



Full wwPDB EM Validation Report ⓘ

Nov 26, 2022 – 07:50 PM EST

PDB ID : 7SZK
EMDB ID : EMD-25571
Title : Cryo-EM structure of 27a bound to E. coli RNAP and rrnBP1 promoter complex
Authors : Shin, Y.; Murakami, K.S.
Deposited on : 2021-11-28
Resolution : 2.94 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

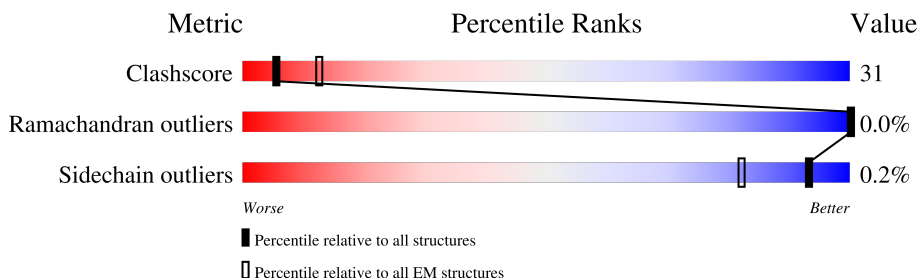
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.94 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	
1	B	329	
2	C	1342	
3	D	1407	
4	E	91	
5	F	613	
6	X	64	
7	Y	64	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	D9X	C	3001	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 29840 atoms, of which 81 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	231	Total	C	N	O	S	0	0
			1794	1117	318	353	6		
1	B	230	Total	C	N	O	S	0	0
			1786	1112	317	351	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0
			10570	6631	1841	2055	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1340	Total	C	N	O	S	0	0
			10382	6522	1849	1962	49		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	76	Total	C	N	O	S	0	0
			605	368	115	121	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	466	Total	C	N	O	S	0	0
			3799	2384	679	713	23		

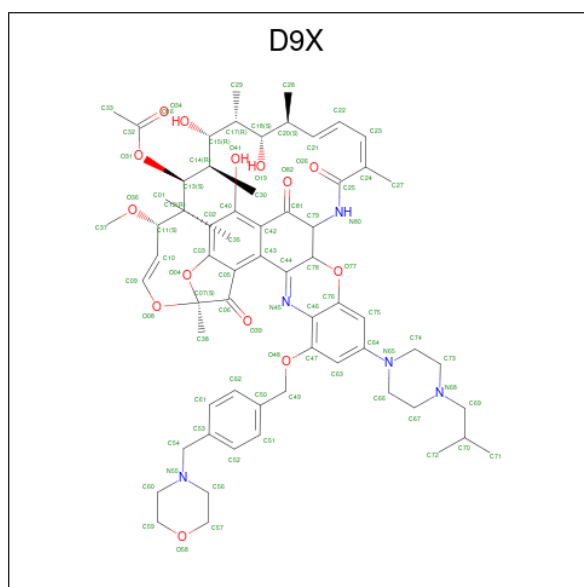
- Molecule 6 is a DNA chain called DNA (5'-D(P*CP*TP*CP*GP*TP*AP*GP*AP*GP*TP*CP*CP*GP*TP*GP*TP*CP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	18	Total	C	N	O	P	0	0
			370	175	71	106	18		

- Molecule 7 is a DNA chain called DNA (5'-D(P*CP*TP*CP*GP*TP*AP*GP*AP*GP*TP*CP*CP*GP*TP*GP*TP*CP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	18	Total	C	N	O	P	0	0
			368	175	65	110	18		

- Molecule 8 is (2S,7R,7aR,13aP,16Z,18E,20S,21S,22R,23R,24R,25S,26R,27S,28E)-5,21,23-trihydroxy-27-methoxy-2,4,16,20,22,24,26-heptamethyl-10-[4-(2-methylpropyl)piperazin-1-yl]-12-({4-[(morpholin-4-yl)methyl]phenyl}methoxy)-1,6,15-trioxo-1,2,7,7a-tetrahydro-6H-2,7-(epoxypentadeca[1,11,13]trienoimino)[1]benzofuro[4,5-a]phenoxazin-25-yl acetate (three-letter code: D9X) (formula: C₆₃H₈₁N₅O₁₄).



Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total	C	H	N	O	0
			163	63	81	5	14	

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	D	1	Total	Mg	0
			1	1	

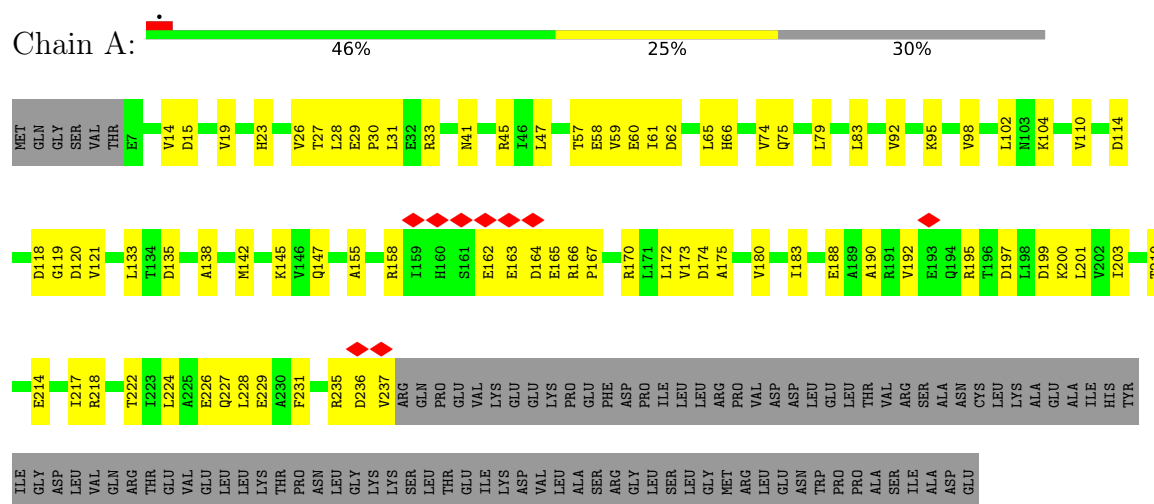
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Zn	0
			2	2	

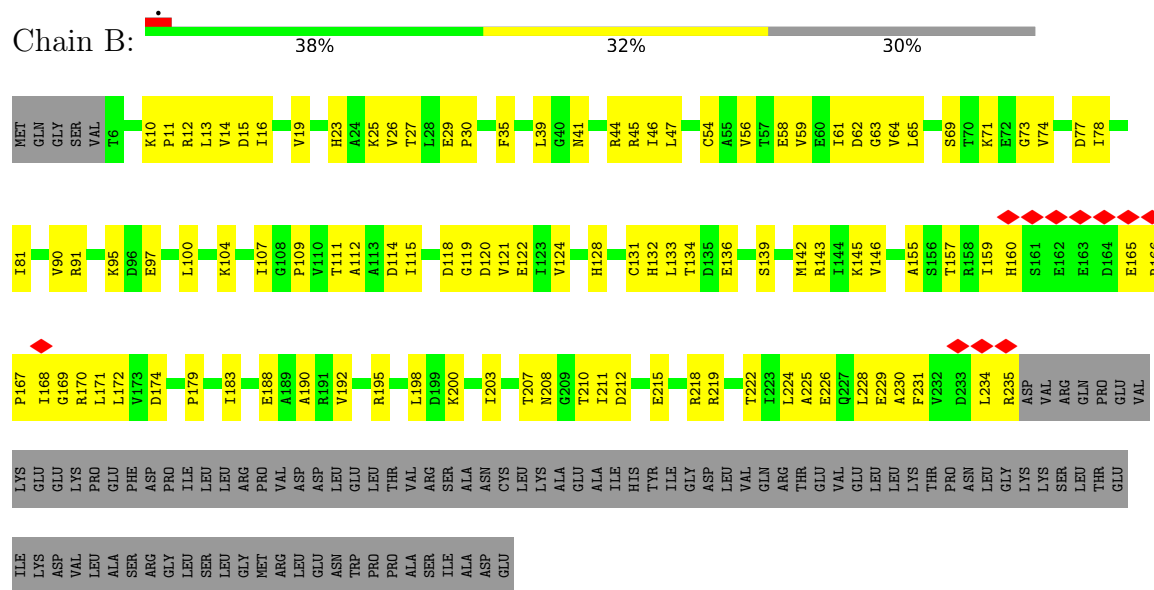
3 Residue-property plots

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

• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha



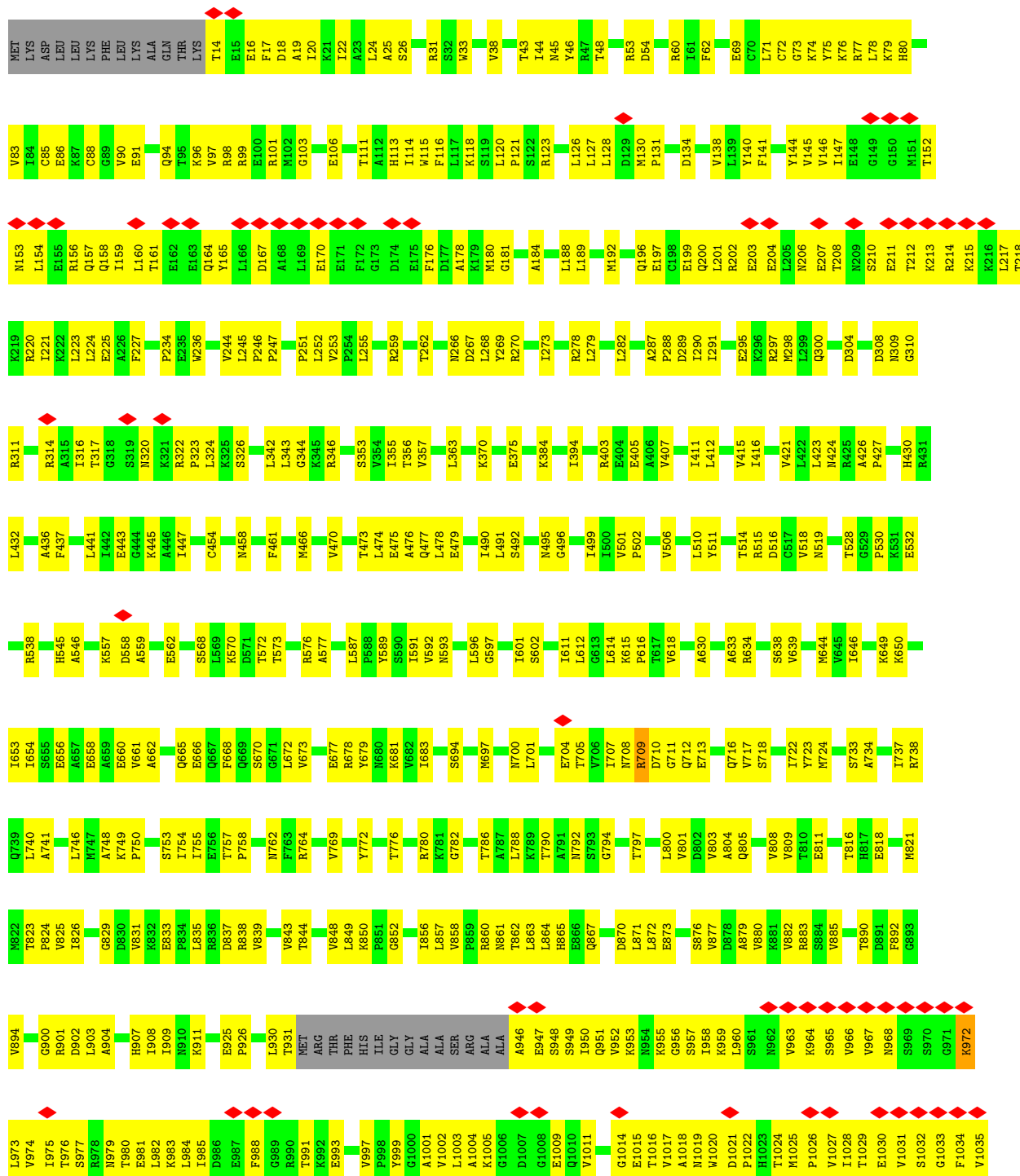
• Molecule 2: DNA-directed RNA polymerase subunit beta

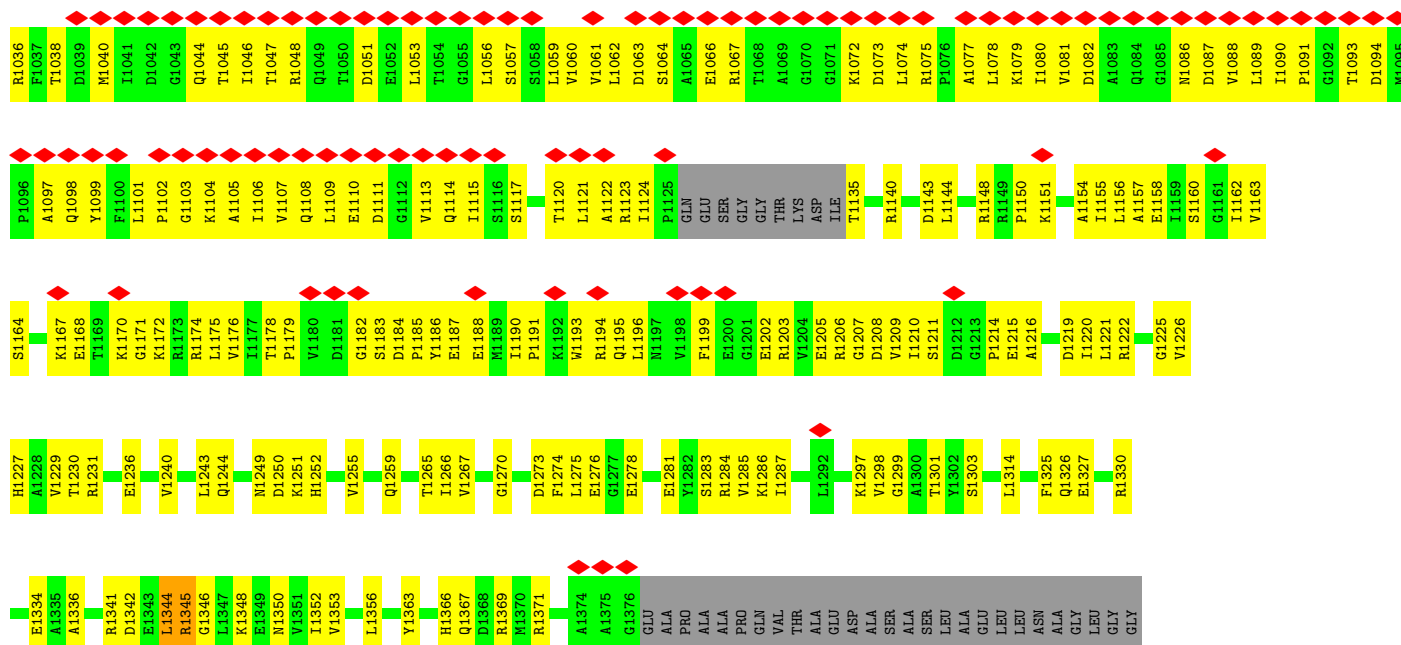


I1182	A1183	T1184	V1186	F1187	D1188	G1189	E1192	A1193	K1196	E1197	L1198	L1201	T1206	Y1213	T1217	E1218	G1219	Q1220	V1225	T1226	G1228	Y1229	K1234	L1235	N1236	H1244	A1245	R1246	S1252	V1253	V1254	T1255	P1258	L1259	G1260	G1261	K1262	Q1263	F1265	G1266	R1269	F1270	G1271											
M1066	G1071	N1072	K1073	I1076	S1077	K1078	I1082	P1093	V1103	P1104	R1106	M1107	I1108	T1109	T1115	K1122	G1125	Q1134	Y1135	Q1136	E1137	K1140	L1141	R1142	L1151	D1154	Q1157	K1158	V1159	D1160	L1161	S1162	T1163	F1164	S1165	D1166	E1167	E1168	M1169	M1170	G1179	M1180	P1181											
E985	A986	E987	K988	L989	D990	K991	L992	P993	R994	D995	R996	W997	L998	E999	L1000	G1001	T1003	D1004	E1005	E1006	K914	K1007	Q1008	N1009	Q1010	L1011	E1012	Q1013	A1015	E1016	Q1017	Y1018	D1019	E1020	L1021	K1022	H1023	E1024	F1025	E1026	K1027	K1028	A1031	R1034	L1035	T1036	T1037	Q1038	L1042	A1043	P1044	G1045	V1046	R1058
G879	K886	V887	T888	P889	K890	G891	E892	L895	T896	P897	E898	R899	K900	R903	G907	E908	K909	D912	V913	D915	P921	V924	I929	D937	G938	K943	A956	L960	S961	E962	T965	Q965	E968	R974	I975	R976	A977	V978	L979	V980	A981	G982	G983	V984										
I734	E738	M741	I748	N760	Q761	N762	Q767	E778	D781	V782	L783	A784	Q798	N799	M800	N808	E813	L817	Q1010	L1011	E1012	Q1013	L1014	R827	H832	K944	L845	E849	I850	T851	A852	D853	I854	P855	N856	D866	A716	E867	S868	G869	Y872	T878												
T616	S621	D624	E625	E626	F629	D632	L633	V634	T635	C636	R637	S638	E641	L644	R647	D648	Q649	V650	D651	M653	V660	V661	S662	A665	S666	R678	M685	V690	R694	A695	D696	K697	P698	L699	V714	T715	A716	V717	V724	V727	D728	A729												
R528	R529	I530	L533	R540	E541	A543	G544	F545	R548	D549	V550	T553	V558	I561	E562	T563	Q564	E565	N568	L571	I572	N573	S574	S576	V577	Q580	L581	N582	G585	F586	L587	E588	T589	P590	K593	V594	T595	D596	G597	V598	V599	T600	D601	E602	V615									
D434	I435	R436	K439	L448	I453	V456	M459	Q463	F464	R465	L468	V471	E472	R473	A474	V475	K476	E477	L479	S480	L481	G482	D483	L484	D485	T486	M488	P489	M492	I493	M494	A495	K496	P497	I498	F505	L511	S512	Q513	F514	L521	I524	T525											
S328	G329	K331	R332	I333	E334	L336	F337	T338	N339	D340	Y346	T350	L351	R352	V353	D358	R359	L360	S361	A362	L363	Y367	R368	N369	G373	E379	A380	A381	N387	S391	D396	L397	S398	G401	M406	R411	G418	K422	I425	M429														
V263	E264	K265	G266	R267	D268	I269	T270	L271	R272	H273	I274	R275	Q276	L277	E278	K279	D281	V282	K283	L284	I285	E286	V287	P288	V289	Y291	I292	A293	G294	D300	Y301	I302	D303	E304	S305	T306	G307	E308	L309	I310	C311	A312	M315	E316	L317	S318	L319	D320	L321	L322	K324	L325	S326	Q327
R200	K203	L204	P205	T206	T207	I208	I209	T210	L213	N214	Y215	T216	T217	Q219	T220	D222	L223	E226	K227	V228	I229	F230	G231	L232	R233	D234	N235	K236	L237	Q238	M239	E240	L241	V242	P243	E244	R245	L246	R247	G248	E249	T250	A251	S252	K253	D254	T255	E256	A257	V258	K260	V261	Y262	
T91	V98	L102	V103	I104	Y105	E106	R107	K108	A109	P110	V114	K115	D116	I117	K118	E119	Q120	E121	V122	Y123	M124	G125	E126	I127	I138	I145	K163	H165	S166	K169	V170	L171	P178	Y179	D185	F186	D189	P190	K191	D192	N193	E194	F195	V196	R197	I198	D199							

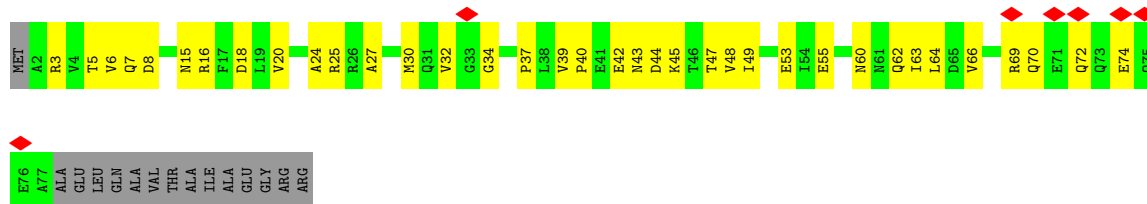


● Molecule 3: DNA-directed RNA polymerase subunit beta'

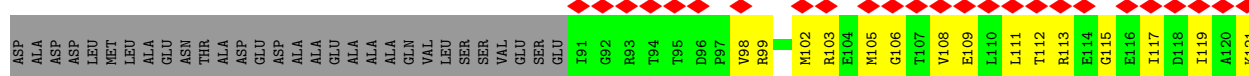


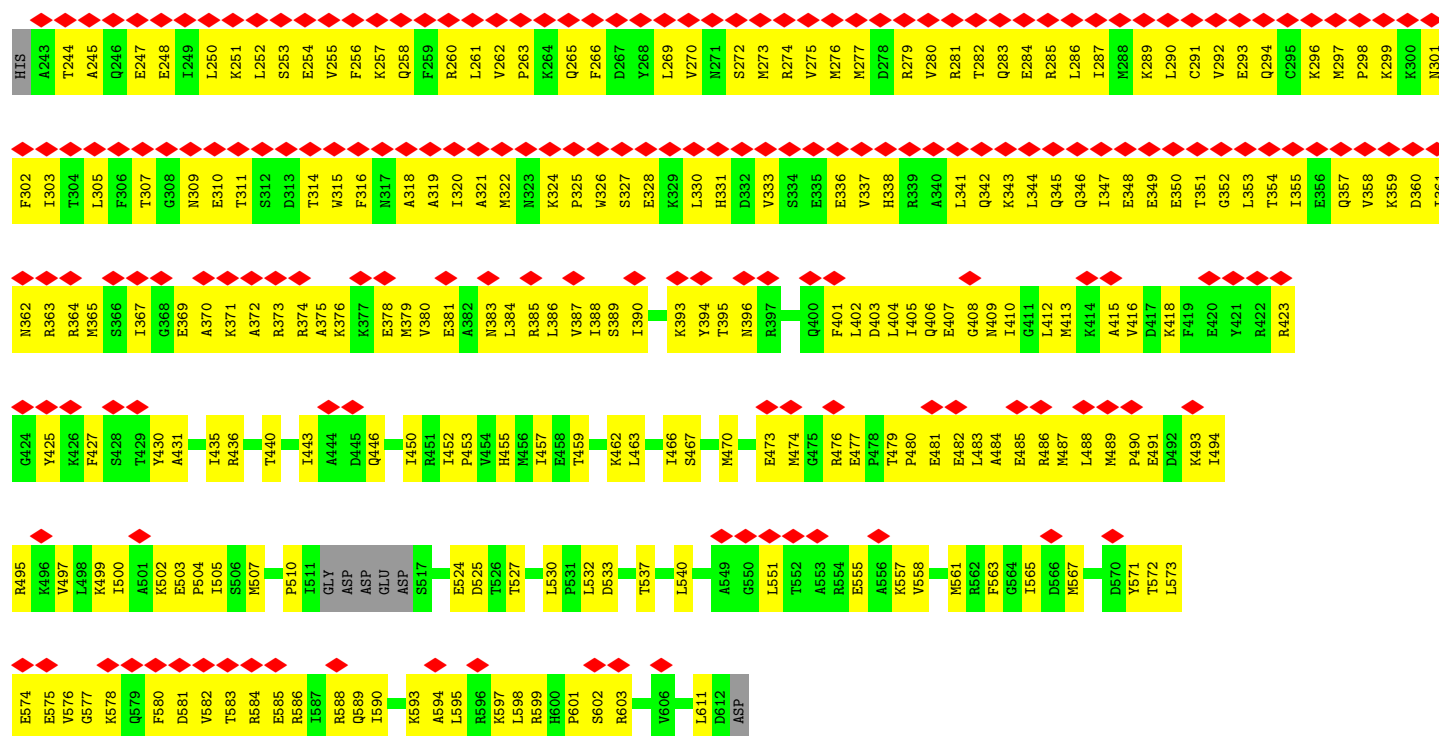


• Molecule 4: DNA-directed RNA polymerase subunit omega

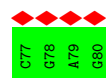
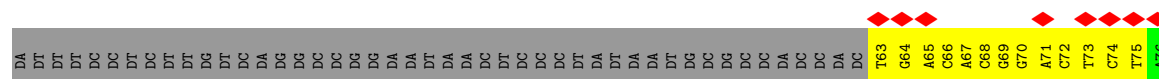


• Molecule 5: RNA polymerase sigma factor RpoD

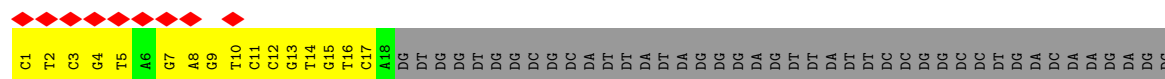




• Molecule 6: DNA (5'-D(P*CP*TP*CP*GP*TP*AP*GP*AP*GP*TP*CP*CP*GP*TP*GP*T
P*CP*A)-3')



• Molecule 7: DNA (5'-D(P*CP*TP*CP*GP*TP*AP*GP*AP*GP*TP*CP*CP*GP*TP*GP*T
P*CP*A)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	285262	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.617	Depositor
Minimum map value	-2.879	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	403.2, 403.2, 403.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, D9X, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/1816	0.51	0/2461
1	B	0.24	0/1808	0.50	0/2450
2	C	0.25	0/10739	0.49	0/14489
3	D	0.24	0/10539	0.49	0/14234
4	E	0.23	0/607	0.49	0/817
5	F	0.24	0/3849	0.49	0/5171
6	X	0.43	0/415	0.81	0/638
7	Y	0.49	0/411	0.89	0/632
All	All	0.25	0/30184	0.51	0/40892

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
3	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	1344	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1794	0	1819	81	0
1	B	1786	0	1813	93	0
2	C	10570	0	10582	529	0
3	D	10382	0	10570	719	0
4	E	605	0	612	34	0
5	F	3799	0	3885	408	0
6	X	370	0	202	29	0
7	Y	368	0	204	27	0
8	C	82	81	0	1	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
All	All	29759	81	29687	1837	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 31.

