD22	2.17	0.45
2:B:523:THR:HA	2:B:555:MET:SD	2.57	0.45
2:B:694:PHE:HZ	2:B:737:LEU:HD13	1.81	0.45
2:B:1075:LYS:HE3	2:B:1075:LYS:HB3	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:CYS:SG	3:C:79:LEU:HD23	2.56	0.45
2:E:151:LYS:HA	2:E:197:LYS:HZ3	1.81	0.45
2:E:319:ARG:NH2	2:E:511:GLU:OE2	2.39	0.45
2:E:718:THR:O	2:E:722:LYS:HE2	2.17	0.45
2:E:821:PRO:O	2:E:824:ILE:HG12	2.16	0.45
2:E:883:THR:HA	2:E:886:LEU:HG	1.99	0.45
2:E:1372:PHE:N	2:E:1424:GLN:HG2	2.31	0.45
2:B:10:GLN:CG	2:B:37:ILE:HB	2.47	0.45
2:B:119:GLN:HA	2:B:122:TYR:CD1	2.52	0.45
2:B:390:LYS:HD2	2:B:390:LYS:HA	1.75	0.45
2:B:1167:GLN:CD	2:B:1167:GLN:H	2.24	0.45
3:C:2:GLN:HE21	3:C:51:VAL:CG1	2.29	0.45
2:E:10:GLN:CG	2:E:37:ILE:HB	2.47	0.45
2:E:333:ILE:O	2:E:405:LEU:HD22	2.17	0.45
2:E:1224:THR:HA	2:E:1227:VAL:HG12	1.98	0.45
2:B:88:VAL:O	2:B:91:LEU:HG	2.15	0.45
2:B:89:GLN:O	2:B:92:THR:OG1	2.28	0.45
2:B:165:VAL:HG23	2:B:175:PRO:HD3	1.99	0.45
2:B:1056:HIS:HD1	2:B:1057:GLU:CD	2.25	0.45
2:B:1368:TYR:O	2:B:1425:TYR:N	2.40	0.45
2:B:1386:LYS:HG3	2:B:1387:GLU:OE1	2.17	0.45
2:B:670:GLN:HA	2:B:673:LEU:HD12	1.97	0.45
2:B:957:MET:O	2:B:961:LEU:HG	2.17	0.45
2:B:961:LEU:HA	2:B:964:MET:CE	2.46	0.45
2:B:1067:ALA:HB1	2:B:1071:LYS:HG3	1.99	0.45
3:C:129:LEU:O	3:C:134:LEU:N	2.45	0.45
1:D:584:LYS:O	1:D:607:LYS:NZ	2.46	0.45
2:E:771:ARG:NH2	2:E:784:GLY:HA2	2.32	0.45
2:E:876:GLU:HA	2:E:924:HIS:HE2	1.81	0.45
2:E:1107:GLY:HA2	2:E:1110:LEU:HD13	1.98	0.45
2:B:718:THR:O	2:B:722:LYS:HE2	2.17	0.45
2:B:720:ILE:HG12	2:B:766:PHE:CE1	2.52	0.45
2:B:794:LEU:HB3	2:B:798:PHE:CZ	2.52	0.45
2:B:1079:MET:HA	2:B:1082:GLU:OE2	2.17	0.45
2:B:1519:ILE:O	2:B:1523:GLU:OE1	2.35	0.45
2:B:1551:LEU:HB3	2:B:1622:LEU:HD13	2.00	0.45
1:D:541:GLN:O	1:D:544:ILE:HG22	2.17	0.45
2:E:187:HIS:NE2	2:E:1008:VAL:HB	2.31	0.45
2:E:720:ILE:HG12	2:E:766:PHE:CE1	2.52	0.45
2:E:790:SER:O	2:E:794:LEU:HD23	2.17	0.45
2:E:1056:HIS:HD1	2:E:1057:GLU:CD	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1065:SER:OG	2:E:1068:LYS:HE3	2.15	0.45
2:E:1466:ARG:O	2:E:1484:ILE:HA	2.17	0.45
2:B:172:ILE:HA	2:B:175:PRO:HG2	1.99	0.44
2:B:792:ARG:NE	2:B:835:GLU:OE1	2.43	0.44
2:B:936:ILE:O	2:B:940:VAL:HG12	2.16	0.44
2:B:1006:TRP:CD1	2:B:1006:TRP:N	2.84	0.44
2:B:1359:GLN:HG3	2:B:1456:ALA:HB2	1.98	0.44
2:B:1362:TYR:HE2	2:B:1459:VAL:HG21	1.82	0.44
2:B:1491:THR:HG23	2:B:1493:TYR:O	2.18	0.44
2:B:1514:PRO:HA	2:B:1517:ASN:HD22	1.81	0.44
3:C:80:ILE:O	3:C:113:VAL:HG22	2.17	0.44
1:D:680:ASP:OD1	1:D:681:LEU:N	2.48	0.44
2:E:1006:TRP:CD1	2:E:1006:TRP:N	2.84	0.44
2:E:1061:LEU:HA	2:E:1064:PHE:CZ	2.51	0.44
2:E:1218:GLU:OE1	2:E:1218:GLU:N	2.35	0.44
3:F:80:ILE:O	3:F:113:VAL:HG22	2.17	0.44
2:B:23:GLN:HB2	2:B:26:GLU:HB2	2.00	0.44
2:B:1065:SER:OG	2:B:1068:LYS:HB2	2.16	0.44
2:B:1412:THR:HB	2:B:1413:PRO:HD3	2.00	0.44
2:B:1623:SER:HB3	2:B:1627:ARG:NH2	2.32	0.44
3:C:80:ILE:HG23	3:C:112:LEU:HD12	1.98	0.44
2:E:3:ARG:NH2	2:E:42:GLU:H	2.13	0.44
2:E:4:TRP:CE3	2:E:46:ARG:HG2	2.52	0.44
2:B:12:TYR:HB3	2:B:67:LYS:HD3	1.98	0.44
2:B:678:ASN:O	2:B:682:GLU:HG2	2.18	0.44
2:B:771:ARG:NH2	2:B:784:GLY:HA2	2.32	0.44
2:B:960:LEU:O	2:B:964:MET:HG3	2.18	0.44
2:B:1375:PHE:O	2:B:1379:LYS:HG3	2.18	0.44
2:B:1623:SER:HB3	2:B:1627:ARG:HH22	1.82	0.44
1:D:658:ASP:CG	1:D:660:HIS:HD1	2.25	0.44
2:E:493:ILE:HD11	2:E:496:TYR:HD1	1.82	0.44
2:E:678:ASN:O	2:E:682:GLU:HG2	2.18	0.44
2:E:795:PHE:CD2	2:E:839:LEU:HD13	2.53	0.44
2:E:957:MET:O	2:E:961:LEU:HG	2.17	0.44
2:E:1061:LEU:HA	2:E:1064:PHE:CE2	2.53	0.44
2:E:1205:LEU:HA	2:E:1208:ARG:HD3	1.97	0.44
2:E:1412:THR:HB	2:E:1413:PRO:HD3	2.00	0.44
1:A:575:TRP:CZ3	1:A:588:TYR:HB2	2.40	0.44
2:B:730:TYR:HB3	2:B:770:SER:HB3	2.00	0.44
2:B:904:GLN:OE1	2:B:908:ASN:ND2	2.25	0.44
2:B:910:LEU:HA	2:B:913:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1373:PRO:HD2	2:B:1376:LEU:HD12	1.98	0.44
3:C:164:GLY:O	3:C:168:VAL:N	2.36	0.44
2:E:112:THR:OG1	2:E:113:LEU:N	2.49	0.44
2:E:119:GLN:HA	2:E:122:TYR:CD1	2.52	0.44
2:E:327:MET:HG3	2:E:346:ILE:HG12	2.00	0.44
2:E:486:PRO:HB3	2:E:496:TYR:HE1	1.81	0.44
2:E:662:GLY:HA3	2:E:703:LEU:HD13	2.00	0.44
2:E:943:MET:HG2	2:E:953:PHE:CD2	2.53	0.44
2:E:1545:HIS:N	2:E:1546:PRO:HD2	2.33	0.44
2:E:1549:MET:HE1	3:F:39:ASN:OD1	2.18	0.44
2:E:1623:SER:HB3	2:E:1627:ARG:HH22	1.82	0.44
2:B:4:TRP:CE3	2:B:46:ARG:HG2	2.52	0.44
2:B:486:PRO:HB3	2:B:496:TYR:HE1	1.81	0.44
2:B:493:ILE:HD11	2:B:496:TYR:HD1	1.82	0.44
2:B:1488:THR:OG1	2:B:1508:SER:HB2	2.18	0.44
1:D:580:SER:HB2	1:D:585:VAL:CG2	2.48	0.44
2:E:165:VAL:HG23	2:E:175:PRO:HD3	1.99	0.44
2:E:466:VAL:CG1	2:E:531:PHE:HB3	2.47	0.44
2:E:901:ALA:O	2:E:905:LEU:HG	2.16	0.44
2:E:960:LEU:O	2:E:964:MET:HG3	2.17	0.44
2:E:1362:TYR:HE2	2:E:1459:VAL:HG21	1.82	0.44
2:E:1370:GLN:N	2:E:1421:SER:O	2.51	0.44
2:E:1386:LYS:HG3	2:E:1387:GLU:OE1	2.17	0.44
3:F:93:VAL:O	3:F:98:TYR:HB3	2.18	0.44
1:A:541:GLN:O	1:A:544:ILE:HG22	2.17	0.44
1:A:690:LEU:O	1:A:694:ILE:HG12	2.18	0.44
2:B:1061:LEU:HA	2:B:1064:PHE:CE2	2.53	0.44
3:C:110:ILE:O	3:C:152:VAL:HG12	2.18	0.44
2:E:545:ARG:HH11	2:E:546:ALA:HB3	1.80	0.44
2:E:642:ASN:O	2:E:646:ASN:N	2.50	0.44
2:E:868:LEU:O	2:E:871:GLN:HG3	2.18	0.44
2:E:1058:SER:HA	2:E:1080:ARG:NH1	2.32	0.44
2:E:1495:PHE:CE1	2:E:1502:PHE:HD2	2.35	0.44
2:E:1613:GLU:OE2	2:E:1614:GLN:HG3	2.17	0.44
2:B:327:MET:HG3	2:B:346:ILE:HG12	2.00	0.44
2:B:697:LEU:O	2:B:701:ILE:HG12	2.18	0.44
2:B:795:PHE:CD2	2:B:839:LEU:HD13	2.53	0.44
2:B:994:LYS:HZ2	2:B:1048:HIS:HB3	1.81	0.44
2:B:1058:SER:HA	2:B:1080:ARG:NH1	2.32	0.44
2:B:1096:PRO:O	2:B:1100:LYS:NZ	2.40	0.44
2:B:1460:GLN:HG3	2:B:1493:TYR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1466:ARG:O	2:B:1484:ILE:HA	2.17	0.44
1:D:721:ASP:OD1	1:D:721:ASP:N	2.50	0.44
2:E:12:TYR:HB3	2:E:67:LYS:HD3	1.98	0.44
2:E:659:GLU:OE1	2:E:659:GLU:N	2.43	0.44
2:E:718:THR:O	2:E:722:LYS:HB2	2.17	0.44
2:E:730:TYR:HB3	2:E:770:SER:HB3	2.00	0.44
2:E:794:LEU:HB3	2:E:798:PHE:CZ	2.52	0.44
2:E:1067:ALA:HB1	2:E:1071:LYS:HG3	1.99	0.44
2:E:1328:TYR:O	2:E:1333:PHE:N	2.44	0.44
1:A:537:LYS:HE2	1:A:690:LEU:HD23	1.98	0.44
2:B:3:ARG:NH2	2:B:42:GLU:H	2.13	0.44
2:B:743:ASN:HB3	2:B:749:LYS:HD2	2.00	0.44
2:B:857:LEU:HB3	2:B:905:LEU:HD21	2.00	0.44
2:B:1613:GLU:OE2	2:B:1614:GLN:HG3	2.17	0.44
3:C:128:LYS:O	3:C:131:GLU:HG2	2.18	0.44
2:E:1081:LYS:HA	2:E:1120:LEU:HD23	2.00	0.44
2:E:1314:TRP:HZ3	2:E:1357:ARG:HH11	1.66	0.44
2:E:1551:LEU:HB3	2:E:1622:LEU:HD13	2.00	0.44
1:A:707:PRO:HB2	1:A:709:ALA:O	2.17	0.44
2:B:166:ARG:NH1	2:B:168:ASP:H	2.16	0.44
2:B:258:TYR:HA	2:B:488:ALA:HB3	2.00	0.44
2:B:466:VAL:CG1	2:B:531:PHE:HB3	2.47	0.44
2:B:879:LEU:O	2:B:880:PRO:C	2.59	0.44
2:B:1043:TRP:CE3	2:B:1043:TRP:N	2.86	0.44
3:C:65:ASP:HA	3:C:68:ARG:HG2	1.99	0.44
3:C:93:VAL:O	3:C:98:TYR:HB3	2.18	0.44
2:E:179:SER:OG	2:E:182:ALA:HB3	2.18	0.44
2:E:573:LYS:HE3	2:E:616:THR:HG21	2.00	0.44
2:E:790:SER:O	2:E:793:GLN:HG2	2.18	0.44
2:E:1146:MET:SD	2:E:1146:MET:N	2.84	0.44
2:E:1154:LYS:O	2:E:1155:LEU:C	2.61	0.44
2:E:1367:TYR:N	2:E:1379:LYS:O	2.50	0.44
3:F:69:PRO:HA	3:F:72:TYR:CD2	2.53	0.44
3:F:110:ILE:O	3:F:152:VAL:HG12	2.18	0.44
1:A:584:LYS:NZ	2:B:1403:PRO:HA	2.33	0.43
1:A:658:ASP:CG	1:A:660:HIS:HD1	2.25	0.43
