Full wwPDB EM Validation Report ⓘ

Mar 20, 2024 – 04:03 PM JST

PDB ID	:	7DU2
EMDB ID	:	EMD-30865
Title	:	RNA polymerase III EC complex in post-translocation state
Authors	:	Li, L.; Yu, Z.; Zhao, D.; Ren, Y.; Hou, H.; Xu, Y.
Deposited on	:	2021-01-07
Resolution	:	3.35 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:

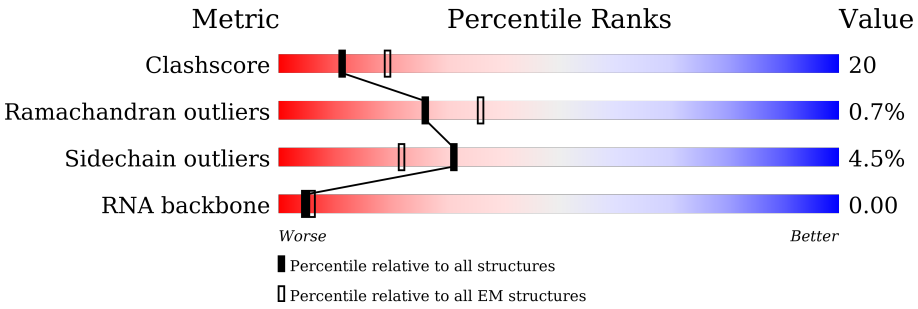
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.35 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
RNA backbone	4643	859

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 <=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	1390	70% 22% • 7%
2	B	1133	65% 25% • 8%
3	C	346	65% 26% • 5%
4	G	204	54% 26% 19%
5	K	133	48% 27% • 23%
6	L	58	52% 21% • 24%
7	P	316	7% 28% 12% • 59%

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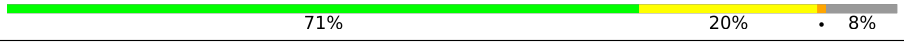
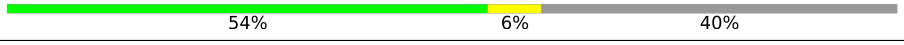
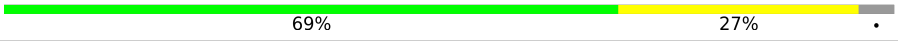
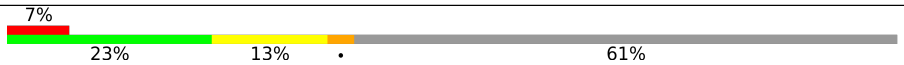
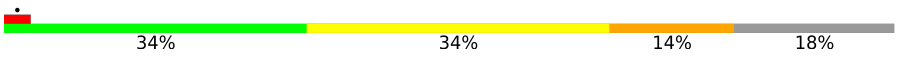
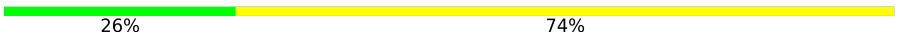
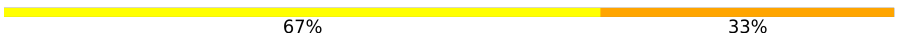
Mol	Chain	Length	Quality of chain
8	E	210	
9	F	127	
10	H	150	
11	J	67	
12	O	534	
13	Q	223	
14	D	148	
15	M	708	
16	N	398	
17	I	108	
18	X	14	
19	Y	19	
20	R	3	

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
23	SF4	P	401	-	-	X	-

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 36616 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1293	10152	6430	1776	1875	71	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1044	8254	5238	1434	1514	68	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	330	2641	1667	469	494	11	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	166	1337	876	211	245	5	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	K	103	822	513	145	157	7	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L	44	372	231	72	63	6	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	130	Total	C	N	O	S	0	0
			1008	636	166	196	10		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	194	Total	C	N	O	S	0	0
			1590	1014	276	292	8		

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	76	Total	C	N	O	S	0	0
			610	392	103	110	5		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	122	Total	C	N	O	S	0	0
			1002	645	167	185	5		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 12 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	443	Total	C	N	O	S	0	0
			3546	2233	620	673	20		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	86	Total	C	N	O	S	0	0
			724	463	124	131	6		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	122	Total	C	N	O	S	0	0
			985	614	172	196	3		

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	154	Total	C	N	O	S	0	0
			1272	809	226	232	5		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	92	Total	C	N	O	S	0	0
			697	445	117	131	4		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	47	Total	C	N	O	S	0	0
			340	210	65	60	5		

- Molecule 18 is a DNA chain called DNA (5'-D(P*GP*TP*CP*TP*GP*AP*TP*CP*TP*CP*GP*GP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	14	Total	C	N	O	P	0	0
			288	137	52	85	14		

- Molecule 19 is a DNA chain called DNA (5'-D(P*TP*TP*CP*CP*GP*AP*GP*AP*TP*CP*AP*GP*AP*CP*GP*AP*GP*AP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Y	19	Total	C	N	O	P	0	0
			392	186	75	112	19		

- Molecule 20 is a RNA chain called RNA (5'-R(P*AP*UP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	3	Total	C	N	O	P	0	0
			62	28	10	21	3		

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Lig-

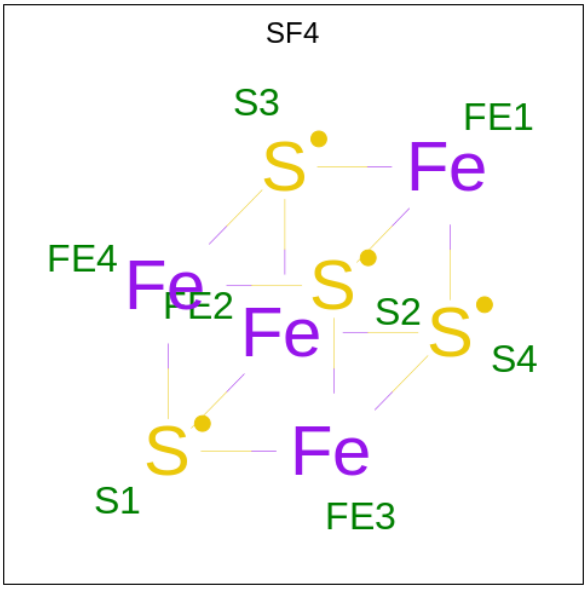
and of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total Mg 1 1	0

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 23 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



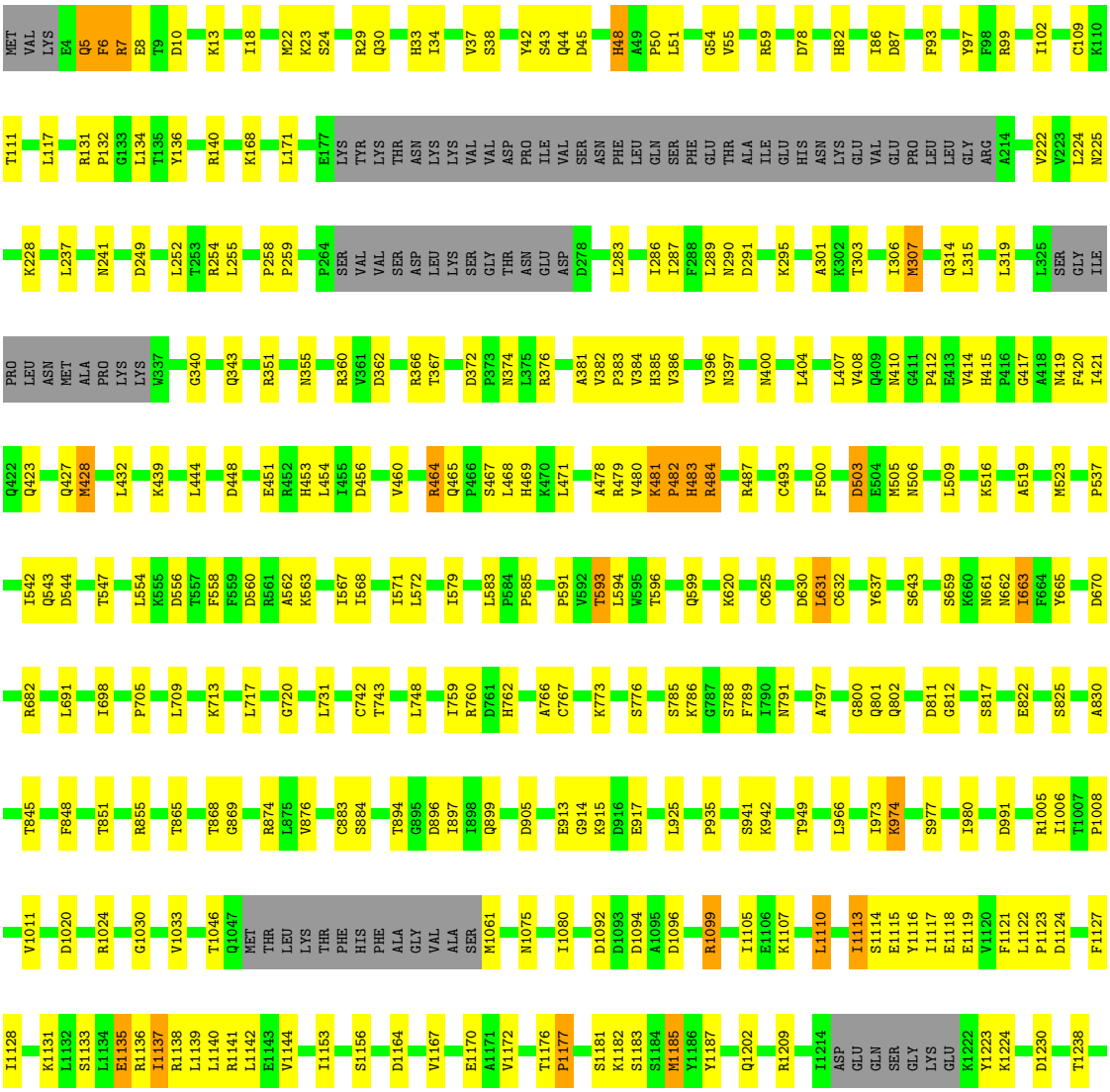
Mol	Chain	Residues	Atoms	AltConf
23	P	1	Total Fe S 8 4 4	0

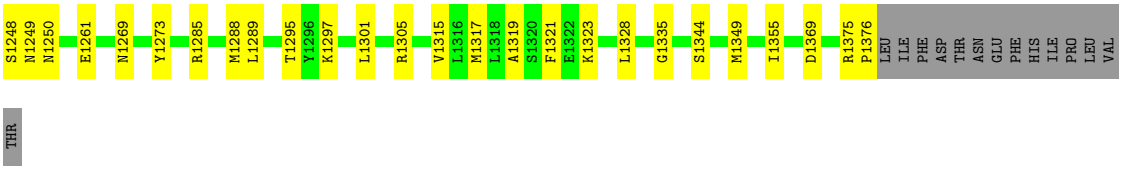
3 Residue-property plots (i)

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 III subunit RPC1

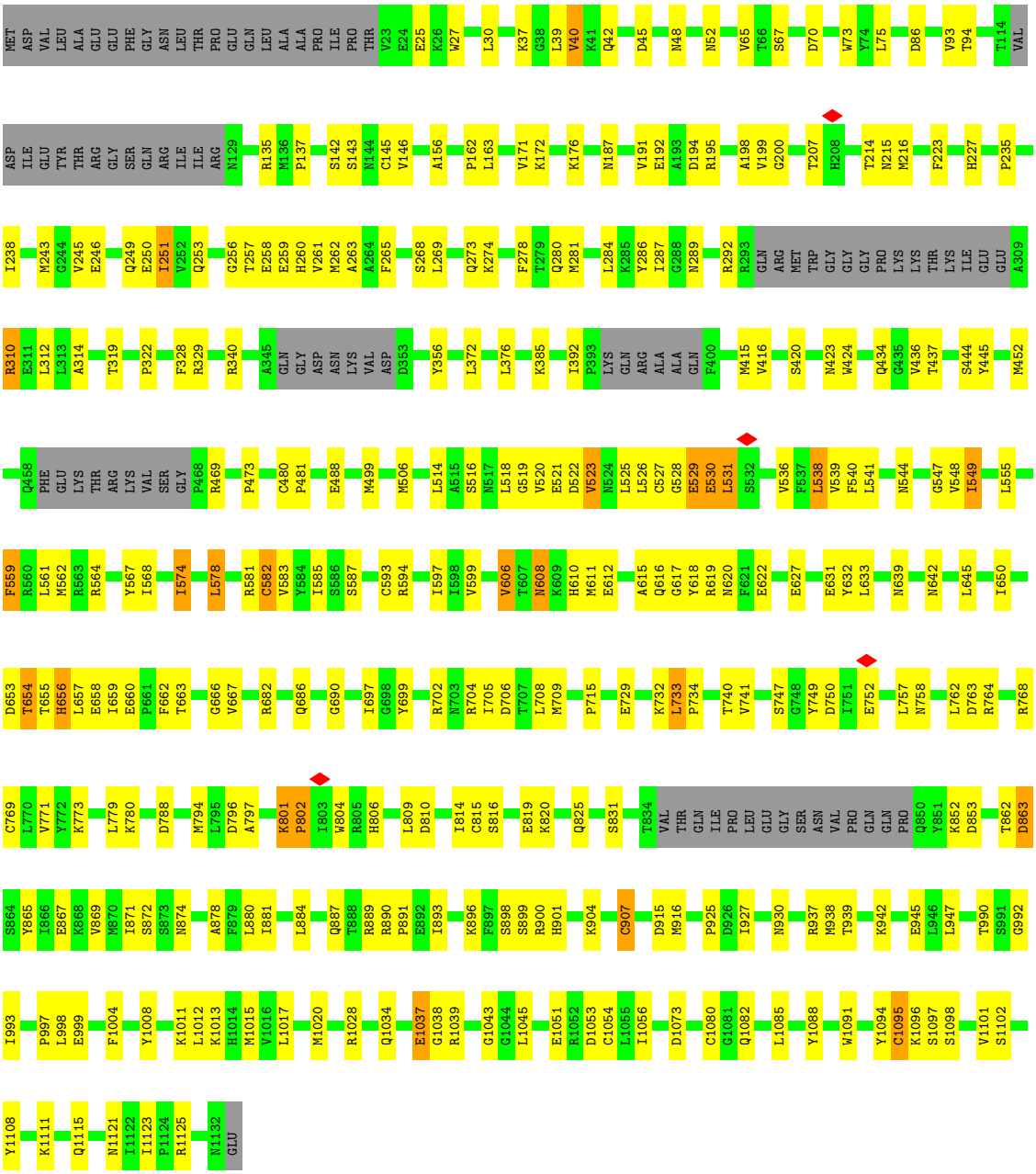
Chain A:





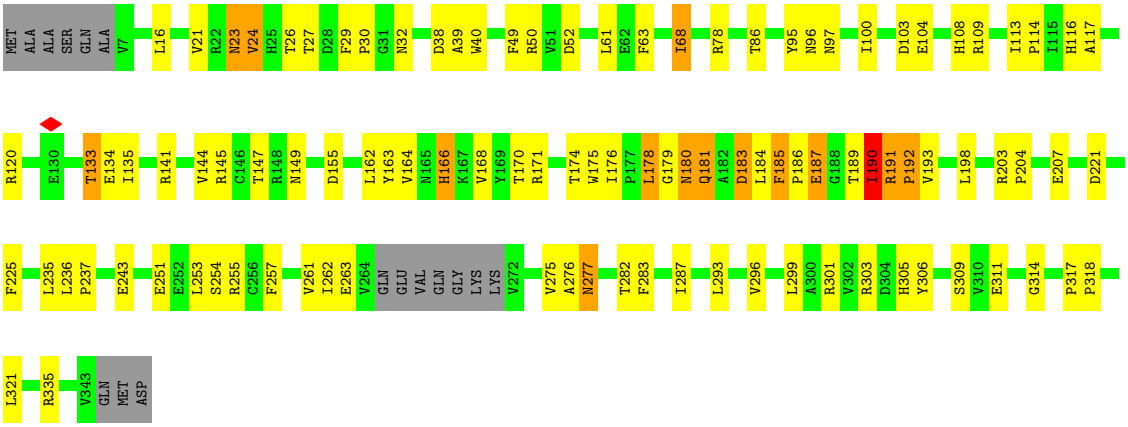
• Molecule 2: DNA-directed RNA polymerase III subunit RPC2

Chain B:



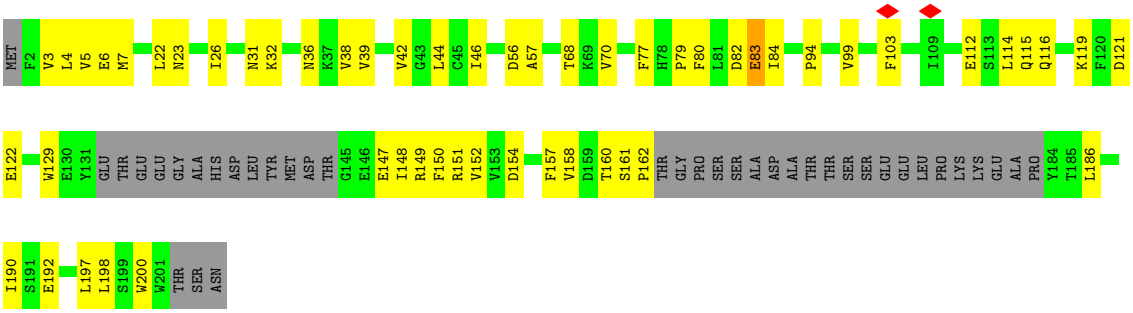
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C:



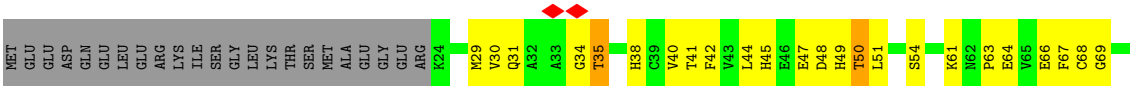
• Molecule 4: DNA-directed RNA polymerase III subunit RPC8

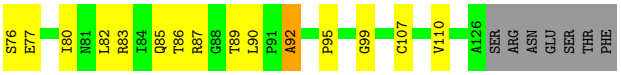
Chain G:



• Molecule 5: DNA-directed RNA polymerases I and III subunit RPAC2

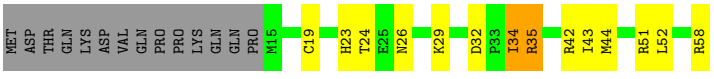
Chain K:





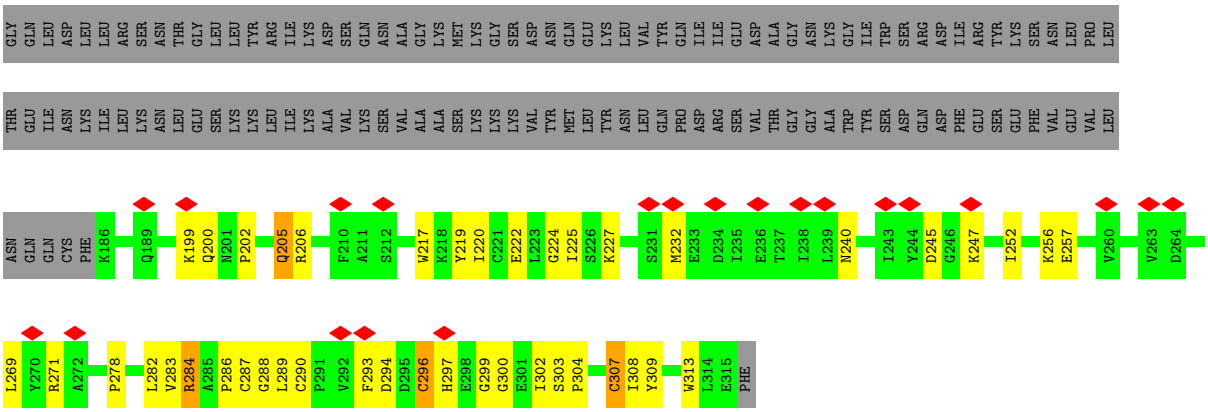
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



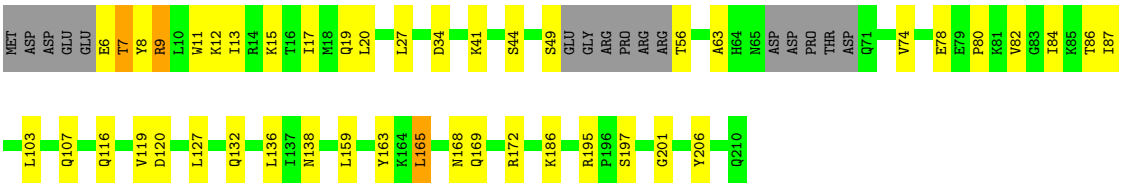
• Molecule 7: DNA-directed RNA polymerase III subunit RPC6

Chain P:



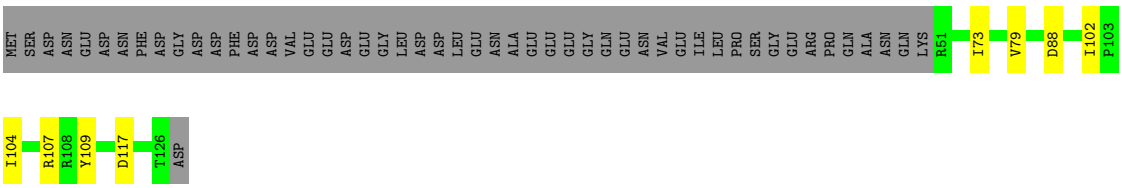
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



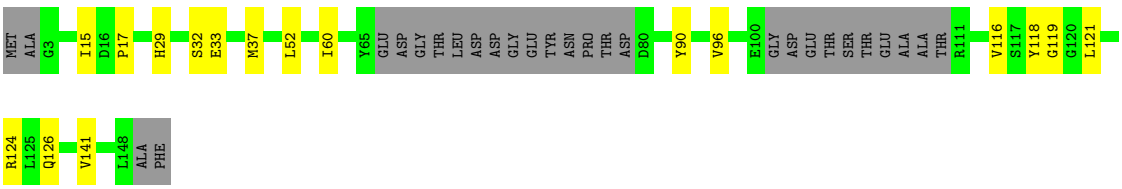
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:

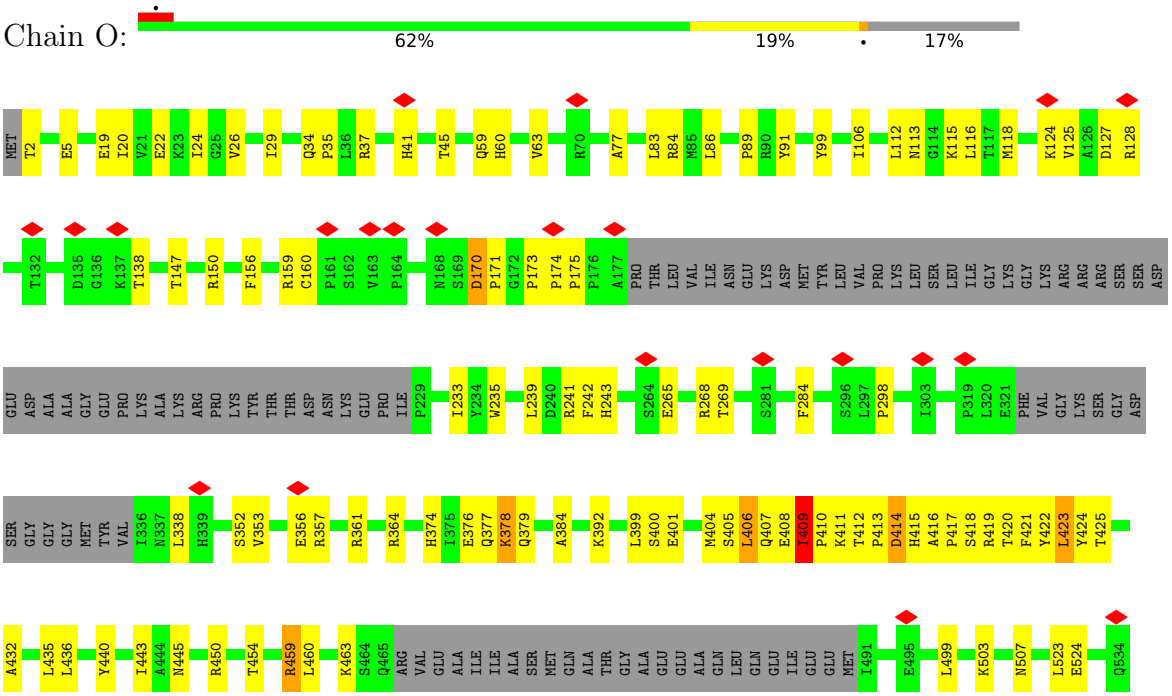


• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:

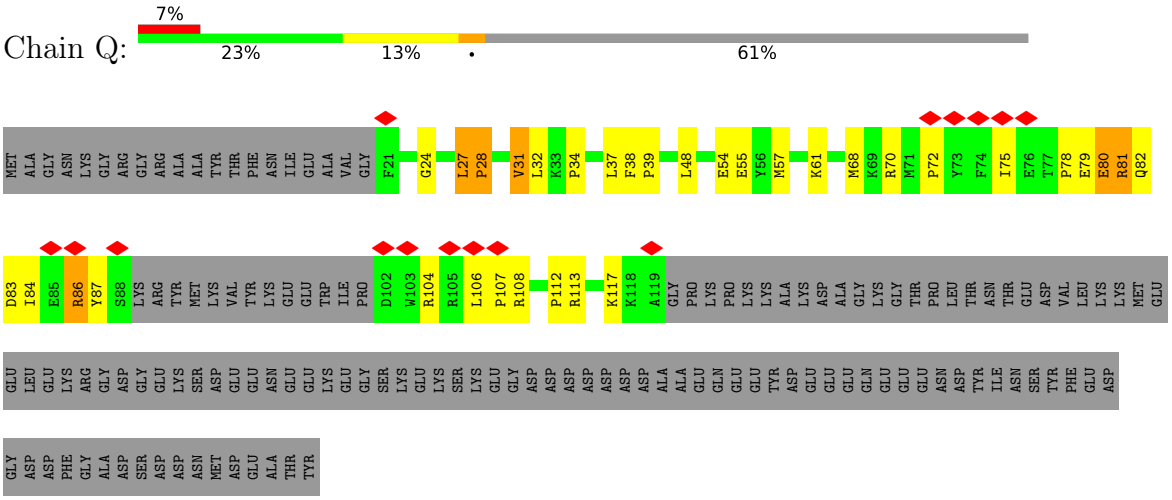
• Molecule 12: DNA-directed RNA polymerase III subunit RPC3

Chain O:



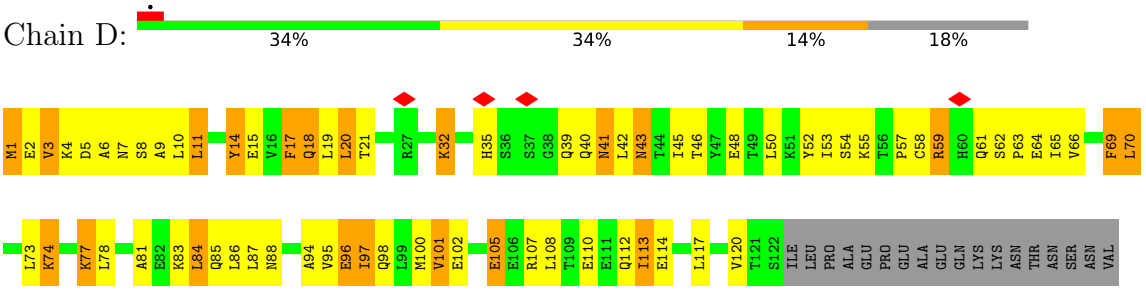
• Molecule 13: DNA-directed RNA polymerase III subunit RPC7

Chain Q:



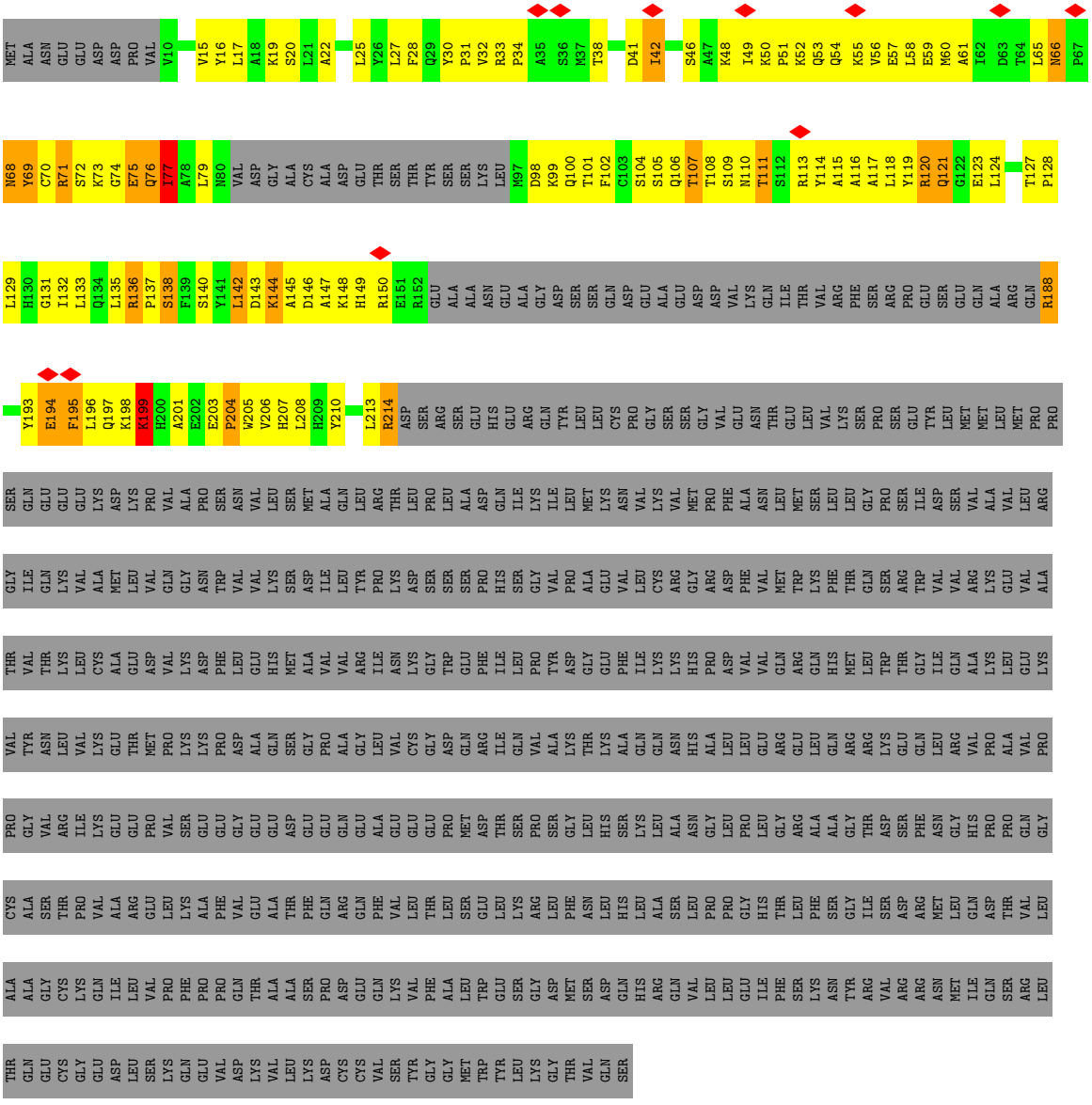
• Molecule 14: DNA-directed RNA polymerase III subunit RPC9

Chain D:



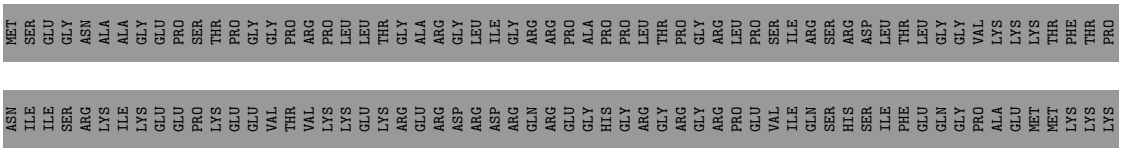
• Molecule 15: DNA-directed RNA polymerase III subunit RPC5

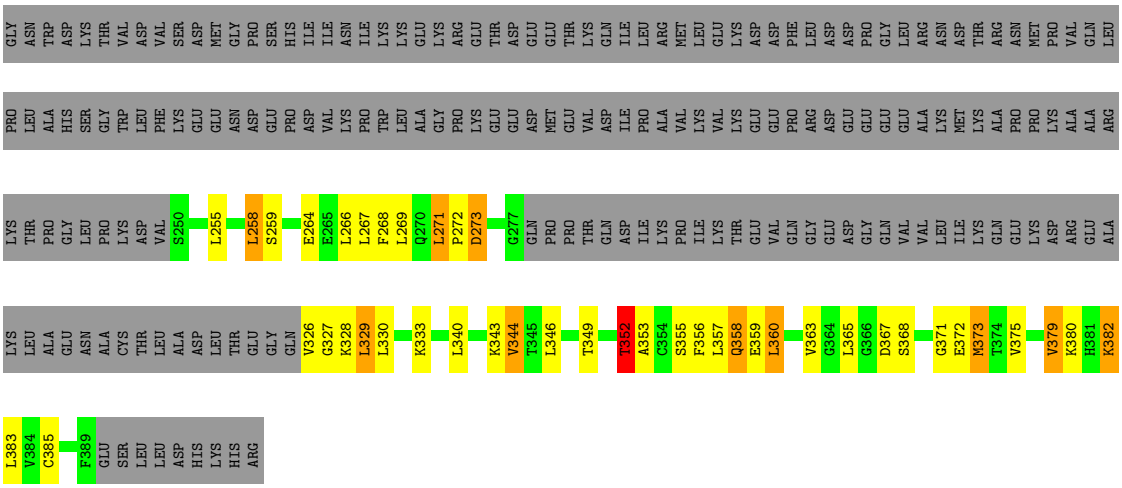
Chain M:



• Molecule 16: DNA-directed RNA polymerase III subunit RPC4

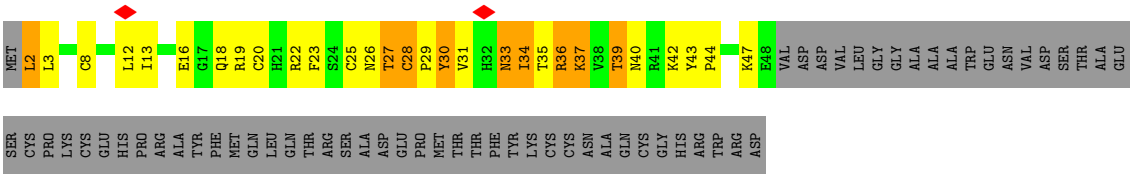
Chain N:





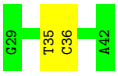
• Molecule 17: DNA-directed RNA polymerase III subunit RPC10

Chain I:



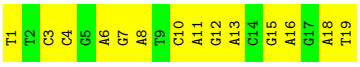
• Molecule 18: DNA (5'-D(P*GP*TP*CP*TP*GP*AP*TP*CP*TP*CP*GP*GP*AP*A)-3')

Chain X:



• Molecule 19: DNA (5'-D(P*TP*TP*CP*CP*GP*AP*GP*AP*TP*CP*AP*GP*AP*CP*GP* AP*GP*AP*T)-3')

Chain Y:



• Molecule 20: RNA (5'-R(P*AP*UP*C)-3')

Chain R:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64111	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.189	Depositor
Minimum map value	-0.778	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	337.28, 337.28, 337.28	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.054, 1.054, 1.054	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, SF4

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	0.54	0/10329	0.65	0/13920
2	B	0.61	0/8410	0.68	0/11338
3	C	0.63	0/2694	0.69	0/3653
4	G	0.50	0/1374	0.69	0/1868
5	K	0.63	0/837	0.67	0/1129
6	L	0.60	0/377	0.64	0/500
7	P	0.44	0/1028	0.72	0/1391
8	E	0.53	0/1616	0.61	0/2180
9	F	0.60	0/620	0.64	0/839
10	H	0.60	0/1019	0.68	0/1366
11	J	0.68	0/516	0.70	0/696
12	O	0.40	0/3604	0.60	0/4872
13	Q	0.45	0/742	0.69	0/996
14	D	0.58	0/997	0.79	0/1343
15	M	0.63	0/1301	0.95	0/1754
16	N	0.59	0/703	0.90	0/946
17	I	0.61	0/346	0.92	0/469
18	X	0.67	0/322	1.05	0/495
19	Y	0.48	0/440	0.81	0/677
20	R	0.21	0/68	0.70	0/103
All	All	0.56	0/37343	0.69	0/50535

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10152	0	10382	325	0
2	B	8254	0	8364	312	0
3	C	2641	0	2615	152	0
4	G	1337	0	1306	104	0
5	K	822	0	810	61	0
6	L	372	0	382	21	0
7	P	1008	0	998	64	0
8	E	1590	0	1630	41	0
9	F	610	0	642	5	0
10	H	1002	0	999	12	0
11	J	507	0	524	24	0
12	O	3546	0	3585	143	0
13	Q	724	0	734	44	0
14	D	985	0	1006	117	0
15	M	1272	0	1264	154	0
16	N	697	0	742	69	0
17	I	340	0	306	63	0
18	X	288	0	159	1	0
19	Y	392	0	214	22	0
20	R	62	0	33	4	0
21	A	1	0	0	0	0
22	A	2	0	0	0	0
22	B	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0
22	L	1	0	0	0	0
23	P	8	0	0	4	0
All	All	36616	0	36695	1469	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 20.