All (1837) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:344:LEU:HD12	5:F:347:ILE:HD11	1.30	1.13
5:F:151:VAL:HG22	5:F:156:ALA:HB3	1.30	1.12
5:F:383:ASN:HB3	5:F:412:LEU:HD11	1.33	1.09
3:D:201:LEU:HB2	3:D:221:ILE:HD11	1.35	1.09
6:X:63:DT:H2''	6:X:64:DG:H5'	1.32	1.08
3:D:126:LEU:HD11	3:D:223:LEU:HD13	1.39	1.04
3:D:317:THR:HG22	3:D:324:LEU:HD23	1.36	1.04
2:C:292:ILE:HD11	2:C:333:ILE:HD11	1.40	1.03
3:D:1079:LYS:HE3	3:D:1087:ASP:HB2	1.35	1.03
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.38	1.03
3:D:161:THR:HG22	3:D:164:GLN:HG3	1.36	1.02
3:D:1062:LEU:HD12	3:D:1066:GLU:HG3	1.42	1.01
7:Y:10:DT:H2''	7:Y:11:DC:H5'	1.38	1.01
3:D:1162:ILE:HD13	3:D:1203:ARG:HD3	1.42	1.01
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.40	1.00
2:C:238:GLN:HB3	2:C:284:LEU:HD21	1.42	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:301:TYR:HB2	2:C:311:CYS:HB3	1.44	1.00
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.43	0.99
3:D:950:ILE:HD11	3:D:982:LEU:HD23	1.45	0.99
2:C:993:PRO:HD2	2:C:996:ARG:HG3	1.43	0.98
2:C:1244:HIS:HB2	2:C:1262:LYS:HE2	1.41	0.97
5:F:462:LYS:HE2	5:F:487:MET:HE2	1.44	0.97
2:C:102:LEU:HD23	2:C:117:ILE:HD11	1.44	0.97
5:F:292:VAL:HG12	5:F:296:LYS:HD2	1.48	0.95
3:D:709:ARG:HD3	3:D:710:ASP:H	1.30	0.95
5:F:387:VAL:HG23	5:F:412:LEU:HD13	1.47	0.93
3:D:863:LEU:HD11	3:D:901:ARG:HB2	1.49	0.93
2:C:28:LEU:HD21	2:C:524:ILE:HD13	1.53	0.91
1:B:231:PHE:HA	1:B:234:LEU:HD22	1.52	0.91
2:C:1159:VAL:HG12	2:C:1160:ASP:H	1.35	0.91
3:D:1101:LEU:HD22	3:D:1105:ALA:HB1	1.53	0.91
3:D:952:VAL:HG21	3:D:1011:VAL:HG12	1.52	0.91
5:F:161:LEU:HD12	5:F:162:ILE:HB	1.53	0.91
5:F:379:MET:HG2	5:F:416:VAL:HG21	1.53	0.90
2:C:471:VAL:HG21	2:C:498:ILE:HD11	1.51	0.90
2:C:238:GLN:HG3	2:C:286:GLU:HG3	1.54	0.89
6:X:68:DC:H2''	6:X:69:DG:H5'	1.54	0.89
1:A:14:VAL:HG12	1:A:15:ASP:H	1.36	0.89
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.51	0.89
3:D:356:THR:HG22	3:D:357:VAL:H	1.36	0.89
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.53	0.89
2:C:595:THR:HG22	2:C:596:ASP:H	1.38	0.88
3:D:19:ALA:HB1	3:D:1341:ARG:HE	1.37	0.88
5:F:119:ILE:HG23	5:F:375:ALA:HB1	1.55	0.88
5:F:98:VAL:HG22	5:F:402:LEU:HD11	1.56	0.88
5:F:584:ARG:HE	5:F:586:ARG:HD3	1.39	0.88
2:C:75:LEU:HD21	2:C:127:ILE:HD11	1.54	0.88
5:F:466:ILE:HG22	5:F:470:MET:HE2	1.57	0.87
5:F:276:MET:CE	5:F:347:ILE:HD12	2.04	0.87
5:F:130:VAL:HG23	5:F:365:MET:HG3	1.55	0.87
2:C:237:LEU:HD11	2:C:289:VAL:HG22	1.58	0.86
2:C:985:GLU:HG3	2:C:988:LYS:HE2	1.57	0.86
2:C:633:LEU:HB3	2:C:644:LEU:HD12	1.55	0.85
3:D:1021:ASP:HB3	3:D:1024:THR:HB	1.58	0.85
3:D:1062:LEU:HD13	3:D:1104:LYS:H	1.40	0.85
1:A:218:ARG:HH12	1:B:234:LEU:H	1.23	0.85
2:C:253:PHE:HE2	2:C:291:TYR:HB2	1.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1160:ASP:CB	2:C:1161:LEU:HA	2.06	0.84
5:F:224:LEU:HD21	5:F:255:VAL:HG21	1.59	0.84
3:D:825:VAL:HG12	3:D:833:GLU:HB3	1.60	0.83
3:D:960:LEU:HB3	3:D:963:VAL:HG11	1.58	0.83
3:D:114:ILE:HD11	3:D:311:ARG:HD2	1.60	0.83
2:C:844:LYS:HG3	2:C:845:LEU:HD12	1.60	0.83
3:D:959:LYS:HB3	3:D:983:LYS:HB2	1.59	0.83
3:D:295:GLU:HA	3:D:298:MET:HE3	1.60	0.82
5:F:310:GLU:HB3	5:F:355:ILE:HD13	1.61	0.82
3:D:964:LYS:HG2	3:D:977:SER:HB2	1.60	0.82
2:C:615:VAL:HG12	2:C:638:SER:HB3	1.60	0.81
2:C:528:ARG:NH2	2:C:576:SER:O	2.13	0.81
3:D:826:ILE:HG22	3:D:831:VAL:HG12	1.62	0.81
2:C:1297:ASP:O	2:C:1301:ARG:HG3	1.80	0.81
4:E:3:ARG:NH1	4:E:55:GLU:OE1	2.13	0.81
2:C:1024:GLU:OE1	2:C:1028:LYS:NZ	2.14	0.81
5:F:127:ILE:O	5:F:130:VAL:HG12	1.80	0.81
5:F:151:VAL:HG11	5:F:161:LEU:HD23	1.62	0.81
2:C:813:GLU:HB2	3:D:461:PHE:HD2	1.46	0.80
3:D:959:LYS:HB2	3:D:985:ILE:HG12	1.63	0.80
3:D:1046:ILE:HD12	3:D:1059:LEU:HD22	1.63	0.80
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.63	0.80
5:F:298:PRO:HD2	5:F:301:ASN:HD21	1.45	0.80
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.62	0.80
3:D:677:GLU:O	3:D:681:LYS:HG2	1.81	0.80
3:D:1160:SER:OG	3:D:1203:ARG:NH1	2.13	0.79
5:F:250:LEU:O	5:F:253:SER:OG	1.98	0.79
1:B:14:VAL:HG12	1:B:15:ASP:H	1.47	0.79
3:D:266:ASN:O	3:D:270:ARG:HG3	1.83	0.79
2:C:120:GLN:OE1	2:C:120:GLN:N	2.14	0.79
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.61	0.79
2:C:660:VAL:HG21	3:D:769:VAL:HG11	1.63	0.79
5:F:158:LEU:HA	5:F:161:LEU:CD2	2.11	0.79
2:C:122:VAL:HB	2:C:493:ILE:HD11	1.65	0.79
3:D:1140:ARG:HG2	3:D:1240:VAL:HG21	1.65	0.79
5:F:466:ILE:HG22	5:F:470:MET:CE	2.12	0.79
3:D:701:LEU:HD21	3:D:723:TYR:HB2	1.64	0.79
5:F:309:ASN:ND2	5:F:314:THR:OG1	2.16	0.79
1:A:58:GLU:HG2	1:A:172:LEU:HD23	1.65	0.78
1:B:95:LYS:NZ	1:B:120:ASP:OD2	2.12	0.78
3:D:1298:VAL:H	3:D:1299:GLY:HA3	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:128:ASN:HA	5:F:131:GLN:OE1	1.83	0.78
2:C:36:GLN:O	2:C:40:GLU:HB2	1.83	0.78
2:C:65:ASN:O	2:C:105:TYR:N	2.12	0.78
2:C:550:VAL:HG22	3:D:780:ARG:HH21	1.48	0.77
2:C:976:ARG:HH11	2:C:980:VAL:HG21	1.49	0.77
1:A:145:LYS:NZ	1:A:147:GLN:OE1	2.17	0.77
2:C:312:ALA:H	2:C:315:MET:HE1	1.47	0.77
1:A:164:ASP:HA	1:A:166:ARG:HH11	1.49	0.77
1:B:225:ALA:O	1:B:229:GLU:HG2	1.84	0.77
3:D:1005:LYS:NZ	3:D:1015:GLU:OE2	2.17	0.77
3:D:1056:LEU:HD12	3:D:1108:GLN:HB2	1.66	0.77
2:C:84:GLU:OE1	2:C:88:ARG:NH1	2.18	0.77
3:D:1044:GLN:OE1	3:D:1045:THR:OG1	2.03	0.76
2:C:119:GLU:CB	2:C:489:PRO:HG2	2.15	0.76
2:C:241:LEU:HD11	2:C:246:LEU:HD21	1.65	0.76
3:D:746:LEU:HG	3:D:758:PRO:HB3	1.66	0.76
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.14	0.76
2:C:119:GLU:HB2	2:C:489:PRO:HG2	1.68	0.76
2:C:276:GLN:HA	2:C:279:LYS:HE2	1.66	0.76
5:F:292:VAL:HG13	5:F:296:LYS:HA	1.66	0.76
3:D:1158:GLU:O	3:D:1206:ARG:NH1	2.19	0.76
2:C:488:MET:SD	2:C:489:PRO:HD2	2.25	0.76
3:D:694:SER:HB3	3:D:738:ARG:HH11	1.50	0.76
3:D:973:LEU:HD22	3:D:1003:LEU:HD13	1.65	0.76
5:F:597:LYS:O	5:F:603:ARG:NH2	2.19	0.76
3:D:201:LEU:HB2	3:D:221:ILE:CD1	2.15	0.75
5:F:220:LYS:O	5:F:223:GLU:HG3	1.84	0.75
2:C:895:LEU:HD13	2:C:903:ARG:NH1	2.01	0.75
3:D:755:ILE:HG22	3:D:757:THR:H	1.51	0.75
5:F:582:VAL:HG23	5:F:586:ARG:NH2	2.01	0.75
6:X:72:DC:H2''	6:X:73:DT:H5'	1.68	0.75
5:F:418:LYS:O	5:F:430:TYR:OH	2.04	0.75
1:A:226:GLU:O	1:B:10:LYS:NZ	2.20	0.75
3:D:1109:LEU:HG	3:D:1113:VAL:HG11	1.68	0.75
5:F:533:ASP:O	5:F:537:THR:HG23	1.86	0.75
3:D:964:LYS:O	3:D:976:THR:OG1	2.01	0.75
5:F:473:GLU:OE2	5:F:486:ARG:NH2	2.19	0.75
5:F:355:ILE:O	5:F:359:LYS:HG2	1.87	0.74
5:F:401:PHE:O	5:F:405:ILE:HG23	1.86	0.74
3:D:1090:ILE:HB	3:D:1093:THR:CG2	2.17	0.74
5:F:283:GLN:O	5:F:286:LEU:HG	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:813:GLU:HB2	3:D:461:PHE:CD2	2.22	0.74
3:D:734:ALA:O	3:D:738:ARG:HG3	1.87	0.74
3:D:259:ARG:HG2	5:F:502:LYS:HE3	1.69	0.74
2:C:255:ILE:HB	2:C:263:VAL:HB	1.68	0.74
1:A:228:LEU:HD11	1:B:224:LEU:HD23	1.70	0.74
2:C:728:ASP:OD1	2:C:729:ALA:N	2.20	0.74
3:D:1314:LEU:HG	3:D:1326:GLN:HE22	1.52	0.74
5:F:281:ARG:HD3	5:F:285:ARG:HH21	1.52	0.74
5:F:363:ARG:O	5:F:367:ILE:HG12	1.87	0.74
2:C:1184:THR:HG23	2:C:1189:GLY:HA3	1.68	0.74
3:D:128:LEU:HD23	3:D:192:MET:HE1	1.70	0.74
3:D:1020:TRP:CZ3	3:D:1022:PRO:HA	2.23	0.74
1:B:165:GLU:HB3	1:B:170:ARG:NE	2.02	0.73
3:D:811:GLU:OE1	3:D:890:THR:OG1	2.03	0.73
3:D:203:GLU:HA	3:D:206:ASN:HD21	1.51	0.73
5:F:311:THR:HG23	5:F:348:GLU:OE1	1.89	0.73
3:D:19:ALA:HA	3:D:1342:ASP:O	1.87	0.73
5:F:354:THR:HG22	5:F:357:GLN:OE1	1.88	0.73
1:B:74:VAL:HG12	1:B:133:LEU:HD23	1.70	0.73
2:C:545:PHE:CZ	3:D:788:LEU:HD13	2.24	0.73
3:D:857:LEU:HD11	3:D:871:LEU:HD21	1.70	0.73
5:F:261:LEU:HB3	5:F:266:PHE:CE1	2.24	0.73
2:C:189:ASP:OD1	2:C:193:ASN:N	2.17	0.73
5:F:383:ASN:HB2	5:F:412:LEU:HD21	1.71	0.73
3:D:46:TYR:HB3	5:F:450:ILE:CG2	2.19	0.73
5:F:148:TYR:CE1	5:F:161:LEU:HD13	2.23	0.73
3:D:201:LEU:CB	3:D:221:ILE:HD11	2.18	0.72
3:D:972:LYS:HG3	3:D:1002:VAL:HG13	1.70	0.72
3:D:1078:LEU:HD13	3:D:1101:LEU:HD21	1.71	0.72
4:E:39:VAL:CG2	4:E:40:PRO:HD2	2.19	0.72
2:C:91:THR:OG1	2:C:138:ILE:O	2.05	0.72
2:C:472:GLU:OE2	2:C:476:LYS:HD2	1.89	0.72
3:D:309:ASN:HB2	3:D:326:SER:HB3	1.71	0.72
1:A:162:GLU:OE1	1:A:162:GLU:N	2.22	0.72
2:C:1043:ALA:O	2:C:1046:VAL:HG22	1.89	0.72
2:C:1192:GLU:O	2:C:1196:LYS:HG2	1.90	0.72
5:F:359:LYS:HA	5:F:362:ASN:ND2	2.05	0.72
2:C:331:LYS:HB3	2:C:332:ARG:NH1	2.04	0.72
2:C:65:ASN:CB	2:C:105:TYR:HB2	2.17	0.72
2:C:1196:LYS:HD2	2:C:1206:THR:CG2	2.19	0.72
5:F:302:PHE:O	5:F:305:LEU:HG	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ARG:NH2	1:A:173:VAL:O	2.23	0.72
5:F:225:ARG:O	5:F:229:VAL:HG13	1.90	0.72
3:D:709:ARG:HD3	3:D:710:ASP:N	2.02	0.72
3:D:786:THR:O	3:D:790:THR:HG23	1.90	0.72
2:C:896:THR:OG1	2:C:897:PRO:HD2	1.90	0.71
2:C:196:VAL:HG21	2:C:209:ILE:CD1	2.20	0.71
2:C:471:VAL:HG21	2:C:498:ILE:CD1	2.20	0.71
2:C:1244:HIS:NE2	2:C:1265:PHE:O	2.22	0.71
3:D:952:VAL:CG2	3:D:1011:VAL:HG12	2.20	0.71
5:F:216:LEU:O	5:F:219:GLU:HG3	1.90	0.71
3:D:120:LEU:HB3	3:D:121:PRO:CD	2.19	0.71
2:C:979:LEU:CD1	2:C:997:TRP:HB3	2.20	0.71
2:C:106:GLU:OE2	2:C:109:ALA:HB3	1.90	0.71
2:C:1010:GLN:O	2:C:1014:LEU:HG	1.91	0.71
4:E:44:ASP:HB3	4:E:48:VAL:CG1	2.21	0.71
3:D:1325:PHE:CE1	3:D:1326:GLN:HG3	2.25	0.71
5:F:119:ILE:CG2	5:F:375:ALA:HB1	2.20	0.71
1:B:11:PRO:O	1:B:12:ARG:NH1	2.23	0.71
2:C:367:TYR:HD2	2:C:381:ALA:HA	1.56	0.71
3:D:298:MET:HE1	5:F:406:GLN:HG3	1.73	0.71
3:D:45:ASN:HB3	3:D:48:THR:O	1.89	0.71
3:D:1062:LEU:HD13	3:D:1104:LYS:N	2.05	0.71
3:D:1184:ASP:N	3:D:1185:PRO:HD2	2.06	0.71
5:F:292:VAL:O	5:F:296:LYS:N	2.24	0.71
3:D:126:LEU:HD11	3:D:223:LEU:CD1	2.17	0.70
3:D:1026:PRO:HB3	3:D:1120:THR:HA	1.70	0.70
1:B:231:PHE:HA	1:B:234:LEU:CD2	2.20	0.70
5:F:136:GLU:OE2	5:F:361:ILE:HG12	1.89	0.70
3:D:1040:MET:CE	3:D:1059:LEU:HD13	2.22	0.70
6:X:72:DC:O2	7:Y:9:DG:N2	2.24	0.70
3:D:196:GLN:O	3:D:200:GLN:HG2	1.92	0.70
1:A:104:LYS:HG2	1:A:110:VAL:HG22	1.72	0.70
1:B:235:ARG:NH1	1:B:235:ARG:O	2.23	0.70
5:F:355:ILE:O	5:F:358:VAL:HG12	1.92	0.70
3:D:310:GLY:HA2	3:D:314:ARG:HG2	1.74	0.70
3:D:973:LEU:HB2	3:D:1003:LEU:HD13	1.74	0.69
2:C:471:VAL:CG2	2:C:497:PRO:HG2	2.21	0.69
3:D:79:LYS:HG3	3:D:80:HIS:CD2	2.27	0.69
2:C:896:THR:HG22	2:C:899:GLU:OE1	1.91	0.69
3:D:701:LEU:CD2	3:D:723:TYR:HB2	2.22	0.69
3:D:980:THR:OG1	3:D:997:VAL:HG23	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1122:ALA:O	3:D:1123:ARG:HD3	1.93	0.69
1:B:136:GLU:OE1	1:B:136:GLU:N	2.24	0.69
3:D:1163:VAL:HG23	3:D:1175:LEU:HD21	1.74	0.69
5:F:245:ALA:HA	5:F:248:GLU:OE2	1.92	0.69
3:D:872:LEU:HB3	3:D:877:VAL:HG21	1.75	0.69
3:D:902:ASP:O	3:D:903:LEU:HG	1.92	0.69
2:C:256:GLU:HB3	2:C:261:VAL:HG12	1.73	0.69
2:C:483:ASP:OD1	2:C:484:LEU:N	2.26	0.69
2:C:231:GLU:HA	2:C:331:LYS:O	1.92	0.69
3:D:473:THR:HG23	3:D:476:ALA:H	1.55	0.69
3:D:958:ILE:HD11	3:D:1011:VAL:HB	1.73	0.69
5:F:254:GLU:O	5:F:258:GLN:HG3	1.93	0.69
5:F:563:PHE:HB2	5:F:565:ILE:HD12	1.74	0.69
1:A:19:VAL:CG2	1:A:23:HIS:HB3	2.23	0.69
3:D:403:ARG:NH2	3:D:405:GLU:OE2	2.26	0.69
2:C:694:ARG:O	2:C:798:GLN:NE2	2.26	0.68
6:X:65:DA:H2''	6:X:66:DC:H5'	1.75	0.68
1:A:165:GLU:HA	1:A:170:ARG:HH21	1.58	0.68
3:D:80:HIS:HB3	3:D:83:VAL:CG1	2.23	0.68
5:F:346:GLN:O	5:F:349:GLU:HG2	1.93	0.68
2:C:1160:ASP:HB2	2:C:1162:SER:H	1.56	0.68
3:D:72:CYS:SG	3:D:74:LYS:HG3	2.34	0.68
3:D:203:GLU:HA	3:D:206:ASN:ND2	2.08	0.68
3:D:221:ILE:HG22	3:D:225:GLU:OE1	1.92	0.68
3:D:1072:LYS:O	3:D:1075:ARG:NH1	2.24	0.68
5:F:269:LEU:O	5:F:273:MET:HG3	1.94	0.68
5:F:344:LEU:HA	5:F:347:ILE:HG12	1.75	0.68
3:D:829:GLY:HA2	3:D:993:GLU:HB2	1.76	0.68
3:D:972:LYS:HD3	3:D:1003:LEU:H	1.59	0.68
1:A:236:ASP:OD2	1:B:218:ARG:NH1	2.22	0.68
2:C:1252:SER:HB3	2:C:1255:THR:O	1.94	0.68
3:D:568:SER:OG	3:D:570:LYS:NZ	2.26	0.68
3:D:282:LEU:HD13	3:D:291:ILE:HG22	1.75	0.68
3:D:950:ILE:CD1	3:D:982:LEU:HD23	2.22	0.68
5:F:132:CYS:HA	5:F:257:LYS:HE3	1.76	0.68
5:F:151:VAL:HG11	5:F:161:LEU:CD2	2.23	0.68
5:F:355:ILE:HA	5:F:358:VAL:HG12	1.76	0.68
3:D:856:ILE:O	3:D:856:ILE:HG13	1.94	0.68
5:F:115:GLY:O	5:F:119:ILE:HG13	1.93	0.68
1:A:19:VAL:HG22	1:A:23:HIS:HB3	1.76	0.67
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:949:SER:HB2	3:D:1016:THR:CG2	2.23	0.67
3:D:211:GLU:HG2	3:D:212:THR:N	2.08	0.67
3:D:259:ARG:HG2	5:F:502:LYS:CD	2.23	0.67
3:D:342:LEU:HD13	3:D:1352:ILE:HG23	1.76	0.67
3:D:1162:ILE:CD1	3:D:1203:ARG:HD3	2.22	0.67
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.76	0.67
2:C:974:ARG:HH11	2:C:978:VAL:HG21	1.58	0.67
3:D:1077:ALA:HB1	3:D:1098:GLN:NE2	2.10	0.67
3:D:1144:LEU:HD11	3:D:1236:GLU:HB3	1.74	0.67
2:C:564:PRO:HG2	2:C:568:ASN:O	1.93	0.67
5:F:360:ASP:O	5:F:364:ARG:HG2	1.93	0.67
2:C:57:PHE:CD2	2:C:70:TYR:HB2	2.30	0.67
3:D:317:THR:HG23	3:D:322:ARG:O	1.93	0.67
5:F:117:ILE:HG22	5:F:121:LYS:HE2	1.77	0.67
5:F:138:PRO:HD2	5:F:353:LEU:HD23	1.76	0.67
5:F:333:VAL:O	5:F:337:VAL:HG23	1.95	0.67
2:C:276:GLN:HA	2:C:279:LYS:HG2	1.77	0.67
2:C:398:SER:HB2	2:C:401:GLY:H	1.58	0.67
3:D:94:GLN:NE2	3:D:96:LYS:HE3	2.09	0.67
3:D:111:THR:HG23	3:D:300:GLN:HG2	1.77	0.67
3:D:825:VAL:CG1	3:D:833:GLU:HB3	2.24	0.67
3:D:980:THR:OG1	3:D:997:VAL:O	2.12	0.67
3:D:1029:THR:O	3:D:1117:SER:OG	2.08	0.67
5:F:341:LEU:O	5:F:345:GLN:HG3	1.95	0.67
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.76	0.67
4:E:60:ASN:OD1	4:E:63:ILE:HG12	1.94	0.67
1:A:231:PHE:HE1	1:B:39:LEU:HD13	1.59	0.66
3:D:322:ARG:HH11	5:F:510:PRO:HD3	1.60	0.66
3:D:474:LEU:HD21	4:E:27:ALA:HB3	1.74	0.66
5:F:226:ALA:O	5:F:229:VAL:HG22	1.95	0.66
2:C:46:GLN:O	2:C:51:ALA:HB2	1.94	0.66
3:D:145:VAL:HG11	3:D:184:ALA:HB1	1.76	0.66
2:C:238:GLN:HG3	2:C:286:GLU:CG	2.23	0.66
3:D:416:ILE:HG21	3:D:441:LEU:HD21	1.78	0.66
5:F:281:ARG:HD3	5:F:285:ARG:NH2	2.09	0.66
2:C:965:GLN:O	2:C:968:GLU:HG2	1.96	0.66
3:D:201:LEU:HD11	3:D:220:ARG:NH1	2.10	0.66
3:D:161:THR:CG2	3:D:164:GLN:HG3	2.19	0.66
5:F:98:VAL:HG22	5:F:402:LEU:CD1	2.25	0.66
3:D:949:SER:HB2	3:D:1016:THR:HG23	1.76	0.66
3:D:131:PRO:HG2	3:D:134:ASP:OD2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1082:ASP:HB3	3:D:1088:VAL:CG1	2.25	0.66
3:D:1160:SER:OG	3:D:1205:GLU:HA	1.95	0.66
2:C:1160:ASP:HB2	2:C:1161:LEU:CA	2.22	0.66
5:F:355:ILE:HG23	5:F:359:LYS:HE3	1.76	0.66
2:C:198:ILE:HG22	2:C:199:ASP:H	1.59	0.66
3:D:279:LEU:HD13	3:D:295:GLU:HB3	1.78	0.66
3:D:528:THR:HG22	3:D:532:GLU:OE1	1.96	0.66
2:C:478:ARG:NH1	2:C:482:GLY:HA3	2.12	0.66
3:D:835:LEU:O	3:D:839:VAL:HG12	1.96	0.66
2:C:593:LYS:O	2:C:600:THR:OG1	2.12	0.65
3:D:126:LEU:CD1	3:D:223:LEU:HD13	2.20	0.65
3:D:697:MET:CE	3:D:738:ARG:HA	2.26	0.65
5:F:144:LEU:HD11	5:F:148:TYR:HE2	1.61	0.65
1:B:192:VAL:HG12	1:B:198:LEU:HD11	1.78	0.65
2:C:685:MET:CE	2:C:1071:GLY:HA2	2.25	0.65
3:D:1026:PRO:CB	3:D:1120:THR:HA	2.26	0.65
5:F:148:TYR:CZ	5:F:161:LEU:HD13	2.31	0.65
5:F:482:GLU:HA	5:F:485:GLU:OE1	1.95	0.65
1:A:92:VAL:HG22	1:A:121:VAL:HG12	1.76	0.65
3:D:1156:LEU:HD12	3:D:1219:ASP:HB3	1.77	0.65
7:Y:4:DG:H2'	7:Y:5:DT:C6	2.31	0.65
3:D:267:ASP:OD2	3:D:268:LEU:N	2.29	0.65
5:F:147:GLN:O	5:F:151:VAL:HG23	1.96	0.65
5:F:473:GLU:HG3	5:F:474:MET:HG3	1.79	0.65
5:F:482:GLU:HA	5:F:485:GLU:CD	2.16	0.65
6:X:63:DT:C2'	6:X:64:DG:H5'	2.20	0.65
2:C:895:LEU:HD11	2:C:900:LYS:HD3	1.79	0.65
3:D:1188:GLU:HB2	3:D:1190:ILE:HD11	1.79	0.65
3:D:650:LYS:O	3:D:654:ILE:HG12	1.97	0.65
3:D:976:THR:HA	3:D:999:TYR:CE1	2.32	0.65
3:D:1046:ILE:HG22	3:D:1061:VAL:HG22	1.79	0.65
3:D:1080:ILE:HG12	3:D:1097:ALA:O	1.96	0.65
1:B:207:THR:HG21	1:B:211:ILE:O	1.97	0.65
3:D:848:VAL:HG12	3:D:858:VAL:HB	1.78	0.65
2:C:1137:GLU:OE2	2:C:1140:LYS:HE3	1.97	0.65
3:D:1109:LEU:HD23	3:D:1115:ILE:CD1	2.27	0.65
5:F:158:LEU:HA	5:F:161:LEU:HD21	1.77	0.65
5:F:213:ASP:O	5:F:216:LEU:HG	1.97	0.65
5:F:261:LEU:HD21	5:F:265:GLN:HB3	1.79	0.65
3:D:384:LYS:HG3	3:D:415:VAL:CG1	2.27	0.65
3:D:839:VAL:HG23	3:D:882:VAL:HG11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:44:ASP:HB3	4:E:48:VAL:HG11	1.79	0.65
5:F:141:ILE:O	5:F:145:LEU:HD23	1.97	0.65
5:F:279:ARG:NH2	5:F:347:ILE:HD13	2.11	0.65
5:F:380:VAL:O	5:F:384:LEU:HG	1.97	0.65
2:C:301:TYR:OH	2:C:333:ILE:HA	1.97	0.64
3:D:16:GLU:OE2	3:D:1369:ARG:HD2	1.96	0.64
5:F:440:THR:O	5:F:443:ILE:HG22	1.96	0.64
1:A:118:ASP:HB3	1:A:121:VAL:HG22	1.79	0.64
1:A:226:GLU:O	1:A:229:GLU:HG2	1.97	0.64
5:F:152:GLU:HG2	5:F:218:ARG:NH1	2.12	0.64
1:B:215:GLU:O	1:B:219:ARG:HG3	1.97	0.64
2:C:1298:VAL:HG12	2:C:1301:ARG:NH2	2.11	0.64
3:D:800:LEU:O	3:D:803:VAL:HG12	1.97	0.64
5:F:158:LEU:O	5:F:161:LEU:HG	1.97	0.64
5:F:344:LEU:HA	5:F:347:ILE:CD1	2.27	0.64
5:F:390:ILE:HG21	5:F:435:ILE:HG21	1.78	0.64
2:C:1159:VAL:HG12	2:C:1160:ASP:N	2.11	0.64
3:D:1048:ARG:HA	3:D:1059:LEU:HD23	1.80	0.64
3:D:1273:ASP:HB3	3:D:1276:GLU:OE1	1.98	0.64
5:F:436:ARG:O	5:F:440:THR:HG23	1.97	0.64
2:C:453:ILE:HG22	2:C:585:GLY:O	1.97	0.64
3:D:114:ILE:HD13	3:D:308:ASP:HB3	1.80	0.64
5:F:141:ILE:HG23	5:F:256:PHE:CZ	2.32	0.64
5:F:582:VAL:O	5:F:586:ARG:NH2	2.31	0.64
2:C:45:GLY:O	2:C:46:GLN:NE2	2.30	0.64
2:C:207:THR:HG21	2:C:351:LEU:HD23	1.80	0.64
3:D:202:ARG:HE	3:D:221:ILE:HG21	1.62	0.64
3:D:1048:ARG:HG3	3:D:1059:LEU:HD21	1.80	0.64
3:D:1057:SER:H	3:D:1108:GLN:HA	1.61	0.64
3:D:1140:ARG:NH2	3:D:1236:GLU:OE1	2.29	0.64
3:D:829:GLY:HA2	3:D:993:GLU:CB	2.28	0.64
1:B:100:LEU:HD23	1:B:115:ILE:HG21	1.78	0.64
2:C:251:ALA:HB3	2:C:267:ARG:O	1.98	0.64
2:C:256:GLU:HB3	2:C:261:VAL:HA	1.79	0.64
2:C:302:ILE:HA	2:C:310:ILE:HG22	1.79	0.64
3:D:518:VAL:HG11	3:D:707:ILE:HG23	1.79	0.64
4:E:25:ARG:HH12	4:E:64:LEU:HB3	1.62	0.64
4:E:25:ARG:NH1	4:E:64:LEU:HB3	2.12	0.64
5:F:144:LEU:HD23	5:F:256:PHE:CE1	2.33	0.64
5:F:479:THR:OG1	5:F:480:PRO:HD2	1.98	0.64
3:D:572:THR:HG21	3:D:589:TYR:CE2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1062:LEU:HD12	3:D:1066:GLU:CG	2.25	0.63
2:C:283:LYS:HD2	2:C:284:LEU:HB2	1.79	0.63
2:C:473:ARG:NH1	2:C:477:GLU:HB2	2.14	0.63
3:D:1298:VAL:N	3:D:1299:GLY:HA3	2.08	0.63
1:A:66:HIS:NE2	2:C:929:ILE:HG22	2.14	0.63
1:A:218:ARG:NH1	1:B:234:LEU:HD23	2.13	0.63
1:A:236:ASP:HA	1:B:16:ILE:HD12	1.81	0.63
2:C:178:PRO:HB3	2:C:397:LEU:HD23	1.79	0.63
2:C:1260:GLY:HA3	3:D:346:ARG:NH1	2.13	0.63
2:C:1269:ARG:NH1	3:D:344:GLY:O	2.31	0.63
3:D:826:ILE:CG2	3:D:831:VAL:HG12	2.28	0.63
3:D:1030:GLU:OE1	3:D:1099:TYR:OH	2.17	0.63
5:F:359:LYS:HA	5:F:362:ASN:HD21	1.62	0.63
1:B:46:ILE:HD11	1:B:224:LEU:HD13	1.79	0.63
3:D:977:SER:HB3	3:D:980:THR:CG2	2.28	0.63
5:F:253:SER:O	5:F:257:LYS:HG3	1.97	0.63
2:C:471:VAL:HG22	2:C:497:PRO:HG2	1.80	0.63
2:C:1286:THR:HG23	3:D:479:GLU:OE1	1.98	0.63
3:D:167:ASP:O	3:D:170:GLU:HG3	1.99	0.63
3:D:694:SER:HB3	3:D:738:ARG:NH1	2.11	0.63
5:F:385:ARG:O	5:F:388:ILE:HG22	1.98	0.63
5:F:467:SER:HA	5:F:470:MET:HE3	1.80	0.63
2:C:59:ILE:HG12	2:C:472:GLU:HG2	1.80	0.63
2:C:60:GLN:HG2	2:C:67:GLU:OE1	1.98	0.63
3:D:353:SER:OG	3:D:445:LYS:O	2.14	0.63
3:D:1034:PHE:HB2	3:D:1081:VAL:HG23	1.80	0.63
5:F:361:ILE:HG12	5:F:364:ARG:HH21	1.62	0.63
5:F:572:THR:HG23	5:F:575:GLU:H	1.64	0.63
2:C:115:LYS:HD3	2:C:116:ASP:N	2.13	0.63
2:C:867:GLU:HG3	2:C:943:LYS:NZ	2.14	0.63
3:D:860:ARG:HG2	3:D:861:ASN:H	1.64	0.63
1:B:120:ASP:OD1	1:B:121:VAL:HG23	1.99	0.63
2:C:106:GLU:H	2:C:114:VAL:HG21	1.64	0.62
3:D:308:ASP:OD2	3:D:311:ARG:NE	2.24	0.62
3:D:1032:SER:HB2	3:D:1115:ILE:O	1.98	0.62
5:F:289:LYS:O	5:F:293:GLU:HG2	1.99	0.62
3:D:259:ARG:HG2	5:F:502:LYS:CE	2.28	0.62
3:D:1160:SER:CB	3:D:1205:GLU:HA	2.30	0.62
3:D:1252:HIS:O	3:D:1255:VAL:HG22	1.99	0.62
5:F:348:GLU:O	5:F:352:GLY:N	2.25	0.62
2:C:245:ARG:HB3	2:C:337:PHE:CE1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:268:ARG:CZ	2:C:270:THR:HG22	2.30	0.62
2:C:1025:PHE:HA	2:C:1028:LYS:NZ	2.14	0.62
2:C:1254:VAL:O	3:D:99:ARG:NH2	2.29	0.62
3:D:210:SER:HB3	3:D:213:LYS:HE2	1.80	0.62
3:D:967:VAL:HG12	3:D:973:LEU:CD1	2.30	0.62
1:A:118:ASP:OD1	1:A:119:GLY:N	2.33	0.62
2:C:57:PHE:HD2	2:C:70:TYR:HB2	1.62	0.62
2:C:593:LYS:HB3	2:C:602:GLU:HG3	1.80	0.62
2:C:976:ARG:O	2:C:980:VAL:HG23	2.00	0.62
3:D:310:GLY:HA2	3:D:314:ARG:CG	2.29	0.62
3:D:974:VAL:CG1	3:D:1028:ILE:HD13	2.30	0.62
2:C:56:VAL:HG21	2:C:468:LEU:HB3	1.80	0.62
2:C:598:VAL:HG23	2:C:626:GLU:O	1.99	0.62
3:D:80:HIS:HB3	3:D:83:VAL:HG12	1.81	0.62
3:D:1064:SER:O	3:D:1072:LYS:NZ	2.33	0.62
3:D:1183:SER:C	3:D:1185:PRO:HD2	2.20	0.62
3:D:1345:ARG:HG3	3:D:1345:ARG:O	1.99	0.62
5:F:151:VAL:HG22	5:F:156:ALA:CB	2.19	0.62
6:X:71:DA:H2''	6:X:72:DC:C5'	2.30	0.62
3:D:279:LEU:HB2	3:D:295:GLU:HG3	1.82	0.62
3:D:1057:SER:HB3	3:D:1107:VAL:O	1.99	0.62
5:F:161:LEU:HD12	5:F:162:ILE:CB	2.28	0.62
2:C:300:ASP:HB2	2:C:312:ALA:HA	1.81	0.62
2:C:660:VAL:HG21	3:D:769:VAL:CG1	2.30	0.62
3:D:156:ARG:O	3:D:156:ARG:HD3	1.99	0.62
3:D:215:LYS:O	3:D:218:THR:HG22	1.98	0.62
3:D:963:VAL:HA	3:D:980:THR:HG22	1.81	0.62
5:F:252:LEU:HA	5:F:255:VAL:HG12	1.80	0.62
3:D:952:VAL:HG12	3:D:993:GLU:OE2	1.98	0.62
2:C:253:PHE:CE2	2:C:291:TYR:HB2	2.30	0.62
2:C:976:ARG:NH1	2:C:977:ALA:HA	2.14	0.62
3:D:901:ARG:HG2	3:D:907:HIS:O	2.00	0.62
3:D:1011:VAL:HG13	3:D:1015:GLU:OE1	2.00	0.61