1:A:721:ASP:OD1	1:A:721:ASP:N	2.50	0.43
2:B:156:ASN:HB3	2:B:161:LEU:HB2	2.00	0.43
2:B:166:ARG:HD2	2:B:166:ARG:HA	1.85	0.43
2:B:508:CYS:HB3	2:B:510:TYR:CE2	2.51	0.43
2:B:879:LEU:HG	2:B:931:ARG:HH12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1545:HIS:N	2:B:1546:PRO:HD2	2.33	0.43
2:E:166:ARG:NH1	2:E:168:ASP:H	2.16	0.43
2:E:431:MET:HG2	2:E:625:LEU:HD23	2.00	0.43
2:E:1488:THR:OG1	2:E:1508:SER:HB2	2.18	0.43
2:E:1611:LEU:HD11	2:E:1616:LYS:HA	2.00	0.43
3:F:21:ILE:HD11	3:F:35:THR:HG23	2.00	0.43
3:F:128:LYS:O	3:F:131:GLU:HG2	2.18	0.43
2:B:285:SER:N	2:B:288:ASP:OD2	2.44	0.43
2:B:471:SER:O	2:B:528:ARG:N	2.26	0.43
2:B:790:SER:O	2:B:794:LEU:HD23	2.17	0.43
2:B:1081:LYS:HA	2:B:1120:LEU:HD23	2.00	0.43
1:D:537:LYS:HE2	1:D:690:LEU:HD23	1.98	0.43
1:D:697:ARG:HE	2:E:30:GLN:CD	2.26	0.43
2:E:1185:TYR:O	2:E:1188:SER:OG	2.24	0.43
2:E:1313:MET:HE2	2:E:1313:MET:HB2	1.87	0.43
2:E:1519:ILE:O	2:E:1523:GLU:OE1	2.35	0.43
2:B:302:ARG:HD3	2:B:322:PHE:HD1	1.84	0.43
2:B:718:THR:O	2:B:722:LYS:HB2	2.17	0.43
2:B:1121:ARG:HG2	2:B:1125:ILE:HD11	2.00	0.43
3:C:69:PRO:HA	3:C:72:TYR:CD2	2.53	0.43
1:D:714:PRO:HG2	2:E:44:TRP:CZ2	2.53	0.43
2:E:23:GLN:HB2	2:E:26:GLU:HB2	1.99	0.43
2:E:380:THR:HG21	2:E:510:TYR:CD2	2.53	0.43
2:E:572:TYR:OH	2:E:589:PRO:O	2.17	0.43
2:E:737:LEU:HD12	2:E:737:LEU:HA	1.83	0.43
2:E:743:ASN:HB3	2:E:749:LYS:HD2	2.00	0.43
2:E:879:LEU:HG	2:E:931:ARG:HH12	1.83	0.43
2:E:1633:VAL:O	2:E:1639:VAL:N	2.50	0.43
3:F:49:LYS:NZ	3:F:50:PRO:O	2.31	0.43
2:B:248:PRO:HD2	2:B:293:ARG:HG3	1.99	0.43
2:B:886:LEU:HD12	2:B:887:SER:N	2.34	0.43
2:B:1063:THR:HA	2:B:1069:ARG:CD	2.47	0.43
2:B:1328:TYR:O	2:B:1333:PHE:N	2.44	0.43
3:C:163:ARG:C	3:C:165:LEU:H	2.26	0.43
1:D:707:PRO:HB2	1:D:709:ALA:O	2.17	0.43
2:E:1373:PRO:HD2	2:E:1376:LEU:HD12	1.98	0.43
3:F:87:PRO:HG2	3:F:134:LEU:HB3	2.01	0.43
1:A:570:ARG:O	1:A:570:ARG:NH1	2.51	0.43
1:A:694:ILE:HG13	1:A:695:LYS:N	2.33	0.43
1:A:726:CYS:CA	2:B:46:ARG:HH22	2.31	0.43
2:B:185:LYS:HE2	2:B:185:LYS:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:589:PRO:HD3	2:B:598:LYS:NZ	2.33	0.43
2:B:662:GLY:HA3	2:B:703:LEU:HD13	2.00	0.43
2:B:683:MET:HE1	2:B:689:TYR:CG	2.54	0.43
2:B:868:LEU:O	2:B:871:GLN:HG3	2.18	0.43
2:B:1079:MET:N	2:B:1079:MET:SD	2.92	0.43
3:C:21:ILE:HD11	3:C:35:THR:HG23	2.00	0.43
2:E:156:ASN:HD22	2:E:161:LEU:HD12	1.83	0.43
2:E:156:ASN:HB3	2:E:161:LEU:HB2	2.00	0.43
2:E:172:ILE:HA	2:E:175:PRO:HG2	1.99	0.43
2:E:222:TYR:HB3	2:E:405:LEU:HD11	2.01	0.43
2:E:429:ARG:HE	2:E:429:ARG:HB2	1.58	0.43
2:E:683:MET:HE1	2:E:689:TYR:CD2	2.54	0.43
2:E:792:ARG:NE	2:E:835:GLU:OE1	2.43	0.43
2:E:1344:LYS:O	2:E:1347:SER:OG	2.25	0.43
2:E:1491:THR:HG23	2:E:1493:TYR:O	2.18	0.43
1:A:668:GLY:O	1:A:672:LEU:HG	2.19	0.43
2:B:112:THR:OG1	2:B:113:LEU:N	2.49	0.43
2:B:179:SER:OG	2:B:182:ALA:HB3	2.18	0.43
2:B:267:MET:HG3	2:B:268:PRO:HD2	2.00	0.43
2:B:380:THR:HG21	2:B:510:TYR:CD2	2.53	0.43
2:B:642:ASN:O	2:B:646:ASN:N	2.50	0.43
2:B:695:ASP:OD1	2:B:740:TYR:OH	2.37	0.43
2:B:943:MET:HG2	2:B:953:PHE:CD2	2.53	0.43
1:D:668:GLY:O	1:D:672:LEU:HG	2.19	0.43
2:E:679:ILE:HG22	2:E:680:MET:HE2	2.01	0.43
2:E:683:MET:HE1	2:E:689:TYR:CG	2.54	0.43
2:E:724:PHE:CZ	2:E:726:ALA:HB3	2.54	0.43
2:E:857:LEU:HB3	2:E:905:LEU:HD21	2.00	0.43
2:E:972:TYR:O	2:E:975:THR:N	2.47	0.43
2:E:1079:MET:N	2:E:1079:MET:SD	2.92	0.43
2:E:1221:MET:HA	2:E:1224:THR:HG22	2.01	0.43
1:A:580:SER:HB2	1:A:585:VAL:CG2	2.48	0.43
2:B:438:LEU:HD12	2:B:439:PRO:HD2	2.01	0.43
2:B:724:PHE:CZ	2:B:726:ALA:HB3	2.54	0.43
2:B:790:SER:O	2:B:793:GLN:HG2	2.18	0.43
2:B:1197:VAL:O	2:B:1201:LEU:HG	2.19	0.43
2:B:1283:LEU:HD11	2:B:1291:TYR:HB2	2.00	0.43
2:B:1370:GLN:N	2:B:1421:SER:O	2.51	0.43
3:C:9:VAL:HG22	3:C:78:PHE:CZ	2.46	0.43
2:E:202:LYS:H	2:E:202:LYS:HG2	1.49	0.43
2:E:267:MET:HG3	2:E:268:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:886:LEU:HD12	2:E:887:SER:N	2.34	0.43
3:F:14:VAL:HB	3:F:16:LYS:HZ2	1.84	0.43
3:F:163:ARG:C	3:F:165:LEU:H	2.27	0.43
2:E:327:MET:HE3	2:E:327:MET:HB3	1.70	0.43
2:E:1375:PHE:O	2:E:1379:LYS:HG3	2.18	0.43
2:E:1432:LYS:HB3	2:E:1432:LYS:HE3	1.82	0.43
2:B:431:MET:HG2	2:B:625:LEU:HD23	2.00	0.43
3:C:49:LYS:HZ2	3:C:51:VAL:HG12	1.83	0.43
3:C:63:ASP:C	3:C:66:ARG:HH11	2.27	0.43
1:D:569:ARG:O	1:D:571:GLN:HG3	2.19	0.43
2:E:102:TRP:CZ2	2:E:118:GLN:HG3	2.54	0.43
2:E:910:LEU:HA	2:E:913:LEU:HD12	2.00	0.43
2:E:1063:THR:HA	2:E:1069:ARG:CD	2.47	0.43
2:E:1086:ARG:HA	2:E:1089:ASP:OD2	2.19	0.43
1:A:670:ASN:HB2	1:A:678:MET:HE1	2.01	0.43
2:B:151:LYS:HA	2:B:197:LYS:HZ3	1.83	0.43
2:B:222:TYR:HB3	2:B:405:LEU:HD11	2.01	0.43
2:B:302:ARG:HD3	2:B:322:PHE:CD1	2.53	0.43
2:B:545:ARG:HH11	2:B:546:ALA:HB3	1.81	0.43
2:B:683:MET:HE1	2:B:689:TYR:CD2	2.54	0.43
2:B:1105:MET:HA	2:B:1108:PRO:HG2	2.01	0.43
2:B:1495:PHE:CE1	2:B:1502:PHE:HD2	2.35	0.43
1:D:690:LEU:O	1:D:694:ILE:HG12	2.18	0.43
2:E:302:ARG:HD3	2:E:322:PHE:CD1	2.53	0.43
2:E:697:LEU:O	2:E:701:ILE:HG12	2.18	0.43
2:E:1634:GLU:OE2	2:E:1641:THR:HB	2.19	0.43
3:F:21:ILE:HD13	3:F:34:PRO:HA	2.01	0.43
3:F:63:ASP:C	3:F:66:ARG:HH11	2.27	0.43
2:B:194:ILE:O	2:B:198:ILE:HG23	2.19	0.42
2:B:456:ASP:H	2:B:618:ASP:CG	2.27	0.42
2:B:630:LYS:HG2	2:B:668:PHE:CZ	2.54	0.42
2:B:945:ARG:NH1	2:B:947:SER:H	2.16	0.42
2:B:955:ALA:HA	2:B:958:ILE:HG12	2.01	0.42
2:B:1086:ARG:HA	2:B:1089:ASP:OD2	2.19	0.42
2:B:1550:LEU:O	2:B:1551:LEU:C	2.62	0.42
1:D:570:ARG:O	1:D:570:ARG:NH1	2.51	0.42
1:D:694:ILE:HG13	1:D:695:LYS:N	2.34	0.42
2:E:113:LEU:HA	2:E:116:GLN:CD	2.44	0.42
2:E:143:GLU:HG3	2:E:147:LYS:HZ2	1.83	0.42
2:E:564:ASP:OD1	2:E:633:GLN:NE2	2.42	0.42
2:E:589:PRO:HD3	2:E:598:LYS:NZ	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1460:GLN:HG3	2:E:1493:TYR:O	2.18	0.42
2:E:1515:LEU:HD11	2:E:1575:TYR:HE2	1.84	0.42
2:B:113:LEU:HA	2:B:116:GLN:CD	2.44	0.42
2:B:156:ASN:HD22	2:B:161:LEU:HD12	1.83	0.42
2:B:306:MET:SD	2:B:536:SER:HA	2.59	0.42
2:B:656:LYS:N	2:B:656:LYS:HD2	2.35	0.42
2:B:737:LEU:HD12	2:B:737:LEU:HA	1.83	0.42
2:B:1135:GLU:HG3	2:B:1144:PHE:HA	2.01	0.42
2:B:1146:MET:SD	2:B:1146:MET:N	2.84	0.42
1:D:564:LYS:HE3	1:D:590:ASP:HA	2.01	0.42
1:D:609:PRO:HB2	1:D:612:ASP:OD1	2.19	0.42
2:E:258:TYR:HA	2:E:488:ALA:HB3	2.00	0.42
2:E:285:SER:N	2:E:288:ASP:OD2	2.44	0.42
2:E:306:MET:SD	2:E:536:SER:HA	2.59	0.42
2:E:443:ARG:O	2:E:628:SER:HA	2.19	0.42
2:E:1197:VAL:O	2:E:1201:LEU:HG	2.19	0.42
1:A:569:ARG:O	1:A:571:GLN:HG3	2.19	0.42
1:A:633:GLN:OE1	1:A:637:VAL:HG21	2.20	0.42
1:A:692:MET:O	1:A:696:LEU:HG	2.19	0.42
2:B:1153:THR:O	2:B:1156:ASP:HB3	2.19	0.42
2:B:1221:MET:HA	2:B:1224:THR:HG22	2.01	0.42
2:B:1567:GLU:HA	2:B:1571:PHE:HB2	2.00	0.42
1:D:692:MET:O	1:D:696:LEU:HG	2.19	0.42
2:E:248:PRO:HD2	2:E:293:ARG:HG3	1.99	0.42
2:E:302:ARG:HD3	2:E:322:PHE:HD1	1.84	0.42
2:E:465:ASN:HB2	2:E:534:ARG:HB2	2.01	0.42
2:B:222:TYR:CG	2:B:289:LEU:HD11	2.54	0.42
2:B:443:ARG:O	2:B:628:SER:HA	2.19	0.42
2:B:1044:ASN:OD1	2:B:1048:HIS:NE2	2.53	0.42
2:B:1314:TRP:CZ3	2:B:1357:ARG:HD3	2.55	0.42
2:B:1314:TRP:HZ3	2:B:1357:ARG:HH11	1.66	0.42
2:B:1463:ARG:HA	2:B:1487:THR:O	2.20	0.42
2:B:1515:LEU:HD11	2:B:1575:TYR:HE2	1.84	0.42
1:D:541:GLN:N	1:D:542:PRO:HD3	2.35	0.42