All (1469) 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)
15:M:31:PRO:HG2	15:M:136:ARG:CD	1.57	1.32
16:N:357:LEU:HD23	16:N:358:GLN:NE2	1.43	1.29
3:C:191:ARG:CB	3:C:192:PRO:HD3	1.61	1.27
12:O:356:GLU:OE1	13:Q:39:PRO:HD3	1.33	1.26
1:A:484:ARG:HH21	2:B:1017:LEU:CD2	1.49	1.26
5:K:40:VAL:CG2	5:K:92:ALA:HB1	1.64	1.25
5:K:40:VAL:HG22	5:K:92:ALA:CB	1.65	1.25
12:O:409:ILE:CG1	12:O:423:LEU:HD11	1.67	1.23
12:O:409:ILE:CD1	12:O:423:LEU:HD11	1.68	1.22
12:O:374:HIS:HB3	12:O:423:LEU:CD1	1.70	1.21
12:O:409:ILE:CG2	12:O:423:LEU:HD21	1.72	1.19
3:C:181:GLN:HE21	3:C:181:GLN:HA	1.03	1.18
12:O:374:HIS:HB3	12:O:423:LEU:HD12	1.18	1.17
12:O:410:PRO:HB2	12:O:419:ARG:NH2	1.60	1.17
12:O:409:ILE:N	12:O:410:PRO:HD2	1.58	1.17
1:A:483:HIS:CD2	2:B:893:ILE:HB	1.80	1.16
4:G:103:PHE:HB3	14:D:48:GLU:HB3	1.25	1.16
3:C:191:ARG:HG3	3:C:192:PRO:CD	1.76	1.15
12:O:409:ILE:HG13	12:O:423:LEU:CD1	1.76	1.15
12:O:410:PRO:CB	12:O:419:ARG:HH21	1.63	1.11
1:A:383:PRO:HB3	1:A:483:HIS:O	1.50	1.11
12:O:409:ILE:H	12:O:410:PRO:CD	1.60	1.11
3:C:191:ARG:HG3	3:C:192:PRO:HD2	1.17	1.10
13:Q:106:LEU:HD12	13:Q:107:PRO:HD2	1.25	1.10
12:O:409:ILE:HG13	12:O:423:LEU:HD11	1.28	1.10
1:A:29:ARG:HH12	7:P:302:ILE:HD11	1.04	1.09
1:A:29:ARG:HH12	7:P:302:ILE:CD1	1.64	1.09
3:C:191:ARG:HB2	3:C:192:PRO:HD3	1.13	1.09
3:C:191:ARG:CG	3:C:192:PRO:HD3	1.81	1.09
16:N:357:LEU:CD2	16:N:358:GLN:NE2	2.14	1.09
3:C:116:HIS:CD2	3:C:190:ILE:HD11	1.87	1.09
4:G:32:LYS:HZ3	14:D:39:GLN:HG3	1.17	1.09
1:A:571:ILE:HD11	1:A:682:ARG:HG2	1.28	1.08
15:M:31:PRO:CG	15:M:136:ARG:HD2	1.83	1.08
2:B:518:LEU:HD21	2:B:555:LEU:HA	1.29	1.08
12:O:409:ILE:CB	12:O:423:LEU:HD21	1.83	1.08
3:C:191:ARG:CG	3:C:192:PRO:CD	2.31	1.08
12:O:410:PRO:HB2	12:O:419:ARG:HH21	0.93	1.08
6:L:34:ILE:HD12	6:L:34:ILE:H	1.16	1.07
3:C:170:THR:HB	3:C:192:PRO:HG3	1.36	1.06
12:O:352:SER:O	12:O:356:GLU:HG2	1.51	1.06
4:G:148:ILE:HG23	4:G:190:ILE:CG2	1.83	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ARG:HH21	2:B:1017:LEU:HD23	0.99	1.06
15:M:32:VAL:HG11	15:M:137:PRO:HD3	1.35	1.06
15:M:140:SER:O	15:M:144:LYS:HG3	1.56	1.06
7:P:284:ARG:HB2	12:O:356:GLU:HG3	1.32	1.04
3:C:191:ARG:CB	3:C:192:PRO:CD	2.36	1.03
1:A:481:LYS:HB3	1:A:487:ARG:HH21	1.20	1.02
16:N:357:LEU:CD2	16:N:358:GLN:HE22	1.70	1.02
12:O:407:GLN:HB3	12:O:422:TYR:HB3	1.41	1.02
12:O:409:ILE:HG21	12:O:423:LEU:HD21	1.39	1.02
14:D:11:LEU:HD23	14:D:11:LEU:H	1.19	1.02
15:M:116:ALA:HB2	16:N:269:LEU:HB2	1.04	1.02
7:P:299:GLY:HA2	7:P:303:SER:CB	1.89	1.01
7:P:304:PRO:HG3	12:O:445:ASN:ND2	1.76	1.01
4:G:32:LYS:CB	14:D:39:GLN:HG3	1.90	1.01
15:M:31:PRO:CG	15:M:136:ARG:CD	2.37	1.00
1:A:1116:TYR:HB3	17:I:40:ASN:CB	1.91	1.00
1:A:484:ARG:NH2	2:B:1017:LEU:CD2	2.22	1.00
1:A:571:ILE:CD1	1:A:682:ARG:HG2	1.92	1.00
3:C:170:THR:O	3:C:191:ARG:HD2	1.60	1.00
12:O:377:GLN:HB3	12:O:421:PHE:HZ	1.26	1.00
4:G:148:ILE:HG23	4:G:190:ILE:HG23	1.41	0.99
4:G:32:LYS:HB3	14:D:39:GLN:HG3	0.99	0.99
15:M:31:PRO:HG2	15:M:136:ARG:HD2	1.00	0.99
3:C:116:HIS:CB	3:C:190:ILE:HG13	1.91	0.98
4:G:84:ILE:H	14:D:85:GLN:HE22	1.06	0.98
2:B:599:VAL:HB	2:B:655:THR:O	1.63	0.98
4:G:32:LYS:HB3	14:D:39:GLN:CG	1.92	0.98
13:Q:27:LEU:HD22	13:Q:27:LEU:H	1.27	0.97
6:L:23:HIS:NE2	11:J:64:PRO:HB2	1.78	0.97
15:M:115:ALA:HB1	15:M:128:PRO:HA	1.44	0.96
3:C:116:HIS:HB3	3:C:190:ILE:HG13	1.46	0.96
7:P:300:GLY:H	7:P:303:SER:HB3	1.30	0.96
1:A:1099:ARG:CG	1:A:1141:ARG:HB2	1.96	0.96
3:C:117:ALA:HB2	3:C:189:THR:HG22	1.47	0.96
12:O:409:ILE:H	12:O:410:PRO:HD2	0.79	0.96
17:I:20:CYS:SG	17:I:22:ARG:NH1	2.39	0.95
2:B:312:LEU:HD22	15:M:188:ARG:HG2	1.49	0.95
19:Y:1:DT:H5”	19:Y:1:DT:C6	2.01	0.95
1:A:1099:ARG:HG2	1:A:1141:ARG:CG	1.95	0.95
1:A:456:ASP:HA	1:A:478:ALA:O	1.67	0.94
1:A:484:ARG:NH2	2:B:1017:LEU:HD23	1.82	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:412:THR:HB	12:O:419:ARG:HA	1.50	0.94
1:A:1099:ARG:HG2	1:A:1141:ARG:HG2	1.50	0.94
15:M:31:PRO:HG2	15:M:136:ARG:NE	1.81	0.93
3:C:299:LEU:H	3:C:299:LEU:HD23	1.30	0.93
2:B:530:GLU:HA	2:B:536:VAL:HG21	1.51	0.93
1:A:481:LYS:HB3	1:A:487:ARG:NH2	1.84	0.93
4:G:83:GLU:HA	14:D:85:GLN:NE2	1.83	0.93
15:M:116:ALA:HB2	16:N:269:LEU:CB	1.96	0.93
17:I:28:CYS:O	17:I:28:CYS:SG	2.27	0.92
7:P:284:ARG:HA	7:P:284:ARG:NE	1.81	0.92
7:P:284:ARG:HA	7:P:284:ARG:HE	1.34	0.92
12:O:409:ILE:HD12	12:O:423:LEU:HD11	1.48	0.92
2:B:802:PRO:HG2	2:B:806:HIS:HD2	1.35	0.92
4:G:32:LYS:HZ3	14:D:39:GLN:CG	1.82	0.92
1:A:483:HIS:HD2	2:B:893:ILE:HB	1.31	0.91
3:C:170:THR:HB	3:C:192:PRO:CG	1.99	0.91
12:O:409:ILE:HB	12:O:423:LEU:HD21	1.49	0.91
1:A:1099:ARG:NH1	1:A:1099:ARG:HB2	1.86	0.91
2:B:660:GLU:OE1	2:B:660:GLU:HA	1.70	0.91
14:D:17:PHE:HB2	14:D:53:ILE:HG21	1.53	0.91
14:D:11:LEU:H	14:D:11:LEU:CD2	1.84	0.91
3:C:134:GLU:HG3	3:C:179:GLY:N	1.86	0.90
14:D:97:ILE:HA	14:D:101:VAL:HB	1.54	0.90
7:P:299:GLY:HA2	7:P:303:SER:HB3	1.51	0.90
1:A:481:LYS:HD2	1:A:482:PRO:HD3	1.50	0.90
3:C:181:GLN:HA	3:C:181:GLN:NE2	1.87	0.90
13:Q:106:LEU:HD12	13:Q:107:PRO:CD	2.00	0.90
2:B:156:ALA:HA	11:J:62:TYR:CE1	2.07	0.89
17:I:27:THR:HG22	17:I:29:PRO:HD3	1.55	0.89
8:E:27:LEU:CD2	8:E:63:ALA:O	2.21	0.88
14:D:4:LYS:HE2	14:D:4:LYS:HA	1.52	0.88
15:M:71:ARG:CZ	15:M:71:ARG:HA	2.03	0.88
1:A:484:ARG:NH2	2:B:1017:LEU:HD21	1.88	0.88
16:N:357:LEU:HD23	16:N:358:GLN:HE22	1.06	0.88
15:M:49:ILE:HG23	15:M:54:GLN:HG3	1.56	0.88
2:B:801:LYS:H	2:B:801:LYS:CE	1.87	0.88
15:M:136:ARG:H	15:M:136:ARG:HH21	1.19	0.88
12:O:407:GLN:O	12:O:410:PRO:HD2	1.73	0.87
1:A:1117:ILE:O	17:I:40:ASN:HA	1.73	0.87
12:O:377:GLN:HB3	12:O:421:PHE:CZ	2.09	0.87
1:A:29:ARG:NH1	7:P:302:ILE:HD11	1.88	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:801:LYS:H	2:B:801:LYS:HE2	1.39	0.86
4:G:103:PHE:HB3	14:D:48:GLU:CB	2.04	0.86
4:G:103:PHE:O	14:D:48:GLU:HB3	1.74	0.86
13:Q:27:LEU:H	13:Q:27:LEU:CD2	1.87	0.86
3:C:191:ARG:HB2	3:C:192:PRO:CD	2.00	0.86
5:K:40:VAL:HG22	5:K:92:ALA:HB1	0.86	0.86
15:M:69:TYR:HB3	17:I:27:THR:HB	1.56	0.86
3:C:113:ILE:CG2	3:C:192:PRO:HB3	2.06	0.86
12:O:407:GLN:O	12:O:410:PRO:CD	2.24	0.86
1:A:1099:ARG:HG2	1:A:1141:ARG:HB2	1.55	0.86
19:Y:3:DC:OP2	19:Y:3:DC:H2'	1.77	0.85
1:A:1099:ARG:HG2	1:A:1141:ARG:CB	2.06	0.85
3:C:183:ASP:OD1	3:C:183:ASP:N	2.07	0.85
8:E:27:LEU:HD23	8:E:27:LEU:H	1.40	0.85
17:I:22:ARG:HG2	17:I:29:PRO:HB3	1.58	0.85
14:D:43:ASN:H	14:D:43:ASN:HD22	1.25	0.85
5:K:86:THR:HG21	5:K:90:LEU:HB2	1.58	0.84
14:D:11:LEU:HD23	14:D:11:LEU:N	1.91	0.84
1:A:171:LEU:H	1:A:171:LEU:HD23	1.39	0.84
15:M:31:PRO:CG	15:M:136:ARG:NE	2.39	0.84
5:K:64:GLU:HB3	5:K:90:LEU:HD21	1.59	0.84
4:G:148:ILE:HG23	4:G:190:ILE:HG21	1.60	0.84
12:O:374:HIS:CB	12:O:423:LEU:HD12	2.06	0.84
1:A:1099:ARG:HB2	1:A:1099:ARG:CZ	2.07	0.84
1:A:1137:ILE:HD12	1:A:1142:LEU:HD21	1.58	0.84
12:O:409:ILE:HG13	12:O:423:LEU:CG	2.06	0.84
2:B:25:GLU:O	2:B:611:MET:HG2	1.78	0.83
4:G:3:VAL:HA	14:D:11:LEU:HD21	1.58	0.83
6:L:34:ILE:HD12	6:L:34:ILE:N	1.92	0.83
1:A:483:HIS:NE2	2:B:893:ILE:HD12	1.94	0.83
12:O:409:ILE:HB	12:O:423:LEU:CD2	2.09	0.83
7:P:299:GLY:HA2	7:P:303:SER:HB2	1.61	0.83
12:O:415:HIS:O	12:O:419:ARG:HG3	1.78	0.83
2:B:814:ILE:HD13	2:B:814:ILE:N	1.94	0.82
3:C:113:ILE:HG21	3:C:192:PRO:HB3	1.61	0.82
4:G:84:ILE:N	14:D:85:GLN:HE22	1.77	0.82
14:D:58:CYS:HA	14:D:61:GLN:HB2	1.60	0.82
4:G:32:LYS:NZ	14:D:39:GLN:CG	2.43	0.82
1:A:568:ILE:O	1:A:571:ILE:HG22	1.79	0.81
1:A:383:PRO:CB	1:A:483:HIS:O	2.27	0.81