5:F:158:LEU:HD12	5:F:161:LEU:HD11	1.81	0.61
1:A:14:VAL:HG12	1:A:15:ASP:N	2.13	0.61
2:C:221:LEU:HD12	2:C:336:LEU:HD21	1.81	0.61
3:D:518:VAL:HG12	3:D:707:ILE:HD13	1.81	0.61
3:D:572:THR:HG21	3:D:589:TYR:HE2	1.65	0.61
3:D:1215:GLU:CG	3:D:1220:ILE:HD11	2.30	0.61
4:E:70:GLN:O	4:E:74:GLU:HG2	2.00	0.61
5:F:144:LEU:HD23	5:F:256:PHE:CD1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:74:DC:H2"	6:X:75:DT:C5	2.35	0.61
2:C:921:PRO:O	2:C:924:VAL:HG12	2.00	0.61
2:C:979:LEU:HD13	2:C:997:TRP:HB3	1.82	0.61
3:D:972:LYS:HE2	3:D:1002:VAL:HG22	1.81	0.61
3:D:1040:MET:HE1	3:D:1059:LEU:HD13	1.80	0.61
5:F:162:ILE:HG12	5:F:165:PHE:CZ	2.34	0.61
3:D:88:CYS:SG	3:D:90:VAL:HG12	2.40	0.61
3:D:474:LEU:HD21	4:E:27:ALA:CB	2.31	0.61
5:F:390:ILE:HD13	5:F:435:ILE:HB	1.81	0.61
1:A:190:ALA:HB2	1:A:200:LYS:HB3	1.82	0.61
1:B:19:VAL:CG2	1:B:23:HIS:HB3	2.29	0.61
3:D:1075:ARG:HH21	3:D:1168:GLU:HG2	1.64	0.61
3:D:1265:THR:OG1	3:D:1303:SER:OG	2.16	0.61
2:C:1335:ILE:HD12	3:D:1336:ALA:HB2	1.83	0.61
3:D:490:ILE:HD12	3:D:614:LEU:HD11	1.83	0.61
3:D:1040:MET:HB2	3:D:1046:ILE:HG21	1.83	0.61
5:F:281:ARG:HA	5:F:284:GLU:HG2	1.83	0.61
5:F:348:GLU:HA	5:F:351:THR:HG22	1.80	0.61
2:C:734:ILE:O	2:C:748:ILE:HG23	2.00	0.61
2:C:850:ILE:HG22	2:C:850:ILE:O	2.00	0.61
2:C:1193:ALA:O	2:C:1197:GLU:HG3	2.00	0.61
3:D:201:LEU:HD11	3:D:220:ARG:HH11	1.65	0.61
3:D:960:LEU:HB3	3:D:963:VAL:CG1	2.29	0.61
3:D:1020:TRP:HZ3	3:D:1022:PRO:HA	1.63	0.61
1:B:62:ASP:OD1	1:B:63:GLY:N	2.34	0.61
5:F:214:PRO:HB2	5:F:218:ARG:HE	1.64	0.61
5:F:525:ASP:OD1	5:F:527:THR:HG22	2.00	0.61
2:C:615:VAL:HG12	2:C:638:SER:CB	2.28	0.61
2:C:715:THR:HG23	2:C:784:ALA:O	2.01	0.61
3:D:145:VAL:CG1	3:D:184:ALA:HB1	2.31	0.61
5:F:99:ARG:O	5:F:103:ARG:HG3	2.01	0.61
5:F:319:ALA:HA	5:F:322:MET:CE	2.30	0.61
1:A:95:LYS:NZ	1:A:120:ASP:OD2	2.20	0.61
1:B:61:ILE:HG12	1:B:142:MET:HB3	1.83	0.61
2:C:549:ASP:OD1	2:C:550:VAL:N	2.33	0.61
3:D:77:ARG:HG2	3:D:79:LYS:NZ	2.16	0.61
5:F:247:GLU:O	5:F:251:LYS:HG2	1.99	0.61
5:F:324:LYS:HB3	5:F:325:PRO:HD2	1.82	0.61
5:F:413:MET:O	5:F:416:VAL:HG12	2.01	0.61
2:C:75:LEU:HD21	2:C:127:ILE:CD1	2.28	0.60
2:C:1157:GLN:HG3	2:C:1159:VAL:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:996:ARG:O	2:C:999:GLU:HG2	2.00	0.60
2:C:82:VAL:HG23	2:C:83:GLN:OE1	2.02	0.60
2:C:714:VAL:O	2:C:767:GLN:NE2	2.34	0.60
3:D:559:ALA:HB3	3:D:562:GLU:HB2	1.83	0.60
5:F:402:LEU:O	5:F:405:ILE:HG12	2.01	0.60
2:C:962:GLU:O	2:C:965:GLN:HG3	2.02	0.60
2:C:1246:ARG:HA	3:D:375:GLU:OE2	2.01	0.60
3:D:342:LEU:O	3:D:343:LEU:HD23	2.00	0.60
3:D:749:LYS:HB2	3:D:750:PRO:HD2	1.82	0.60
3:D:1046:ILE:CG2	3:D:1061:VAL:HG22	2.31	0.60
3:D:1284:ARG:HA	3:D:1287:ILE:HG22	1.81	0.60
5:F:253:SER:HB2	5:F:257:LYS:NZ	2.17	0.60
5:F:489:MET:HG2	5:F:493:LYS:CE	2.31	0.60
2:C:434:ASP:OD1	2:C:439:LYS:HB2	2.01	0.60
2:C:898:GLU:HA	2:C:898:GLU:OE2	2.01	0.60
3:D:71:LEU:H	3:D:90:VAL:HG11	1.65	0.60
2:C:1151:LEU:HD12	2:C:1201:LEU:HD22	1.84	0.60
3:D:316:ILE:HA	3:D:323:PRO:HA	1.84	0.60
3:D:423:LEU:HB3	3:D:466:MET:SD	2.41	0.60
5:F:585:GLU:O	5:F:589:GLN:HG2	2.01	0.60
7:Y:4:DG:H2'	7:Y:5:DT:H6	1.65	0.60
2:C:231:GLU:HB2	2:C:332:ARG:NH1	2.16	0.60
5:F:111:LEU:HD23	5:F:112:THR:O	2.02	0.60
2:C:185:ASP:O	2:C:196:VAL:HG23	2.01	0.60
2:C:898:GLU:HB3	5:F:540:LEU:HD22	1.84	0.60
3:D:197:GLU:O	3:D:201:LEU:HG	2.01	0.60
3:D:1101:LEU:HB3	3:D:1105:ALA:HB3	1.84	0.60
5:F:262:VAL:HG13	5:F:265:GLN:H	1.67	0.60
5:F:337:VAL:O	5:F:341:LEU:HD23	2.01	0.60
2:C:37:LYS:HD2	2:C:47:TYR:CE2	2.37	0.60
2:C:310:ILE:HD11	2:C:324:LYS:HG2	1.82	0.60
3:D:1036:ARG:HH22	3:D:1038:THR:HB	1.67	0.60
1:B:12:ARG:NE	1:B:12:ARG:HA	2.17	0.59
2:C:104:ILE:HD11	2:C:115:LYS:HB3	1.82	0.59
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.37	0.59
5:F:141:ILE:HG12	5:F:252:LEU:CD2	2.32	0.59
2:C:284:LEU:HD23	2:C:285:ILE:N	2.17	0.59
2:C:1023:HIS:O	2:C:1027:LYS:HG2	2.01	0.59
3:D:123:ARG:NH2	3:D:1334:GLU:OE2	2.35	0.59
3:D:430:HIS:NE2	3:D:432:LEU:HB2	2.17	0.59
3:D:860:ARG:O	3:D:862:THR:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:595:LEU:O	5:F:599:ARG:HG3	2.02	0.59
3:D:44:ILE:HG22	3:D:46:TYR:H	1.67	0.59
3:D:317:THR:HA	3:D:324:LEU:HD21	1.84	0.59
2:C:276:GLN:HG2	2:C:279:LYS:HE2	1.82	0.59
7:Y:11:DC:H2"	7:Y:12:DC:C6	2.37	0.59
2:C:52:ALA:HA	2:C:465:ARG:HD3	1.83	0.59
2:C:238:GLN:HB3	2:C:284:LEU:CD2	2.27	0.59
2:C:1164:PHE:HB2	2:C:1168:GLU:OE2	2.02	0.59
3:D:289:ASP:OD1	3:D:290:ILE:N	2.36	0.59
3:D:298:MET:CE	5:F:406:GLN:HG3	2.32	0.59
3:D:965:SER:OG	3:D:975:ILE:HD13	2.03	0.59
3:D:282:LEU:HD21	5:F:410:ILE:HD11	1.84	0.59
3:D:473:THR:O	3:D:477:GLN:HG3	2.03	0.59
3:D:709:ARG:CD	3:D:710:ASP:H	2.08	0.59
1:A:235:ARG:HG3	1:A:236:ASP:N	2.18	0.59
2:C:1253:LEU:CD2	3:D:253:VAL:HG11	2.33	0.59
3:D:208:THR:HG23	3:D:214:ARG:HG2	1.85	0.59
3:D:356:THR:HG22	3:D:357:VAL:N	2.13	0.59
3:D:975:ILE:HG22	3:D:999:TYR:HA	1.85	0.59
5:F:390:ILE:CG2	5:F:435:ILE:HG21	2.32	0.59
2:C:65:ASN:HB3	2:C:105:TYR:CB	2.24	0.59
3:D:1035:VAL:CG2	3:D:1111:ASP:HA	2.32	0.59
3:D:1174:ARG:NH2	3:D:1187:GLU:HG2	2.18	0.59
3:D:268:LEU:HD21	3:D:324:LEU:HD13	1.85	0.59
3:D:1063:ASP:OD1	3:D:1064:SER:N	2.33	0.59
1:B:230:ALA:O	1:B:234:LEU:HD13	2.03	0.58
2:C:1103:VAL:HB	2:C:1104:PRO:HD3	1.84	0.58
3:D:782:GLY:O	3:D:786:THR:HG23	2.03	0.58
5:F:147:GLN:OE1	5:F:265:GLN:NE2	2.35	0.58
1:A:214:GLU:O	1:A:218:ARG:HG3	2.03	0.58
2:C:251:ALA:HB1	2:C:255:ILE:CD1	2.33	0.58
2:C:580:GLN:O	2:C:587:LEU:HD23	2.03	0.58
2:C:895:LEU:HD13	2:C:903:ARG:HH12	1.68	0.58
5:F:250:LEU:O	5:F:254:GLU:OE1	2.21	0.58
3:D:1167:LYS:HB3	3:D:1170:LYS:HE3	1.85	0.58
5:F:327:SER:O	5:F:331:HIS:ND1	2.23	0.58
5:F:390:ILE:HD13	5:F:435:ILE:CG2	2.32	0.58
2:C:596:ASP:OD1	2:C:597:GLY:N	2.32	0.58
2:C:621:SER:HB2	2:C:653:MET:CE	2.34	0.58
3:D:1175:LEU:HD23	3:D:1176:VAL:N	2.18	0.58
5:F:161:LEU:CD1	5:F:162:ILE:HB	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:315:TRP:HZ2	5:F:341:LEU:HD21	1.68	0.58
1:B:107:ILE:HD11	1:B:136:GLU:HB3	1.85	0.58
2:C:179:TYR:HB2	2:C:397:LEU:O	2.03	0.58
2:C:545:PHE:HZ	3:D:788:LEU:HD13	1.66	0.58
2:C:820:GLU:O	2:C:823:VAL:HG12	2.03	0.58
2:C:1021:LEU:HA	2:C:1024:GLU:CG	2.33	0.58
3:D:794:GLY:O	3:D:797:THR:HG22	2.03	0.58
4:E:16:ARG:O	4:E:16:ARG:HG2	2.02	0.58
5:F:563:PHE:HB2	5:F:565:ILE:CD1	2.33	0.58
1:A:102:LEU:HD11	1:A:114:ASP:HB2	1.85	0.58
2:C:1186:VAL:HG23	2:C:1187:PHE:H	1.68	0.58
3:D:317:THR:OG1	3:D:320:ASN:HB2	2.04	0.58
3:D:1051:ASP:HB2	3:D:1056:LEU:O	2.04	0.58
3:D:1226:VAL:O	3:D:1229:VAL:HG12	2.04	0.58
5:F:374:ARG:O	5:F:378:GLU:OE1	2.21	0.58
6:X:66:DC:H1'	6:X:67:DA:H5'	1.86	0.58
1:B:192:VAL:HG12	1:B:198:LEU:CD1	2.33	0.58
3:D:128:LEU:HD23	3:D:192:MET:CE	2.33	0.58
3:D:416:ILE:HD13	3:D:441:LEU:HD21	1.85	0.58
5:F:102:MET:O	5:F:105:MET:HG3	2.03	0.58
5:F:383:ASN:HB3	5:F:412:LEU:CD1	2.20	0.58
6:X:72:DC:H1'	6:X:73:DT:C5'	2.33	0.58
6:X:72:DC:C2'	6:X:73:DT:H5'	2.32	0.58
3:D:384:LYS:HG3	3:D:415:VAL:HG12	1.85	0.58
3:D:876:SER:OG	3:D:988:PHE:O	2.15	0.58
1:A:27:THR:C	1:A:28:LEU:HD12	2.24	0.58
2:C:237:LEU:HD11	2:C:289:VAL:CG2	2.33	0.58
3:D:981:GLU:OE2	3:D:983:LYS:HD3	2.04	0.58
3:D:1244:GLN:O	3:D:1244:GLN:HG3	2.03	0.58
3:D:1327:GLU:HG2	3:D:1327:GLU:O	2.03	0.58
3:D:1367:GLN:O	3:D:1371:ARG:HG3	2.04	0.58
5:F:150:ARG:HB3	5:F:155:GLU:HG2	1.86	0.58
2:C:398:SER:CB	2:C:401:GLY:H	2.16	0.58
3:D:615:LYS:O	3:D:618:VAL:HG22	2.04	0.58
3:D:1002:VAL:O	3:D:1018:ALA:HA	2.03	0.58
2:C:272:ARG:HG3	2:C:275:ARG:HH21	1.69	0.57
2:C:453:ILE:HD11	2:C:530:ILE:HD12	1.86	0.57
2:C:1018:TYR:O	2:C:1022:LYS:HG2	2.03	0.57
3:D:1075:ARG:NH2	3:D:1168:GLU:HG2	2.19	0.57
3:D:1278:GLU:OE2	3:D:1283:SER:HB2	2.04	0.57
5:F:133:SER:HA	5:F:136:GLU:OE1	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:895:LEU:HD21	2:C:900:LYS:HD3	1.85	0.57
3:D:204:GLU:HB3	3:D:217:LEU:HD21	1.86	0.57
2:C:993:PRO:HB2	2:C:995:ASP:OD1	2.04	0.57
2:C:1304:MET:HE2	2:C:1308:ILE:HD11	1.86	0.57
3:D:118:LYS:HG3	3:D:118:LYS:O	2.05	0.57
3:D:220:ARG:O	3:D:224:LEU:HD13	2.04	0.57
3:D:656:GLU:O	3:D:660:GLU:HG3	2.04	0.57
5:F:491:GLU:HA	5:F:494:ILE:HD13	1.86	0.57
1:A:41:ASN:O	1:A:45:ARG:HG2	2.05	0.57
2:C:595:THR:HG22	2:C:596:ASP:N	2.15	0.57
2:C:1157:GLN:HG3	2:C:1159:VAL:CG2	2.34	0.57
3:D:77:ARG:HG3	3:D:78:LEU:N	2.19	0.57
3:D:733:SER:O	3:D:737:ILE:HG12	2.03	0.57
5:F:370:ALA:O	5:F:374:ARG:HD3	2.04	0.57
7:Y:10:DT:C2'	7:Y:11:DC:H5'	2.24	0.57
1:A:188:GLU:HG3	1:A:200:LYS:HE3	1.87	0.57
1:A:231:PHE:CE1	1:B:39:LEU:HD13	2.38	0.57
1:B:107:ILE:CD1	1:B:136:GLU:HB3	2.34	0.57
2:C:301:TYR:CB	2:C:311:CYS:HB3	2.29	0.57
2:C:985:GLU:CG	2:C:988:LYS:HE2	2.32	0.57
2:C:1339:LEU:HD23	3:D:20:ILE:HG12	1.87	0.57
4:E:3:ARG:HG2	4:E:48:VAL:HG23	1.86	0.57
5:F:320:ILE:HA	5:F:327:SER:OG	2.04	0.57
5:F:386:LEU:O	5:F:390:ILE:HG22	2.05	0.57
5:F:503:GLU:CD	5:F:504:PRO:HD2	2.25	0.57
3:D:210:SER:CB	3:D:213:LYS:HE2	2.34	0.57
5:F:466:ILE:O	5:F:470:MET:HE2	2.05	0.57
5:F:481:GLU:O	5:F:485:GLU:OE1	2.21	0.57
1:A:228:LEU:HD11	1:B:224:LEU:CD2	2.33	0.57
2:C:1002:LEU:HD12	2:C:1007:LYS:HB3	1.86	0.57
2:C:1186:VAL:HG23	2:C:1187:PHE:N	2.18	0.57
3:D:1178:THR:OG1	3:D:1184:ASP:OD1	2.11	0.57
3:D:1278:GLU:OE1	3:D:1278:GLU:N	2.38	0.57
2:C:230:PHE:O	2:C:332:ARG:HA	2.04	0.57
3:D:1221:LEU:HA	3:D:1225:GLY:O	2.05	0.57
5:F:286:LEU:HD12	5:F:287:ILE:N	2.20	0.57
5:F:573:LEU:HD12	5:F:574:GLU:N	2.18	0.57
2:C:993:PRO:CD	2:C:996:ARG:HG3	2.26	0.57
3:D:120:LEU:CB	3:D:121:PRO:HD3	2.30	0.57
6:X:72:DC:H1'	6:X:73:DT:H5'	1.87	0.57
2:C:475:VAL:HG22	2:C:492:MET:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:813:GLU:HA	2:C:813:GLU:OE1	2.05	0.57
5:F:387:VAL:CG2	5:F:412:LEU:HD13	2.31	0.57
1:B:230:ALA:O	1:B:234:LEU:HD22	2.04	0.56
2:C:169:LYS:O	2:C:171:LEU:HD12	2.05	0.56
2:C:233:ARG:HB2	2:C:238:GLN:CD	2.25	0.56
2:C:1270:PHE:O	3:D:344:GLY:HA2	2.05	0.56
2:C:1335:ILE:HG21	3:D:22:ILE:HD11	1.87	0.56
3:D:146:VAL:HG23	3:D:176:PHE:HE1	1.70	0.56
3:D:1078:LEU:HB3	3:D:1099:TYR:O	2.05	0.56
5:F:161:LEU:HD12	5:F:162:ILE:N	2.19	0.56
5:F:474:MET:HE1	5:F:482:GLU:OE1	2.05	0.56
2:C:196:VAL:HG21	2:C:209:ILE:HD11	1.87	0.56
2:C:221:LEU:HD12	2:C:336:LEU:CD2	2.35	0.56
2:C:1021:LEU:HA	2:C:1024:GLU:HG3	1.87	0.56
3:D:146:VAL:HG12	3:D:158:GLN:O	2.05	0.56
3:D:788:LEU:HD23	3:D:792:ASN:ND2	2.20	0.56
3:D:1025:MET:O	3:D:1122:ALA:HB3	2.04	0.56
2:C:104:ILE:HG12	2:C:115:LYS:O	2.06	0.56
3:D:611:ILE:CG2	3:D:612:LEU:HD12	2.34	0.56
3:D:824:PRO:HD3	3:D:835:LEU:HD13	1.86	0.56
3:D:833:GLU:OE2	3:D:837:ASP:HB2	2.06	0.56
3:D:955:LYS:HD3	3:D:956:GLY:H	1.69	0.56
3:D:1057:SER:OG	3:D:1059:LEU:HG	2.06	0.56
3:D:1267:VAL:HG22	3:D:1267:VAL:O	2.04	0.56
5:F:276:MET:HE1	5:F:347:ILE:HD12	1.83	0.56
6:X:68:DC:H1'	6:X:69:DG:H5''	1.88	0.56
1:A:26:VAL:HG11	1:A:217:ILE:CD1	2.35	0.56
2:C:301:TYR:N	2:C:311:CYS:O	2.35	0.56
2:C:634:VAL:HG23	2:C:636:CYS:SG	2.45	0.56
3:D:557:LYS:HA	3:D:562:GLU:O	2.05	0.56
3:D:843:VAL:HG13	3:D:883:ARG:HD3	1.86	0.56
3:D:957:SER:HB3	3:D:985:ILE:O	2.06	0.56
5:F:164:GLY:O	5:F:260:ARG:HB3	2.05	0.56
3:D:1143:ASP:OD1	3:D:1148:ARG:NH1	2.37	0.56
5:F:127:ILE:O	5:F:131:GLN:OE1	2.23	0.56
3:D:144:TYR:HB2	3:D:160:LEU:O	2.06	0.56
3:D:202:ARG:NE	3:D:221:ILE:HG21	2.20	0.56
3:D:984:LEU:HD12	3:D:993:GLU:OE2	2.06	0.56
3:D:1163:VAL:CG2	3:D:1175:LEU:HD11	2.36	0.56
4:E:5:THR:HG22	4:E:7:GLN:H	1.71	0.56
6:X:70:DG:N2	7:Y:11:DC:O2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:17:LYS:HG3	2:C:1154:ASP:O	2.06	0.56
3:D:31:ARG:NH1	3:D:106:GLU:OE2	2.37	0.56
3:D:973:LEU:HD13	3:D:1003:LEU:HD22	1.88	0.56
3:D:977:SER:HB3	3:D:980:THR:HG23	1.86	0.56
5:F:132:CYS:O	5:F:135:ALA:HB3	2.06	0.56
5:F:316:PHE:O	5:F:320:ILE:HD12	2.06	0.56
5:F:324:LYS:HB2	5:F:326:TRP:CD1	2.41	0.56
1:B:97:GLU:OE2	1:B:145:LYS:HE3	2.06	0.56
2:C:231:GLU:OE1	2:C:231:GLU:N	2.39	0.56
2:C:247:ARG:HA	2:C:274:ILE:HD11	1.88	0.56
2:C:289:VAL:HG11	2:C:319:LEU:HD13	1.88	0.56
2:C:1160:ASP:HB2	2:C:1162:SER:N	2.21	0.56
3:D:75:TYR:OH	3:D:86:GLU:OE1	2.24	0.56
3:D:948:SER:HB2	3:D:1020:TRP:O	2.06	0.56
3:D:1160:SER:HB2	3:D:1206:ARG:H	1.70	0.56
5:F:291:CYS:SG	5:F:292:VAL:HG23	2.46	0.56
5:F:344:LEU:HA	5:F:347:ILE:CG1	2.36	0.56
2:C:109:ALA:HB1	2:C:110:PRO:HD2	1.88	0.56
2:C:264:GLU:OE1	2:C:264:GLU:N	2.38	0.56
2:C:1005:GLU:OE2	2:C:1006:GLU:HG2	2.06	0.56
3:D:130:MET:HG2	3:D:157:GLN:CD	2.27	0.56
3:D:492:SER:HB3	3:D:495:ASN:O	2.06	0.56
3:D:826:ILE:O	3:D:826:ILE:HG13	2.05	0.56
3:D:1061:VAL:HG11	3:D:1101:LEU:HD12	1.89	0.56
3:D:1281:GLU:O	3:D:1285:VAL:HG23	2.06	0.56
5:F:292:VAL:CG1	5:F:296:LYS:HD2	2.31	0.56
1:B:71:LYS:NZ	1:B:139:SER:O	2.26	0.55
2:C:106:GLU:N	2:C:114:VAL:HG21	2.20	0.55
2:C:1151:LEU:HD12	2:C:1201:LEU:CD2	2.36	0.55
3:D:705:THR:OG1	3:D:718:SER:HA	2.06	0.55
3:D:973:LEU:HD22	3:D:1003:LEU:CD1	2.34	0.55
3:D:984:LEU:O	3:D:991:THR:HA	2.06	0.55
5:F:131:GLN:O	5:F:134:VAL:HG22	2.06	0.55
5:F:502:LYS:HG2	5:F:503:GLU:N	2.21	0.55
2:C:185:ASP:OD1	2:C:186:PHE:N	2.39	0.55
2:C:210:LEU:O	2:C:215:TYR:HB2	2.06	0.55
2:C:217:THR:O	2:C:221:LEU:HD23	2.06	0.55
2:C:621:SER:HB2	2:C:653:MET:HE3	1.87	0.55
3:D:823:THR:HG22	3:D:879:ALA:CB	2.36	0.55
3:D:1044:GLN:NE2	3:D:1074:LEU:HD23	2.21	0.55
3:D:1284:ARG:HA	3:D:1287:ILE:CG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:319:ALA:HA	5:F:322:MET:HE2	1.87	0.55
5:F:574:GLU:HB3	5:F:578:LYS:NZ	2.21	0.55
2:C:1164:PHE:HB3	2:C:1168:GLU:HB2	1.87	0.55
3:D:902:ASP:H	3:D:1251:LYS:HZ2	1.52	0.55
3:D:1243:LEU:O	3:D:1243:LEU:HD23	2.06	0.55
2:C:367:TYR:CD2	2:C:381:ALA:HA	2.37	0.55
2:C:273:HIS:O	2:C:277:LEU:HD23	2.07	0.55
3:D:43:THR:HG21	3:D:252:LEU:HD22	1.89	0.55
4:E:32:VAL:HG23	4:E:34:GLY:H	1.72	0.55
5:F:333:VAL:HG22	5:F:336:GLU:HG3	1.89	0.55
1:A:26:VAL:HG21	1:A:217:ILE:HD11	1.89	0.55
3:D:950:ILE:HG13	3:D:950:ILE:O	2.05	0.55
3:D:1044:GLN:HE22	3:D:1074:LEU:HB2	1.71	0.55
5:F:102:MET:HA	5:F:105:MET:HG3	1.88	0.55
5:F:144:LEU:HD11	5:F:148:TYR:CE2	2.41	0.55
1:A:162:GLU:HG2	1:A:163:GLU:N	2.21	0.55
2:C:8:LYS:HD3	2:C:1168:GLU:OE1	2.07	0.55
3:D:821:MET:HE3	3:D:879:ALA:HB1	1.88	0.55
3:D:967:VAL:HG12	3:D:973:LEU:HD12	1.89	0.55
5:F:283:GLN:HA	5:F:286:LEU:CD2	2.36	0.55
5:F:285:ARG:O	5:F:289:LYS:HD3	2.06	0.55
5:F:585:GLU:OE1	5:F:588:ARG:HD2	2.06	0.55
3:D:278:ARG:NH2	5:F:403:ASP:OD2	2.38	0.55
3:D:966:VAL:O	3:D:974:VAL:HG23	2.07	0.55
4:E:69:ARG:NH2	4:E:72:GLN:OE1	2.40	0.55
2:C:1142:ARG:NH2	2:C:1165:SER:O	2.37	0.55
2:C:1159:VAL:CG1	2:C:1160:ASP:H	2.15	0.55
6:X:69:DG:H1	7:Y:12:DC:H42	1.55	0.55
1:B:64:VAL:HG23	1:B:69:SER:OG	2.06	0.55
1:B:73:GLY:O	1:B:134:THR:OG1	2.18	0.55
2:C:994:ARG:H	2:C:994:ARG:HD2	1.71	0.55
3:D:1107:VAL:HG12	3:D:1109:LEU:O	2.07	0.55
5:F:358:VAL:HG13	5:F:359:LYS:HE2	1.89	0.55
2:C:145:ILE:HD13	2:C:512:SER:HA	1.89	0.54
3:D:1356:LEU:O	3:D:1366:HIS:NE2	2.26	0.54
1:A:98:VAL:HG11	1:A:121:VAL:HG11	1.90	0.54
1:A:224:LEU:HD23	1:B:228:LEU:HD11	1.90	0.54
2:C:301:TYR:O	2:C:311:CYS:N	2.28	0.54
2:C:988:LYS:HB3	2:C:992:LEU:HD12	1.87	0.54
3:D:77:ARG:HG2	3:D:79:LYS:HZ2	1.72	0.54
5:F:497:VAL:HA	5:F:500:ILE:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:30:MET:HE3	4:E:37:PRO:HB3	1.88	0.54
5:F:482:GLU:HA	5:F:485:GLU:OE2	2.07	0.54
6:X:71:DA:H2"	6:X:72:DC:H5"	1.90	0.54
2:C:122:VAL:CB	2:C:493:ILE:HD11	2.37	0.54
3:D:77:ARG:HG3	3:D:78:LEU:H	1.72	0.54
3:D:972:LYS:CE	3:D:1002:VAL:HA	2.36	0.54
5:F:394:TYR:O	5:F:404:LEU:HD13	2.07	0.54
2:C:397:LEU:O	2:C:398:SER:OG	2.25	0.54
2:C:406:ASN:ND2	2:C:411:ARG:HD2	2.22	0.54
2:C:817:LEU:HD12	2:C:1078:LYS:HB3	1.89	0.54
2:C:996:ARG:HA	2:C:999:GLU:HG2	1.88	0.54
2:C:1021:LEU:O	2:C:1024:GLU:HG3	2.07	0.54
3:D:662:ALA:O	3:D:666:GLU:HG2	2.07	0.54
3:D:948:SER:O	3:D:1019:ASN:HA	2.07	0.54
1:B:14:VAL:HG12	1:B:15:ASP:N	2.19	0.54
1:B:188:GLU:OE1	1:B:200:LYS:HD3	2.08	0.54
3:D:152:THR:HG22	3:D:153:ASN:N	2.23	0.54
3:D:1067:ARG:HB2	3:D:1072:LYS:HZ2	1.72	0.54
7:Y:11:DC:H2"	7:Y:12:DC:C5	2.42	0.54
3:D:121:PRO:HB2	3:D:123:ARG:HH12	1.72	0.54
3:D:426:ALA:CB	3:D:427:PRO:HD3	2.26	0.54
3:D:701:LEU:HD23	3:D:701:LEU:O	2.08	0.54
5:F:344:LEU:CA	5:F:347:ILE:HG12	2.38	0.54
5:F:489:MET:HB3	5:F:490:PRO:CD	2.37	0.54
2:C:448:LEU:HB2	2:C:553:THR:HG21	1.90	0.54
3:D:857:LEU:CD1	3:D:871:LEU:HD21	2.38	0.54
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.90	0.54
5:F:387:VAL:HG11	5:F:409:ASN:OD1	2.07	0.54
2:C:898:GLU:HB3	5:F:540:LEU:CD2	2.38	0.54
2:C:1109:ILE:HG22	2:C:1109:ILE:O	2.07	0.54
3:D:103:GLY:C	3:D:244:VAL:HG22	2.28	0.54
3:D:885:VAL:CG2	3:D:894:VAL:HG11	2.37	0.54
3:D:946:ALA:HA	3:D:1022:PRO:HG2	1.90	0.54
3:D:1078:LEU:CD1	3:D:1101:LEU:HD21	2.38	0.54
3:D:1090:ILE:HB	3:D:1093:THR:HG22	1.89	0.54
1:A:166:ARG:N	1:A:167:PRO:HD2	2.23	0.54
1:B:41:ASN:O	1:B:45:ARG:HG2	2.07	0.54
3:D:697:MET:HE3	3:D:738:ARG:HA	1.90	0.54
1:A:158:ARG:HG2	1:A:163:GLU:OE1	2.08	0.53
2:C:127:ILE:O	2:C:127:ILE:HG13	2.08	0.53
3:D:902:ASP:H	3:D:1251:LYS:NZ	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1209:VAL:HG12	3:D:1211:SER:O	2.08	0.53
4:E:30:MET:HE3	4:E:49:ILE:HG21	1.89	0.53
5:F:561:MET:HA	5:F:567:MET:CE	2.37	0.53
2:C:1220:GLN:HG3	2:C:1220:GLN:O	2.08	0.53
3:D:1046:ILE:O	3:D:1046:ILE:HG13	2.07	0.53
5:F:141:ILE:H	5:F:141:ILE:HD12	1.73	0.53
5:F:292:VAL:CG1	5:F:296:LYS:HA	2.34	0.53
5:F:343:LYS:O	5:F:347:ILE:HG23	2.08	0.53
1:B:77:ASP:O	1:B:81:ILE:HG12	2.09	0.53
2:C:228:VAL:HB	2:C:335:THR:OG1	2.09	0.53
2:C:244:GLU:O	2:C:247:ARG:HG2	2.08	0.53
3:D:848:VAL:CG1	3:D:858:VAL:HB	2.39	0.53
3:D:1106:ILE:HD11	3:D:1123:ARG:HG2	1.90	0.53
5:F:379:MET:HG2	5:F:416:VAL:CG2	2.33	0.53
2:C:230:PHE:CE1	2:C:292:ILE:HD12	2.43	0.53
3:D:279:LEU:HD13	3:D:295:GLU:CG	2.39	0.53
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.91	0.53
3:D:1027:VAL:CG2	3:D:1121:LEU:HB3	2.37	0.53
3:D:1030:GLU:HG2	3:D:1031:VAL:HG13	1.89	0.53
5:F:113:ARG:H	5:F:113:ARG:HD3	1.72	0.53
1:B:64:VAL:HG11	1:B:78:ILE:HD11	1.91	0.53
2:C:563:THR:HG21	3:D:780:ARG:NH1	2.23	0.53
2:C:690:VAL:HG12	2:C:1234:LYS:O	2.08	0.53
3:D:1158:GLU:HG2	3:D:1186:TYR:CZ	2.44	0.53
7:Y:9:DG:H2''	7:Y:10:DT:H5'	1.91	0.53
2:C:67:GLU:N	2:C:103:VAL:O	2.29	0.53
3:D:502:PRO:HB3	3:D:506:VAL:HB	1.91	0.53
4:E:15:ASN:HB3	4:E:18:ASP:OD1	2.08	0.53
5:F:379:MET:CG	5:F:416:VAL:HG21	2.34	0.53
5:F:586:ARG:O	5:F:590:ILE:HG13	2.09	0.53
2:C:903:ARG:O	2:C:907:GLY:N	2.33	0.53
2:C:908:GLU:HG2	5:F:611:LEU:HD11	1.91	0.53
2:C:976:ARG:HH11	2:C:980:VAL:CG2	2.19	0.53
3:D:411:ILE:O	3:D:415:VAL:HG13	2.08	0.53
3:D:709:ARG:NH1	3:D:710:ASP:HB3	2.23	0.53
3:D:821:MET:CE	3:D:879:ALA:HB1	2.39	0.53
5:F:133:SER:HB3	5:F:361:ILE:HG23	1.90	0.53
1:B:58:GLU:HB2	1:B:171:LEU:O	2.09	0.53
3:D:157:GLN:HG2	3:D:157:GLN:O	2.08	0.53
3:D:407:VAL:O	3:D:411:ILE:HG12	2.08	0.53
5:F:270:VAL:CG1	5:F:274:ARG:HE	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:5:TYR:O	2:C:9:LYS:HG3	2.09	0.53
2:C:119:GLU:HB3	2:C:489:PRO:HG2	1.88	0.53
2:C:632:ASP:OD1	2:C:633:LEU:N	2.42	0.53
3:D:957:SER:O	3:D:958:ILE:HD13	2.09	0.53
3:D:1330:ARG:O	3:D:1334:GLU:OE1	2.27	0.53
2:C:309:LEU:HD21	2:C:312:ALA:HB2	1.90	0.53
2:C:985:GLU:HG3	2:C:988:LYS:CE	2.36	0.53
3:D:1150:PRO:O	3:D:1151:LYS:HG2	2.08	0.53
3:D:1164:SER:O	3:D:1175:LEU:HG	2.09	0.53
1:B:44:ARG:HH11	1:B:44:ARG:HG2	1.74	0.52
1:B:165:GLU:HB3	1:B:170:ARG:CD	2.38	0.52
2:C:448:LEU:HB2	2:C:553:THR:CG2	2.40	0.52
3:D:363:LEU:HD12	3:D:363:LEU:O	2.09	0.52
5:F:299:LYS:O	5:F:303:ILE:HG13	2.09	0.52
5:F:302:PHE:HA	5:F:305:LEU:HD21	1.91	0.52
1:B:159:ILE:HG12	1:B:172:LEU:HD12	1.90	0.52
2:C:248:GLY:O	2:C:249:GLU:HG3	2.08	0.52
2:C:629:PHE:HB2	2:C:647:ARG:HG3	1.90	0.52
3:D:46:TYR:HB3	5:F:450:ILE:HG22	1.87	0.52
3:D:1190:ILE:H	3:D:1190:ILE:HD12	1.73	0.52
1:B:159:ILE:CG1	1:B:172:LEU:HD12	2.39	0.52
2:C:178:PRO:CB	2:C:397:LEU:HD23	2.39	0.52
2:C:250:THR:HA	2:C:268:ARG:HA	1.91	0.52
2:C:256:GLU:CB	2:C:261:VAL:HA	2.40	0.52
2:C:309:LEU:HD23	2:C:309:LEU:O	2.09	0.52
2:C:832:HIS:CD2	2:C:1058:ARG:HG3	2.44	0.52
3:D:43:THR:CG2	3:D:252:LEU:HD22	2.38	0.52
3:D:801:VAL:O	3:D:805:GLN:HB3	2.09	0.52
3:D:1215:GLU:HG2	3:D:1220:ILE:HD11	1.91	0.52
5:F:369:GLU:O	5:F:373:ARG:HG2	2.10	0.52
5:F:383:ASN:CB	5:F:412:LEU:HD21	2.38	0.52
3:D:154:LEU:HA	3:D:158:GLN:NE2	2.25	0.52
3:D:1004:ALA:C	3:D:1005:LYS:HD3	2.30	0.52
3:D:1266:ILE:HG23	3:D:1274:PHE:HA	1.92	0.52
5:F:265:GLN:O	5:F:269:LEU:HD23	2.09	0.52
5:F:292:VAL:HG22	5:F:297:MET:SD	2.50	0.52
2:C:903:ARG:HD3	2:C:908:GLU:O	2.10	0.52
2:C:974:ARG:HD2	2:C:974:ARG:O	2.10	0.52
2:C:1007:LYS:O	2:C:1011:LEU:HG	2.09	0.52
3:D:394:ILE:HG12	5:F:532:LEU:HD11	1.91	0.52
5:F:347:ILE:HG13	5:F:348:GLU:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:ARG:HG3	2:C:1181:PRO:HB2	1.90	0.52
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.92	0.52
2:C:276:GLN:HA	2:C:279:LYS:CE	2.37	0.52
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.92	0.52
2:C:564:PRO:HG3	2:C:572:ILE:HG13	1.92	0.52
3:D:43:THR:HG22	3:D:44:ILE:HG12	1.91	0.52
3:D:967:VAL:HA	3:D:972:LYS:O	2.09	0.52