2:E:446:ILE:HG23	2:E:626:ILE:HG12	2.01	0.42
2:E:695:ASP:OD1	2:E:740:TYR:OH	2.37	0.42
2:E:795:PHE:CE2	2:E:839:LEU:HD13	2.55	0.42
2:E:1044:ASN:OD1	2:E:1048:HIS:NE2	2.53	0.42
2:E:1283:LEU:HD11	2:E:1291:TYR:HB2	2.00	0.42
2:E:1392:GLU:OE1	2:E:1392:GLU:N	2.50	0.42
2:B:143:GLU:HG3	2:B:147:LYS:HZ2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:746:ASP:CG	2:B:748:SER:HG	2.25	0.42
2:B:1110:LEU:O	2:B:1114:LEU:N	2.51	0.42
2:B:1617:PRO:O	2:B:1620:GLU:HG3	2.20	0.42
2:E:166:ARG:HA	2:E:166:ARG:HD2	1.85	0.42
2:E:1121:ARG:HG2	2:E:1125:ILE:HD11	2.00	0.42
2:E:1361:GLU:OE2	2:E:1388:TYR:HA	2.20	0.42
3:F:96:LYS:C	3:F:99:PRO:HD2	2.45	0.42
1:A:541:GLN:N	1:A:542:PRO:HD3	2.35	0.42
1:A:677:MET:CB	1:A:682:THR:HG21	2.49	0.42
2:B:573:LYS:HE3	2:B:616:THR:HG21	2.00	0.42
2:B:1611:LEU:HD13	2:B:1619:HIS:HB2	2.02	0.42
2:B:1611:LEU:HD11	2:B:1616:LYS:HA	2.00	0.42
1:D:677:MET:CB	1:D:682:THR:HG21	2.49	0.42
2:E:656:LYS:N	2:E:656:LYS:HD2	2.35	0.42
2:E:945:ARG:NH1	2:E:947:SER:H	2.16	0.42
1:A:617:VAL:HG23	1:A:622:CYS:SG	2.59	0.42
2:B:156:ASN:HA	2:B:161:LEU:HD12	2.02	0.42
2:B:355:THR:HG22	2:B:355:THR:O	2.20	0.42
2:B:1041:GLN:O	2:B:1043:TRP:N	2.52	0.42
2:B:1361:GLU:OE2	2:B:1388:TYR:HA	2.20	0.42
1:D:617:VAL:HG23	1:D:622:CYS:SG	2.59	0.42
1:D:633:GLN:OE1	1:D:637:VAL:HG21	2.20	0.42
2:E:222:TYR:CG	2:E:289:LEU:HD11	2.54	0.42
2:E:630:LYS:HG2	2:E:668:PHE:CZ	2.54	0.42
2:E:1372:PHE:CE2	2:E:1424:GLN:HB3	2.54	0.42
2:E:1532:CYS:SG	2:E:1550:LEU:HD12	2.60	0.42
2:E:1567:GLU:HA	2:E:1571:PHE:HB2	2.00	0.42
1:A:609:PRO:HB2	1:A:612:ASP:OD1	2.19	0.42
2:B:102:TRP:CZ2	2:B:118:GLN:HG3	2.54	0.42
2:B:446:ILE:HG23	2:B:626:ILE:HG12	2.01	0.42
2:B:1154:LYS:O	2:B:1155:LEU:C	2.61	0.42
2:B:1185:TYR:O	2:B:1188:SER:OG	2.24	0.42
3:C:87:PRO:HG2	3:C:134:LEU:HB3	2.01	0.42
2:E:456:ASP:H	2:E:618:ASP:CG	2.27	0.42
2:E:842:LYS:HB2	2:E:842:LYS:HE3	1.85	0.42
2:E:1276:LYS:HD2	2:E:1277:PRO:HD2	2.02	0.42
2:B:187:HIS:CD2	2:B:1009:MET:HG2	2.55	0.42
2:B:972:TYR:O	2:B:975:THR:N	2.47	0.42
2:B:1039:GLU:O	2:B:1040:LEU:HD23	2.19	0.42
2:B:1232:LYS:HB2	2:B:1240:TYR:CE2	2.55	0.42
2:B:1372:PHE:CE2	2:B:1424:GLN:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:563:ARG:HB2	1:D:655:ILE:O	2.20	0.42
2:E:185:LYS:HE2	2:E:185:LYS:HA	2.01	0.42
2:E:231:PHE:CE2	2:E:241:LEU:HD21	2.55	0.42
2:E:842:LYS:HA	2:E:845:GLN:HE21	1.84	0.42
2:E:932:LEU:H	2:E:935:ARG:HH21	1.64	0.42
2:E:1513:SER:N	2:E:1516:GLU:OE1	2.30	0.42
2:E:1613:GLU:CD	2:E:1614:GLN:HG3	2.45	0.42
2:B:80:VAL:HG22	2:B:85:LEU:HD11	2.01	0.42
2:B:465:ASN:HB2	2:B:534:ARG:HB2	2.01	0.42
2:B:679:ILE:HG22	2:B:680:MET:HE2	2.01	0.42
2:B:1432:LYS:HB3	2:B:1432:LYS:HE3	1.82	0.42
2:B:1532:CYS:SG	2:B:1550:LEU:HD12	2.60	0.42
2:B:1634:GLU:OE2	2:B:1641:THR:HB	2.19	0.42
3:C:21:ILE:HD13	3:C:34:PRO:HA	2.01	0.42
3:C:96:LYS:C	3:C:99:PRO:HD2	2.45	0.42
1:D:670:ASN:HB2	1:D:678:MET:HE1	2.01	0.42
2:E:44:TRP:CZ3	2:E:60:PRO:HG3	2.55	0.42
2:E:222:TYR:HD2	2:E:284:LEU:O	2.03	0.42
2:E:355:THR:HG22	2:E:355:THR:O	2.20	0.42
2:E:438:LEU:HD12	2:E:439:PRO:HD2	2.01	0.42
2:E:508:CYS:HB3	2:E:510:TYR:CE2	2.51	0.42
2:E:642:ASN:OD1	2:E:645:SER:OG	2.36	0.42
2:E:1039:GLU:O	2:E:1040:LEU:HD23	2.19	0.42
2:E:1046:TYR:HE2	2:E:1090:MET:HG2	1.85	0.42
2:E:1112:VAL:HA	2:E:1115:THR:HG23	2.02	0.42
2:E:1221:MET:HE2	2:E:1250:LEU:HB3	2.02	0.42
2:E:1280:PRO:HA	2:E:1283:LEU:HD23	2.02	0.42
2:E:1550:LEU:O	2:E:1551:LEU:C	2.62	0.42
2:E:1611:LEU:HD13	2:E:1619:HIS:HB2	2.02	0.42
2:B:44:TRP:CZ3	2:B:60:PRO:HG3	2.55	0.41
2:B:417:PHE:HB3	2:B:420:LEU:HB2	2.02	0.41
2:B:842:LYS:HA	2:B:845:GLN:HE21	1.84	0.41
2:B:1022:ASN:O	2:B:1026:GLU:OE1	2.38	0.41
2:B:1633:VAL:O	2:B:1639:VAL:N	2.50	0.41
3:C:6:CYS:HA	3:C:77:VAL:O	2.20	0.41
3:C:110:ILE:O	3:C:151:ALA:HB1	2.20	0.41
1:D:543:GLU:H	1:D:543:GLU:CD	2.25	0.41
1:D:551:GLN:CD	1:D:552:ARG:HH21	2.28	0.41
1:D:643:SER:OG	1:D:653:ASN:ND2	2.45	0.41
1:D:658:ASP:OD1	1:D:661:GLU:HG2	2.20	0.41
2:E:173:LEU:O	2:E:176:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:321:PRO:HB2	2:B:351:ILE:HD11	2.02	0.41
2:B:1108:PRO:HA	2:B:1111:GLU:OE2	2.20	0.41
2:B:1617:PRO:HA	2:B:1620:GLU:HG3	2.02	0.41
1:D:565:LEU:HD21	1:D:624:HIS:CE1	2.55	0.41
2:E:382:VAL:O	2:E:386:VAL:HG23	2.21	0.41
2:E:1110:LEU:O	2:E:1114:LEU:HD23	2.20	0.41
2:E:1314:TRP:CZ3	2:E:1357:ARG:HD3	2.55	0.41
2:B:196:GLU:O	2:B:199:GLN:NE2	2.54	0.41
2:B:222:TYR:HD2	2:B:284:LEU:O	2.03	0.41
2:B:378:PRO:HA	2:B:501:TYR:CE1	2.56	0.41
2:B:468:VAL:HG13	2:B:531:PHE:CE1	2.55	0.41
2:B:642:ASN:OD1	2:B:645:SER:OG	2.36	0.41
2:B:1136:PHE:HB2	2:B:1186:LEU:HD23	2.02	0.41
2:B:1221:MET:HE2	2:B:1250:LEU:HB3	2.02	0.41
2:E:3:ARG:HH22	2:E:42:GLU:CB	2.33	0.41
2:E:140:GLU:OE1	2:E:140:GLU:N	2.54	0.41
2:E:771:ARG:O	2:E:775:LEU:HG	2.20	0.41
2:E:959:ALA:O	2:E:963:GLN:HG3	2.20	0.41
2:E:1095:GLY:HA3	2:E:1096:PRO:HD3	1.93	0.41
2:E:1153:THR:O	2:E:1156:ASP:HB3	2.19	0.41
2:E:1232:LYS:HB2	2:E:1240:TYR:CE2	2.55	0.41
3:F:129:LEU:O	3:F:134:LEU:N	2.45	0.41
1:A:569:ARG:HD3	1:A:569:ARG:H	1.85	0.41
2:B:130:GLN:NE2	2:B:144:LEU:HD11	2.35	0.41
2:B:231:PHE:CE2	2:B:241:LEU:HD21	2.55	0.41
2:B:959:ALA:O	2:B:963:GLN:HG3	2.20	0.41
2:B:1306:SER:O	2:B:1310:LYS:HG2	2.21	0.41
2:B:1470:LYS:HD3	2:B:1483:TRP:CG	2.55	0.41
1:D:700:ASP:CB	2:E:32:GLY:HA2	2.46	0.41
2:E:772:VAL:HA	2:E:775:LEU:HD12	2.03	0.41
2:E:955:ALA:HA	2:E:958:ILE:HG12	2.01	0.41
2:E:1041:GLN:O	2:E:1043:TRP:N	2.52	0.41
2:E:1043:TRP:N	2:E:1043:TRP:CE3	2.86	0.41
2:E:1463:ARG:HA	2:E:1487:THR:O	2.20	0.41
2:E:1470:LYS:HD3	2:E:1483:TRP:CG	2.55	0.41
2:B:140:GLU:N	2:B:140:GLU:OE1	2.54	0.41
2:B:255:SER:HA	2:B:430:LYS:HA	2.02	0.41
2:B:932:LEU:H	2:B:935:ARG:HH21	1.64	0.41
2:B:1200:LEU:O	2:B:1204:LEU:HD23	2.21	0.41
2:E:945:ARG:HH11	2:E:946:GLN:N	2.19	0.41
2:E:1066:GLN:OE1	2:E:1069:ARG:NH1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1200:LEU:O	2:E:1204:LEU:HD23	2.21	0.41
2:E:1515:LEU:O	2:E:1519:ILE:HG13	2.21	0.41
2:E:1617:PRO:O	2:E:1620:GLU:HG3	2.20	0.41
3:F:110:ILE:O	3:F:151:ALA:HB1	2.20	0.41
2:B:146:LYS:HB2	2:B:146:LYS:HE2	1.82	0.41
2:B:1154:LYS:O	2:B:1157:GLN:N	2.54	0.41
2:B:1399:LEU:HD13	2:B:1405:ALA:HB1	2.02	0.41
1:D:530:SER:O	1:D:534:LEU:N	2.37	0.41
1:D:569:ARG:H	1:D:569:ARG:HD3	1.85	0.41
2:E:13:GLY:HA3	2:E:35:VAL:HG22	2.02	0.41
2:E:187:HIS:CD2	2:E:1009:MET:HG2	2.55	0.41
2:E:196:GLU:O	2:E:199:GLN:NE2	2.54	0.41
2:E:321:PRO:HB2	2:E:351:ILE:HD11	2.02	0.41
2:E:564:ASP:OD1	2:E:626:ILE:HB	2.21	0.41
2:E:1105:MET:HA	2:E:1108:PRO:HG2	2.01	0.41
2:E:1236:ARG:HA	2:E:1236:ARG:HD3	1.76	0.41
2:E:1440:SER:C	2:E:1441:TYR:HD1	2.29	0.41
2:B:1110:LEU:O	2:B:1114:LEU:HD23	2.21	0.41
3:C:7:VAL:HB	3:C:78:PHE:HD2	1.86	0.41
2:E:194:ILE:O	2:E:198:ILE:HG23	2.19	0.41
2:E:255:SER:HA	2:E:430:LYS:HA	2.03	0.41
2:E:378:PRO:HA	2:E:501:TYR:CE1	2.56	0.41
2:E:1135:GLU:HG3	2:E:1144:PHE:HA	2.01	0.41
2:E:1306:SER:O	2:E:1310:LYS:HG2	2.21	0.41
2:B:98:TRP:HH2	2:B:155:GLY:CA	2.28	0.41
2:B:99:ALA:O	2:B:103:ARG:HG2	2.21	0.41
2:B:663:GLY:O	2:B:666:VAL:HG12	2.20	0.41
2:B:795:PHE:CE2	2:B:839:LEU:HD13	2.55	0.41
2:B:1046:TYR:HE2	2:B:1090:MET:HG2	1.85	0.41
2:B:1276:LYS:HD2	2:B:1277:PRO:HD2	2.02	0.41