2:B:1091:TRP:HE1	4:G:162:PRO:CD	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:LYS:CB	1:A:487:ARG:HH21	1.93	0.81
1:A:483:HIS:CE1	2:B:893:ILE:HD12	2.16	0.81
1:A:1099:ARG:HG3	1:A:1141:ARG:HB2	1.63	0.80
15:M:199:LYS:HB2	15:M:199:LYS:NZ	1.96	0.80
1:A:785:SER:O	1:A:786:LYS:HD2	1.80	0.80
12:O:407:GLN:CB	12:O:422:TYR:HB3	2.11	0.80
15:M:136:ARG:HH21	15:M:136:ARG:N	1.80	0.80
5:K:86:THR:HG21	5:K:90:LEU:CB	2.11	0.79
2:B:650:ILE:HG23	2:B:654:THR:HG21	1.65	0.79
3:C:162:LEU:CD1	3:C:204:PRO:HD3	2.12	0.79
5:K:40:VAL:CG2	5:K:92:ALA:CB	2.41	0.79
2:B:256:GLY:HA2	2:B:531:LEU:HD11	1.62	0.79
17:I:18:GLN:O	17:I:19:ARG:HG2	1.82	0.79
4:G:103:PHE:CG	14:D:48:GLU:OE1	2.36	0.79
1:A:500:PHE:CD2	2:B:752:GLU:HB2	2.18	0.78
4:G:32:LYS:HZ3	4:G:32:LYS:HB3	1.48	0.78
1:A:383:PRO:HB3	1:A:484:ARG:HA	1.64	0.78
7:P:300:GLY:N	7:P:303:SER:HB3	1.97	0.78
2:B:802:PRO:HG2	2:B:806:HIS:CD2	2.19	0.78
3:C:162:LEU:HD11	3:C:203:ARG:HD2	1.65	0.78
3:C:185:PHE:CB	3:C:186:PRO:CD	2.62	0.77
15:M:48:LYS:HB2	15:M:57:GLU:HB2	1.65	0.77
4:G:32:LYS:NZ	14:D:39:GLN:HG3	1.97	0.77
17:I:34:ILE:HG13	17:I:36:ARG:HE	1.49	0.77
2:B:156:ALA:HA	11:J:62:TYR:CD1	2.20	0.77
2:B:1038:GLY:O	2:B:1043:GLY:HA2	1.84	0.77
1:A:483:HIS:NE2	2:B:893:ILE:CG1	2.48	0.77
3:C:185:PHE:HB3	3:C:186:PRO:HD3	1.65	0.77
23:P:401:SF4:S2	12:O:445:ASN:OD1	2.43	0.77
2:B:245:VAL:CG2	2:B:250:GLU:HG2	2.14	0.76
4:G:36:ASN:OD1	14:D:45:ILE:HB	1.85	0.76
4:G:151:ARG:HD2	4:G:151:ARG:O	1.85	0.76
14:D:54:SER:HA	14:D:59:ARG:NH1	2.00	0.76
15:M:32:VAL:HG11	15:M:137:PRO:CD	2.14	0.76
14:D:10:LEU:HD23	14:D:10:LEU:O	1.84	0.76
13:Q:27:LEU:HD22	13:Q:27:LEU:N	2.00	0.75
2:B:253:GLN:HB3	2:B:527:CYS:HB2	1.68	0.75
7:P:293:PHE:HE2	7:P:307:CYS:HB2	1.51	0.75
2:B:1091:TRP:HE1	4:G:162:PRO:N	1.84	0.75
16:N:352:THR:HG21	16:N:382:LYS:HB2	1.68	0.75
2:B:530:GLU:HG3	2:B:548:VAL:HG21	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ASP:HB2	1:A:479:ARG:HD3	1.69	0.75
7:P:284:ARG:HB2	12:O:356:GLU:CG	2.13	0.74
6:L:35:ARG:HE	6:L:42:ARG:HH21	1.33	0.74
8:E:27:LEU:HD23	8:E:63:ALA:O	1.86	0.74
12:O:356:GLU:OE1	13:Q:39:PRO:CD	2.26	0.74
15:M:115:ALA:CB	15:M:128:PRO:HA	2.15	0.74
1:A:1110:LEU:HD12	1:A:1110:LEU:O	1.87	0.74
1:A:412:PRO:HB3	1:A:419:ASN:HB3	1.70	0.74
4:G:103:PHE:O	14:D:48:GLU:CB	2.35	0.74
5:K:86:THR:HB	5:K:90:LEU:HD22	1.69	0.74
1:A:483:HIS:CD2	2:B:893:ILE:CB	2.67	0.74
2:B:526:LEU:HG	16:N:358:GLN:HE21	1.53	0.73
2:B:539:VAL:HA	2:B:583:VAL:HG22	1.70	0.73
2:B:67:SER:HG	2:B:73:TRP:HE1	1.33	0.73
2:B:620:ASN:HB3	2:B:622:GLU:OE1	1.88	0.73
12:O:409:ILE:HG21	12:O:423:LEU:CD2	2.18	0.73
6:L:34:ILE:H	6:L:34:ILE:CD1	1.97	0.73
12:O:409:ILE:CG1	12:O:423:LEU:CD1	2.47	0.73
1:A:385:HIS:CD2	1:A:484:ARG:NH1	2.57	0.73
1:A:415:HIS:NE2	1:A:480:VAL:HG21	2.04	0.73
1:A:428:MET:CE	1:A:428:MET:HA	2.19	0.73
15:M:56:VAL:HG12	15:M:135:LEU:HD22	1.69	0.73
13:Q:82:GLN:CD	14:D:107:ARG:HH21	1.93	0.72
3:C:68:ILE:N	3:C:68:ILE:HD12	2.05	0.72
5:K:86:THR:CG2	5:K:90:LEU:HB2	2.19	0.72
4:G:79:PRO:HG2	4:G:150:PHE:CE2	2.24	0.72
1:A:29:ARG:NH1	7:P:302:ILE:CD1	2.46	0.72
4:G:99:VAL:HG21	4:G:148:ILE:HD11	1.70	0.72
15:M:136:ARG:NH2	15:M:136:ARG:HB2	2.04	0.72
17:I:3:LEU:HB2	17:I:12:LEU:HD12	1.72	0.72
5:K:42:PHE:HZ	5:K:92:ALA:O	1.73	0.72
7:P:288:GLY:O	12:O:357:ARG:NH1	2.23	0.72
2:B:1091:TRP:HE1	4:G:162:PRO:CG	2.02	0.71
5:K:42:PHE:CZ	5:K:92:ALA:O	2.43	0.71
2:B:519:GLY:O	2:B:549:ILE:HG23	1.90	0.71
7:P:284:ARG:CB	12:O:356:GLU:HG3	2.18	0.71
15:M:118:LEU:HD23	15:M:118:LEU:O	1.90	0.71
5:K:86:THR:CB	5:K:90:LEU:HB2	2.20	0.71
15:M:136:ARG:H	15:M:136:ARG:NH2	1.88	0.71
15:M:15:VAL:HA	15:M:124:LEU:HB2	1.71	0.71
17:I:34:ILE:HG13	17:I:34:ILE:O	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:HIS:NE2	2:B:893:ILE:CD1	2.53	0.70
2:B:608:ASN:ND2	2:B:612:GLU:OE2	2.24	0.70
2:B:522:ASP:HB2	2:B:547:GLY:HA2	1.72	0.70
2:B:526:LEU:N	2:B:526:LEU:HD22	2.06	0.70
4:G:103:PHE:CB	14:D:48:GLU:HB3	2.15	0.70
1:A:1133:SER:HB3	1:A:1136:ARG:HG2	1.73	0.70
3:C:170:THR:O	3:C:191:ARG:CD	2.37	0.70
16:N:368:SER:HA	16:N:371:GLY:C	2.12	0.70
14:D:77:LYS:O	14:D:77:LYS:HG3	1.90	0.70
2:B:801:LYS:CD	2:B:801:LYS:N	2.55	0.70
2:B:257:THR:H	2:B:531:LEU:HG	1.57	0.70
2:B:289:ASN:HD21	2:B:310:ARG:HE	1.39	0.70
2:B:163:LEU:HD11	2:B:732:LYS:HD2	1.74	0.69
2:B:801:LYS:N	2:B:801:LYS:HD3	2.07	0.69
15:M:76:GLN:HE21	15:M:76:GLN:HA	1.57	0.69
3:C:116:HIS:CG	3:C:190:ILE:HD11	2.26	0.69
2:B:594:ARG:NH1	2:B:658:GLU:OE2	2.24	0.69
6:L:23:HIS:NE2	11:J:64:PRO:CB	2.55	0.69
1:A:1137:ILE:HG13	1:A:1144:VAL:HG22	1.74	0.69
2:B:526:LEU:HD22	2:B:526:LEU:H	1.56	0.69
3:C:299:LEU:H	3:C:299:LEU:CD2	2.06	0.69
12:O:409:ILE:CB	12:O:423:LEU:CD2	2.67	0.69
14:D:1:MET:O	14:D:1:MET:SD	2.51	0.69
1:A:29:ARG:HH22	7:P:302:ILE:HD12	1.58	0.68
1:A:464:ARG:NH1	1:A:503:ASP:OD1	2.26	0.68
2:B:245:VAL:HG23	2:B:250:GLU:HG2	1.75	0.68
1:A:483:HIS:NE2	2:B:893:ILE:HG13	2.08	0.68
2:B:802:PRO:HD2	2:B:806:HIS:HB2	1.75	0.68
16:N:357:LEU:HD23	16:N:358:GLN:HE21	1.51	0.68
2:B:191:VAL:HA	2:B:199:VAL:HG22	1.74	0.68
4:G:32:LYS:NZ	14:D:39:GLN:HG2	2.07	0.68
15:M:30:TYR:HB2	16:N:359:GLU:O	1.93	0.68
3:C:114:PRO:O	3:C:192:PRO:HA	1.94	0.68
8:E:41:LYS:HA	8:E:44:SER:HB3	1.76	0.68
16:N:365:LEU:HD22	16:N:373:MET:HG3	1.75	0.68
1:A:1118:GLU:HB3	17:I:39:THR:C	2.14	0.68
2:B:733:LEU:N	2:B:733:LEU:HD23	2.09	0.68
15:M:71:ARG:HA	15:M:71:ARG:NH1	2.09	0.68
16:N:271:LEU:HG	16:N:272:PRO:HD2	1.75	0.68
5:K:90:LEU:HD12	5:K:90:LEU:H	1.59	0.68
15:M:116:ALA:CB	16:N:269:LEU:HB2	2.00	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:I:34:ILE:O	17:I:36:ARG:NE	2.26	0.67
2:B:1038:GLY:O	2:B:1043:GLY:CA	2.42	0.67
8:E:168:ASN:O	8:E:169:GLN:HB3	1.92	0.67
1:A:1096:ASP:O	1:A:1099:ARG:HB3	1.93	0.67
3:C:187:GLU:HG3	3:C:187:GLU:O	1.95	0.67
1:A:1121:PHE:CD2	17:I:37:LYS:HB2	2.30	0.67
1:A:171:LEU:H	1:A:171:LEU:CD2	2.07	0.67
1:A:897:ILE:HD11	8:E:165:LEU:HD11	1.76	0.67
1:A:1141:ARG:HA	1:A:1141:ARG:NE	2.10	0.67
6:L:35:ARG:HE	6:L:42:ARG:NH2	1.93	0.67
3:C:181:GLN:HE21	3:C:181:GLN:CA	1.86	0.66
12:O:409:ILE:HG13	12:O:423:LEU:HG	1.76	0.66
2:B:1038:GLY:O	2:B:1043:GLY:N	2.27	0.66
1:A:785:SER:O	1:A:786:LYS:CD	2.42	0.66
2:B:901:HIS:NE2	2:B:945:GLU:OE2	2.27	0.66
15:M:56:VAL:HG11	15:M:135:LEU:HD13	1.77	0.66
17:I:22:ARG:CG	17:I:29:PRO:HB3	2.26	0.66
17:I:33:ASN:O	17:I:35:THR:N	2.28	0.66
17:I:8:CYS:HG	17:I:25:CYS:HG	1.42	0.66
1:A:896:ASP:HA	8:E:169:GLN:HG3	1.77	0.66
1:A:897:ILE:HD12	8:E:165:LEU:HD21	1.76	0.66
13:Q:106:LEU:CD1	13:Q:107:PRO:HD2	2.14	0.66
1:A:43:SER:HB2	1:A:54:GLY:HA3	1.78	0.66
2:B:200:GLY:HA2	2:B:215:ASN:HA	1.77	0.66
3:C:21:VAL:HG23	3:C:24:VAL:HG13	1.77	0.66
14:D:73:LEU:HD13	14:D:83:LYS:HB2	1.78	0.66
7:P:289:LEU:HA	12:O:357:ARG:HG2	1.76	0.66
15:M:118:LEU:HD23	15:M:118:LEU:C	2.16	0.65
3:C:162:LEU:CD1	3:C:204:PRO:CD	2.75	0.65
3:C:277:ASN:N	3:C:277:ASN:OD1	2.30	0.65
7:P:304:PRO:HG3	12:O:445:ASN:HD22	1.59	0.65
1:A:1121:PHE:O	17:I:36:ARG:NH2	2.28	0.65
2:B:278:PHE:HB3	2:B:284:LEU:HD21	1.77	0.65
3:C:263:GLU:HB2	3:C:276:ALA:HB2	1.78	0.65
15:M:16:TYR:N	15:M:124:LEU:O	2.25	0.65
15:M:147:ALA:O	15:M:150:ARG:HB2	1.97	0.65
1:A:1136:ARG:HH11	17:I:47:LYS:CB	2.10	0.65
2:B:916:MET:HG2	2:B:925:PRO:HD2	1.79	0.65
15:M:205:TRP:O	16:N:368:SER:HB2	1.97	0.65
15:M:206:VAL:HA	16:N:368:SER:HB2	1.79	0.65
2:B:1091:TRP:NE1	4:G:162:PRO:N	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:365:LEU:N	16:N:365:LEU:HD23	2.11	0.65