3:D:1172:LYS:HD2	3:D:1191:PRO:HG3	1.92	0.52
2:C:59:ILE:CD1	2:C:472:GLU:HG2	2.40	0.52
2:C:715:THR:CG2	2:C:782:VAL:HG13	2.40	0.52
2:C:895:LEU:HD23	2:C:895:LEU:H	1.75	0.52
3:D:145:VAL:HG21	3:D:188:LEU:HD21	1.90	0.52
4:E:3:ARG:HG2	4:E:48:VAL:CG2	2.40	0.52
5:F:481:GLU:O	5:F:484:ALA:HB3	2.09	0.52
1:A:135:ASP:HB3	1:A:138:ALA:HB2	1.91	0.52
3:D:127:LEU:HD23	3:D:189:LEU:CD2	2.40	0.52
3:D:630:ALA:O	3:D:634:ARG:HG3	2.09	0.52
3:D:903:LEU:HD21	3:D:909:ILE:HD12	1.92	0.52
5:F:303:ILE:O	5:F:307:THR:N	2.39	0.52
5:F:344:LEU:O	5:F:347:ILE:HG12	2.10	0.52
2:C:854:ILE:HG23	2:C:855:PRO:HD2	1.92	0.52
3:D:227:PHE:CE2	3:D:234:PRO:HG3	2.45	0.52
3:D:478:LEU:HD21	4:E:47:THR:HG23	1.92	0.52
3:D:870:ASP:HA	3:D:873:GLU:HG2	1.92	0.52
5:F:219:GLU:OE2	5:F:220:LYS:HG2	2.10	0.52
7:Y:9:DG:H2'	7:Y:10:DT:C6	2.44	0.52
2:C:163:LYS:H	2:C:163:LYS:HD3	1.75	0.52
2:C:294:GLY:HA2	2:C:316:GLU:OE2	2.10	0.52
3:D:146:VAL:HG23	3:D:176:PHE:CE1	2.45	0.52
3:D:972:LYS:HD3	3:D:1002:VAL:HA	1.91	0.52
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.45	0.51
5:F:124:GLU:O	5:F:127:ILE:HG22	2.09	0.51
6:X:74:DC:H2''	6:X:75:DT:C4	2.44	0.51
1:A:14:VAL:HG21	1:A:29:GLU:HB2	1.92	0.51
2:C:565:GLU:HG2	2:C:565:GLU:O	2.10	0.51
2:C:1160:ASP:CB	2:C:1161:LEU:CA	2.85	0.51
2:C:1269:ARG:HH12	3:D:344:GLY:HA3	1.75	0.51
2:C:1335:ILE:HD12	3:D:1336:ALA:CB	2.40	0.51
3:D:62:PHE:O	3:D:98:ARG:HA	2.10	0.51
3:D:697:MET:HE1	3:D:738:ARG:HA	1.91	0.51
3:D:844:THR:O	3:D:861:ASN:HA	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1038:THR:HG23	3:D:1077:ALA:HB3	1.92	0.51
3:D:1106:ILE:HD11	3:D:1123:ARG:CG	2.40	0.51
3:D:1208:ASP:OD1	3:D:1209:VAL:N	2.43	0.51
5:F:166:VAL:HG13	5:F:258:GLN:O	2.11	0.51
5:F:244:THR:O	5:F:248:GLU:HG2	2.10	0.51
7:Y:13:DG:H2"	7:Y:14:DT:H71	1.91	0.51
2:C:59:ILE:HG12	2:C:472:GLU:CG	2.41	0.51
2:C:119:GLU:OE1	2:C:119:GLU:HA	2.10	0.51
2:C:406:ASN:HD22	2:C:411:ARG:HD2	1.74	0.51
2:C:1021:LEU:HG	2:C:1024:GLU:OE2	2.10	0.51
3:D:227:PHE:HE2	3:D:234:PRO:HG3	1.74	0.51
2:C:339:ASN:OD1	2:C:340:ASP:N	2.44	0.51
2:C:624:ASP:OD1	2:C:624:ASP:O	2.28	0.51
3:D:251:PRO:HG2	5:F:507:MET:CE	2.39	0.51
3:D:646:ILE:HD12	3:D:762:ASN:HD21	1.74	0.51
3:D:712:GLN:H	3:D:712:GLN:CD	2.13	0.51
3:D:1184:ASP:N	3:D:1185:PRO:CD	2.72	0.51
5:F:272:SER:O	5:F:275:VAL:HG12	2.10	0.51
5:F:316:PHE:HE1	5:F:330:LEU:HD21	1.75	0.51
6:X:72:DC:H42	7:Y:8:DA:H61	1.58	0.51
1:B:179:PRO:O	1:B:207:THR:HG23	2.09	0.51
2:C:1244:HIS:HB2	2:C:1262:LYS:CE	2.29	0.51
3:D:24:LEU:HD21	3:D:116:PHE:CE2	2.45	0.51
3:D:1082:ASP:HB3	3:D:1088:VAL:HG11	1.93	0.51
5:F:141:ILE:HG21	5:F:252:LEU:HD21	1.92	0.51
2:C:28:LEU:HD21	2:C:524:ILE:CD1	2.34	0.51
2:C:678:ARG:CZ	2:C:1106:ARG:HD2	2.40	0.51
3:D:14:THR:O	3:D:14:THR:HG22	2.10	0.51
3:D:515:ARG:HH22	3:D:717:VAL:HB	1.75	0.51
3:D:946:ALA:O	3:D:947:GLU:HG2	2.10	0.51
5:F:479:THR:HG23	5:F:482:GLU:H	1.75	0.51
2:C:5:TYR:HE2	2:C:778:GLU:HG2	1.74	0.51
2:C:914:LYS:HG2	2:C:915:ASP:N	2.26	0.51
3:D:1035:VAL:HG23	3:D:1111:ASP:HA	1.92	0.51
3:D:1057:SER:O	3:D:1108:GLN:HA	2.11	0.51
5:F:453:PRO:HB2	5:F:455:HIS:CD2	2.45	0.51
5:F:488:LEU:HD23	5:F:488:LEU:H	1.76	0.51
2:C:303:ASP:HB3	2:C:306:THR:OG1	2.11	0.51
3:D:1179:PRO:HB2	3:D:1182:GLY:N	2.26	0.51
5:F:148:TYR:OH	5:F:162:ILE:HD13	2.10	0.51
5:F:252:LEU:O	5:F:255:VAL:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:333:VAL:HG13	5:F:337:VAL:CG2	2.40	0.51
5:F:412:LEU:HB2	5:F:435:ILE:HD11	1.93	0.51
5:F:503:GLU:CG	5:F:504:PRO:HD2	2.41	0.51
2:C:272:ARG:HA	2:C:275:ARG:HE	1.76	0.51
2:C:514:PHE:CE2	2:C:760:ASN:HB3	2.46	0.51
2:C:533:LEU:HD21	2:C:571:LEU:HD13	1.91	0.51
2:C:685:MET:HE1	2:C:1071:GLY:HA2	1.92	0.51
2:C:1151:LEU:HD13	2:C:1198:LEU:HD12	1.92	0.51
3:D:649:LYS:O	3:D:653:ILE:HG13	2.11	0.51
3:D:964:LYS:CG	3:D:977:SER:HB2	2.38	0.51
3:D:973:LEU:CB	3:D:1003:LEU:HD13	2.40	0.51
3:D:976:THR:HA	3:D:999:TYR:HE1	1.76	0.51
2:C:109:ALA:HB1	2:C:110:PRO:CD	2.42	0.51
2:C:115:LYS:HD3	2:C:116:ASP:H	1.74	0.51
2:C:312:ALA:C	2:C:315:MET:HE2	2.32	0.51
2:C:436:ARG:HD2	2:C:436:ARG:O	2.11	0.51
3:D:965:SER:HA	3:D:974:VAL:O	2.11	0.51
2:C:1115:THR:CG2	2:C:1228:GLY:HA3	2.41	0.50
3:D:54:ASP:OD2	3:D:60:ARG:NH2	2.43	0.50
3:D:946:ALA:O	3:D:1022:PRO:HG3	2.11	0.50
5:F:330:LEU:HD12	5:F:333:VAL:HG11	1.93	0.50
2:C:60:GLN:HG2	2:C:67:GLU:CD	2.30	0.50
3:D:196:GLN:N	3:D:196:GLN:OE1	2.44	0.50
3:D:268:LEU:HD21	3:D:324:LEU:CD1	2.41	0.50
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.93	0.50
3:D:1344:LEU:O	3:D:1346:GLY:N	2.44	0.50
5:F:282:THR:O	5:F:285:ARG:HG2	2.10	0.50
2:C:1151:LEU:CD1	2:C:1198:LEU:HD12	2.40	0.50
2:C:1269:ARG:NH1	3:D:344:GLY:HA3	2.26	0.50
3:D:749:LYS:HG2	3:D:753:SER:O	2.10	0.50
3:D:839:VAL:O	3:D:839:VAL:HG22	2.11	0.50
3:D:1030:GLU:OE2	3:D:1031:VAL:HG22	2.11	0.50
3:D:1040:MET:HG3	3:D:1040:MET:O	2.12	0.50
3:D:1063:ASP:HB2	3:D:1103:GLY:N	2.27	0.50
5:F:132:CYS:O	5:F:136:GLU:OE1	2.29	0.50
5:F:163:THR:OG1	5:F:260:ARG:HG2	2.11	0.50
2:C:1336:ASN:HB2	3:D:25:ALA:HB2	1.93	0.50
3:D:772:TYR:O	3:D:776:THR:HG23	2.12	0.50
3:D:1196:LEU:HD12	3:D:1196:LEU:H	1.77	0.50
4:E:8:ASP:N	4:E:8:ASP:OD1	2.45	0.50
5:F:489:MET:HG2	5:F:493:LYS:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ILE:HD12	1:B:131:CYS:HB3	1.93	0.50
2:C:237:LEU:CD1	2:C:289:VAL:HA	2.41	0.50
2:C:800:MET:HE1	2:C:827:ARG:HD3	1.94	0.50
3:D:46:TYR:CZ	5:F:453:PRO:HD3	2.46	0.50
3:D:165:TYR:CE1	3:D:178:ALA:HB3	2.47	0.50
3:D:343:LEU:HD21	3:D:1352:ILE:CD1	2.42	0.50
3:D:1160:SER:HG	3:D:1203:ARG:HH12	1.55	0.50
2:C:270:THR:HB	2:C:272:ARG:NH1	2.27	0.50
2:C:485:ASP:OD1	2:C:486:THR:N	2.44	0.50
3:D:75:TYR:HE1	3:D:85:CYS:HA	1.76	0.50
5:F:252:LEU:HA	5:F:255:VAL:CG1	2.41	0.50
1:A:31:LEU:HB2	1:A:199:ASP:O	2.12	0.50
1:A:222:THR:O	1:A:226:GLU:HG3	2.11	0.50
2:C:245:ARG:HD3	2:C:337:PHE:CE1	2.47	0.50
2:C:542:ARG:HD2	6:X:63:DT:O4'	2.12	0.50
3:D:707:ILE:HG21	3:D:716:GLN:NE2	2.27	0.50
5:F:122:ARG:HH21	5:F:375:ALA:HB2	1.77	0.50
2:C:699:LEU:HG	2:C:799:ASN:ND2	2.26	0.50
3:D:201:LEU:CD1	3:D:220:ARG:HG2	2.42	0.50
3:D:665:GLN:HA	3:D:665:GLN:OE1	2.12	0.50
5:F:261:LEU:HG	5:F:265:GLN:HB2	1.94	0.50
2:C:164:THR:OG1	2:C:171:LEU:HD13	2.12	0.50
2:C:241:LEU:HG	2:C:246:LEU:HD11	1.93	0.50
2:C:974:ARG:HH11	2:C:978:VAL:CG2	2.23	0.50
3:D:644:MET:O	3:D:764:ARG:NE	2.44	0.50
3:D:658:GLU:O	3:D:661:VAL:HG22	2.12	0.50
3:D:1004:ALA:O	3:D:1005:LYS:HD3	2.11	0.50
3:D:1249:ASN:OD1	3:D:1250:ASP:N	2.44	0.50
4:E:62:GLN:O	4:E:66:VAL:HG23	2.12	0.50
2:C:550:VAL:HG23	3:D:780:ARG:HE	1.77	0.49
3:D:91:GLU:OE2	3:D:101:ARG:NH2	2.24	0.49
3:D:287:ALA:HB1	3:D:288:PRO:HD2	1.94	0.49
3:D:511:TYR:HE2	3:D:724:MET:HG3	1.75	0.49
3:D:1036:ARG:HH21	3:D:1079:LYS:HD3	1.76	0.49
3:D:1109:LEU:CG	3:D:1113:VAL:HG11	2.39	0.49
5:F:127:ILE:HG12	5:F:131:GLN:NE2	2.27	0.49
5:F:142:THR:O	5:F:146:GLU:HG3	2.11	0.49
6:X:67:DA:H2''	6:X:68:DC:C6	2.47	0.49
7:Y:4:DG:H2''	7:Y:5:DT:C5'	2.41	0.49
2:C:245:ARG:HD3	2:C:337:PHE:CD1	2.47	0.49
2:C:563:THR:OG1	2:C:564:PRO:HD2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1304:MET:O	2:C:1308:ILE:HG12	2.12	0.49
3:D:849:LEU:HD23	3:D:856:ILE:HA	1.94	0.49
3:D:1216:ALA:O	3:D:1220:ILE:HD12	2.12	0.49
5:F:294:GLN:HE22	5:F:325:PRO:HB2	1.78	0.49
5:F:338:HIS:O	5:F:342:GLN:HG2	2.13	0.49
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.94	0.49
2:C:493:ILE:HG13	2:C:493:ILE:O	2.11	0.49
2:C:891:GLY:O	2:C:892:GLU:HG2	2.12	0.49
2:C:1115:THR:HG23	2:C:1228:GLY:HA3	1.93	0.49
5:F:315:TRP:HE1	5:F:341:LEU:HD11	1.77	0.49
5:F:344:LEU:O	5:F:347:ILE:CG1	2.60	0.49
5:F:494:ILE:HD12	5:F:494:ILE:H	1.77	0.49
7:Y:8:DA:H2'	7:Y:8:DA:OP2	2.11	0.49
1:B:109:PRO:HB3	1:B:132:HIS:CE1	2.48	0.49
1:B:166:ARG:N	1:B:167:PRO:HD2	2.27	0.49
2:C:199:ASP:OD1	2:C:200:ARG:N	2.42	0.49
2:C:540:ARG:O	2:C:548:ARG:NH2	2.44	0.49
2:C:1037:THR:HG22	2:C:1037:THR:O	2.12	0.49
3:D:426:ALA:HB3	3:D:427:PRO:CD	2.30	0.49
3:D:697:MET:SD	3:D:741:ALA:HB3	2.52	0.49
3:D:749:LYS:HD2	3:D:753:SER:OG	2.13	0.49
3:D:816:THR:OG1	3:D:818:GLU:OE1	2.31	0.49
3:D:892:PHE:N	3:D:1281:GLU:OE1	2.45	0.49
3:D:903:LEU:HD11	3:D:909:ILE:HA	1.94	0.49
3:D:1048:ARG:HA	3:D:1059:LEU:CD2	2.42	0.49
3:D:1163:VAL:HG12	3:D:1202:GLU:O	2.12	0.49
5:F:390:ILE:HD13	5:F:435:ILE:CB	2.43	0.49
2:C:1271:GLY:N	2:C:1274:GLU:OE1	2.43	0.49
3:D:658:GLU:HA	3:D:661:VAL:HG22	1.95	0.49
3:D:973:LEU:CD2	3:D:1003:LEU:HD13	2.38	0.49
3:D:1179:PRO:HB2	3:D:1182:GLY:H	1.76	0.49
5:F:277:MET:HA	5:F:280:VAL:HG22	1.93	0.49
5:F:302:PHE:HA	5:F:305:LEU:CD2	2.42	0.49
5:F:395:THR:HG23	5:F:396:ASN:N	2.27	0.49
1:A:65:LEU:HD23	1:A:65:LEU:H	1.77	0.49
2:C:14:ASP:HB3	2:C:1157:GLN:OE1	2.13	0.49
2:C:207:THR:HG23	2:C:350:THR:CG2	2.43	0.49
2:C:257:ALA:HB3	2:C:262:TYR:HE2	1.76	0.49
2:C:373:GLY:O	5:F:103:ARG:HD2	2.11	0.49
2:C:738:GLU:HA	2:C:741:MET:CE	2.42	0.49
2:C:995:ASP:OD1	2:C:995:ASP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:197:GLU:OE2	3:D:220:ARG:NH1	2.39	0.49
3:D:259:ARG:CG	5:F:502:LYS:HE3	2.39	0.49
3:D:930:LEU:O	3:D:931:THR:HB	2.12	0.49
3:D:1078:LEU:HB2	3:D:1101:LEU:HG	1.94	0.49
3:D:1273:ASP:O	3:D:1274:PHE:HB3	2.12	0.49
5:F:283:GLN:HA	5:F:286:LEU:HD21	1.94	0.49
2:C:980:VAL:O	2:C:984:VAL:HG22	2.12	0.49
3:D:491:LEU:HD22	3:D:496:GLY:O	2.12	0.49
3:D:1004:ALA:HB3	3:D:1017:VAL:HA	1.94	0.49
3:D:1122:ALA:C	3:D:1123:ARG:HD3	2.33	0.49
1:A:164:ASP:HA	1:A:166:ARG:NH1	2.23	0.49
2:C:1005:GLU:OE1	2:C:1007:LYS:N	2.33	0.49
3:D:295:GLU:HA	3:D:298:MET:CE	2.37	0.49
3:D:1005:LYS:HB3	3:D:1009:GLU:HB2	1.95	0.49
3:D:1227:HIS:O	3:D:1230:THR:HG22	2.12	0.49
5:F:162:ILE:HG12	5:F:165:PHE:CE2	2.48	0.49
5:F:230:VAL:O	5:F:234:THR:HG22	2.13	0.49
5:F:479:THR:CG2	5:F:482:GLU:HG3	2.42	0.49
5:F:487:MET:HB3	5:F:489:MET:CE	2.42	0.49
1:B:29:GLU:OE2	1:B:190:ALA:HB1	2.13	0.49
2:C:1298:VAL:HG23	2:C:1299:ASN:N	2.28	0.49
2:C:117:ILE:CD1	2:C:489:PRO:HD3	2.42	0.49
2:C:996:ARG:HD3	2:C:999:GLU:OE2	2.13	0.49
2:C:1137:GLU:HG3	2:C:1140:LYS:HG2	1.95	0.49
2:C:1192:GLU:OE2	3:D:764:ARG:NH1	2.46	0.49
5:F:315:TRP:CZ2	5:F:341:LEU:HD11	2.48	0.49
5:F:344:LEU:HA	5:F:347:ILE:HD11	1.95	0.49
2:C:219:GLN:O	2:C:223:LEU:HD13	2.13	0.48
3:D:289:ASP:OD1	3:D:290:ILE:HG12	2.12	0.48
3:D:638:SER:OG	3:D:639:VAL:N	2.46	0.48
5:F:224:LEU:HD21	5:F:255:VAL:CG2	2.36	0.48
1:B:212:ASP:N	1:B:212:ASP:OD1	2.45	0.48
3:D:670:SER:HB2	3:D:672:LEU:HD23	1.95	0.48
5:F:367:ILE:HG22	5:F:371:LYS:HE2	1.95	0.48
2:C:263:VAL:HG22	2:C:273:HIS:CG	2.48	0.48
3:D:1029:THR:HG22	3:D:1099:TYR:CD2	2.48	0.48
5:F:133:SER:HA	5:F:136:GLU:CD	2.34	0.48
5:F:347:ILE:HA	5:F:350:GLU:HG2	1.94	0.48
2:C:4:SER:OG	2:C:7:GLU:HB2	2.13	0.48
2:C:230:PHE:CD1	2:C:292:ILE:HD12	2.48	0.48
2:C:233:ARG:HB2	2:C:238:GLN:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:301:TYR:HB2	2:C:311:CYS:CB	2.29	0.48
2:C:302:ILE:CG2	2:C:309:LEU:HA	2.36	0.48
3:D:708:ASN:HA	3:D:713:GLU:HA	1.95	0.48
3:D:1086:ASN:OD1	3:D:1087:ASP:N	2.46	0.48
5:F:524:GLU:HG2	5:F:525:ASP:N	2.27	0.48
2:C:276:GLN:CA	2:C:279:LYS:HE2	2.41	0.48
2:C:849:GLU:O	2:C:886:LYS:HG3	2.13	0.48
3:D:53:ARG:NH2	3:D:60:ARG:HH11	2.11	0.48
3:D:184:ALA:O	3:D:188:LEU:HD13	2.14	0.48
3:D:755:ILE:H	3:D:755:ILE:HD12	1.78	0.48
3:D:823:THR:HG22	3:D:879:ALA:HB2	1.95	0.48
3:D:1157:ALA:O	3:D:1207:GLY:N	2.32	0.48
3:D:1195:GLN:HG2	3:D:1195:GLN:O	2.13	0.48
6:X:68:DC:H2''	6:X:69:DG:C5'	2.34	0.48
1:B:44:ARG:HG2	1:B:44:ARG:NH1	2.28	0.48
1:B:91:ARG:NH2	1:B:124:VAL:HG22	2.29	0.48
1:B:111:THR:HG22	1:B:112:ALA:N	2.28	0.48
2:C:117:ILE:HD12	2:C:489:PRO:HD3	1.95	0.48
2:C:1217:THR:HG22	2:C:1219:GLU:HG3	1.95	0.48
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.49	0.48
3:D:1314:LEU:HD23	3:D:1314:LEU:O	2.12	0.48
5:F:276:MET:HE1	5:F:347:ILE:CD1	2.43	0.48
5:F:301:ASN:OD1	5:F:302:PHE:N	2.46	0.48
5:F:357:GLN:O	5:F:361:ILE:HG13	2.14	0.48
5:F:557:LYS:O	5:F:561:MET:HG2	2.14	0.48
5:F:573:LEU:HA	5:F:576:VAL:HG22	1.96	0.48
2:C:761:GLN:O	2:C:762:ASN:HB2	2.13	0.48
3:D:97:VAL:O	3:D:101:ARG:HG3	2.14	0.48
3:D:490:ILE:HD12	3:D:614:LEU:CD1	2.43	0.48
3:D:839:VAL:HG21	3:D:880:VAL:HG11	1.95	0.48
5:F:385:ARG:HH12	5:F:389:SER:HB2	1.79	0.48
3:D:279:LEU:HD13	3:D:295:GLU:CB	2.43	0.48
3:D:282:LEU:HD21	5:F:410:ILE:CD1	2.44	0.48
2:C:241:LEU:HD21	2:C:246:LEU:HD13	1.95	0.48
2:C:301:TYR:HB3	2:C:325:LEU:HD11	1.95	0.48
5:F:102:MET:HA	5:F:105:MET:CG	2.43	0.48
5:F:261:LEU:HD21	5:F:265:GLN:CB	2.43	0.48
5:F:466:ILE:HG22	5:F:470:MET:HE1	1.93	0.48
2:C:75:LEU:CD2	2:C:127:ILE:HD11	2.37	0.48
2:C:358:ASP:OD1	2:C:361:SER:OG	2.31	0.48
2:C:359:ARG:HE	2:C:363:LEU:HD11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:738:GLU:HA	2:C:741:MET:HE2	1.96	0.48
2:C:1166:ASP:O	2:C:1170:MET:HG2	2.14	0.48
5:F:261:LEU:HD11	5:F:265:GLN:HG3	1.96	0.48
1:A:74:VAL:HG22	1:A:133:LEU:HD23	1.96	0.47
1:B:19:VAL:HG23	1:B:23:HIS:HB3	1.94	0.47
1:B:111:THR:HG23	1:B:128:HIS:O	2.13	0.47
1:B:118:ASP:OD1	1:B:119:GLY:N	2.47	0.47
2:C:575:LEU:HG	2:C:576:SER:N	2.29	0.47
2:C:1164:PHE:HB2	2:C:1168:GLU:CD	2.34	0.47
3:D:199:GLU:OE1	3:D:199:GLU:HA	2.14	0.47
3:D:1154:ALA:N	3:D:1214:PRO:O	2.47	0.47
5:F:319:ALA:HA	5:F:322:MET:HE1	1.95	0.47
1:B:222:THR:O	1:B:226:GLU:HG3	2.14	0.47
2:C:74:ARG:HG2	2:C:75:LEU:N	2.29	0.47
2:C:333:ILE:HG13	2:C:333:ILE:O	2.13	0.47
3:D:1188:GLU:O	3:D:1190:ILE:HD12	2.14	0.47
5:F:221:PHE:HA	5:F:224:LEU:HD12	1.96	0.47
2:C:57:PHE:HB3	2:C:58:PRO:HA	1.96	0.47
2:C:208:ILE:H	2:C:208:ILE:HD12	1.79	0.47
3:D:863:LEU:CD1	3:D:901:ARG:HB2	2.35	0.47
5:F:558:VAL:HG22	5:F:580:PHE:HE2	1.79	0.47
2:C:888:THR:CG2	2:C:889:PRO:HD2	2.45	0.47
2:C:937:ASP:OD2	2:C:938:GLY:N	2.47	0.47
3:D:974:VAL:HG11	3:D:1028:ILE:CG2	2.44	0.47
3:D:975:ILE:HB	3:D:1001:ALA:H	1.79	0.47
5:F:315:TRP:CZ2	5:F:341:LEU:HD21	2.50	0.47
5:F:462:LYS:HE2	5:F:487:MET:CE	2.31	0.47
5:F:551:LEU:HD21	5:F:598:LEU:HD21	1.95	0.47
2:C:268:ARG:NH1	2:C:270:THR:HG22	2.29	0.47
2:C:398:SER:HB2	2:C:401:GLY:N	2.28	0.47
3:D:269:TYR:O	3:D:273:ILE:HG13	2.15	0.47
3:D:959:LYS:HG3	3:D:985:ILE:HG13	1.97	0.47
3:D:1205:GLU:OE2	3:D:1206:ARG:HG2	2.14	0.47
5:F:250:LEU:HD23	5:F:251:LYS:HD3	1.97	0.47
5:F:252:LEU:HG	5:F:256:PHE:CE2	2.50	0.47
5:F:299:LYS:HG2	5:F:303:ILE:CD1	2.44	0.47
2:C:198:ILE:HG22	2:C:199:ASP:N	2.26	0.47
2:C:975:ILE:HG22	2:C:997:TRP:HE3	1.78	0.47
3:D:213:LYS:O	3:D:217:LEU:HD13	2.13	0.47
5:F:252:LEU:CA	5:F:255:VAL:HG12	2.45	0.47
5:F:358:VAL:HG13	5:F:359:LYS:CE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:229:ILE:HB	2:C:240:GLU:HB3	1.95	0.47
2:C:1045:GLY:H	5:F:495:ARG:HH21	1.62	0.47
3:D:53:ARG:HA	3:D:54:ASP:HA	1.50	0.47
3:D:475:GLU:HG3	4:E:24:ALA:HB1	1.95	0.47
3:D:1048:ARG:NH1	3:D:1059:LEU:HD11	2.29	0.47
3:D:1053:LEU:HD23	3:D:1053:LEU:H	1.80	0.47
5:F:227:GLN:HA	5:F:230:VAL:HG22	1.96	0.47
5:F:348:GLU:HA	5:F:351:THR:CG2	2.45	0.47
5:F:582:VAL:HG23	5:F:586:ARG:CZ	2.44	0.47
1:B:59:VAL:HG23	1:B:143:ARG:O	2.15	0.47
2:C:542:ARG:HG2	2:C:542:ARG:O	2.15	0.47
3:D:872:LEU:O	3:D:877:VAL:HG22	2.15	0.47
3:D:984:LEU:HD13	3:D:993:GLU:HG2	1.97	0.47
3:D:1170:LYS:HG3	3:D:1170:LYS:O	2.15	0.47
2:C:241:LEU:CG	2:C:246:LEU:HD11	2.44	0.47
2:C:696:ASP:O	2:C:697:LYS:HB3	2.15	0.47
2:C:1125:GLY:HA3	2:C:1179:GLY:HA2	1.97	0.47
2:C:1151:LEU:O	2:C:1151:LEU:HD23	2.15	0.47
3:D:710:ASP:OD1	3:D:711:GLY:N	2.48	0.47
3:D:1044:GLN:NE2	3:D:1074:LEU:HB2	2.30	0.47
3:D:1251:LYS:O	3:D:1255:VAL:HG13	2.15	0.47
5:F:299:LYS:HG2	5:F:303:ILE:HD11	1.96	0.47
5:F:333:VAL:HG13	5:F:337:VAL:HG21	1.96	0.47
1:B:192:VAL:HG13	1:B:195:ARG:HG3	1.97	0.47
2:C:302:ILE:HB	2:C:308:GLU:O	2.15	0.47
3:D:210:SER:O	3:D:214:ARG:HB2	2.15	0.47
3:D:901:ARG:HD2	3:D:901:ARG:C	2.36	0.47
5:F:291:CYS:SG	5:F:292:VAL:N	2.88	0.47
1:A:162:GLU:CG	1:A:163:GLU:N	2.78	0.46
1:B:65:LEU:HD23	1:B:168:ILE:CG2	2.45	0.46
2:C:321:LEU:O	2:C:325:LEU:HD23	2.15	0.46
3:D:1109:LEU:HD23	3:D:1115:ILE:HD11	1.97	0.46
5:F:231:THR:O	5:F:235:ILE:HG23	2.15	0.46
5:F:427:PHE:CE2	5:F:431:ALA:HB2	2.50	0.46
1:A:33:ARG:NH2	1:A:197:ASP:HA	2.29	0.46
1:A:235:ARG:HG2	1:B:13:LEU:HD22	1.97	0.46
3:D:208:THR:CG2	3:D:214:ARG:HG2	2.44	0.46
3:D:416:ILE:HG21	3:D:441:LEU:CD2	2.43	0.46
3:D:454:CYS:O	3:D:458:ASN:N	2.48	0.46
3:D:974:VAL:HG12	3:D:1028:ILE:HD13	1.95	0.46
5:F:105:MET:SD	5:F:106:GLY:N	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:231:THR:HG23	5:F:248:GLU:CD	2.36	0.46
5:F:583:THR:HA	5:F:586:ARG:HH12	1.79	0.46
7:Y:7:DG:H2''	7:Y:8:DA:OP2	2.15	0.46
1:A:57:THR:HG22	1:A:175:ALA:HB2	1.96	0.46
2:C:52:ALA:CB	2:C:465:ARG:HD3	2.46	0.46
3:D:74:LYS:HB3	3:D:74:LYS:HE2	1.68	0.46
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.95	0.46
3:D:206:ASN:OD1	3:D:207:GLU:N	2.48	0.46
3:D:1108:GLN:HG2	3:D:1109:LEU:N	2.30	0.46
5:F:319:ALA:HB1	5:F:326:TRP:CH2	2.51	0.46
5:F:502:LYS:HG2	5:F:503:GLU:H	1.80	0.46
1:B:166:ARG:HA	1:B:166:ARG:NE	2.30	0.46
2:C:486:THR:O	2:C:486:THR:HG22	2.15	0.46
3:D:423:LEU:HD12	3:D:437:PHE:CD2	2.50	0.46
3:D:788:LEU:CD2	3:D:792:ASN:ND2	2.79	0.46
3:D:949:SER:HB2	3:D:1016:THR:HG21	1.97	0.46
3:D:1155:ILE:HD12	3:D:1155:ILE:H	1.81	0.46
3:D:1194:ARG:HD2	3:D:1211:SER:OG	2.16	0.46
5:F:105:MET:O	5:F:108:VAL:HG12	2.15	0.46
5:F:279:ARG:HH22	5:F:347:ILE:HD13	1.81	0.46
5:F:393:LYS:NZ	5:F:436:ARG:HH12	2.14	0.46
7:Y:4:DG:H2''	7:Y:5:DT:O4'	2.15	0.46
1:A:66:HIS:CE1	2:C:929:ILE:HG22	2.50	0.46
1:B:192:VAL:HG13	1:B:192:VAL:O	2.15	0.46
2:C:249:GLU:O	2:C:269:ILE:HB	2.16	0.46
2:C:261:VAL:HG23	2:C:261:VAL:O	2.15	0.46
2:C:303:ASP:O	2:C:307:GLY:N	2.41	0.46
2:C:304:GLU:HG2	2:C:305:SER:N	2.30	0.46
2:C:589:THR:OG1	2:C:590:PRO:HD2	2.16	0.46
3:D:252:LEU:HG	3:D:252:LEU:O	2.15	0.46
3:D:518:VAL:HG11	3:D:707:ILE:CG2	2.45	0.46
3:D:1029:THR:HG22	3:D:1099:TYR:CE2	2.51	0.46
3:D:1047:THR:H	3:D:1060:VAL:HG22	1.79	0.46
5:F:262:VAL:HG22	5:F:263:PRO:HD2	1.97	0.46
5:F:333:VAL:HG22	5:F:336:GLU:CG	2.45	0.46
7:Y:9:DG:H2''	7:Y:10:DT:C5'	2.46	0.46
1:A:192:VAL:O	1:A:192:VAL:HG22	2.15	0.46
2:C:241:LEU:CD1	2:C:246:LEU:HD11	2.46	0.46
2:C:660:VAL:O	2:C:660:VAL:HG12	2.16	0.46
2:C:890:LYS:NZ	2:C:914:LYS:HE3	2.30	0.46
3:D:44:ILE:HG22	3:D:45:ASN:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:121:PRO:HB2	3:D:123:ARG:NH1	2.30	0.46
3:D:279:LEU:HA	3:D:295:GLU:HG2	1.97	0.46
3:D:530:PRO:HB3	3:D:577:ALA:O	2.16	0.46
3:D:562:GLU:OE1	3:D:562:GLU:HA	2.16	0.46
3:D:804:ALA:CB	3:D:1259:GLN:HG3	2.46	0.46
3:D:974:VAL:HG11	3:D:1028:ILE:HG21	1.97	0.46
3:D:1215:GLU:HG2	3:D:1215:GLU:O	2.15	0.46
3:D:1283:SER:O	3:D:1286:LYS:HG2	2.16	0.46
2:C:1184:THR:HG23	2:C:1189:GLY:CA	2.40	0.46
3:D:146:VAL:HG11	3:D:158:GLN:HG2	1.98	0.46
3:D:972:LYS:CD	3:D:1002:VAL:HA	2.45	0.46
3:D:1120:THR:HG23	3:D:1120:THR:O	2.15	0.46
5:F:361:ILE:HA	5:F:364:ARG:NE	2.30	0.46
1:B:207:THR:HG22	1:B:208:ASN:N	2.30	0.46
2:C:234:ASP:O	2:C:235:ASN:HB2	2.15	0.46
2:C:289:VAL:HG11	2:C:319:LEU:CD1	2.45	0.46
2:C:315:MET:HA	2:C:352:ARG:HH12	1.81	0.46
3:D:478:LEU:CD2	4:E:47:THR:HG23	2.45	0.46
3:D:1030:GLU:OE1	3:D:1030:GLU:N	2.48	0.46
3:D:1048:ARG:HH12	3:D:1059:LEU:HD11	1.80	0.46
3:D:1167:LYS:CB	3:D:1174:ARG:HD3	2.45	0.46
5:F:152:GLU:HG2	5:F:218:ARG:HH11	1.81	0.46
5:F:164:GLY:HA3	5:F:260:ARG:NH2	2.31	0.46
5:F:572:THR:HG22	5:F:575:GLU:CD	2.35	0.46
1:B:120:ASP:OD1	1:B:121:VAL:N	2.48	0.46
2:C:576:SER:OG	2:C:577:VAL:N	2.49	0.46
2:C:895:LEU:HD12	2:C:899:GLU:CB	2.45	0.46
3:D:18:ASP:OD1	3:D:18:ASP:N	2.49	0.46
3:D:72:CYS:SG	3:D:73:GLY:N	2.89	0.46
3:D:159:ILE:HG13	3:D:159:ILE:O	2.15	0.46
5:F:133:SER:HA	5:F:136:GLU:OE2	2.16	0.46
7:Y:1:DC:C2'	7:Y:2:DT:H72	2.46	0.46
2:C:213:LEU:HD23	2:C:422:LYS:CG	2.46	0.46
2:C:582:ASN:HB2	2:C:586:PHE:O	2.16	0.46
2:C:615:VAL:HG23	2:C:615:VAL:O	2.16	0.46
3:D:516:ASP:HA	3:D:545:HIS:HB2	1.98	0.46
3:D:1172:LYS:HB3	3:D:1191:PRO:HA	1.98	0.46
3:D:1348:LYS:O	3:D:1352:ILE:HG12	2.16	0.46
5:F:290:LEU:HD23	5:F:330:LEU:CD1	2.46	0.46
5:F:362:ASN:OD1	5:F:363:ARG:N	2.49	0.46
5:F:446:GLN:HG3	5:F:446:GLN:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLN:HG3	1:B:35:PHE:CE2	2.51	0.45
3:D:255:LEU:N	3:D:259:ARG:O	2.33	0.45
3:D:951:GLN:OE1	3:D:1014:GLY:HA2	2.16	0.45
3:D:1314:LEU:HG	3:D:1326:GLN:NE2	2.24	0.45
5:F:355:ILE:CA	5:F:358:VAL:HG12	2.44	0.45
5:F:401:PHE:HA	5:F:404:LEU:HD12	1.98	0.45
6:X:71:DA:H2''	6:X:72:DC:H5'	1.97	0.45
2:C:107:ARG:HA	2:C:108:GLU:HA	1.52	0.45
2:C:196:VAL:HG11	2:C:209:ILE:CD1	2.46	0.45
2:C:230:PHE:HB2	2:C:333:ILE:CG1	2.46	0.45
2:C:253:PHE:O	2:C:255:ILE:HD12	2.16	0.45
5:F:503:GLU:HG3	5:F:504:PRO:HD2	1.98	0.45
7:Y:12:DC:H2''	7:Y:13:DG:O5'	2.17	0.45
2:C:890:LYS:N	2:C:912:ASP:O	2.49	0.45
3:D:46:TYR:HB3	5:F:450:ILE:HG21	1.95	0.45
3:D:964:LYS:O	3:D:964:LYS:HG3	2.16	0.45
3:D:968:ASN:ND2	3:D:974:VAL:HG22	2.31	0.45
3:D:980:THR:HG1	3:D:997:VAL:HG23	1.79	0.45
3:D:1034:PHE:N	3:D:1081:VAL:O	2.50	0.45
3:D:1047:THR:HG23	3:D:1060:VAL:CG2	2.46	0.45
3:D:1196:LEU:HG	3:D:1210:ILE:CG2	2.46	0.45
5:F:311:THR:HG23	5:F:348:GLU:CD	2.36	0.45
2:C:543:ALA:CB	2:C:548:ARG:HE	2.29	0.45