2:B:1280:PRO:HA	2:B:1283:LEU:HD23	2.02	0.41
2:B:1499:LEU:HD23	2:B:1499:LEU:HA	1.88	0.41
2:E:417:PHE:HB3	2:E:420:LEU:HB2	2.02	0.41
2:E:640:LEU:CD1	2:E:657:LEU:HD11	2.51	0.41
2:E:1068:LYS:HB2	2:E:1068:LYS:HE3	1.87	0.41
2:E:1108:PRO:HA	2:E:1111:GLU:OE2	2.20	0.41
1:A:551:GLN:CD	1:A:552:ARG:HH21	2.28	0.41
1:A:563:ARG:HB2	1:A:655:ILE:O	2.20	0.41
1:A:564:LYS:O	1:A:573:LYS:NZ	2.29	0.41
1:A:567:ALA:HB3	1:A:573:LYS:HD3	2.03	0.41
2:B:1:MET:HE1	2:B:44:TRP:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:VAL:C	2:B:171:ASN:HD22	2.21	0.41
2:B:222:TYR:CD1	2:B:289:LEU:HD11	2.55	0.41
2:B:382:VAL:O	2:B:386:VAL:HG23	2.21	0.41
2:B:561:THR:HG22	2:B:632:THR:O	2.21	0.41
2:B:564:ASP:OD1	2:B:626:ILE:HB	2.21	0.41
2:B:945:ARG:HH11	2:B:946:GLN:N	2.19	0.41
2:B:1033:MET:C	2:B:1035:GLN:N	2.79	0.41
2:B:1546:PRO:HA	2:B:1549:MET:HB2	2.03	0.41
2:B:1613:GLU:CD	2:B:1614:GLN:HG3	2.45	0.41
2:B:1629:LEU:O	2:B:1633:VAL:HG22	2.21	0.41
3:C:1:MET:HE2	3:C:43:ASN:HD21	1.86	0.41
2:E:144:LEU:O	2:E:148:VAL:HG22	2.21	0.41
2:E:222:TYR:CD1	2:E:289:LEU:HD11	2.55	0.41
2:E:468:VAL:HG13	2:E:531:PHE:CE1	2.55	0.41
2:E:663:GLY:O	2:E:666:VAL:HG12	2.20	0.41
2:E:752:LEU:HD23	2:E:752:LEU:HA	1.95	0.41
2:E:841:CYS:O	2:E:845:GLN:HG3	2.21	0.41
2:E:853:VAL:O	2:E:856:LYS:HG2	2.21	0.41
2:E:875:ARG:NH1	2:E:921:THR:HB	2.36	0.41
2:E:1033:MET:C	2:E:1035:GLN:N	2.79	0.41
2:E:1051:VAL:O	2:E:1055:THR:OG1	2.30	0.41
2:E:1075:LYS:HB3	2:E:1075:LYS:HE3	1.64	0.41
2:E:1136:PHE:HB2	2:E:1186:LEU:HD23	2.02	0.41
2:E:1154:LYS:O	2:E:1157:GLN:N	2.54	0.41
2:E:1546:PRO:HA	2:E:1549:MET:HB2	2.03	0.41
2:E:1629:LEU:O	2:E:1633:VAL:HG22	2.21	0.41
3:F:7:VAL:HB	3:F:78:PHE:HD2	1.86	0.41
3:F:69:PRO:HB3	3:F:104:HIS:CD2	2.56	0.41
3:F:121:ASP:HA	3:F:126:ILE:HD11	2.03	0.41
3:F:139:TYR:O	3:F:142:GLY:N	2.54	0.41
1:A:564:LYS:HE3	1:A:590:ASP:CG	2.46	0.41
1:A:565:LEU:HD21	1:A:624:HIS:CE1	2.55	0.41
2:B:145:LYS:O	2:B:149:THR:OG1	2.25	0.41
2:B:640:LEU:CD1	2:B:657:LEU:HD11	2.51	0.41
2:B:764:PHE:HA	2:B:767:ILE:HB	2.03	0.41
2:B:841:CYS:O	2:B:845:GLN:HG3	2.21	0.41
2:B:875:ARG:NH1	2:B:921:THR:HB	2.36	0.41
2:B:1125:ILE:HD12	2:B:1125:ILE:H	1.85	0.41
2:B:1536:HIS:CG	2:B:1542:LEU:HD22	2.55	0.41
2:B:1565:ASN:O	2:B:1568:LYS:HG3	2.21	0.41
3:C:42:ALA:O	3:C:53:LEU:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:594:SER:HB2	1:D:596:GLN:NE2	2.36	0.41
2:E:62:THR:HG23	2:E:63:TYR:HD1	1.86	0.41
2:E:87:LEU:O	2:E:90:GLU:HG3	2.21	0.41
2:E:130:GLN:NE2	2:E:144:LEU:HD11	2.35	0.41
2:E:189:VAL:O	2:E:193:ARG:HG2	2.21	0.41
2:E:746:ASP:OD2	2:E:748:SER:OG	2.31	0.41
2:E:806:LEU:HD12	2:E:813:LYS:HE3	2.02	0.41
2:E:943:MET:HG3	2:E:943:MET:O	2.21	0.41
2:E:1022:ASN:O	2:E:1026:GLU:OE1	2.38	0.41
2:E:1125:ILE:HD12	2:E:1125:ILE:H	1.85	0.41
2:E:1618:LEU:HD13	2:E:1621:ARG:HH21	1.86	0.41
3:F:161:THR:HB	3:F:163:ARG:HG3	2.02	0.41
1:A:564:LYS:HE3	1:A:590:ASP:HA	2.01	0.40
1:A:660:HIS:CG	1:A:661:GLU:N	2.89	0.40
2:B:3:ARG:HH22	2:B:42:GLU:CB	2.33	0.40
2:B:806:LEU:HD12	2:B:813:LYS:HE3	2.02	0.40
2:B:877:VAL:C	2:B:880:PRO:HD2	2.46	0.40
2:B:1112:VAL:HA	2:B:1115:THR:HG23	2.02	0.40
2:B:1236:ARG:HA	2:B:1236:ARG:HD3	1.76	0.40
3:C:171:GLU:HA	3:C:174:ARG:HG2	2.03	0.40
1:D:544:ILE:CD1	1:D:689:LEU:HB2	2.51	0.40
1:D:564:LYS:HE3	1:D:590:ASP:CG	2.46	0.40
1:D:567:ALA:HB3	1:D:573:LYS:HD3	2.03	0.40
2:E:80:VAL:HG22	2:E:85:LEU:HD11	2.01	0.40
2:E:1301:TYR:O	2:E:1305:ILE:HG12	2.21	0.40
3:F:33:ILE:HD13	3:F:33:ILE:HA	1.89	0.40
1:A:544:ILE:CD1	1:A:689:LEU:HB2	2.51	0.40
1:A:658:ASP:OD1	1:A:661:GLU:HG2	2.20	0.40
2:B:116:GLN:HA	2:B:119:GLN:HG3	2.03	0.40
2:B:173:LEU:O	2:B:176:ASP:HB2	2.20	0.40
2:B:1234:LYS:N	2:B:1234:LYS:HD2	2.37	0.40
2:B:1618:LEU:HD13	2:B:1621:ARG:HH21	1.86	0.40
1:D:658:ASP:OD1	1:D:660:HIS:ND1	2.49	0.40
1:D:678:MET:HA	1:D:683:ARG:HH12	1.87	0.40
2:E:25:VAL:HB	2:E:56:LYS:O	2.21	0.40
2:E:394:HIS:HD2	2:E:396:GLY:H	1.70	0.40
2:E:877:VAL:C	2:E:880:PRO:HD2	2.46	0.40
2:E:1368:TYR:N	2:E:1425:TYR:O	2.49	0.40
1:A:594:SER:HB2	1:A:596:GLN:NE2	2.36	0.40
1:A:641:ALA:O	1:A:662:TYR:OH	2.27	0.40
2:B:18:ASN:HA	2:B:29:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:TRP:CZ2	2:B:266:GLY:HA2	2.56	0.40
2:B:435:GLU:O	2:B:708:LYS:HD3	2.21	0.40
2:B:697:LEU:HA	2:B:700:ILE:HD12	2.03	0.40
2:B:821:PRO:HA	2:B:824:ILE:HG23	2.04	0.40
2:B:853:VAL:O	2:B:856:LYS:HG2	2.21	0.40
2:B:866:SER:C	2:B:868:LEU:N	2.79	0.40
2:B:874:CYS:HA	2:B:877:VAL:HG22	2.03	0.40
2:B:1280:PRO:HA	2:B:1283:LEU:HB2	2.03	0.40
3:C:129:LEU:O	3:C:133:LYS:N	2.54	0.40
2:E:18:ASN:HA	2:E:29:LEU:O	2.21	0.40
2:E:147:LYS:O	2:E:151:LYS:HG2	2.21	0.40
2:E:156:ASN:HA	2:E:161:LEU:HD12	2.02	0.40
2:E:1168:TYR:CZ	2:E:1172:LEU:HD11	2.56	0.40
2:E:1305:ILE:HD11	2:E:1320:LEU:HB2	2.02	0.40
2:E:1399:LEU:HD13	2:E:1405:ALA:HB1	2.02	0.40
2:B:189:VAL:O	2:B:193:ARG:HG2	2.21	0.40
2:B:288:ASP:CG	2:B:291:ARG:HH21	2.27	0.40
2:B:636:ASP:OD2	2:B:656:LYS:HB3	2.21	0.40
2:B:761:LYS:HE2	2:B:765:ARG:NE	2.37	0.40
2:B:1066:GLN:CD	2:B:1069:ARG:HH12	2.29	0.40
2:B:1168:TYR:CZ	2:B:1172:LEU:HD11	2.56	0.40
2:B:1305:ILE:HD11	2:B:1320:LEU:HB2	2.02	0.40
2:B:1522:MET:HB3	2:B:1592:LEU:HD23	2.04	0.40
2:E:4:TRP:HZ3	2:E:45:TYR:HA	1.87	0.40
2:E:802:MET:HE1	2:E:846:SER:C	2.46	0.40
2:E:1040:LEU:HD22	2:E:1043:TRP:CH2	2.56	0.40
3:F:6:CYS:HA	3:F:77:VAL:O	2.20	0.40
1:A:564:LYS:H	1:A:573:LYS:HD2	1.86	0.40
2:B:13:GLY:HA3	2:B:35:VAL:HG22	2.02	0.40
2:B:87:LEU:O	2:B:90:GLU:HG3	2.21	0.40
2:B:771:ARG:O	2:B:775:LEU:HG	2.20	0.40
2:B:772:VAL:HA	2:B:775:LEU:HD12	2.03	0.40
2:B:1040:LEU:HD22	2:B:1043:TRP:CH2	2.56	0.40
2:B:1154:LYS:HA	2:B:1157:GLN:OE1	2.21	0.40
3:C:10:GLY:HA3	3:C:16:LYS:HE3	2.04	0.40
3:C:24:THR:HG22	3:C:42:ALA:HB2	2.04	0.40
3:C:139:TYR:O	3:C:142:GLY:N	2.54	0.40
2:E:262:TRP:CZ2	2:E:266:GLY:HA2	2.56	0.40
2:E:561:THR:HG22	2:E:632:THR:O	2.21	0.40
2:E:939:THR:O	2:E:943:MET:N	2.30	0.40
2:E:1465:SER:HA	2:E:1486:ARG:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1523:GLU:O	2:E:1524:LEU:C	2.65	0.40
2:E:1633:VAL:O	2:E:1639:VAL:HG22	2.22	0.40
3:F:100:GLU:O	3:F:104:HIS:ND1	2.48	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	196/733 (27%)	180 (92%)	16 (8%)	0	100	100
1	D	196/733 (27%)	180 (92%)	16 (8%)	0	100	100
2	B	1640/1648 (100%)	1530 (93%)	110 (7%)	0	100	100
2	E	1640/1648 (100%)	1529 (93%)	111 (7%)	0	100	100
3	C	175/184 (95%)	165 (94%)	10 (6%)	0	100	100
3	F	175/184 (95%)	165 (94%)	10 (6%)	0	100	100
All	All	4022/5130 (78%)	3749 (93%)	273 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	183/664 (28%)	183 (100%)	0	100	100
1	D	183/664 (28%)	183 (100%)	0	100	100
2	B	1495/1497 (100%)	1495 (100%)	0	100	100
2	E	1495/1497 (100%)	1495 (100%)	0	100	100
3	C	153/157 (98%)	153 (100%)	0	100	100
3	F	153/157 (98%)	153 (100%)	0	100	100
All	All	3662/4636 (79%)	3662 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	550	GLN
1	A	554	ASN
1	A	624	HIS
2	B	51	GLN
2	B	108	ASN
2	B	118	GLN
2	B	119	GLN
2	B	414	GLN
2	B	444	ASN
2	B	653	ASN
2	B	723	HIS
2	B	738	ASN
2	B	885	GLN
2	B	926	GLN
2	B	1014	ASN
2	B	1143	ASN
2	B	1401	GLN
2	B	1517	ASN
2	B	1619	HIS
3	C	2	GLN
1	D	550	GLN
1	D	554	ASN
1	D	624	HIS
2	E	20	ASN
2	E	51	GLN
2	E	118	GLN
2	E	119	GLN
2	E	130	GLN