1:A:33:HIS:CE1	2:B:1088:TYR:HE2	2.15	0.65
5:K:90:LEU:HD12	5:K:90:LEU:N	2.12	0.65
1:A:45:ASP:HB2	1:A:50:PRO:HD2	1.79	0.65
2:B:1037:GLU:O	2:B:1037:GLU:HG2	1.94	0.65
8:E:197:SER:H	8:E:201:GLY:HA2	1.60	0.65
12:O:412:THR:CB	12:O:419:ARG:HA	2.24	0.65
1:A:1141:ARG:HA	1:A:1141:ARG:HE	1.62	0.64
4:G:151:ARG:HD2	4:G:151:ARG:C	2.16	0.64
13:Q:86:ARG:NH1	13:Q:86:ARG:HB2	2.12	0.64
15:M:199:LYS:HB2	15:M:199:LYS:HZ2	1.60	0.64
1:A:38:SER:HA	13:Q:24:GLY:HA2	1.80	0.64
1:A:572:LEU:HD13	5:K:83:ARG:HD2	1.79	0.64
2:B:521:GLU:HG2	2:B:525:LEU:HD11	1.80	0.64
4:G:32:LYS:HZ3	4:G:32:LYS:CB	2.09	0.64
2:B:1039:ARG:HH21	19:Y:19:DT:H4'	1.60	0.64
2:B:39:LEU:HD21	2:B:667:VAL:HG11	1.78	0.64
2:B:214:THR:HG21	2:B:319:THR:H	1.63	0.64
15:M:71:ARG:HH12	15:M:74:GLY:HA3	1.63	0.64
7:P:220:ILE:HD11	7:P:271:ARG:HD2	1.80	0.64
15:M:27:LEU:HB2	15:M:132:ILE:HG12	1.78	0.64
15:M:106:GLN:HG3	15:M:133:LEU:HG	1.78	0.64
1:A:1114:SER:HA	1:A:1133:SER:H	1.63	0.64
16:N:346:LEU:HD12	16:N:346:LEU:N	2.12	0.64
16:N:368:SER:OG	16:N:373:MET:SD	2.52	0.64
5:K:48:ASP:OD2	5:K:48:ASP:N	2.31	0.63
1:A:625:CYS:CB	1:A:632:CYS:SG	2.85	0.63
2:B:574:ILE:HG23	2:B:585:ILE:HG13	1.78	0.63
7:P:293:PHE:CE1	13:Q:31:VAL:HG12	2.33	0.63
2:B:801:LYS:H	2:B:801:LYS:CD	2.11	0.63
7:P:299:GLY:CA	7:P:303:SER:HB3	2.24	0.63
3:C:185:PHE:CB	3:C:186:PRO:HD3	2.25	0.63
3:C:254:SER:HA	3:C:262:ILE:HG21	1.80	0.63
7:P:293:PHE:CE2	7:P:307:CYS:HB2	2.34	0.63
16:N:357:LEU:CD2	16:N:358:GLN:HE21	2.05	0.63
2:B:245:VAL:HG21	2:B:250:GLU:HG2	1.80	0.63
2:B:258:GLU:HG3	2:B:260:HIS:HD2	1.62	0.63
6:L:29:LYS:O	6:L:32:ASP:HB2	1.99	0.63
12:O:409:ILE:N	12:O:410:PRO:CD	2.34	0.63
13:Q:82:GLN:CG	14:D:107:ARG:HH21	2.12	0.63
15:M:42:ILE:HD12	15:M:42:ILE:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:136:ARG:HH21	15:M:136:ARG:HB2	1.63	0.63
3:C:78:ARG:CD	5:K:50:THR:HG22	2.29	0.63
12:O:159:ARG:HA	12:O:235:TRP:HB3	1.80	0.63
12:O:407:GLN:CG	12:O:422:TYR:HB3	2.29	0.63
3:C:78:ARG:HD3	5:K:50:THR:HG22	1.80	0.62
15:M:147:ALA:O	15:M:150:ARG:N	2.32	0.62
2:B:804:TRP:HB2	2:B:825:GLN:HE21	1.64	0.62
2:B:896:LYS:HD2	2:B:1012:LEU:HD11	1.80	0.62
1:A:742:CYS:SG	1:A:743:THR:N	2.70	0.62
3:C:109:ARG:NH2	3:C:198:LEU:O	2.33	0.62
4:G:79:PRO:CG	4:G:150:PHE:CE2	2.82	0.62
15:M:102:PHE:HD1	15:M:137:PRO:HA	1.64	0.62
19:Y:18:DA:H2	20:R:9:U:H3	1.48	0.62
5:K:89:THR:HG22	5:K:89:THR:O	2.00	0.62
15:M:50:LYS:HE2	15:M:55:LYS:HE3	1.81	0.62
2:B:657:LEU:HG	2:B:658:GLU:N	2.14	0.62
7:P:199:LYS:NZ	7:P:245:ASP:O	2.32	0.62
3:C:116:HIS:CD2	3:C:190:ILE:CD1	2.76	0.62
12:O:91:TYR:OH	12:O:243:HIS:NE2	2.33	0.62
15:M:32:VAL:HG23	15:M:33:ARG:HG2	1.81	0.62
1:A:1110:LEU:HD12	1:A:1110:LEU:C	2.20	0.62
1:A:465:GLN:OE1	1:A:506:ASN:ND2	2.33	0.61
14:D:17:PHE:HB2	14:D:53:ILE:CG2	2.28	0.61
16:N:329:LEU:HD23	16:N:329:LEU:O	2.00	0.61
15:M:75:GLU:HA	15:M:75:GLU:OE2	2.00	0.61
1:A:913:GLU:HB2	1:A:917:GLU:O	1.99	0.61
1:A:1140:LEU:HD21	17:I:47:LYS:CB	2.30	0.61
2:B:657:LEU:HG	2:B:658:GLU:H	1.66	0.61
13:Q:82:GLN:HG2	14:D:107:ARG:NH2	2.13	0.61
14:D:14:TYR:HD2	14:D:18:GLN:HE21	1.47	0.61
15:M:33:ARG:HD2	15:M:38:THR:HG21	1.80	0.61
3:C:116:HIS:CG	3:C:190:ILE:CD1	2.83	0.61
2:B:654:THR:O	2:B:655:THR:OG1	2.18	0.61
1:A:303:THR:H	12:O:377:GLN:HE22	1.47	0.61
7:P:302:ILE:HG22	7:P:302:ILE:O	2.00	0.61
3:C:109:ARG:NH1	11:J:3:ILE:O	2.34	0.61
14:D:20:LEU:HD11	14:D:46:THR:HB	1.82	0.61
15:M:31:PRO:CD	15:M:136:ARG:CD	2.79	0.61
2:B:526:LEU:H	2:B:526:LEU:CD2	2.14	0.61
2:B:862:THR:OG1	2:B:887:GLN:NE2	2.34	0.61
8:E:27:LEU:HD23	8:E:27:LEU:N	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:304:PRO:CG	12:O:445:ASN:ND2	2.59	0.60
4:G:151:ARG:HG3	4:G:152:VAL:HG13	1.82	0.60
2:B:526:LEU:HD11	16:N:358:GLN:HG3	1.84	0.60
14:D:41:ASN:OD1	14:D:41:ASN:N	2.30	0.60
15:M:117:ALA:HB2	15:M:127:THR:OG1	2.01	0.60
16:N:271:LEU:HA	16:N:385:CYS:HB2	1.83	0.60
2:B:526:LEU:HD23	16:N:357:LEU:HD21	1.83	0.60
2:B:733:LEU:HG	2:B:733:LEU:O	2.01	0.60
13:Q:82:GLN:HG2	14:D:107:ARG:HH21	1.66	0.60
14:D:110:GLU:OE2	14:D:110:GLU:HA	2.01	0.60
8:E:7:THR:HG22	8:E:7:THR:O	2.02	0.60
14:D:108:LEU:O	14:D:113:ILE:HG22	2.02	0.60
2:B:617:GLY:C	2:B:619:ARG:H	2.05	0.60
2:B:704:ARG:NH1	2:B:706:ASP:OD2	2.35	0.60
12:O:507:ASN:ND2	13:Q:55:GLU:OE2	2.34	0.60
14:D:18:GLN:OE1	14:D:18:GLN:HA	2.02	0.60
15:M:102:PHE:HA	15:M:138:SER:H	1.66	0.60
3:C:262:ILE:HD12	3:C:275:VAL:HA	1.84	0.60
14:D:43:ASN:H	14:D:43:ASN:ND2	1.96	0.60
1:A:421:ILE:HG13	1:A:432:LEU:HD11	1.84	0.59
3:C:162:LEU:HG	3:C:204:PRO:HD3	1.85	0.59
13:Q:78:PRO:HG3	14:D:7:ASN:HD22	1.67	0.59
2:B:616:GLN:HG3	2:B:618:TYR:H	1.67	0.59
11:J:56:ILE:O	11:J:60:LEU:HG	2.02	0.59
13:Q:80:GLU:HA	13:Q:86:ARG:CD	2.33	0.59
13:Q:113:ARG:HH21	13:Q:117:LYS:HA	1.67	0.59
3:C:170:THR:CB	3:C:192:PRO:HG3	2.23	0.59
4:G:79:PRO:CG	4:G:150:PHE:CD2	2.86	0.59
12:O:364:ARG:NH2	12:O:384:ALA:O	2.35	0.59
15:M:69:TYR:HD1	15:M:73:LYS:HE3	1.67	0.59
1:A:385:HIS:CD2	1:A:484:ARG:HH12	2.19	0.59
1:A:1116:TYR:CD1	17:I:42:LYS:CB	2.84	0.59
15:M:119:TYR:HD2	16:N:267:LEU:HD12	1.68	0.59
15:M:208:LEU:HA	16:N:373:MET:O	2.03	0.59
3:C:50:ARG:NH2	3:C:52:ASP:OD2	2.36	0.59
15:M:68:ASN:O	15:M:68:ASN:ND2	2.23	0.59
3:C:162:LEU:HD23	3:C:162:LEU:O	2.03	0.59
3:C:116:HIS:CG	3:C:190:ILE:HG13	2.38	0.59
12:O:410:PRO:CB	12:O:419:ARG:NH2	2.40	0.59
1:A:404:LEU:HA	1:A:407:LEU:HG	1.85	0.58
1:A:869:GLY:HA3	19:Y:15:DG:H1'	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:23:ASN:OD1	3:C:23:ASN:N	2.34	0.58
7:P:282:LEU:HD22	12:O:356:GLU:OE2	2.03	0.58
12:O:284:PHE:HA	12:O:338:LEU:HB2	1.83	0.58
16:N:344:VAL:HG12	16:N:344:VAL:O	2.03	0.58
2:B:223:PHE:H	2:B:269:LEU:HD11	1.68	0.58
2:B:593:CYS:SG	2:B:632:TYR:HB3	2.42	0.58
3:C:171:ARG:HA	3:C:191:ARG:NE	2.18	0.58
5:K:90:LEU:H	5:K:90:LEU:CD1	2.15	0.58
2:B:145:CYS:SG	2:B:146:VAL:N	2.76	0.58
1:A:1116:TYR:CE1	17:I:42:LYS:CB	2.86	0.58
4:G:114:LEU:HD21	4:G:192:GLU:H	1.68	0.58
4:G:122:GLU:OE2	4:G:129:TRP:NE1	2.37	0.58
15:M:31:PRO:HD2	15:M:136:ARG:HD3	1.85	0.58
15:M:60:MET:HB2	15:M:100:GLN:HB3	1.85	0.58
1:A:905:ASP:OD2	1:A:1285:ARG:NH2	2.36	0.58
2:B:312:LEU:HD22	15:M:188:ARG:N	2.17	0.58
2:B:526:LEU:HG	16:N:358:GLN:HB3	1.85	0.58
1:A:301:ALA:O	12:O:392:LYS:NZ	2.36	0.58
14:D:1:MET:O	14:D:1:MET:CG	2.51	0.58
14:D:54:SER:HA	14:D:59:ARG:CZ	2.34	0.58
1:A:1008:PRO:HA	1:A:1011:VAL:HG12	1.86	0.58
2:B:757:LEU:HD23	2:B:762:LEU:HD21	1.85	0.58
4:G:3:VAL:HG23	14:D:9:ALA:HB2	1.84	0.58
15:M:77:ILE:HD11	15:M:145:ALA:HA	1.84	0.58
1:A:407:LEU:O	1:A:417:GLY:HA2	2.04	0.58
2:B:733:LEU:HD23	2:B:733:LEU:H	1.69	0.58
2:B:814:ILE:HD13	2:B:814:ILE:H	1.69	0.58
5:K:66:GLU:HG2	5:K:87:ARG:HG2	1.86	0.58
5:K:83:ARG:HE	5:K:85:GLN:HE21	1.50	0.58
2:B:65:VAL:HB	2:B:75:LEU:HB3	1.85	0.57
16:N:268:PHE:HB3	16:N:382:LYS:HA	1.85	0.57
1:A:366:ARG:NH2	19:Y:18:DA:OP1	2.37	0.57
2:B:831:SER:HA	2:B:853:ASP:HA	1.86	0.57
1:A:419:ASN:N	1:A:419:ASN:OD1	2.37	0.57
3:C:38:ASP:N	3:C:38:ASP:OD1	2.37	0.57
16:N:357:LEU:HD21	16:N:358:GLN:NE2	2.14	0.57
1:A:791:ASN:ND2	2:B:938:MET:SD	2.73	0.57
5:K:64:GLU:CB	5:K:90:LEU:HD21	2.32	0.57
7:P:202:PRO:O	7:P:205:GLN:NE2	2.37	0.57
15:M:28:PHE:CZ	16:N:365:LEU:HD21	2.39	0.57
12:O:419:ARG:HD2	12:O:422:TYR:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:22:ALA:HB2	15:M:127:THR:HB	1.87	0.57
16:N:357:LEU:CD2	16:N:357:LEU:H	2.17	0.57
1:A:562:ALA:HB2	3:C:29:PHE:CE2	2.38	0.57
1:A:899:GLN:NE2	1:A:1288:MET:O	2.38	0.57