2:C:685:MET:SD	2:C:1073:LYS:HG2	2.57	0.45
2:C:866:ASP:HB3	2:C:872:TYR:CE1	2.51	0.45
5:F:499:LYS:HG3	5:F:499:LYS:O	2.16	0.45
5:F:555:GLU:OE2	5:F:594:ALA:HB2	2.16	0.45
1:B:188:GLU:HB2	1:B:200:LYS:HG2	1.98	0.45
2:C:179:TYR:HB2	2:C:398:SER:HG	1.81	0.45
2:C:199:ASP:O	2:C:200:ARG:HG2	2.16	0.45
2:C:1134:GLN:C	2:C:1135:GLN:HG2	2.36	0.45
3:D:343:LEU:HD21	3:D:1352:ILE:HD11	1.99	0.45
3:D:903:LEU:HD21	3:D:909:ILE:CD1	2.46	0.45
3:D:955:LYS:HD3	3:D:956:GLY:N	2.32	0.45
3:D:972:LYS:CD	3:D:1003:LEU:H	2.28	0.45
6:X:72:DC:H1'	6:X:73:DT:H5''	1.99	0.45
2:C:1035:LYS:O	2:C:1038:GLN:HG2	2.17	0.45
3:D:69:GLU:HB2	3:D:76:LYS:HG2	1.98	0.45
3:D:140:TYR:O	3:D:297:ARG:NH1	2.49	0.45
3:D:510:LEU:HD23	3:D:596:LEU:HD21	1.99	0.45
3:D:668:PHE:HD1	3:D:673:VAL:HG23	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:700:ASN:O	3:D:704:GLU:HB3	2.17	0.45
3:D:833:GLU:HG2	3:D:838:ARG:HD3	1.98	0.45
3:D:1135:THR:O	3:D:1135:THR:HG23	2.15	0.45
5:F:344:LEU:C	5:F:347:ILE:HG12	2.37	0.45
1:B:90:VAL:HG22	1:B:91:ARG:N	2.32	0.45
2:C:30:ILE:HG13	2:C:31:GLN:N	2.32	0.45
2:C:878:THR:HG22	2:C:879:GLY:N	2.31	0.45
3:D:808:VAL:HG12	3:D:809:VAL:N	2.31	0.45
3:D:1199:PHE:HB2	3:D:1202:GLU:HG3	1.99	0.45
5:F:586:ARG:HA	5:F:589:GLN:HG2	1.98	0.45
6:X:64:DG:H2''	6:X:65:DA:C8	2.51	0.45
2:C:59:ILE:CG1	2:C:472:GLU:HG2	2.45	0.45
2:C:276:GLN:HA	2:C:279:LYS:CG	2.46	0.45
2:C:577:VAL:HG23	2:C:661:VAL:O	2.16	0.45
2:C:715:THR:HG22	2:C:716:ALA:N	2.32	0.45
2:C:895:LEU:HD12	2:C:899:GLU:HB2	1.99	0.45
3:D:309:ASN:CB	3:D:326:SER:HB3	2.44	0.45
3:D:1270:GLY:HA3	3:D:1297:LYS:O	2.17	0.45
3:D:1283:SER:O	3:D:1287:ILE:HG22	2.17	0.45
6:X:73:DT:H2''	6:X:74:DC:OP2	2.16	0.45
7:Y:15:DG:H2''	7:Y:16:DT:C6	2.51	0.45
1:B:47:LEU:HD13	1:B:183:ILE:CD1	2.47	0.45
2:C:115:LYS:HA	2:C:115:LYS:HE2	1.99	0.45
2:C:193:ASN:HB2	2:C:195:PHE:HE1	1.82	0.45
2:C:1122:LYS:HG2	2:C:1229:TYR:CE1	2.51	0.45
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.17	0.45
3:D:514:THR:OG1	3:D:596:LEU:HB3	2.17	0.45
5:F:231:THR:HG23	5:F:248:GLU:OE2	2.16	0.45
2:C:1031:ALA:O	2:C:1034:ARG:HG2	2.17	0.45
2:C:1042:LEU:HB3	2:C:1046:VAL:CG2	2.47	0.45
2:C:1330:ILE:HG21	2:C:1337:ILE:HG21	1.99	0.45
3:D:126:LEU:C	3:D:126:LEU:HD12	2.38	0.45
3:D:591:ILE:HG13	3:D:592:VAL:HG13	1.98	0.45
3:D:1179:PRO:HD3	3:D:1184:ASP:HA	1.99	0.45
5:F:148:TYR:O	5:F:152:GLU:HG3	2.17	0.45
5:F:423:ARG:HB2	5:F:425:TYR:CD1	2.52	0.45
1:A:192:VAL:CG1	1:A:195:ARG:H	2.30	0.44
2:C:231:GLU:OE2	2:C:284:LEU:HD11	2.16	0.44
2:C:289:VAL:HG13	2:C:322:LEU:CD2	2.47	0.44
2:C:1264:GLN:OE1	2:C:1264:GLN:N	2.30	0.44
3:D:546:ALA:O	3:D:573:THR:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:804:ALA:HB1	3:D:1259:GLN:HG3	1.99	0.44
3:D:825:VAL:O	3:D:825:VAL:HG13	2.17	0.44
3:D:1167:LYS:HG2	3:D:1170:LYS:HE2	1.99	0.44
5:F:355:ILE:HA	5:F:358:VAL:CG1	2.47	0.44
2:C:124:MET:HA	2:C:495:ALA:HB2	1.98	0.44
2:C:226:GLU:O	2:C:227:LYS:HD3	2.17	0.44
2:C:852:ALA:HB2	2:C:869:GLY:CA	2.48	0.44
2:C:956:ALA:O	2:C:960:LEU:HD13	2.18	0.44
3:D:141:PHE:HA	3:D:180:MET:SD	2.57	0.44
3:D:516:ASP:HB3	3:D:573:THR:HG21	1.99	0.44
3:D:1195:GLN:OE1	3:D:1195:GLN:N	2.51	0.44
5:F:330:LEU:HD12	5:F:333:VAL:CG1	2.47	0.44
1:A:29:GLU:HB3	1:A:30:PRO:CD	2.47	0.44
1:A:162:GLU:CG	1:A:163:GLU:H	2.29	0.44
2:C:82:VAL:O	2:C:86:GLN:HG3	2.18	0.44
2:C:975:ILE:HD11	2:C:1018:TYR:OH	2.17	0.44
3:D:615:LYS:NZ	4:E:7:GLN:HB3	2.33	0.44
3:D:788:LEU:HD23	3:D:792:ASN:HD22	1.81	0.44
3:D:870:ASP:O	3:D:873:GLU:HG2	2.18	0.44
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.99	0.44
3:D:1167:LYS:CB	3:D:1170:LYS:HE3	2.48	0.44
5:F:158:LEU:HA	5:F:161:LEU:HD23	1.97	0.44
1:B:47:LEU:HD13	1:B:183:ILE:HD12	1.99	0.44
2:C:615:VAL:HG23	2:C:650:VAL:HA	1.99	0.44
2:C:1066:MET:SD	2:C:1076:ILE:HD11	2.57	0.44
3:D:576:ARG:HD3	3:D:593:ASN:HA	1.99	0.44
3:D:968:ASN:HD21	3:D:974:VAL:HG22	1.81	0.44
3:D:1109:LEU:CD2	3:D:1113:VAL:HG11	2.48	0.44
3:D:1167:LYS:HG2	3:D:1170:LYS:CE	2.47	0.44
5:F:462:LYS:HG3	5:F:463:LEU:N	2.33	0.44
5:F:483:LEU:O	5:F:483:LEU:HD23	2.17	0.44
2:C:52:ALA:CA	2:C:465:ARG:HD3	2.47	0.44
3:D:1062:LEU:HA	3:D:1103:GLY:HA2	1.99	0.44
3:D:1267:VAL:HG13	3:D:1301:THR:OG1	2.18	0.44
5:F:488:LEU:HG	5:F:488:LEU:O	2.18	0.44
1:A:75:GLN:HG2	1:A:75:GLN:O	2.17	0.44
1:A:224:LEU:CD2	1:B:228:LEU:HD11	2.47	0.44
3:D:518:VAL:HG13	3:D:519:ASN:N	2.33	0.44
5:F:282:THR:HA	5:F:285:ARG:HG2	2.00	0.44
5:F:347:ILE:O	5:F:350:GLU:HG2	2.17	0.44
5:F:572:THR:HG22	5:F:575:GLU:CG	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:589:GLN:O	5:F:593:LYS:HG3	2.17	0.44
2:C:40:GLU:OE1	2:C:40:GLU:HA	2.18	0.44
3:D:421:VAL:O	3:D:436:ALA:HA	2.17	0.44
3:D:559:ALA:CB	3:D:562:GLU:HB2	2.48	0.44
3:D:1274:PHE:C	3:D:1275:LEU:HD12	2.38	0.44
4:E:42:GLU:O	4:E:43:ASN:HB3	2.18	0.44
2:C:107:ARG:HA	2:C:108:GLU:OE1	2.18	0.44
2:C:198:ILE:HG12	2:C:369:MET:HE1	2.00	0.44
2:C:649:GLN:O	2:C:649:GLN:HG2	2.18	0.44
3:D:252:LEU:HD12	3:D:262:THR:HB	1.98	0.44
3:D:282:LEU:HD13	3:D:291:ILE:CG2	2.44	0.44
3:D:665:GLN:OE1	3:D:678:ARG:NH1	2.48	0.44
3:D:1003:LEU:HD21	3:D:1005:LYS:C	2.38	0.44
3:D:1101:LEU:HB3	3:D:1105:ALA:CB	2.47	0.44
5:F:385:ARG:NH1	5:F:389:SER:HB2	2.32	0.44
5:F:408:GLY:HA2	5:F:435:ILE:HG23	2.00	0.44
1:A:180:VAL:HG11	1:A:183:ILE:HD11	1.99	0.44
2:C:189:ASP:OD2	2:C:193:ASN:HB2	2.18	0.44
3:D:479:GLU:HG3	4:E:20:VAL:HG11	1.98	0.44
3:D:1001:ALA:HA	3:D:1020:TRP:HB3	1.99	0.44
5:F:145:LEU:HD21	5:F:256:PHE:HZ	1.83	0.44
5:F:150:ARG:O	5:F:155:GLU:HG3	2.18	0.44
5:F:152:GLU:OE2	5:F:218:ARG:HG2	2.18	0.44
5:F:163:THR:CG2	5:F:262:VAL:HA	2.48	0.44
5:F:584:ARG:HG2	5:F:586:ARG:HH11	1.83	0.44
2:C:1134:GLN:O	2:C:1135:GLN:HG2	2.18	0.43
3:D:154:LEU:HA	3:D:158:GLN:HE22	1.83	0.43
3:D:202:ARG:NH2	3:D:225:GLU:OE2	2.50	0.43
3:D:245:LEU:HD12	3:D:246:PRO:CD	2.48	0.43
3:D:1081:VAL:HG12	3:D:1087:ASP:N	2.33	0.43
3:D:1171:GLY:O	3:D:1172:LYS:HG3	2.18	0.43
5:F:320:ILE:O	5:F:320:ILE:HG22	2.17	0.43
5:F:361:ILE:O	5:F:364:ARG:HG3	2.18	0.43
5:F:561:MET:HA	5:F:567:MET:HE1	1.99	0.43
7:Y:3:DC:H1'	7:Y:4:DG:C8	2.53	0.43
2:C:67:GLU:O	2:C:102:LEU:HD12	2.18	0.43
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.98	0.43
2:C:484:LEU:HA	2:C:487:LEU:HD22	2.00	0.43
5:F:223:GLU:OE2	5:F:224:LEU:HG	2.18	0.43
5:F:245:ALA:HA	5:F:248:GLU:CG	2.49	0.43
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:662:SER:O	2:C:666:SER:HB3	2.19	0.43
2:C:976:ARG:NH1	2:C:980:VAL:HG21	2.27	0.43
3:D:26:SER:HB3	3:D:236:TRP:CZ2	2.53	0.43
3:D:722:ILE:CG2	3:D:737:ILE:HD12	2.48	0.43
3:D:885:VAL:HG11	3:D:1255:VAL:HG12	2.00	0.43
3:D:1040:MET:CE	3:D:1046:ILE:HD13	2.49	0.43
6:X:72:DC:C1'	6:X:73:DT:H5'	2.48	0.43
1:A:66:HIS:HE1	2:C:929:ILE:HB	1.83	0.43
1:B:192:VAL:CG1	1:B:198:LEU:HD11	2.48	0.43
2:C:272:ARG:H	2:C:272:ARG:HD3	1.83	0.43
2:C:808:ASN:H	3:D:633:ALA:HB2	1.83	0.43
1:A:155:ALA:N	1:A:174:ASP:OD1	2.44	0.43
1:B:104:LYS:HD2	1:B:114:ASP:OD2	2.19	0.43
2:C:194:LEU:HD23	2:C:429:MET:CE	2.49	0.43
2:C:724:VAL:CG1	2:C:727:VAL:HG23	2.47	0.43
3:D:130:MET:HG2	3:D:157:GLN:NE2	2.34	0.43
3:D:1210:ILE:O	3:D:1210:ILE:HG22	2.18	0.43
3:D:1219:ASP:OD1	3:D:1222:ARG:NH2	2.52	0.43
5:F:530:LEU:H	5:F:530:LEU:HD12	1.84	0.43
5:F:551:LEU:HD21	5:F:598:LEU:CD2	2.48	0.43
5:F:577:GLY:HA3	5:F:583:THR:HB	2.00	0.43
2:C:1042:LEU:HB3	2:C:1046:VAL:HG21	2.00	0.43
3:D:138:VAL:O	3:D:181:GLY:HA2	2.16	0.43
3:D:300:GLN:NE2	3:D:304:ASP:OD2	2.52	0.43
3:D:1102:PRO:HD2	3:D:1105:ALA:HB2	2.00	0.43
5:F:111:LEU:HD23	5:F:112:THR:N	2.34	0.43
5:F:131:GLN:HA	5:F:134:VAL:HG22	2.01	0.43
5:F:137:TYR:CE1	5:F:353:LEU:HD21	2.53	0.43
1:A:59:VAL:HG21	1:A:142:MET:CE	2.48	0.43
1:A:218:ARG:CZ	1:B:234:LEU:HD23	2.48	0.43
2:C:123:TYR:OH	2:C:126:GLU:HG3	2.18	0.43
2:C:353:VAL:O	2:C:353:VAL:HG12	2.19	0.43
2:C:974:ARG:HD2	2:C:974:ARG:C	2.39	0.43
3:D:45:ASN:O	3:D:46:TYR:CD1	2.72	0.43
3:D:949:SER:HA	3:D:1018:ALA:O	2.19	0.43
5:F:133:SER:OG	5:F:364:ARG:HD2	2.19	0.43
5:F:358:VAL:HA	5:F:361:ILE:HD12	2.00	0.43
5:F:502:LYS:NZ	5:F:505:ILE:HG13	2.34	0.43
6:X:65:DA:H2''	6:X:66:DC:C5'	2.47	0.43
2:C:80:PHE:HB3	2:C:84:GLU:HB2	2.01	0.43
2:C:119:GLU:HB2	2:C:489:PRO:CG	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:203:LYS:O	2:C:204:LEU:HG	2.18	0.43
2:C:256:GLU:CB	2:C:261:VAL:HG12	2.45	0.43
2:C:484:LEU:HG	2:C:484:LEU:O	2.19	0.43
2:C:1005:GLU:CD	2:C:1006:GLU:HG2	2.39	0.43
3:D:1040:MET:HE3	3:D:1046:ILE:HD13	2.00	0.43
3:D:1196:LEU:HA	3:D:1210:ILE:O	2.19	0.43
5:F:108:VAL:HG22	5:F:109:GLU:H	1.83	0.43
5:F:393:LYS:NZ	5:F:436:ARG:HH22	2.16	0.43
2:C:396:ASP:HA	2:C:418:GLY:O	2.19	0.43
3:D:473:THR:HG22	3:D:476:ALA:HB2	2.00	0.43
3:D:490:ILE:HD11	3:D:618:VAL:HG12	2.01	0.43
3:D:843:VAL:HG23	3:D:862:THR:N	2.34	0.43
3:D:850:LYS:HG3	3:D:852:GLY:O	2.18	0.43
3:D:1027:VAL:HB	3:D:1121:LEU:HB3	2.01	0.43
3:D:1033:GLY:HA2	3:D:1114:GLN:NE2	2.34	0.43
3:D:1063:ASP:N	3:D:1103:GLY:HA2	2.34	0.43
3:D:1183:SER:HB2	3:D:1185:PRO:HD2	2.00	0.43
1:A:61:ILE:HG22	1:A:62:ASP:N	2.34	0.43
2:C:561:ILE:HD11	2:C:665:ALA:HB1	2.00	0.43
3:D:432:LEU:CD1	3:D:499:ILE:HD13	2.49	0.43
4:E:39:VAL:HG12	4:E:53:GLU:HG3	2.00	0.43
5:F:220:LYS:HA	5:F:223:GLU:CG	2.48	0.43
5:F:281:ARG:O	5:F:284:GLU:HG2	2.19	0.43
2:C:145:ILE:CD1	2:C:512:SER:HB2	2.49	0.42
2:C:196:VAL:HG21	2:C:209:ILE:HD12	1.96	0.42
2:C:478:ARG:HH12	2:C:482:GLY:HA3	1.84	0.42
2:C:521:LEU:O	2:C:525:THR:HG23	2.19	0.42
3:D:245:LEU:HD12	3:D:246:PRO:HD2	2.00	0.42
3:D:424:ASN:O	3:D:466:MET:HG3	2.18	0.42
3:D:501:VAL:HG11	3:D:602:SER:OG	2.19	0.42
3:D:975:ILE:CG2	3:D:999:TYR:HA	2.48	0.42
3:D:1057:SER:H	3:D:1108:GLN:CA	2.29	0.42
5:F:310:GLU:CD	5:F:355:ILE:HG21	2.39	0.42
5:F:479:THR:HG22	5:F:482:GLU:CG	2.49	0.42
2:C:227:LYS:O	2:C:245:ARG:NH1	2.41	0.42
2:C:484:LEU:HA	2:C:487:LEU:CD2	2.49	0.42
3:D:355:ILE:HA	3:D:447:ILE:O	2.19	0.42
3:D:370:LYS:HE2	3:D:443:GLU:HG3	2.00	0.42
3:D:694:SER:CB	3:D:738:ARG:HH11	2.28	0.42
3:D:959:LYS:HB2	3:D:985:ILE:CG1	2.42	0.42
5:F:213:ASP:HB3	5:F:216:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:372:ALA:O	5:F:376:LYS:HG3	2.19	0.42
1:A:162:GLU:HG2	1:A:163:GLU:H	1.83	0.42
2:C:325:LEU:HA	2:C:328:SER:OG	2.18	0.42
2:C:558:VAL:HG11	2:C:573:ASN:HB3	2.00	0.42
3:D:17:PHE:HZ	3:D:1353:VAL:HG11	1.82	0.42
3:D:145:VAL:CG2	3:D:188:LEU:HD21	2.49	0.42
3:D:679:TYR:O	3:D:683:ILE:HG12	2.19	0.42
3:D:974:VAL:O	3:D:976:THR:HG23	2.19	0.42
3:D:1170:LYS:NZ	3:D:1174:ARG:HH11	2.18	0.42
3:D:1196:LEU:HD12	3:D:1196:LEU:N	2.33	0.42
5:F:415:ALA:O	5:F:430:TYR:HE2	2.01	0.42
1:A:60:GLU:HG3	1:A:60:GLU:O	2.19	0.42
1:A:61:ILE:HG22	1:A:62:ASP:H	1.84	0.42
1:A:201:LEU:CD2	1:A:203:ILE:HG13	2.49	0.42
1:B:54:CYS:SG	1:B:146:VAL:HG12	2.59	0.42
1:B:155:ALA:N	1:B:174:ASP:OD1	2.51	0.42
2:C:205:PRO:HB2	2:C:208:ILE:CD1	2.49	0.42
3:D:950:ILE:HD11	3:D:982:LEU:CD2	2.32	0.42
3:D:977:SER:OG	3:D:979:ASN:OD1	2.37	0.42
3:D:1073:ASP:O	3:D:1075:ARG:NH1	2.52	0.42
3:D:1108:GLN:NE2	3:D:1120:THR:O	2.41	0.42
3:D:1160:SER:HB2	3:D:1205:GLU:HG2	2.02	0.42
5:F:108:VAL:HG22	5:F:109:GLU:N	2.35	0.42
5:F:260:ARG:HB2	5:F:260:ARG:HH11	1.83	0.42
5:F:276:MET:HE2	5:F:347:ILE:HD12	1.97	0.42
5:F:558:VAL:HG22	5:F:580:PHE:CE2	2.55	0.42
1:B:65:LEU:HA	1:B:169:GLY:HA2	2.00	0.42
2:C:125:GLY:N	2:C:495:ALA:HB1	2.34	0.42
2:C:253:PHE:CE2	2:C:288:PRO:HD2	2.55	0.42
2:C:1236:ASN:O	2:C:1236:ASN:OD1	2.37	0.42
2:C:1330:ILE:CG2	2:C:1337:ILE:HG21	2.49	0.42
3:D:1089:LEU:HD22	3:D:1094:ASP:O	2.19	0.42
3:D:1284:ARG:CA	3:D:1287:ILE:HG22	2.46	0.42
4:E:45:LYS:O	4:E:48:VAL:HG12	2.20	0.42
5:F:459:THR:O	5:F:462:LYS:HG2	2.19	0.42
5:F:561:MET:HA	5:F:567:MET:HE3	2.00	0.42
7:Y:8:DA:H1'	7:Y:9:DG:C8	2.54	0.42
1:B:121:VAL:HG12	1:B:122:GLU:N	2.35	0.42
1:B:200:LYS:HE2	1:B:200:LYS:HB2	1.77	0.42
2:C:192:ASP:OD2	2:C:436:ARG:NH2	2.53	0.42
2:C:247:ARG:HB3	2:C:274:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:251:ALA:H	2:C:268:ARG:HA	1.83	0.42
2:C:346:TYR:OH	2:C:436:ARG:NH1	2.52	0.42
2:C:1082:ILE:HD11	2:C:1093:PRO:HG2	2.00	0.42
2:C:1151:LEU:HD13	2:C:1198:LEU:CD1	2.49	0.42
3:D:211:GLU:HG2	3:D:212:THR:HG23	2.02	0.42
3:D:1027:VAL:HG23	3:D:1121:LEU:HB3	2.01	0.42
3:D:1062:LEU:HG	3:D:1066:GLU:O	2.19	0.42
5:F:150:ARG:HB3	5:F:155:GLU:CG	2.49	0.42
5:F:476:ARG:O	5:F:477:GLU:HB3	2.19	0.42
1:B:157:THR:O	1:B:160:HIS:HB3	2.19	0.42
2:C:60:GLN:HG2	2:C:67:GLU:OE2	2.19	0.42
2:C:717:VAL:HG13	2:C:781:ASP:O	2.19	0.42
5:F:124:GLU:HA	5:F:127:ILE:HG22	2.01	0.42
5:F:145:LEU:HD11	5:F:221:PHE:O	2.19	0.42
5:F:235:ILE:HG13	5:F:236:LYS:N	2.35	0.42
2:C:98:VAL:O	2:C:122:VAL:HG22	2.19	0.42
2:C:163:LYS:HD3	2:C:163:LYS:N	2.34	0.42
2:C:276:GLN:CG	2:C:279:LYS:HE2	2.49	0.42
2:C:553:THR:O	2:C:553:THR:HG22	2.19	0.42
2:C:616:ILE:HD13	2:C:652:TYR:HB2	2.02	0.42
3:D:370:LYS:HA	3:D:441:LEU:HD12	2.00	0.42
3:D:843:VAL:CG2	3:D:861:ASN:HB2	2.50	0.42
5:F:117:ILE:H	5:F:117:ILE:HD12	1.84	0.42
5:F:407:GLU:OE1	5:F:407:GLU:HA	2.19	0.42
5:F:423:ARG:HB2	5:F:425:TYR:HD1	1.84	0.42
6:X:67:DA:H2''	6:X:68:DC:C5	2.55	0.42
7:Y:16:DT:H2''	7:Y:17:DC:O4'	2.20	0.42
1:A:47:LEU:HB3	1:A:183:ILE:CD1	2.50	0.42
1:A:167:PRO:HG2	1:A:170:ARG:HE	1.85	0.42
1:B:14:VAL:CG1	1:B:15:ASP:H	2.26	0.42
1:B:81:ILE:CD1	1:B:131:CYS:HB3	2.49	0.42
2:C:325:LEU:O	2:C:330:HIS:HB2	2.20	0.42
3:D:291:ILE:HG23	5:F:406:GLN:HE22	1.84	0.42
3:D:491:LEU:HD12	3:D:904:ALA:O	2.20	0.42
3:D:1220:ILE:HD12	3:D:1220:ILE:H	1.85	0.42
5:F:315:TRP:NE1	5:F:341:LEU:HD11	2.35	0.42
2:C:514:PHE:CZ	2:C:760:ASN:HB3	2.55	0.42
2:C:1253:LEU:HD21	3:D:253:VAL:HG11	1.99	0.42
2:C:1258:PRO:HG2	3:D:346:ARG:HB2	2.02	0.42
3:D:208:THR:HG23	3:D:214:ARG:CG	2.49	0.42
5:F:108:VAL:HG21	5:F:381:GLU:CD	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:500:ILE:O	5:F:500:ILE:HG12	2.20	0.42
1:A:235:ARG:O	1:A:236:ASP:OD1	2.38	0.41
2:C:637:ARG:HB2	2:C:641:GLU:O	2.20	0.41
3:D:75:TYR:CE1	3:D:85:CYS:HA	2.54	0.41
3:D:1048:ARG:NH2	3:D:1110:GLU:HG2	2.34	0.41
5:F:293:GLU:OE1	5:F:293:GLU:HA	2.19	0.41
5:F:452:ILE:HD11	5:F:457:ILE:CD1	2.49	0.41
1:A:158:ARG:HG3	1:A:163:GLU:OE2	2.20	0.41
1:A:165:GLU:HA	1:A:170:ARG:NH2	2.31	0.41
2:C:250:THR:HA	2:C:268:ARG:CA	2.50	0.41
3:D:46:TYR:OH	5:F:453:PRO:HD3	2.19	0.41
3:D:709:ARG:HD3	3:D:710:ASP:CG	2.40	0.41
3:D:903:LEU:HD11	3:D:909:ILE:HD12	2.02	0.41
5:F:158:LEU:HD12	5:F:161:LEU:HD21	2.02	0.41
5:F:573:LEU:O	5:F:576:VAL:HG22	2.20	0.41
2:C:80:PHE:HB2	2:C:85:CYS:SG	2.60	0.41
2:C:104:ILE:O	2:C:114:VAL:HB	2.20	0.41
3:D:245:LEU:CD1	3:D:246:PRO:HD2	2.50	0.41
3:D:953:LYS:HD2	3:D:953:LYS:N	2.36	0.41
3:D:1103:GLY:O	3:D:1124:ILE:HD11	2.20	0.41
3:D:1167:LYS:HB3	3:D:1174:ARG:HG2	2.03	0.41
2:C:178:PRO:HA	2:C:397:LEU:HD23	2.01	0.41
2:C:189:ASP:HB2	2:C:190:PRO:HD2	2.02	0.41
2:C:312:ALA:O	2:C:315:MET:HE2	2.21	0.41
3:D:24:LEU:HD21	3:D:116:PHE:CZ	2.55	0.41
3:D:572:THR:HG22	3:D:593:ASN:ND2	2.36	0.41
3:D:1033:GLY:HA2	3:D:1114:GLN:CD	2.41	0.41
3:D:1036:ARG:HH22	3:D:1038:THR:CB	2.33	0.41
5:F:141:ILE:HG12	5:F:252:LEU:HD23	2.03	0.41
5:F:561:MET:HE3	5:F:571:TYR:CD2	2.56	0.41
7:Y:11:DC:H2'	7:Y:11:DC:OP2	2.20	0.41
1:B:26:VAL:HG12	1:B:27:THR:N	2.35	0.41
1:B:56:VAL:HG22	1:B:146:VAL:HG22	2.03	0.41
2:C:724:VAL:HG11	2:C:727:VAL:CG2	2.51	0.41
3:D:90:VAL:O	3:D:90:VAL:HG13	2.19	0.41
3:D:558:ASP:OD1	3:D:559:ALA:N	2.54	0.41
3:D:860:ARG:O	3:D:861:ASN:C	2.59	0.41
3:D:1024:THR:HG23	3:D:1123:ARG:HD2	2.02	0.41
4:E:3:ARG:CG	4:E:48:VAL:HG23	2.49	0.41
5:F:161:LEU:O	5:F:261:LEU:HD12	2.21	0.41
5:F:216:LEU:HA	5:F:219:GLU:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:328:GLU:O	5:F:331:HIS:HB2	2.19	0.41
2:C:425:ILE:O	2:C:429:MET:HG3	2.19	0.41
2:C:1287:LEU:O	2:C:1291:LEU:HG	2.20	0.41
2:C:1331:ARG:HG2	3:D:33:TRP:CZ3	2.55	0.41
8:C:3001:D9X:N45	8:C:3001:D9X:O39	2.53	0.41
3:D:572:THR:HG21	3:D:589:TYR:OH	2.21	0.41
5:F:236:LYS:HE2	5:F:236:LYS:HA	2.01	0.41
5:F:581:ASP:O	5:F:582:VAL:HG13	2.21	0.41
2:C:699:LEU:HD23	2:C:699:LEU:HA	1.93	0.41
2:C:1044:PRO:HA	5:F:495:ARG:HH21	1.86	0.41
2:C:1151:LEU:O	2:C:1151:LEU:CD2	2.68	0.41
2:C:1184:THR:O	2:C:1184:THR:HG22	2.20	0.41
3:D:974:VAL:CG1	3:D:1028:ILE:HG21	2.50	0.41
3:D:1144:LEU:HD11	3:D:1236:GLU:CB	2.48	0.41
4:E:25:ARG:HH11	4:E:64:LEU:HD13	1.86	0.41
5:F:320:ILE:HG23	5:F:331:HIS:CE1	2.55	0.41
5:F:572:THR:CG2	5:F:575:GLU:H	2.30	0.41
5:F:601:PRO:O	5:F:602:SER:OG	2.29	0.41
2:C:62:TYR:O	2:C:63:SER:OG	2.31	0.41
2:C:459:MET:CE	2:C:511:LEU:HD13	2.50	0.41
2:C:624:ASP:O	2:C:626:GLU:OE1	2.38	0.41
2:C:1008:GLN:O	2:C:1012:GLU:HG2	2.21	0.41
3:D:960:LEU:CB	3:D:963:VAL:HG11	2.41	0.41
3:D:1193:TRP:HD1	3:D:1193:TRP:O	2.03	0.41
5:F:502:LYS:CG	5:F:503:GLU:N	2.84	0.41
1:A:98:VAL:HG11	1:A:121:VAL:CG1	2.51	0.41
2:C:230:PHE:HB2	2:C:333:ILE:HG13	2.03	0.41
2:C:478:ARG:HH11	2:C:482:GLY:HA3	1.85	0.41
2:C:1107:MET:HG3	3:D:740:LEU:HD21	2.02	0.41
2:C:1213:TYR:CD2	2:C:1220:GLN:HB3	2.56	0.41
2:C:1334:GLY:O	3:D:25:ALA:HB3	2.21	0.41
3:D:38:VAL:HG23	3:D:38:VAL:O	2.20	0.41
3:D:147:ILE:HG13	3:D:147:ILE:O	2.21	0.41
3:D:587:LEU:HD23	3:D:591:ILE:CD1	2.51	0.41
3:D:597:GLY:O	3:D:601:ILE:HG13	2.21	0.41
3:D:844:THR:CG2	3:D:864:LEU:HD11	2.51	0.41
3:D:1059:LEU:HD12	3:D:1107:VAL:HB	2.02	0.41
3:D:1179:PRO:HB2	3:D:1182:GLY:CA	2.51	0.41
3:D:1195:GLN:H	3:D:1195:GLN:CD	2.24	0.41
4:E:6:VAL:HG23	4:E:6:VAL:O	2.20	0.41
5:F:166:VAL:HG22	5:F:258:GLN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:260:ARG:HB2	5:F:260:ARG:NH1	2.35	0.41
5:F:262:VAL:HG12	5:F:265:GLN:CG	2.51	0.41
7:Y:9:DG:H2'	7:Y:10:DT:H6	1.84	0.41
1:A:210:THR:O	1:A:210:THR:HG22	2.21	0.41
1:B:61:ILE:HG12	1:B:142:MET:CB	2.49	0.41
2:C:594:VAL:HG12	2:C:595:THR:O	2.21	0.41
3:D:202:ARG:HG2	3:D:221:ILE:HD12	2.01	0.41
3:D:1104:LYS:HB3	3:D:1123:ARG:O	2.20	0.41
5:F:220:LYS:O	5:F:224:LEU:HG	2.21	0.41
2:C:1294:LYS:NZ	3:D:470:VAL:O	2.54	0.40
3:D:803:VAL:HG13	3:D:804:ALA:N	2.36	0.40
5:F:286:LEU:HD12	5:F:287:ILE:HG12	2.03	0.40
5:F:316:PHE:O	5:F:320:ILE:CD1	2.69	0.40
7:Y:13:DG:H2''	7:Y:14:DT:C7	2.51	0.40
1:A:79:LEU:O	1:A:83:LEU:HG	2.20	0.40
1:B:91:ARG:HE	1:B:210:THR:HG23	1.86	0.40
2:C:233:ARG:NE	2:C:233:ARG:HA	2.37	0.40
2:C:890:LYS:HZ2	2:C:914:LYS:HE3	1.84	0.40
2:C:1031:ALA:HA	2:C:1034:ARG:HG2	2.04	0.40
3:D:615:LYS:HB2	3:D:616:PRO:HD3	2.04	0.40
3:D:972:LYS:HE2	3:D:1002:VAL:HG13	2.03	0.40
3:D:1230:THR:HG23	3:D:1231:ARG:N	2.37	0.40
4:E:32:VAL:C	4:E:34:GLY:H	2.24	0.40
5:F:316:PHE:CE1	5:F:320:ILE:HD11	2.56	0.40
5:F:318:ALA:O	5:F:321:ALA:HB3	2.21	0.40
1:A:26:VAL:HG12	1:A:27:THR:N	2.37	0.40
1:A:235:ARG:NH1	1:A:237:VAL:HG12	2.36	0.40
1:B:25:LYS:HA	1:B:203:ILE:O	2.22	0.40
2:C:145:ILE:CG2	2:C:456:VAL:HG22	2.52	0.40
2:C:251:ALA:HB1	2:C:255:ILE:HD13	2.03	0.40
2:C:276:GLN:CA	2:C:279:LYS:HG2	2.50	0.40
2:C:387:ASN:HA	2:C:391:SER:HB3	2.02	0.40
2:C:844:LYS:CG	2:C:845:LEU:HD12	2.42	0.40
2:C:1213:TYR:CE2	2:C:1220:GLN:HB3	2.55	0.40
3:D:370:LYS:HE2	3:D:443:GLU:CG	2.51	0.40
3:D:538:ARG:HA	3:D:538:ARG:HD2	1.86	0.40
3:D:1062:LEU:HB2	3:D:1067:ARG:HA	2.03	0.40
1:A:28:LEU:HD12	1:A:28:LEU:N	2.37	0.40
2:C:1213:TYR:HA	2:C:1220:GLN:HA	2.03	0.40
2:C:1225:VAL:HG12	2:C:1226:THR:N	2.36	0.40
2:C:1260:GLY:HA2	2:C:1266:GLY:CA	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:831:VAL:O	3:D:831:VAL:HG23	2.21	0.40
3:D:911:LYS:NZ	3:D:1363:TYR:OH	2.51	0.40
3:D:1090:ILE:HG23	3:D:1091:PRO:HD2	2.04	0.40
3:D:1167:LYS:HB3	3:D:1174:ARG:CD	2.51	0.40
5:F:291:CYS:C	5:F:297:MET:HE1	2.41	0.40
5:F:425:TYR:HE2	5:F:430:TYR:HB2	1.87	0.40
5:F:530:LEU:HD12	5:F:530:LEU:N	2.37	0.40
6:X:70:DG:H2"	6:X:71:DA:OP2	2.21	0.40
2:C:855:PRO:O	2:C:856:ASN:OD1	2.38	0.40
2:C:890:LYS:HG3	2:C:891:GLY:N	2.37	0.40
2:C:1182:ILE:HG22	2:C:1183:ALA:N	2.37	0.40
3:D:748:ALA:HA	3:D:754:ILE:HA	2.02	0.40
3:D:900:GLY:O	3:D:908:ILE:HG13	2.21	0.40
3:D:1174:ARG:HH21	3:D:1187:GLU:HG2	1.85	0.40
5:F:111:LEU:HD21	5:F:115:GLY:HA3	2.03	0.40
5:F:220:LYS:C	5:F:223:GLU:HG3	2.40	0.40
5:F:355:ILE:C	5:F:358:VAL:HG12	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	229/329 (70%)	216 (94%)	13 (6%)	0	100	100
1	B	228/329 (69%)	216 (95%)	12 (5%)	0	100	100
2	C	1338/1342 (100%)	1235 (92%)	103 (8%)	0	100	100
3	D	1334/1407 (95%)	1253 (94%)	80 (6%)	1 (0%)	51	80
4	E	74/91 (81%)	71 (96%)	3 (4%)	0	100	100
5	F	458/613 (75%)	444 (97%)	14 (3%)	0	100	100
All	All	3661/4111 (89%)	3435 (94%)	225 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	1345	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/286 (70%)	199 (100%)	0	100	100
1	B	198/286 (69%)	198 (100%)	0	100	100
2	C	1155/1157 (100%)	1151 (100%)	4 (0%)	92	97
3	D	1113/1168 (95%)	1111 (100%)	2 (0%)	93	98
4	E	65/75 (87%)	65 (100%)	0	100	100
5	F	415/540 (77%)	415 (100%)	0	100	100
All	All	3145/3512 (90%)	3139 (100%)	6 (0%)	93	98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	272	ARG
2	C	283	LYS
2	C	473	ARG
2	C	478	ARG
3	D	709	ARG
3	D	972	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
2	C	1134	GLN
3	D	157	GLN
3	D	158	GLN
3	D	792	ASN