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Mol	Chain	Res	Type
2	E	414	GLN
2	E	444	ASN
2	E	653	ASN
2	E	723	HIS
2	E	738	ASN
2	E	885	GLN
2	E	926	GLN
2	E	1014	ASN
2	E	1143	ASN
2	E	1401	GLN
2	E	1517	ASN
2	E	1577	GLN
2	E	1614	GLN
2	E	1619	HIS
3	F	2	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](#)

There are no ligands in this entry.

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.

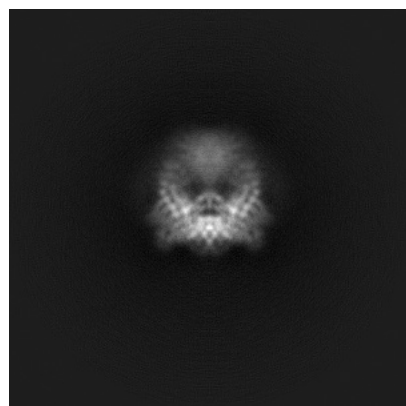
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60147. These allow visual inspection of the internal detail of the map and identification of artifacts.

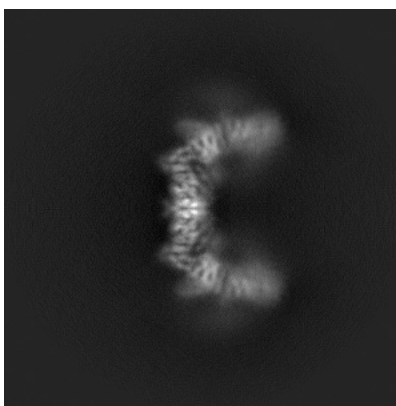
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

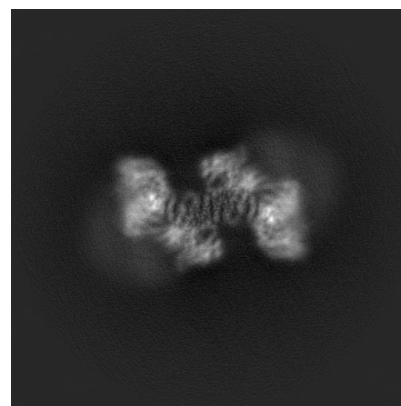
6.1.1 Primary map



X

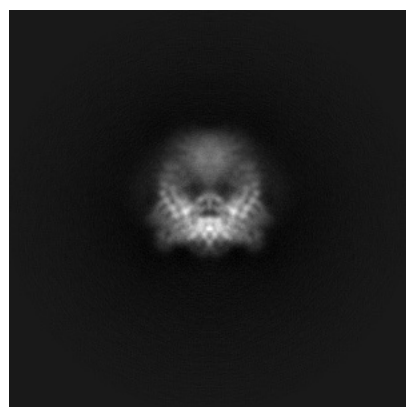


Y

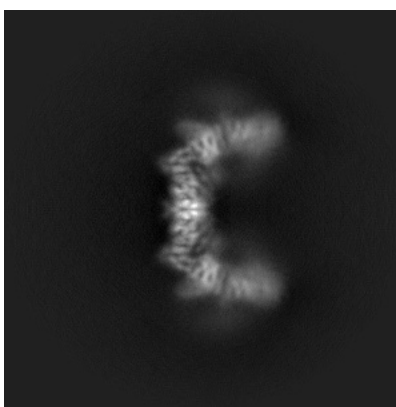


Z

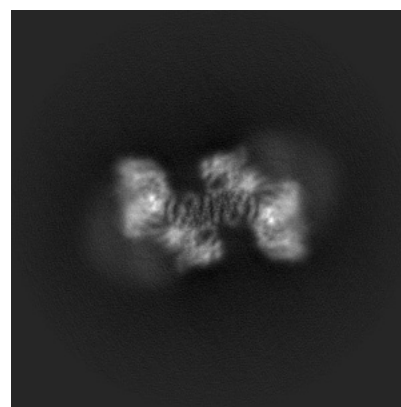
6.1.2 Raw map



X



Y

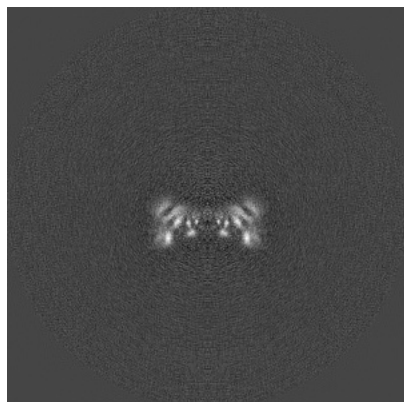


Z

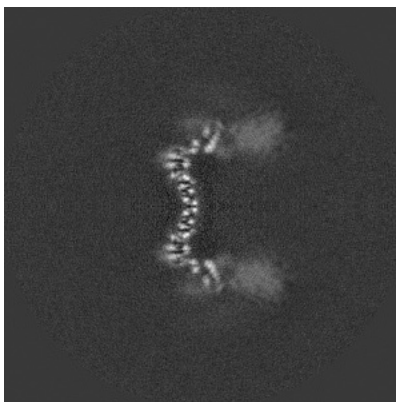
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