2:B:999:GLU:HA	3:C:21:VAL:HG22	1.87	0.57
3:C:116:HIS:HB3	3:C:190:ILE:CG1	2.28	0.57
3:C:184:LEU:HD12	3:C:184:LEU:N	2.20	0.57
4:G:99:VAL:CG2	4:G:148:ILE:HD11	2.34	0.57
7:P:304:PRO:HG3	12:O:445:ASN:HD21	1.64	0.57
12:O:113:ASN:HB2	12:O:116:LEU:HD21	1.86	0.57
15:M:108:THR:OG1	15:M:108:THR:O	2.21	0.57
3:C:180:ASN:OD1	3:C:180:ASN:N	2.37	0.57
6:L:34:ILE:HG22	6:L:44:MET:SD	2.45	0.57
1:A:731:LEU:HD13	1:A:748:LEU:HD22	1.86	0.57
10:H:32:SER:OG	10:H:33:GLU:N	2.37	0.57
8:E:13:ILE:HD11	8:E:132:GLN:HG3	1.87	0.57
17:I:33:ASN:C	17:I:35:THR:H	2.07	0.57
4:G:5:VAL:HG22	14:D:6:ALA:O	2.04	0.56
15:M:31:PRO:HD2	15:M:136:ARG:CD	2.35	0.56
16:N:333:LYS:N	16:N:333:LYS:HD3	2.20	0.56
1:A:23:LYS:HG3	2:B:1123:ILE:HG13	1.86	0.56
5:K:86:THR:OG1	5:K:90:LEU:HB2	2.05	0.56
12:O:374:HIS:HB3	12:O:423:LEU:HD13	1.79	0.56
17:I:20:CYS:SG	17:I:22:ARG:HG3	2.44	0.56
1:A:788:SER:OG	1:A:789:PHE:N	2.38	0.56
1:A:883:CYS:HB3	1:A:1355:ILE:HG23	1.87	0.56
1:A:1119:GLU:HA	1:A:1128:ILE:HA	1.87	0.56
2:B:187:ASN:HD21	2:B:322:PRO:HD3	1.70	0.56
2:B:528:GLY:O	2:B:531:LEU:HB2	2.06	0.56
3:C:162:LEU:HD12	3:C:204:PRO:CD	2.35	0.56
4:G:31:ASN:HB3	14:D:42:LEU:HG	1.87	0.56
14:D:96:GLU:O	14:D:101:VAL:N	2.36	0.56
15:M:73:LYS:HE2	15:M:98:ASP:OD2	2.05	0.56
16:N:357:LEU:HD23	16:N:357:LEU:H	1.69	0.56
19:Y:7:DG:O6	19:Y:8:DA:N6	2.39	0.56
1:A:1122:LEU:HG	1:A:1123:PRO:HD2	1.85	0.56
1:A:1123:PRO:HD3	17:I:34:ILE:HD12	1.88	0.56
1:A:483:HIS:CD2	2:B:893:ILE:HD12	2.40	0.56
7:P:309:TYR:OH	13:Q:32:LEU:O	2.24	0.56
15:M:31:PRO:CG	15:M:136:ARG:HE	2.16	0.56
1:A:558:PHE:HB3	1:A:594:LEU:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:LEU:O	3:C:299:LEU:HD21	2.05	0.56
5:K:34:GLY:O	5:K:35:THR:HB	2.06	0.56
5:K:44:LEU:HD12	5:K:80:ILE:HD11	1.87	0.56
1:A:1121:PHE:CG	17:I:37:LYS:CB	2.89	0.56
2:B:536:VAL:HG22	2:B:536:VAL:O	2.05	0.56
3:C:97:ASN:ND2	3:C:103:ASP:OD1	2.34	0.56
14:D:78:LEU:HD13	14:D:86:LEU:HD11	1.86	0.56
16:N:329:LEU:HD23	16:N:329:LEU:C	2.25	0.56
1:A:303:THR:O	1:A:307:MET:HB2	2.06	0.56
3:C:49:PHE:CE1	3:C:68:ILE:HD11	2.41	0.56
15:M:70:CYS:SG	15:M:71:ARG:N	2.77	0.56
1:A:1136:ARG:O	1:A:1139:LEU:N	2.39	0.56
2:B:518:LEU:HD21	2:B:555:LEU:CA	2.21	0.56
2:B:616:GLN:CD	2:B:618:TYR:HB2	2.26	0.56
17:I:2:LEU:O	17:I:2:LEU:HD23	2.05	0.56
1:A:659:SER:OG	1:A:661:ASN:OD1	2.24	0.56
4:G:112:GLU:OE1	4:G:119:LYS:NZ	2.37	0.56
1:A:855:ARG:NH2	2:B:481:PRO:O	2.39	0.55
1:A:1135:GLU:OE1	1:A:1135:GLU:N	2.39	0.55
2:B:874:ASN:OD1	2:B:874:ASN:N	2.38	0.55
1:A:408:VAL:HG21	1:A:421:ILE:HD11	1.88	0.55
2:B:660:GLU:HG3	2:B:662:PHE:CE2	2.41	0.55
2:B:750:ASP:N	2:B:750:ASP:OD1	2.36	0.55
6:L:23:HIS:CD2	11:J:64:PRO:HB2	2.39	0.55
1:A:367:THR:HG22	2:B:1020:MET:HA	1.87	0.55
2:B:329:ARG:CG	2:B:523:VAL:HG13	2.35	0.55
3:C:171:ARG:HA	3:C:191:ARG:CZ	2.36	0.55
12:O:37:ARG:O	12:O:41:HIS:ND1	2.39	0.55
12:O:265:GLU:OE1	12:O:268:ARG:NH1	2.40	0.55
15:M:31:PRO:HG3	15:M:136:ARG:NE	2.20	0.55
1:A:483:HIS:HB2	1:A:487:ARG:NH1	2.22	0.55
1:A:1138:ARG:O	1:A:1138:ARG:HG2	2.05	0.55
2:B:86:ASP:O	2:B:135:ARG:NH2	2.40	0.55
2:B:1091:TRP:CD1	4:G:162:PRO:HA	2.41	0.55
3:C:100:ILE:HG21	11:J:60:LEU:HD21	1.89	0.55
3:C:179:GLY:H	3:C:181:GLN:HG2	1.71	0.55
15:M:111:THR:HG21	15:M:131:GLY:HA2	1.88	0.55
2:B:70:ASP:HB2	2:B:392:ILE:HG21	1.89	0.55
12:O:410:PRO:HB3	12:O:422:TYR:CE1	2.42	0.55
14:D:2:GLU:OE1	14:D:2:GLU:N	2.27	0.55
15:M:69:TYR:CD2	15:M:69:TYR:N	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:136:ARG:HH21	15:M:136:ARG:CB	2.19	0.55
1:A:851:THR:HG21	2:B:481:PRO:HB2	1.88	0.55
1:A:991:ASP:OD1	1:A:991:ASP:N	2.39	0.55
4:G:44:LEU:HB3	4:G:77:PHE:HB3	1.89	0.55
4:G:147:GLU:OE1	14:D:100:MET:SD	2.64	0.55
2:B:852:LYS:NZ	2:B:853:ASP:O	2.39	0.55
1:A:560:ASP:OD2	3:C:32:ASN:ND2	2.40	0.55
2:B:444:SER:OG	2:B:445:TYR:N	2.40	0.55
7:P:296:CYS:SG	7:P:297:HIS:N	2.79	0.55
15:M:59:GLU:O	15:M:61:ALA:N	2.39	0.55
1:A:1140:LEU:HD21	17:I:47:LYS:HA	1.88	0.55
3:C:162:LEU:CG	3:C:204:PRO:HD3	2.37	0.55
12:O:115:LYS:HE2	12:O:160:CYS:HB2	1.89	0.55
1:A:1133:SER:HB3	1:A:1136:ARG:CG	2.36	0.55
2:B:750:ASP:O	2:B:930:ASN:ND2	2.40	0.55
5:K:50:THR:OG1	5:K:51:LEU:N	2.40	0.55
1:A:1140:LEU:CD2	17:I:47:LYS:HA	2.37	0.54
1:A:1230:ASP:OD1	1:A:1230:ASP:N	2.39	0.54
3:C:237:PRO:HA	3:C:301:ARG:HA	1.89	0.54
7:P:289:LEU:HD13	12:O:357:ARG:HA	1.89	0.54
12:O:99:TYR:OH	12:O:150:ARG:NH1	2.40	0.54
12:O:409:ILE:CD1	12:O:423:LEU:CD1	2.63	0.54
15:M:71:ARG:HA	15:M:71:ARG:NE	2.21	0.54
1:A:537:PRO:HG3	1:A:665:TYR:HB2	1.89	0.54
1:A:571:ILE:HG23	1:A:571:ILE:O	2.08	0.54
1:A:1164:ASP:OD1	1:A:1164:ASP:N	2.40	0.54
2:B:999:GLU:OE1	3:C:24:VAL:HG21	2.07	0.54
3:C:141:ARG:HB2	3:C:176:ILE:HD11	1.90	0.54
5:K:95:PRO:O	5:K:99:GLY:N	2.40	0.54
12:O:86:LEU:HD21	12:O:443:ILE:HD13	1.89	0.54
19:Y:1:DT:H71	19:Y:1:DT:OP1	2.07	0.54
19:Y:1:DT:OP1	19:Y:1:DT:H6	1.89	0.54
2:B:259:GLU:O	2:B:263:ALA:N	2.31	0.54
1:A:30:GLN:NE2	2:B:1094:TYR:CE1	2.75	0.54
1:A:37:VAL:HG11	13:Q:28:PRO:HD3	1.90	0.54
2:B:656:HIS:ND1	2:B:656:HIS:N	2.55	0.54
12:O:239:LEU:HA	12:O:242:PHE:HD2	1.73	0.54
14:D:112:GLN:O	14:D:112:GLN:NE2	2.40	0.54
16:N:360:LEU:HB3	16:N:379:VAL:HB	1.90	0.54
1:A:303:THR:HG1	12:O:424:TYR:HH	1.53	0.54
1:A:340:GLY:N	1:A:343:GLN:OE1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ARG:HA	1:A:355:ASN:HB2	1.89	0.54
1:A:415:HIS:O	1:A:453:HIS:ND1	2.38	0.54
2:B:660:GLU:HG3	2:B:662:PHE:CD2	2.43	0.54
2:B:715:PRO:HB2	2:B:734:PRO:HG2	1.89	0.54
2:B:990:THR:HA	2:B:997:PRO:HA	1.90	0.54
13:Q:82:GLN:OE1	14:D:107:ARG:NH2	2.39	0.54
15:M:65:LEU:C	15:M:65:LEU:HD23	2.28	0.54
17:I:18:GLN:C	17:I:19:ARG:HG2	2.28	0.54
17:I:36:ARG:HA	17:I:36:ARG:CZ	2.38	0.54
2:B:176:LYS:HE3	2:B:420:SER:HA	1.89	0.54
2:B:273:GLN:NE2	2:B:278:PHE:O	2.40	0.54
2:B:612:GLU:OE1	2:B:612:GLU:HA	2.07	0.54
2:B:620:ASN:HB3	2:B:622:GLU:CD	2.28	0.54
7:P:227:LYS:O	7:P:240:ASN:ND2	2.41	0.54
7:P:290:CYS:SG	23:P:401:SF4:S4	3.04	0.54
14:D:62:SER:HB2	14:D:65:ILE:HG23	1.89	0.54
2:B:578:LEU:N	2:B:578:LEU:HD23	2.23	0.54
3:C:95:TYR:HE1	6:L:52:LEU:HD12	1.73	0.54
3:C:184:LEU:HD12	3:C:184:LEU:H	1.73	0.54
14:D:2:GLU:H	14:D:2:GLU:CD	2.07	0.54
1:A:1248:SER:OG	1:A:1249:ASN:N	2.41	0.54
4:G:32:LYS:HE2	14:D:39:GLN:HG2	1.90	0.54
14:D:4:LYS:HE2	14:D:4:LYS:CA	2.31	0.54
15:M:144:LYS:NZ	15:M:144:LYS:HB3	2.21	0.54
1:A:362:ASP:OD2	2:B:1028:ARG:NH2	2.41	0.54
1:A:760:ARG:HD2	1:A:800:GLY:HA3	1.90	0.54
5:K:68:CYS:SG	5:K:69:GLY:N	2.81	0.54
7:P:283:VAL:O	7:P:283:VAL:HG13	2.07	0.54
11:J:33:ASP:OD1	11:J:33:ASP:N	2.41	0.54
18:X:35:DT:H2"	18:X:36:DC:H5"	1.90	0.54
2:B:356:TYR:OH	2:B:639:ASN:ND2	2.41	0.53
2:B:523:VAL:HG12	2:B:523:VAL:O	2.08	0.53
7:P:290:CYS:HB2	7:P:293:PHE:HB2	1.90	0.53
12:O:24:ILE:HD11	12:O:45:THR:HG21	1.90	0.53
12:O:412:THR:OG1	12:O:420:THR:HG23	2.08	0.53
15:M:49:ILE:N	15:M:206:VAL:HG21	2.23	0.53
1:A:630:ASP:N	1:A:630:ASP:OD1	2.40	0.53
3:C:113:ILE:CG2	3:C:192:PRO:CB	2.85	0.53
3:C:117:ALA:CB	3:C:189:THR:HG22	2.29	0.53
12:O:171:PRO:O	12:O:174:PRO:HD2	2.08	0.53
15:M:31:PRO:HG2	15:M:136:ARG:HE	1.68	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:PRO:CG	5:K:76:SER:HB2	2.38	0.53
2:B:142:SER:OG	2:B:143:SER:N	2.41	0.53
2:B:1080:CYS:HB3	2:B:1101:VAL:HG22	1.89	0.53
7:P:286:PRO:HG3	13:Q:38:PHE:CD2	2.44	0.53
14:D:102:GLU:N	14:D:102:GLU:CD	2.62	0.53
1:A:544:ASP:OD2	1:A:544:ASP:C	2.47	0.53
1:A:625:CYS:CB	1:A:632:CYS:HG	2.22	0.53
15:M:28:PHE:HZ	16:N:365:LEU:HD21	1.72	0.53