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Mol	Chain	Res	Type
3	D	962	ASN
3	D	1098	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	D9X	C	3001	-	86,90,90	4.46	39 (45%)	114,133,133	1.53	17 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	D9X	C	3001	-	2/2/27/27	15/72/133/133	0/7/9/9

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	3001	D9X	C47-C46	12.28	1.59	1.40
8	C	3001	D9X	C03-C02	11.88	1.60	1.39
8	C	3001	D9X	C63-C64	9.84	1.57	1.39
8	C	3001	D9X	C75-C76	9.64	1.56	1.38
8	C	3001	D9X	C75-C64	9.54	1.56	1.39
8	C	3001	D9X	C63-C47	9.43	1.56	1.38
8	C	3001	D9X	C43-C05	9.40	1.62	1.41
8	C	3001	D9X	C62-C61	9.20	1.55	1.38
8	C	3001	D9X	C52-C51	9.18	1.55	1.38
8	C	3001	D9X	C25-N80	9.01	1.52	1.34
8	C	3001	D9X	C42-C40	7.95	1.56	1.41
8	C	3001	D9X	C76-C46	7.39	1.52	1.40
8	C	3001	D9X	C40-C02	7.29	1.55	1.40
8	C	3001	D9X	C61-C53	7.17	1.54	1.38
8	C	3001	D9X	C51-C50	7.10	1.54	1.38
8	C	3001	D9X	C62-C50	7.05	1.54	1.38
8	C	3001	D9X	C52-C53	6.96	1.53	1.38
8	C	3001	D9X	O04-C03	6.19	1.49	1.37
8	C	3001	D9X	C43-C44	5.68	1.57	1.47
8	C	3001	D9X	C22-C23	4.88	1.58	1.43
8	C	3001	D9X	C64-N65	4.55	1.51	1.38
8	C	3001	D9X	O77-C76	4.52	1.44	1.38
8	C	3001	D9X	C43-C42	4.36	1.51	1.41
8	C	3001	D9X	C46-N45	3.98	1.46	1.38
8	C	3001	D9X	O31-C32	3.86	1.43	1.35
8	C	3001	D9X	O48-C47	3.85	1.45	1.37
8	C	3001	D9X	C49-C50	3.70	1.59	1.50
8	C	3001	D9X	C42-C81	3.59	1.54	1.46
8	C	3001	D9X	O31-C13	-3.03	1.40	1.44
8	C	3001	D9X	C69-N68	2.84	1.52	1.47
8	C	3001	D9X	C54-C53	2.84	1.56	1.51
8	C	3001	D9X	C05-C03	2.73	1.43	1.39
8	C	3001	D9X	O82-C81	-2.71	1.18	1.22
8	C	3001	D9X	C69-C70	2.61	1.59	1.52
8	C	3001	D9X	O41-C40	2.50	1.42	1.37
8	C	3001	D9X	C33-C32	2.37	1.57	1.49
8	C	3001	D9X	C66-N65	2.30	1.50	1.46
8	C	3001	D9X	C01-C02	2.20	1.56	1.51
8	C	3001	D9X	C74-N65	2.19	1.50	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	3001	D9X	O04-C03-C05	-6.07	110.21	114.36
8	C	3001	D9X	O31-C32-C33	4.85	120.01	111.09
8	C	3001	D9X	C05-C03-C02	-4.02	122.17	125.33
8	C	3001	D9X	O04-C03-C02	3.76	127.61	121.14
8	C	3001	D9X	C74-N65-C66	-3.75	103.23	111.52
8	C	3001	D9X	C40-C42-C81	-3.04	116.98	120.82
8	C	3001	D9X	C20-C21-C22	-2.79	120.29	126.16
8	C	3001	D9X	C70-C69-N68	-2.78	109.86	115.75
8	C	3001	D9X	O04-C07-C06	2.70	108.99	104.55
8	C	3001	D9X	C42-C43-C05	-2.65	116.33	119.90
8	C	3001	D9X	O39-C06-C07	2.63	125.91	120.56
8	C	3001	D9X	C03-C05-C06	2.55	109.67	107.05
8	C	3001	D9X	C22-C23-C24	-2.45	119.42	126.61
8	C	3001	D9X	C42-C81-C79	2.22	118.70	116.24
8	C	3001	D9X	O48-C47-C63	-2.19	118.55	123.58
8	C	3001	D9X	C27-C24-C25	2.15	120.72	115.28
8	C	3001	D9X	C73-N68-C67	2.13	113.63	108.83