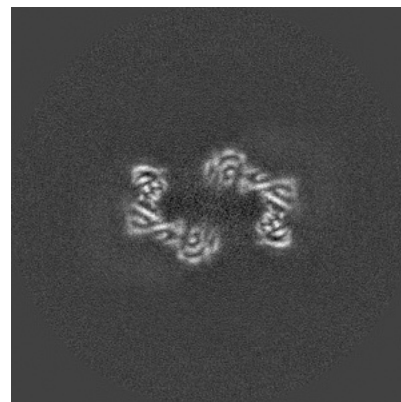
6.2.1 Primary map



X Index: 170

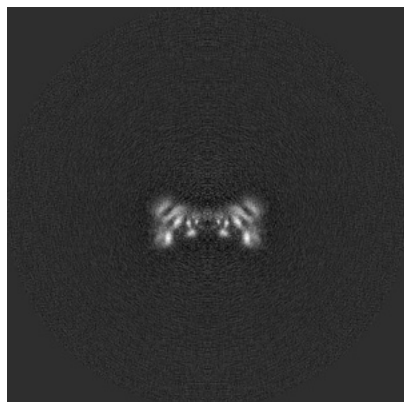


Y Index: 170

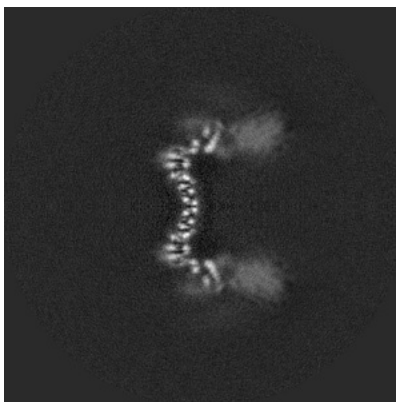


Z Index: 170

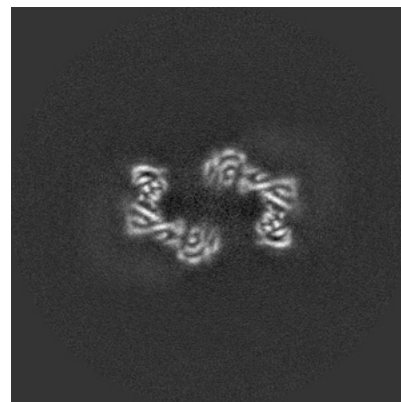
6.2.2 Raw map



X Index: 170



Y Index: 170

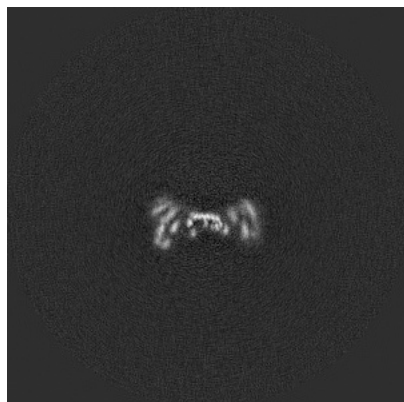


Z Index: 170

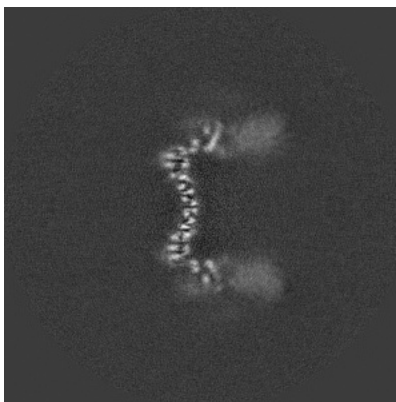
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

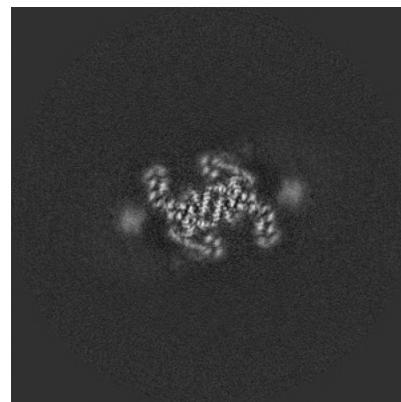
6.3.1 Primary map



X Index: 167

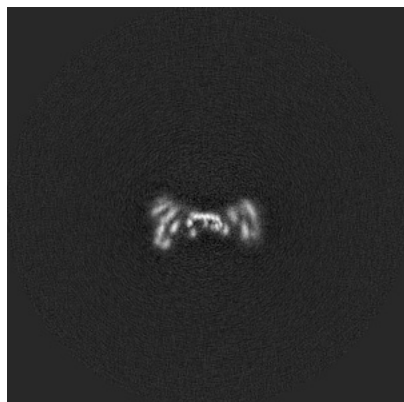


Y Index: 169

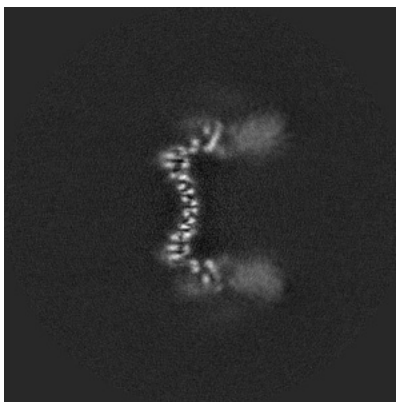


Z Index: 154

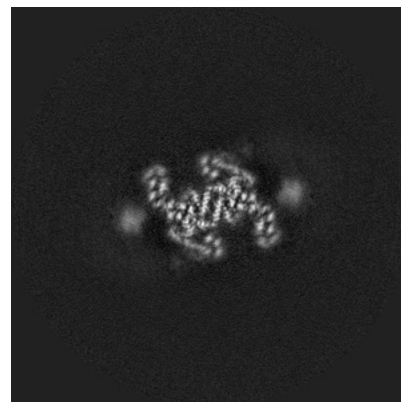
6.3.2 Raw map



X Index: 167



Y Index: 169

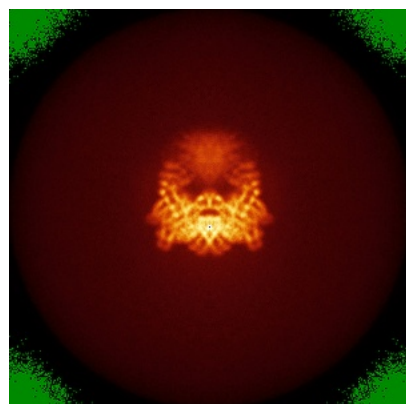


Z Index: 154

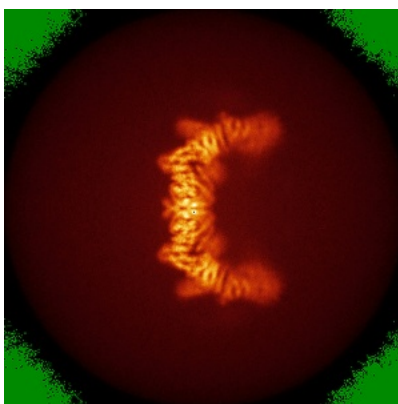
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y



Z

6.4.2 Raw map



X



Y

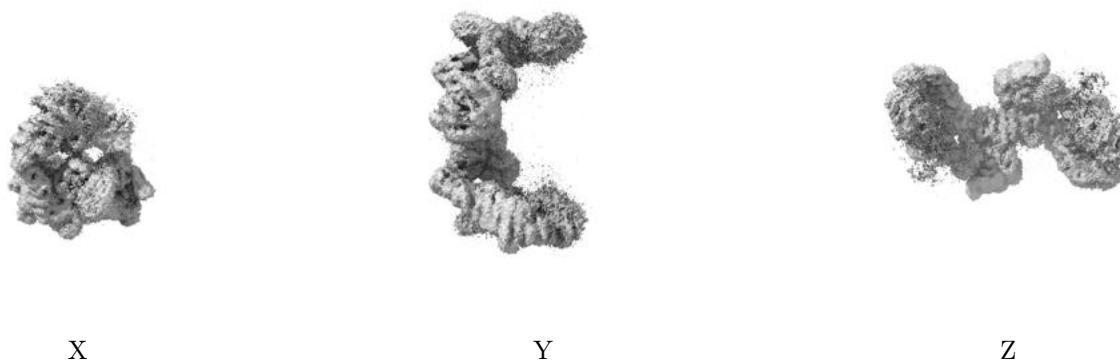


Z

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.

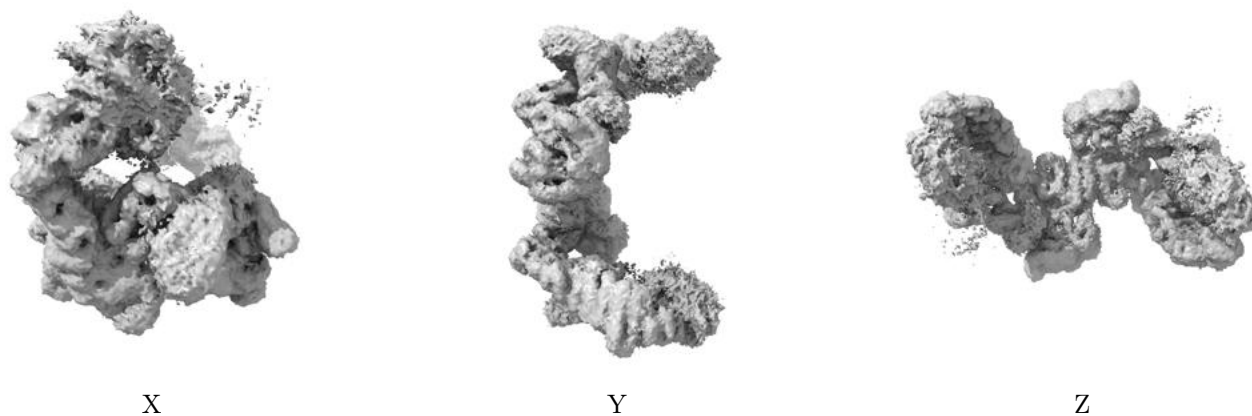
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