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	C	3001	D9X	C79
8	C	3001	D9X	C78

All (15) torsion outliers are listed below:

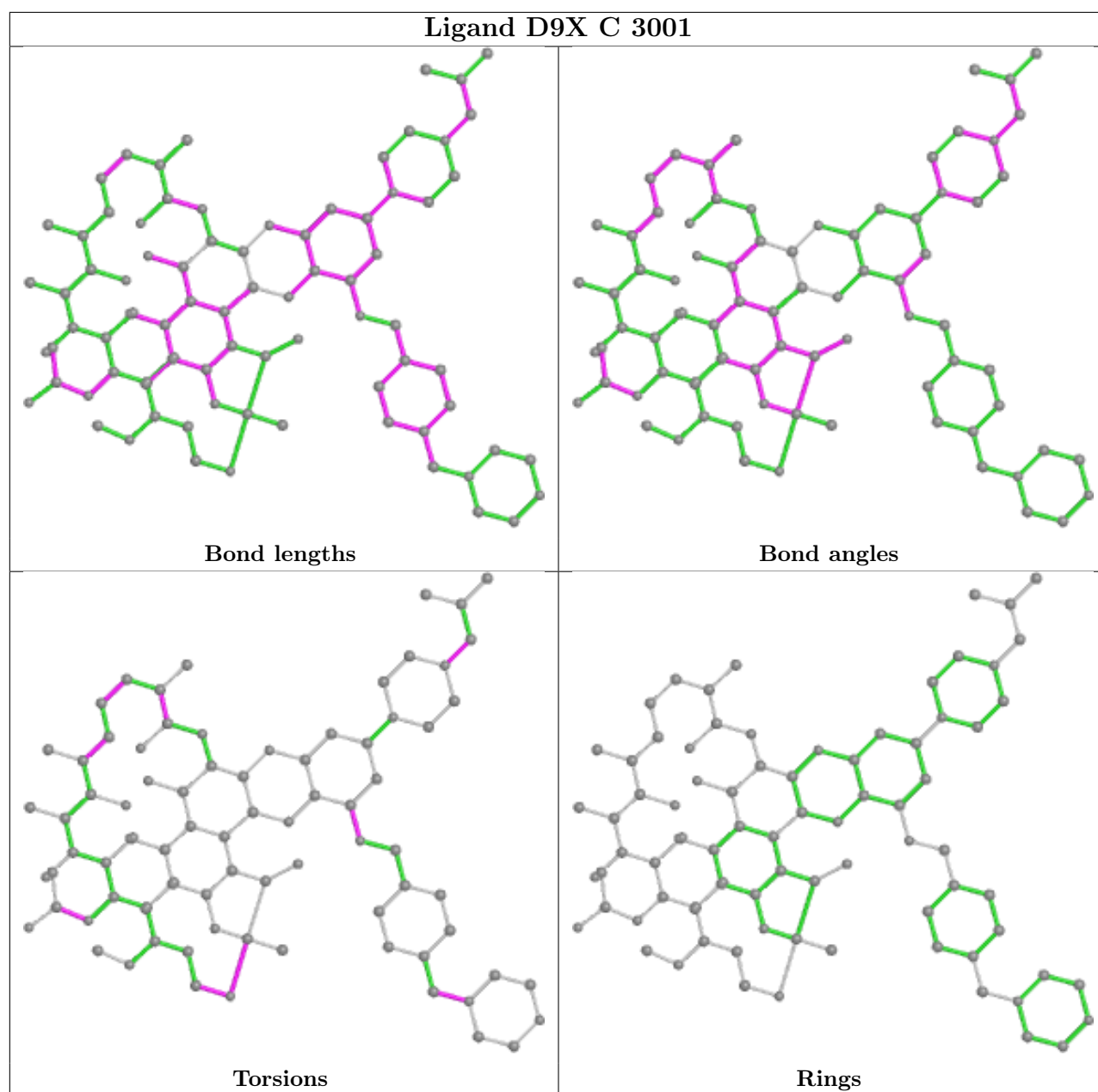
Mol	Chain	Res	Type	Atoms
8	C	3001	D9X	C38-C07-O08-C09
8	C	3001	D9X	O04-C07-O08-C09
8	C	3001	D9X	C33-C32-O31-C13
8	C	3001	D9X	C53-C54-N55-C56
8	C	3001	D9X	C53-C54-N55-C60
8	C	3001	D9X	C21-C22-C23-C24
8	C	3001	D9X	O34-C32-O31-C13
8	C	3001	D9X	C46-C47-O48-C49
8	C	3001	D9X	C06-C07-O08-C09
8	C	3001	D9X	C28-C20-C21-C22
8	C	3001	D9X	C63-C47-O48-C49
8	C	3001	D9X	C70-C69-N68-C67
8	C	3001	D9X	C70-C69-N68-C73
8	C	3001	D9X	C10-C09-O08-C07
8	C	3001	D9X	C27-C24-C25-N80

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	3001	D9X	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

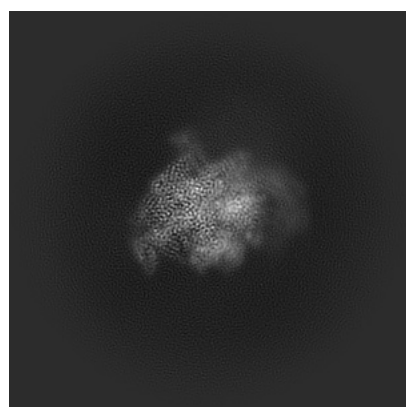
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25571. These allow visual inspection of the internal detail of the map and identification of artifacts.