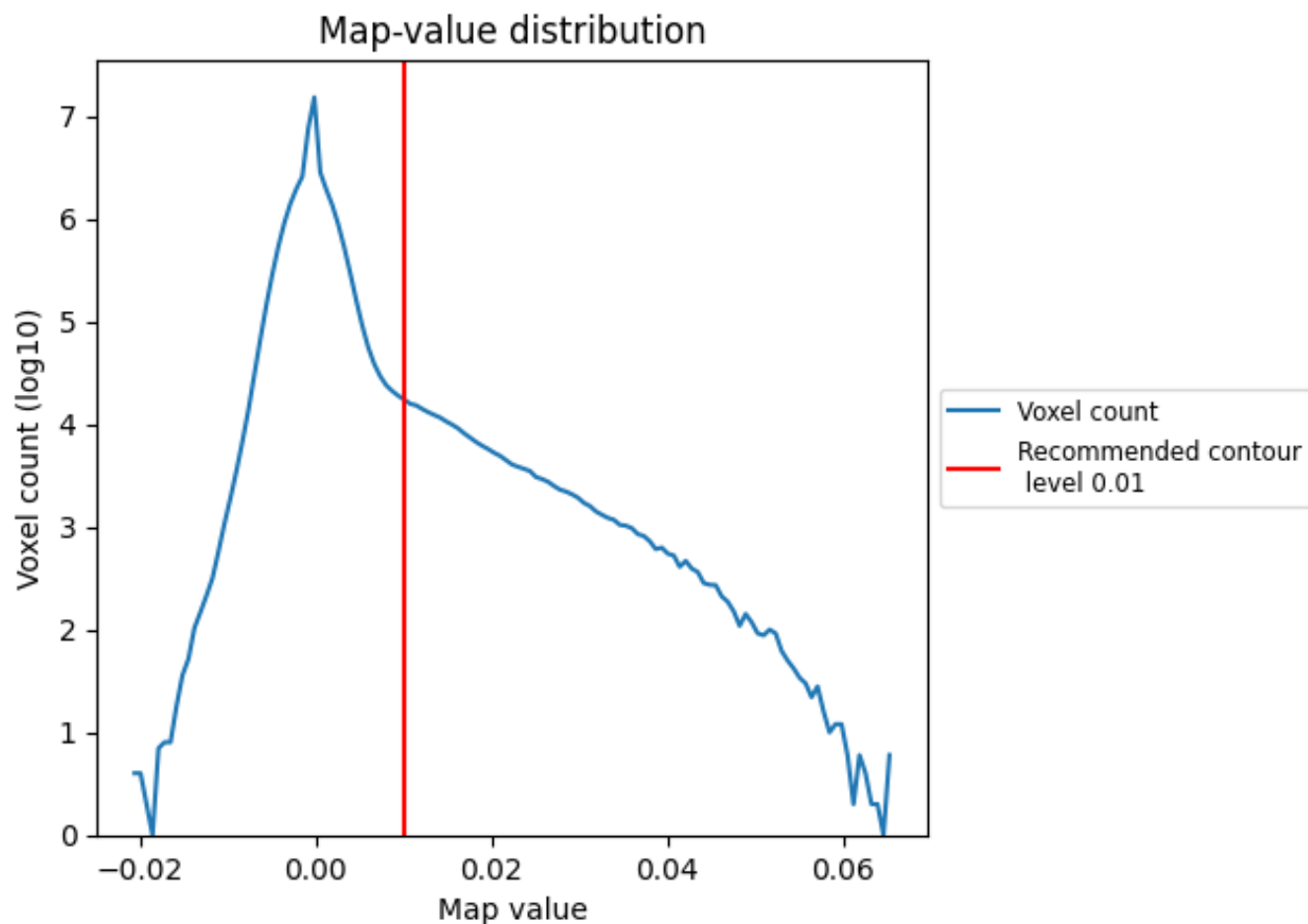
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

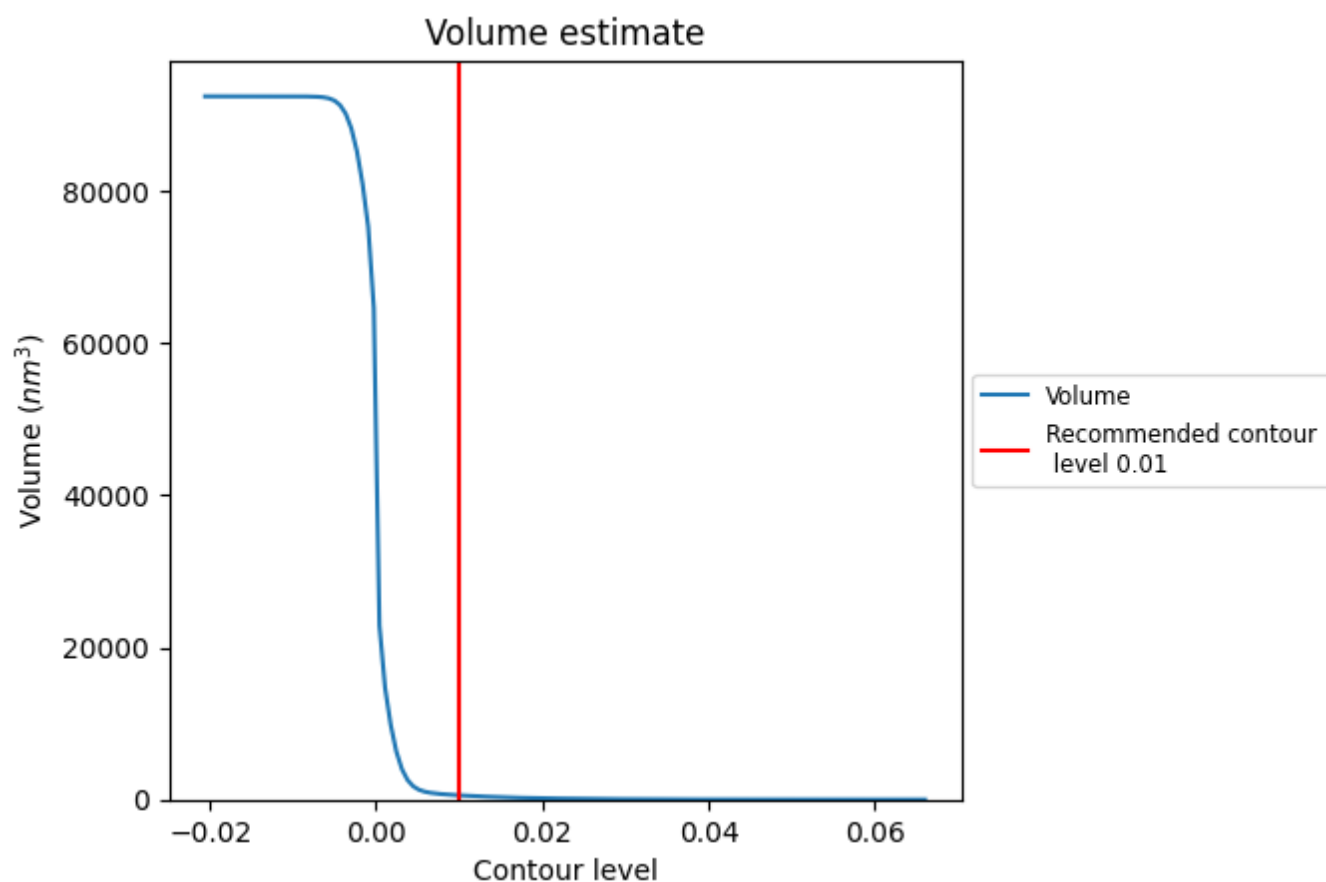
This section contains the results of statistical analysis of the map.

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.

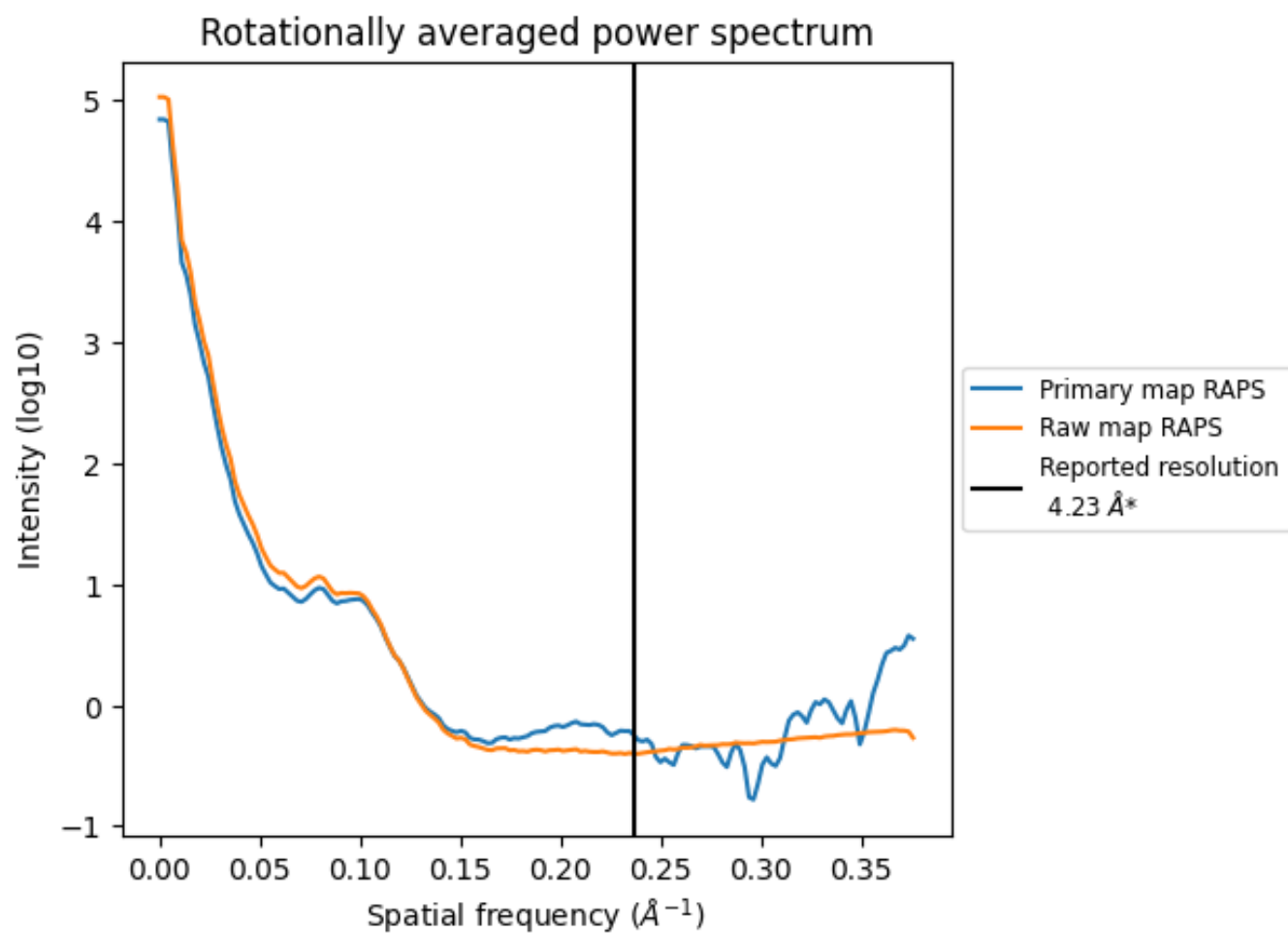
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 555 nm^3 ; this corresponds to an approximate mass of 502 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 ⓘ

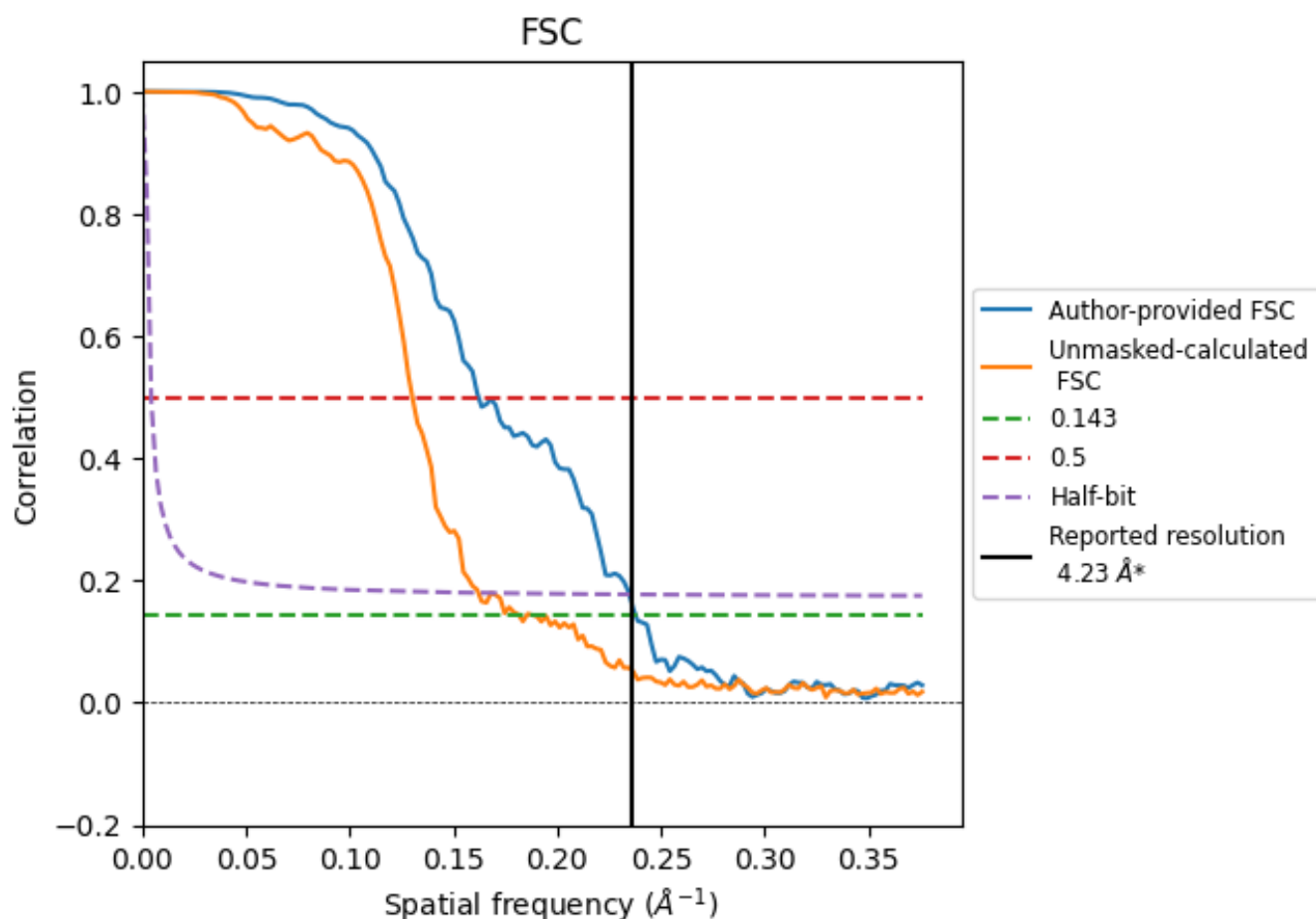


*Reported resolution corresponds to spatial frequency of 0.236 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.236 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

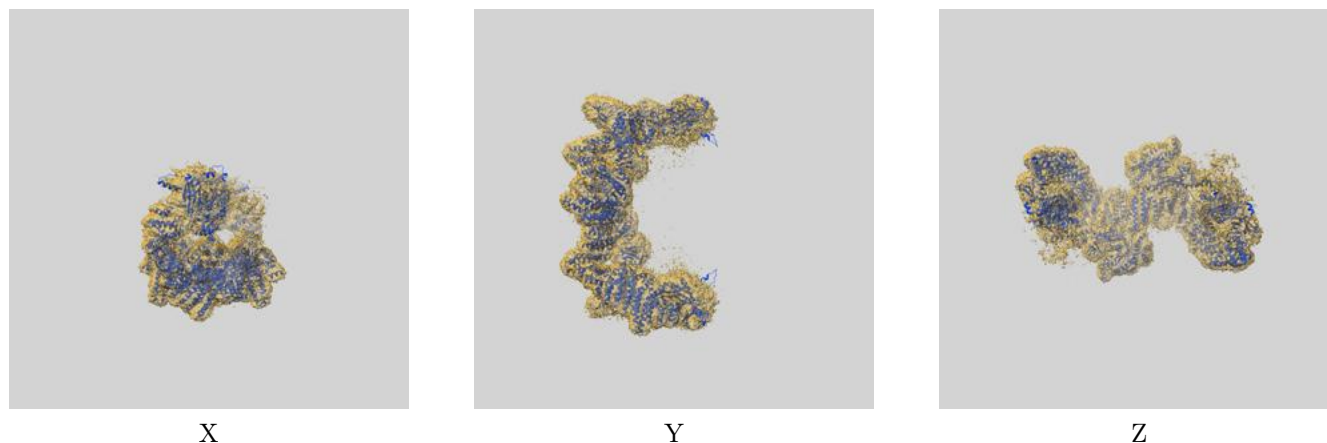
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.23	-	-
Author-provided FSC curve	4.21	6.17	4.26
Unmasked-calculated*	5.51	7.68	6.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.51 differs from the reported value 4.23 by more than 10 %

9 Map-model fit [i](#)

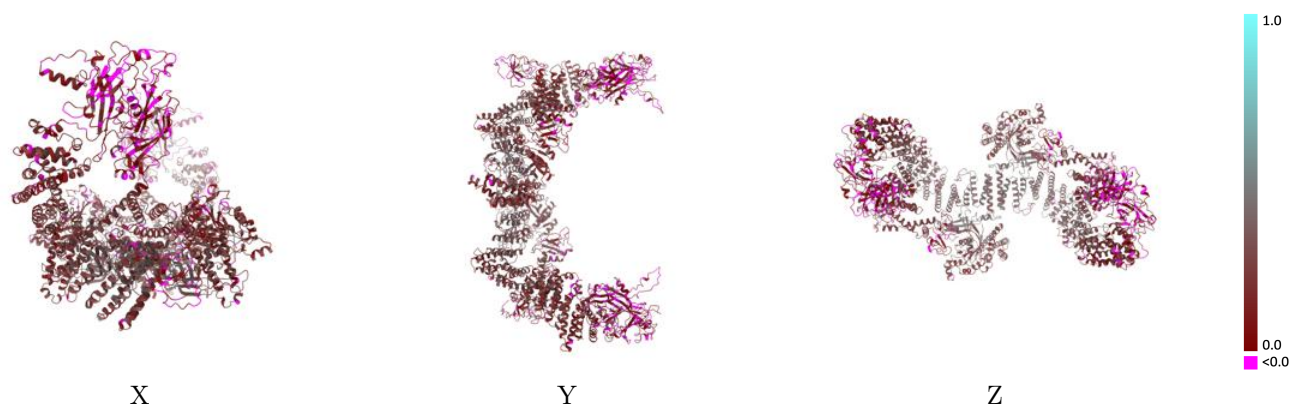
This section contains information regarding the fit between EMDB map EMD-60147 and PDB model 8ZJJ. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



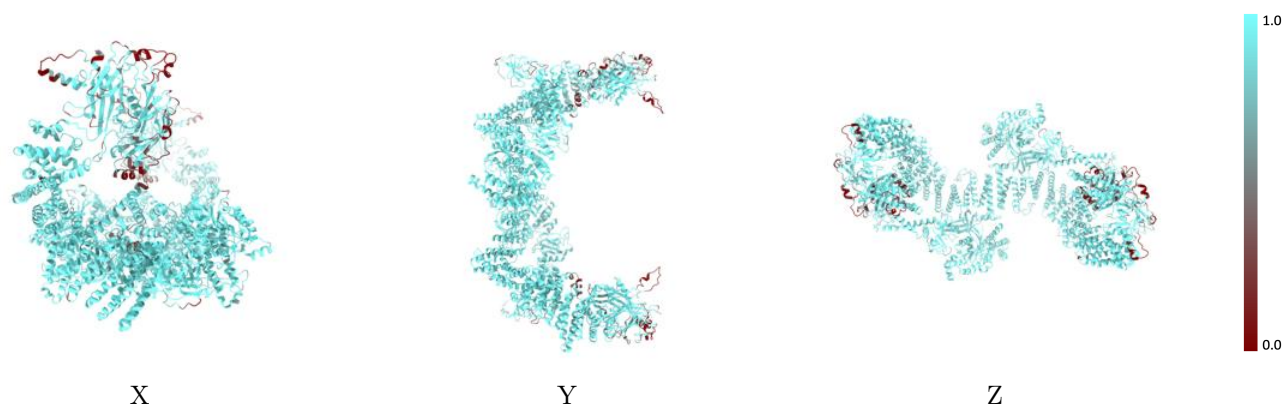
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



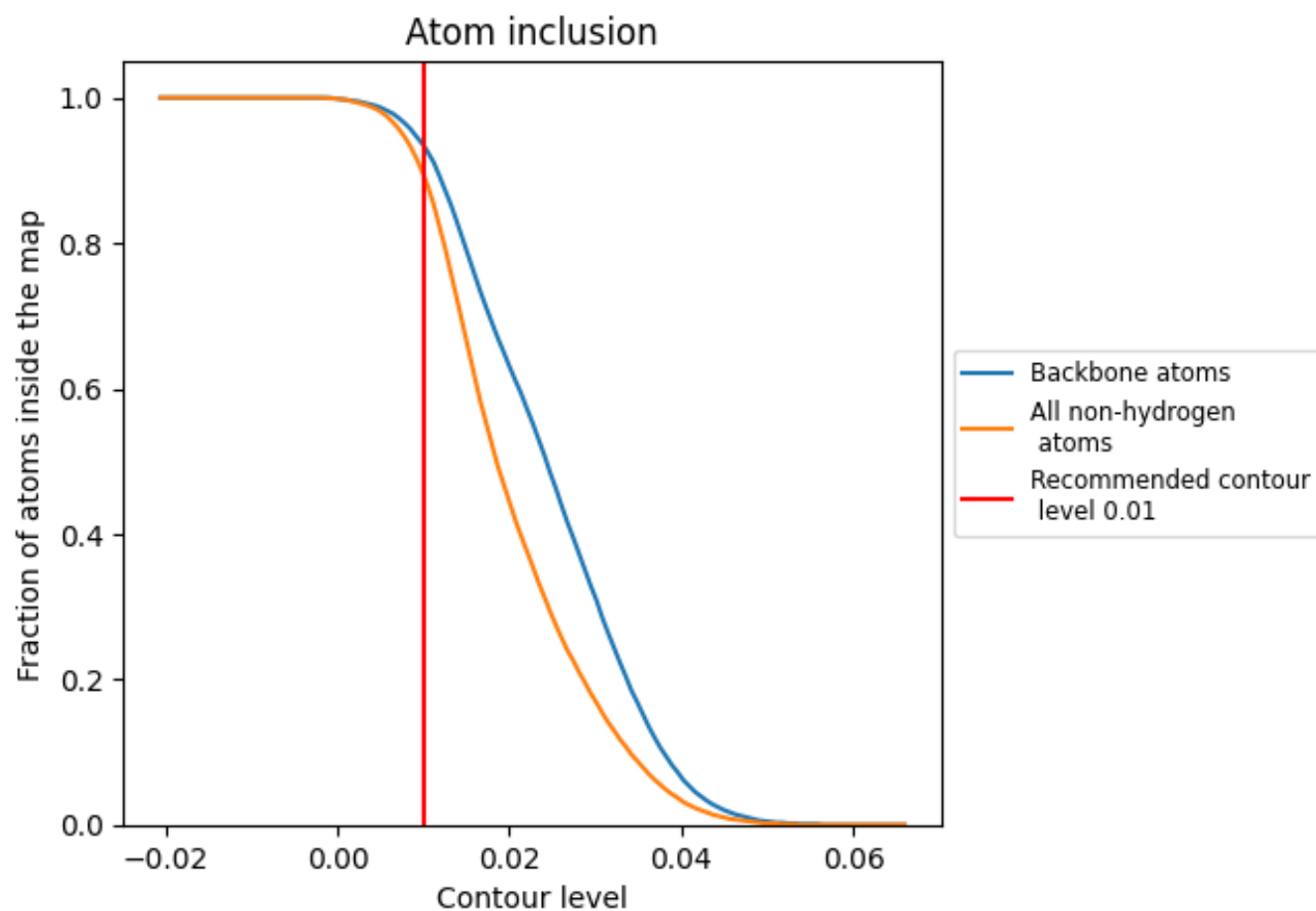
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8950	0.2110
A	0.9390	0.1680
B	0.8870	0.2120
C	0.9630	0.2610
D	0.9160	0.1650
E	0.8810	0.2100
F	0.9640	0.2600

1.0

0.0

<0.0