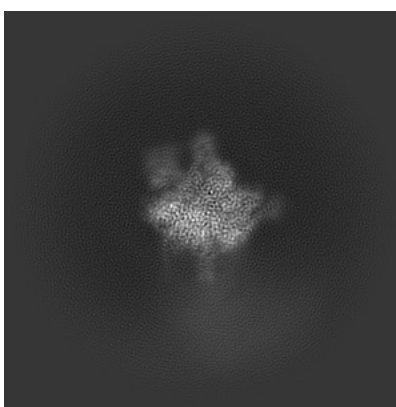
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

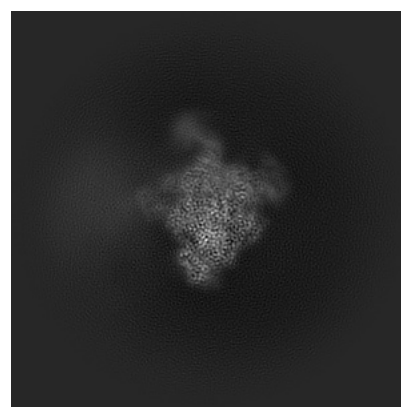
6.1.1 Primary map



X



Y

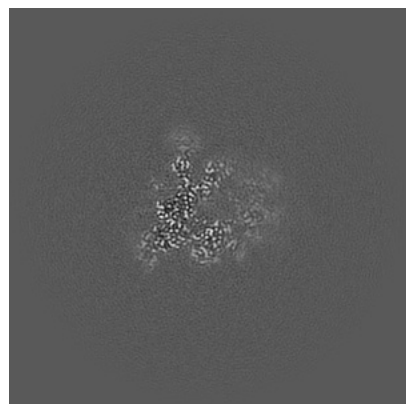


Z

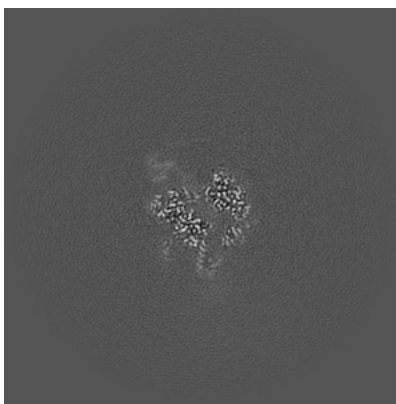
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

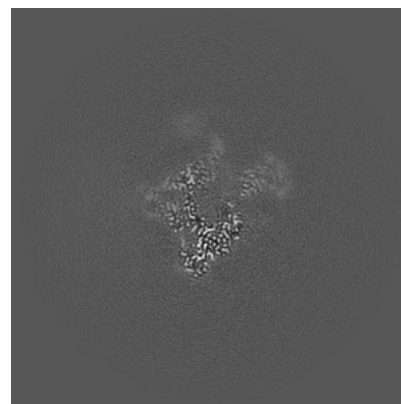
6.2.1 Primary map



X Index: 180



Y Index: 180

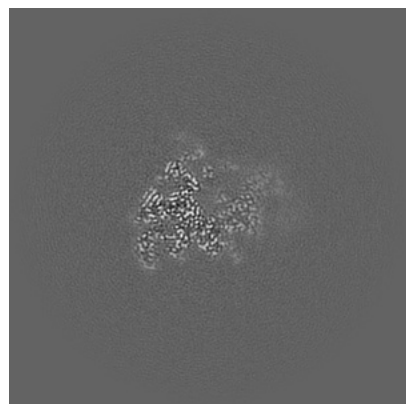


Z Index: 180

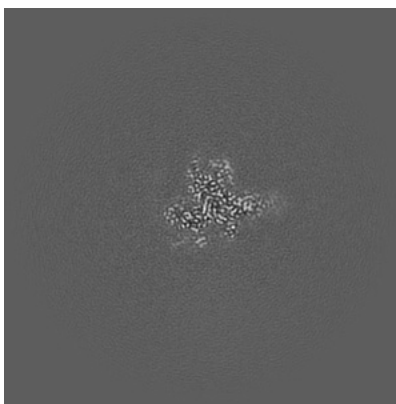
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

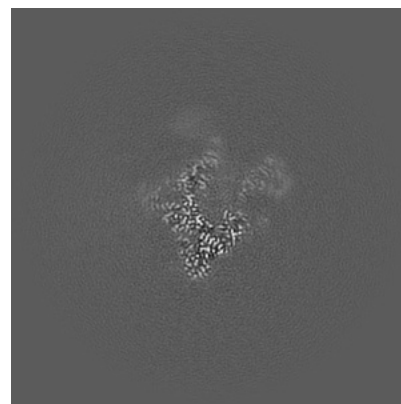
6.3.1 Primary map



X Index: 172



Y Index: 160



Z Index: 178

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

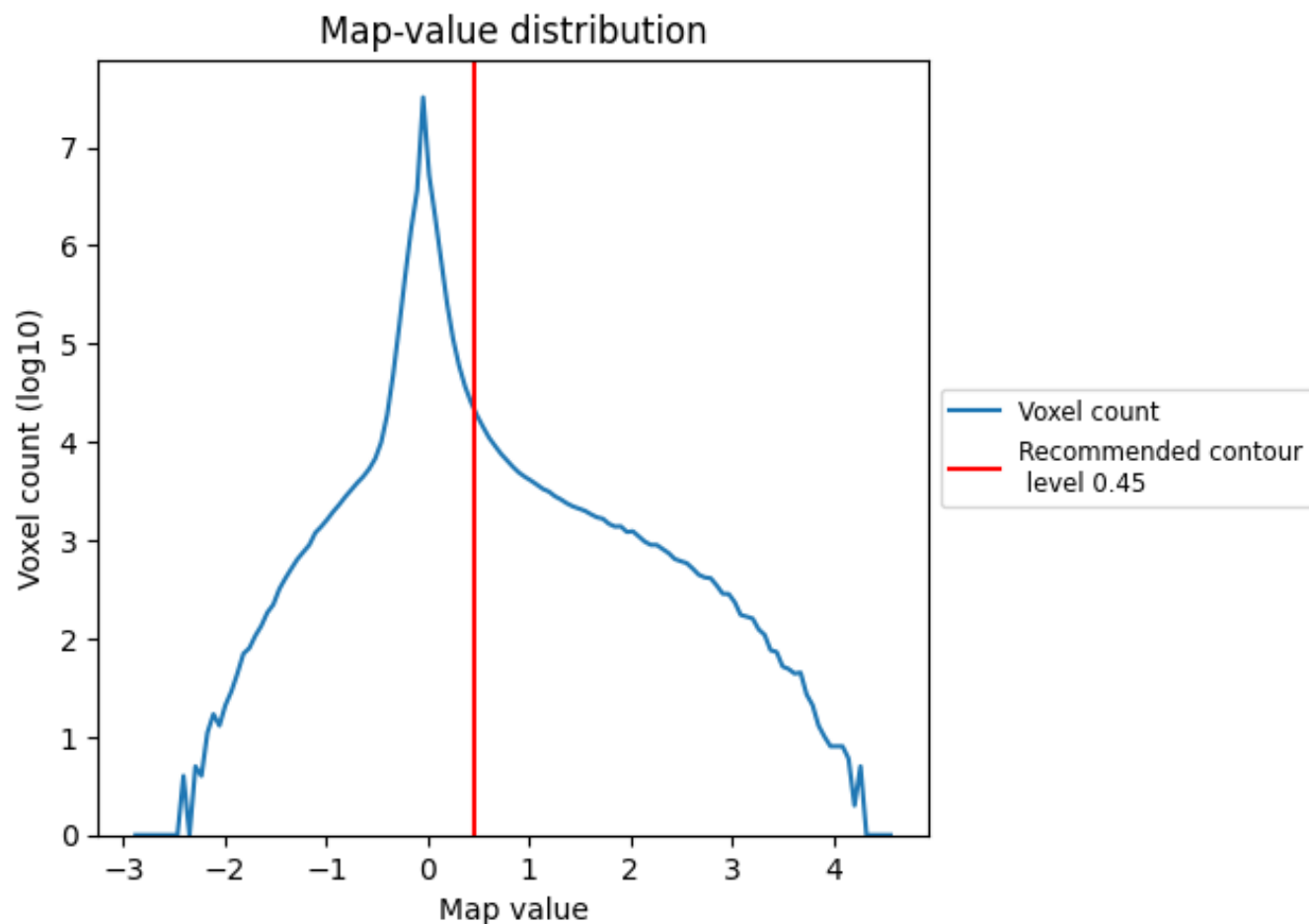
6.5 Mask visualisation

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

7 Map analysis [i](#)

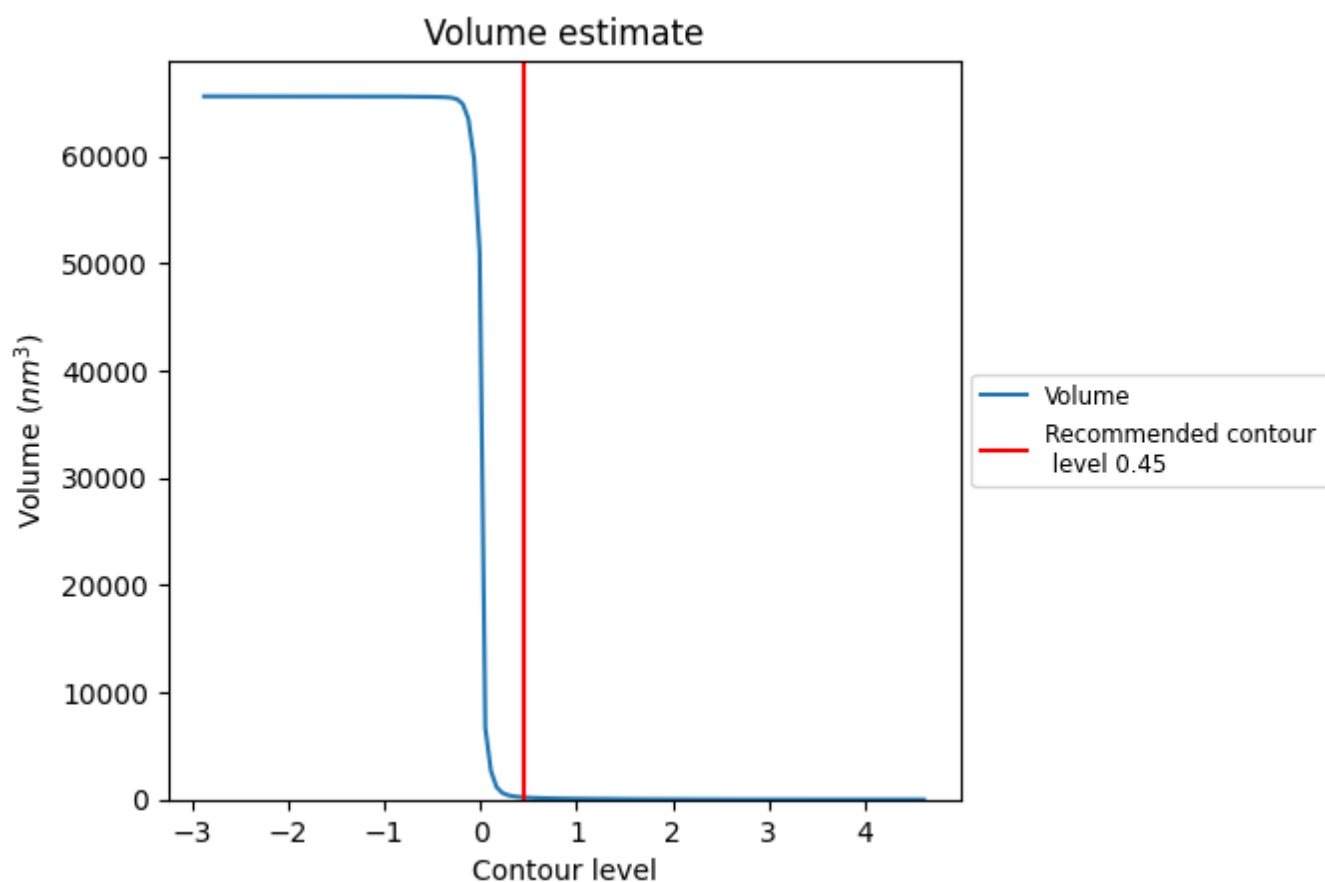
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

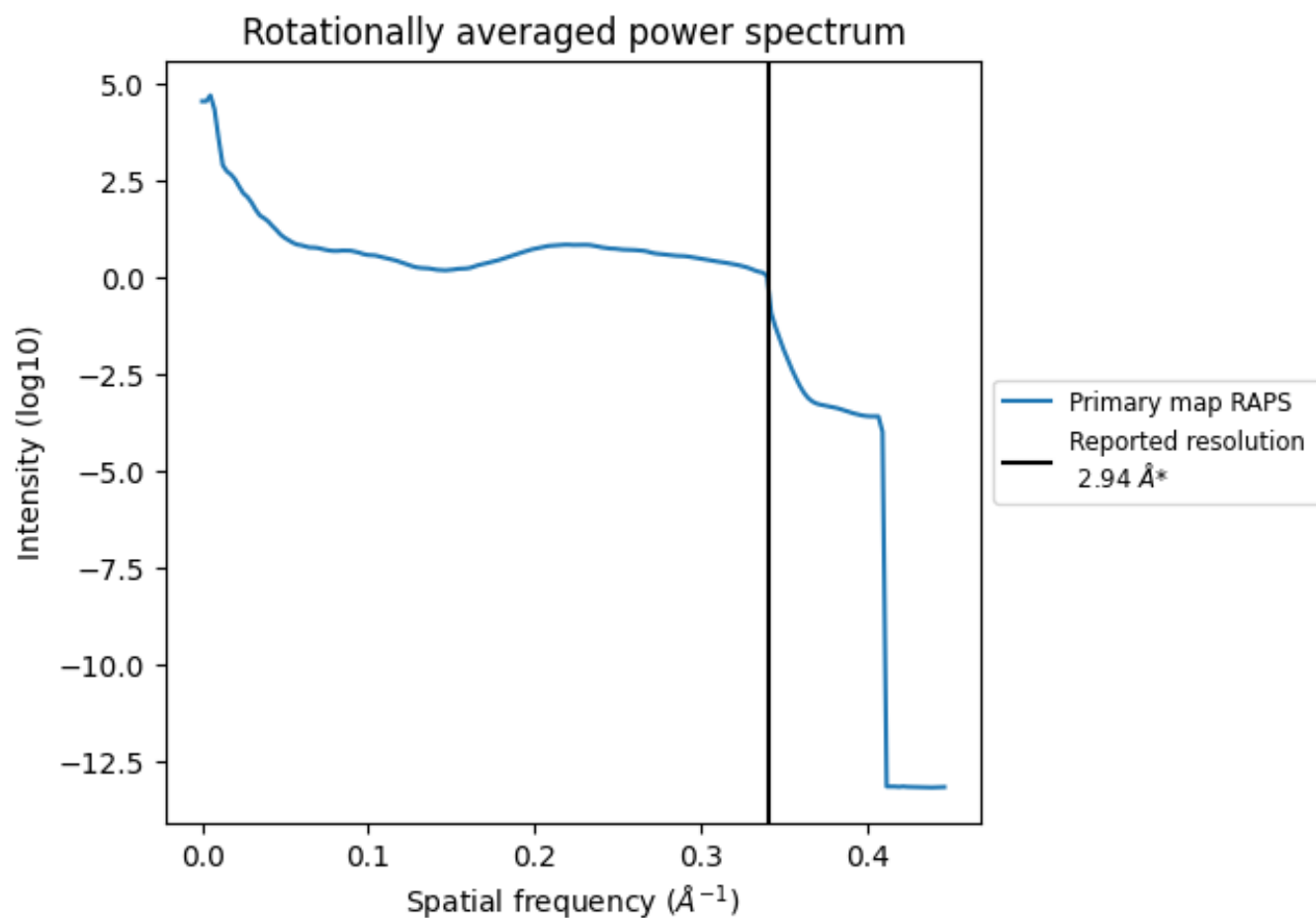
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 208 nm³; this corresponds to an approximate mass of 188 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 0.340 Å⁻¹

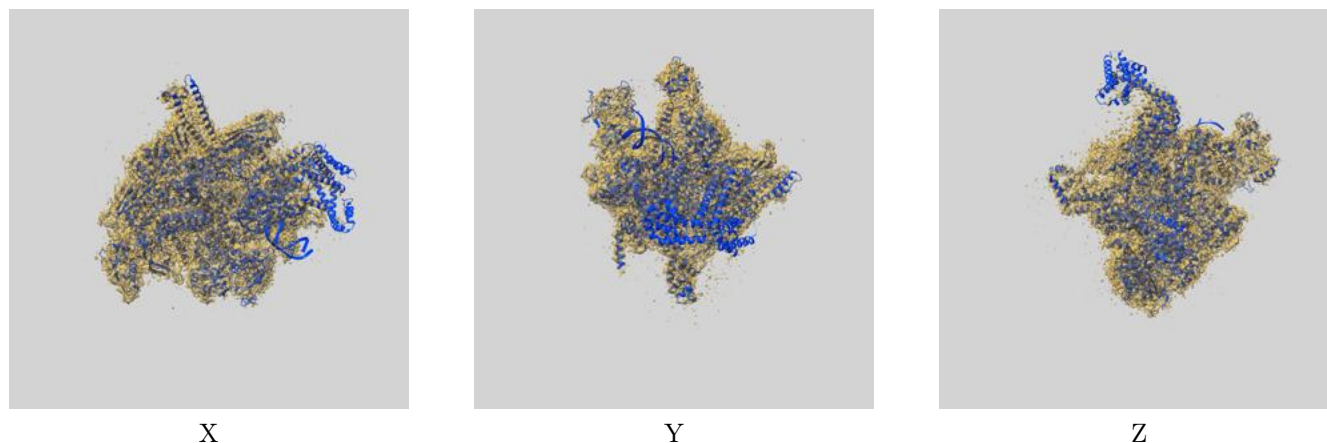
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

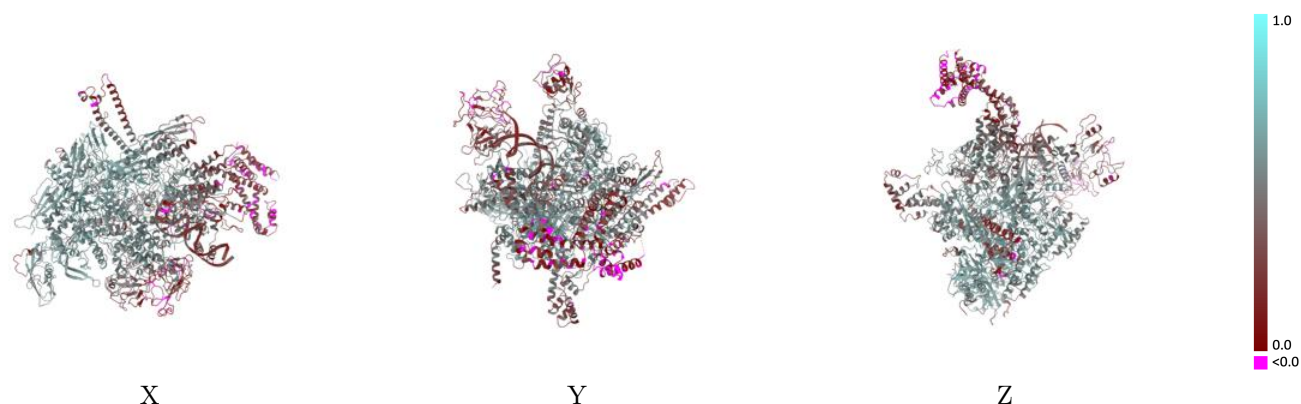
This section contains information regarding the fit between EMDB map EMD-25571 and PDB model 7SZK. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



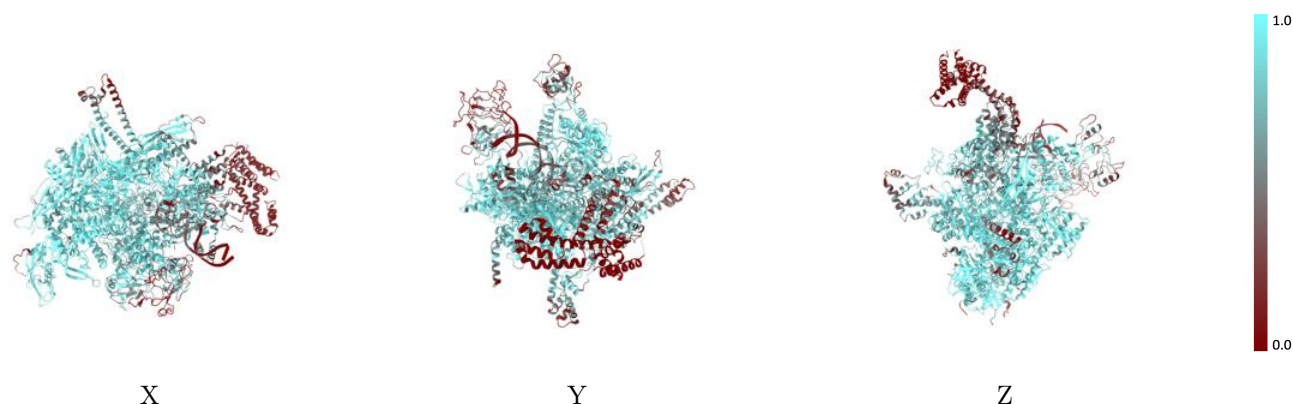
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



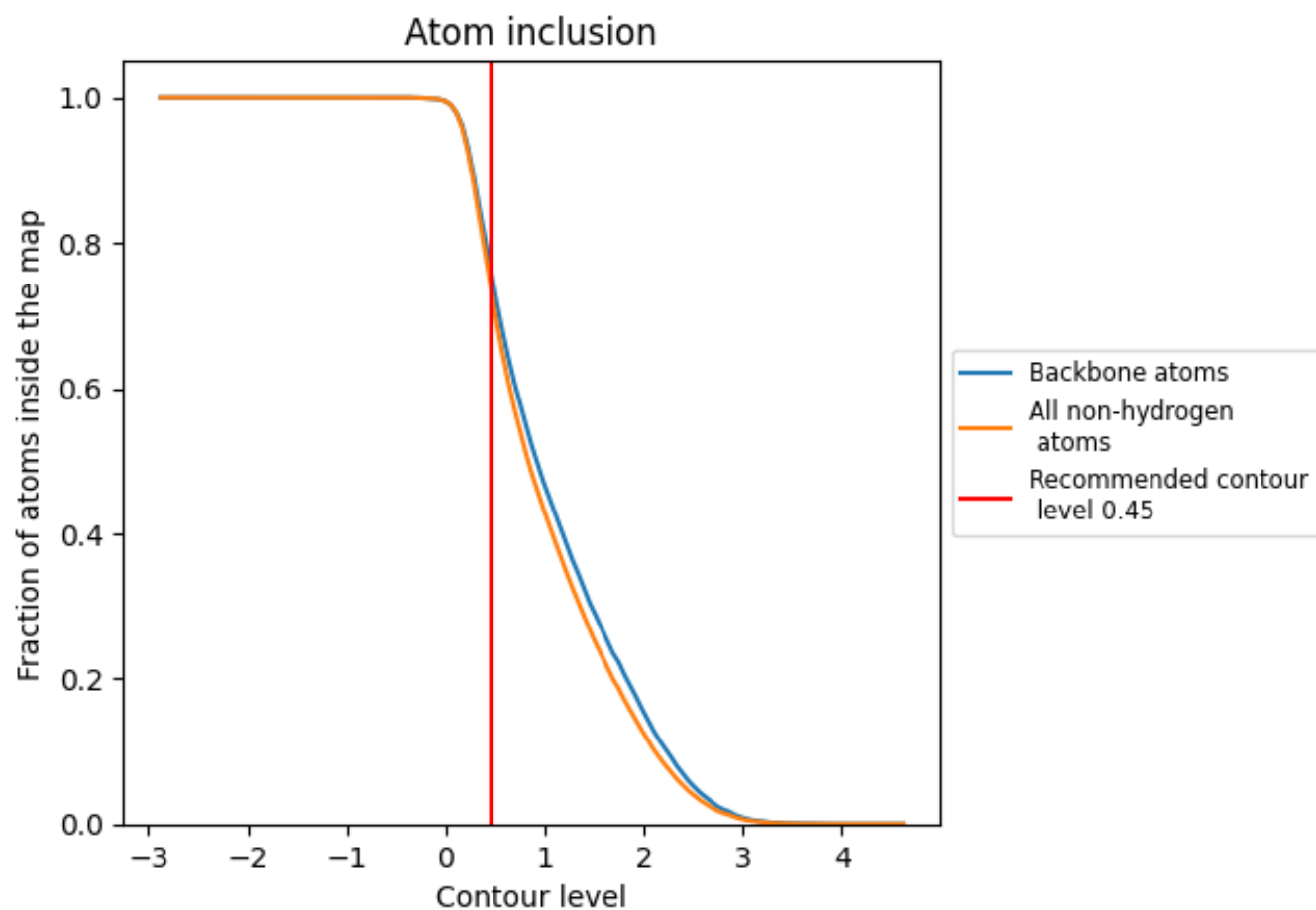
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 74% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7435	<div></div> 0.4620
A	<div></div> 0.8941	<div></div> 0.5550
B	<div></div> 0.8633	<div></div> 0.5260
C	<div></div> 0.8401	<div></div> 0.5060
D	<div></div> 0.7900	<div></div> 0.4750
E	<div></div> 0.7725	<div></div> 0.4880
F	<div></div> 0.3079	<div></div> 0.2590
X	<div></div> 0.3108	<div></div> 0.2910
Y	<div></div> 0.3641	<div></div> 0.3070

1.0

0.0

<0.0