15:M:50:LYS:HD2	15:M:204:PRO:HG3	1.90	0.53
16:N:273:ASP:N	16:N:273:ASP:OD1	2.40	0.53
3:C:235:LEU:HD23	3:C:306:TYR:HB3	1.91	0.53
4:G:32:LYS:HE3	14:D:35:HIS:HD2	1.73	0.53
8:E:17:ILE:HA	8:E:20:LEU:HB3	1.90	0.53
8:E:163:TYR:HB3	8:E:165:LEU:HD13	1.91	0.53
16:N:268:PHE:HD2	16:N:382:LYS:HG2	1.73	0.53
2:B:253:GLN:HB3	2:B:527:CYS:CB	2.37	0.53
15:M:31:PRO:CD	15:M:136:ARG:HD2	2.36	0.53
15:M:107:THR:O	15:M:107:THR:OG1	2.13	0.53
2:B:1091:TRP:HE1	4:G:162:PRO:HG3	1.74	0.53
3:C:134:GLU:HG3	3:C:179:GLY:CA	2.38	0.53
4:G:32:LYS:CE	14:D:39:GLN:HG2	2.38	0.53
12:O:376:GLU:HG3	12:O:424:TYR:HB2	1.91	0.53
14:D:14:TYR:CE2	14:D:18:GLN:HG2	2.43	0.53
1:A:1121:PHE:CG	17:I:37:LYS:HB3	2.43	0.53
2:B:530:GLU:OE2	2:B:530:GLU:N	2.28	0.53
2:B:871:ILE:HG12	2:B:881:ILE:HG12	1.91	0.53
5:K:107:CYS:HA	5:K:110:VAL:HG12	1.90	0.53
1:A:415:HIS:CE1	1:A:480:VAL:HG21	2.44	0.53
1:A:467:SER:HG	2:B:1054:CYS:HG	1.46	0.53
3:C:134:GLU:CG	3:C:178:LEU:HB3	2.39	0.53
3:C:185:PHE:HB3	3:C:186:PRO:CD	2.28	0.53
4:G:154:ASP:OD1	4:G:154:ASP:N	2.39	0.53
1:A:374:ASN:ND2	2:B:749:TYR:OH	2.42	0.53
1:A:482:PRO:HG2	5:K:76:SER:HB2	1.90	0.53
2:B:245:VAL:HG21	2:B:250:GLU:CG	2.39	0.53
2:B:872:SER:O	2:B:880:LEU:N	2.42	0.53
9:F:107:ARG:NE	9:F:117:ASP:OD1	2.42	0.53
12:O:407:GLN:O	12:O:410:PRO:CG	2.57	0.53
13:Q:27:LEU:CD2	13:Q:27:LEU:N	2.63	0.53
1:A:109:CYS:SG	1:A:111:THR:OG1	2.61	0.52
1:A:1153:ILE:O	1:A:1156:SER:OG	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:889:ARG:NH1	2:B:1015:MET:SD	2.81	0.52
5:K:86:THR:HG21	5:K:90:LEU:HB3	1.91	0.52
12:O:419:ARG:HD2	12:O:422:TYR:CZ	2.44	0.52
1:A:241:ASN:HB3	1:A:1335:GLY:HA3	1.92	0.52
3:C:243:GLU:HB3	3:C:296:VAL:HG13	1.91	0.52
12:O:440:TYR:OH	12:O:524:GLU:OE2	2.28	0.52
16:N:367:ASP:O	16:N:371:GLY:N	2.43	0.52
1:A:6:PHE:HE2	4:G:157:PHE:CE2	2.28	0.52
1:A:381:ALA:HB3	1:A:487:ARG:HB2	1.91	0.52
2:B:162:PRO:HD2	2:B:699:TYR:HD2	1.75	0.52
2:B:702:ARG:NH2	2:B:867:GLU:OE2	2.36	0.52
2:B:992:GLY:O	3:C:78:ARG:NH2	2.42	0.52
3:C:191:ARG:CD	3:C:192:PRO:HD3	2.38	0.52
16:N:269:LEU:HD22	16:N:385:CYS:SG	2.49	0.52
16:N:349:THR:O	16:N:349:THR:OG1	2.27	0.52
4:G:103:PHE:CB	14:D:48:GLU:OE1	2.57	0.52
15:M:16:TYR:HA	16:N:326:VAL:HG22	1.91	0.52
15:M:65:LEU:HD23	15:M:65:LEU:O	2.10	0.52
2:B:814:ILE:CD1	2:B:881:ILE:HD13	2.39	0.52
3:C:237:PRO:HB3	3:C:283:PHE:HE2	1.75	0.52
8:E:168:ASN:O	8:E:169:GLN:CB	2.58	0.52
11:J:9:THR:OG1	11:J:44:CYS:SG	2.67	0.52
15:M:52:LYS:HG3	15:M:53:GLN:OE1	2.08	0.52
1:A:1170:GLU:H	1:A:1172:VAL:HG12	1.75	0.52
2:B:810:ASP:CG	2:B:810:ASP:O	2.47	0.52
4:G:148:ILE:CG2	4:G:190:ILE:HG23	2.29	0.52
17:I:19:ARG:O	17:I:19:ARG:HG3	2.08	0.52
1:A:10:ASP:N	1:A:10:ASP:OD1	2.41	0.52
1:A:22:MET:O	2:B:1125:ARG:NH2	2.42	0.52
1:A:383:PRO:CB	1:A:484:ARG:HA	2.37	0.52
1:A:897:ILE:HD12	8:E:165:LEU:CD2	2.39	0.52
2:B:686:GLN:O	2:B:690:GLY:N	2.37	0.52
7:P:286:PRO:HG2	7:P:313:TRP:CG	2.44	0.52
14:D:43:ASN:ND2	14:D:43:ASN:N	2.57	0.52
14:D:102:GLU:N	14:D:102:GLU:OE2	2.40	0.52
1:A:315:LEU:O	1:A:319:LEU:N	2.40	0.52
1:A:428:MET:HA	1:A:428:MET:HE2	1.92	0.52
2:B:898:SER:HA	2:B:904:LYS:HA	1.92	0.52
12:O:127:ASP:HB3	12:O:128:ARG:HH11	1.75	0.52
4:G:32:LYS:CE	14:D:39:GLN:CG	2.87	0.52
4:G:56:ASP:OD1	4:G:56:ASP:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:266:LEU:O	16:N:380:LYS:HB2	2.10	0.52
3:C:163:TYR:CD1	3:C:166:HIS:HB3	2.45	0.52
14:D:59:ARG:NE	14:D:59:ARG:H	2.07	0.52
1:A:5:GLN:HG3	4:G:36:ASN:O	2.09	0.51
1:A:1118:GLU:HG3	17:I:39:THR:H	1.75	0.51
2:B:612:GLU:O	2:B:615:ALA:HB3	2.09	0.51
3:C:68:ILE:HD12	3:C:68:ILE:H	1.75	0.51
15:M:15:VAL:O	16:N:327:GLY:N	2.43	0.51
1:A:1181:SER:OG	1:A:1182:LYS:N	2.42	0.51
2:B:1034:GLN:NE2	2:B:1073:ASP:OD2	2.43	0.51
4:G:103:PHE:CD2	14:D:48:GLU:OE1	2.63	0.51
12:O:5:GLU:HG3	12:O:83:LEU:HD11	1.92	0.51
1:A:6:PHE:HE2	4:G:157:PHE:CD2	2.29	0.51
2:B:246:GLU:OE1	2:B:281:MET:N	2.42	0.51
3:C:221:ASP:OD2	6:L:58:ARG:NH2	2.44	0.51
1:A:407:LEU:C	1:A:407:LEU:HD12	2.30	0.51
1:A:543:GLN:HG2	1:A:786:LYS:HD3	1.92	0.51
1:A:874:ARG:NH1	1:A:1075:ASN:OD1	2.40	0.51
1:A:1136:ARG:NH1	17:I:47:LYS:CB	2.72	0.51
2:B:559:PHE:HB3	2:B:574:ILE:HG13	1.93	0.51
4:G:32:LYS:HG2	14:D:39:GLN:HB2	1.93	0.51
8:E:80:PRO:HA	8:E:107:GLN:HB2	1.92	0.51
2:B:794:MET:O	2:B:802:PRO:HD3	2.09	0.51
1:A:1375:ARG:NH1	1:A:1376:PRO:O	2.43	0.51
2:B:269:LEU:O	2:B:273:GLN:N	2.35	0.51
2:B:516:SER:O	15:M:113:ARG:NH1	2.44	0.51
2:B:611:MET:CE	2:B:611:MET:CA	2.84	0.51
12:O:450:ARG:O	12:O:454:THR:OG1	2.29	0.51
1:A:385:HIS:HD2	1:A:484:ARG:NH1	2.08	0.51
1:A:571:ILE:O	1:A:571:ILE:HG13	2.10	0.51
1:A:1121:PHE:O	17:I:36:ARG:NH1	2.44	0.51
2:B:763:ASP:OD1	2:B:890:ARG:NH1	2.40	0.51
4:G:99:VAL:HG11	4:G:148:ILE:HG12	1.92	0.51
12:O:436:LEU:HB2	12:O:523:LEU:HD22	1.92	0.51
19:Y:10:DC:H2"	19:Y:11:DA:C2	2.46	0.51
2:B:538:LEU:HB3	2:B:548:VAL:HG22	1.93	0.51
3:C:39:ALA:HB1	5:K:63:PRO:HG3	1.91	0.51
8:E:6:GLU:C	8:E:8:TYR:H	2.13	0.51
15:M:79:LEU:HD22	15:M:98:ASP:HB3	1.92	0.51
16:N:333:LYS:HD3	16:N:333:LYS:H	1.74	0.51
17:I:34:ILE:HG13	17:I:36:ARG:NE	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:1:DT:C6	19:Y:1:DT:C5'	2.86	0.51
1:A:7:ARG:NH1	1:A:8:GLU:O	2.43	0.51
2:B:329:ARG:HG2	2:B:523:VAL:HG13	1.93	0.51
2:B:1091:TRP:HA	2:B:1101:VAL:HG21	1.92	0.51
3:C:40:TRP:HB2	5:K:61:LYS:HB3	1.93	0.51
7:P:286:PRO:HA	13:Q:38:PHE:HD2	1.75	0.51
7:P:308:ILE:HD13	13:Q:31:VAL:HG11	1.94	0.51
9:F:73:ILE:HD11	9:F:79:VAL:HG13	1.92	0.51
2:B:258:GLU:HG3	2:B:260:HIS:CD2	2.44	0.50
16:N:268:PHE:O	16:N:383:LEU:N	2.39	0.50
17:I:2:LEU:O	17:I:2:LEU:CG	2.59	0.50
4:G:39:VAL:HB	4:G:42:VAL:HB	1.93	0.50
12:O:409:ILE:CG1	12:O:423:LEU:CG	2.84	0.50
1:A:410:ASN:HB3	1:A:414:VAL:HB	1.93	0.50
8:E:6:GLU:O	8:E:9:ARG:HG3	2.10	0.50
12:O:118:MET:SD	13:Q:108:ARG:NH2	2.75	0.50
15:M:121:GLN:HG2	16:N:259:SER:HA	1.93	0.50
1:A:456:ASP:HB2	1:A:479:ARG:CD	2.39	0.50
2:B:40:VAL:HG12	2:B:40:VAL:O	2.10	0.50
2:B:741:VAL:HG12	2:B:927:ILE:HB	1.93	0.50
4:G:84:ILE:HD11	4:G:149:ARG:HH21	1.77	0.50
12:O:460:LEU:HB3	12:O:499:LEU:HD11	1.92	0.50
14:D:43:ASN:HD22	14:D:43:ASN:N	2.01	0.50
1:A:894:THR:OG1	1:A:896:ASP:OD1	2.27	0.50
1:A:1261:GLU:OE1	8:E:195:ARG:NH1	2.40	0.50
2:B:156:ALA:CA	11:J:62:TYR:CE1	2.88	0.50
2:B:907:CYS:O	2:B:907:CYS:SG	2.70	0.50
3:C:299:LEU:HD23	3:C:299:LEU:N	2.11	0.50
11:J:44:CYS:SG	11:J:45:CYS:N	2.84	0.50
1:A:428:MET:HA	1:A:428:MET:HE3	1.92	0.50
2:B:30:LEU:HD13	2:B:499:MET:HE2	1.93	0.50
2:B:705:ILE:HG23	2:B:884:LEU:HD13	1.92	0.50
3:C:144:VAL:HG21	3:C:168:VAL:HG13	1.93	0.50
3:C:189:THR:O	3:C:191:ARG:N	2.45	0.50
4:G:32:LYS:CB	4:G:32:LYS:NZ	2.72	0.50
13:Q:80:GLU:HA	13:Q:86:ARG:HD3	1.92	0.50
14:D:57:PRO:C	14:D:59:ARG:N	2.64	0.50
1:A:811:ASP:OD1	1:A:811:ASP:N	2.44	0.50
1:A:914:GLY:O	1:A:915:LYS:HB3	2.12	0.50
3:C:116:HIS:HB2	3:C:190:ILE:HG13	1.90	0.50
7:P:252:ILE:HG23	7:P:257:GLU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:15:LYS:HE3	8:E:34:ASP:HA	1.92	0.50
12:O:460:LEU:HA	12:O:463:LYS:HG2	1.94	0.50
16:N:357:LEU:HD23	16:N:357:LEU:N	2.27	0.50
1:A:469:HIS:CD2	1:A:471:LEU:HB2	2.46	0.50
2:B:937:ARG:HB3	2:B:939:THR:HG23	1.93	0.50
4:G:115:GLN:NE2	4:G:192:GLU:O	2.45	0.50
13:Q:27:LEU:O	13:Q:28:PRO:C	2.49	0.50
15:M:105:SER:HB2	15:M:136:ARG:HH12	1.76	0.50
2:B:697:ILE:HD12	2:B:709:MET:HG3	1.93	0.50
15:M:110:ASN:OD1	15:M:110:ASN:N	2.44	0.50
1:A:625:CYS:HB3	1:A:632:CYS:SG	2.51	0.49
1:A:812:GLY:HA3	2:B:473:PRO:HG2	1.93	0.49
1:A:1369:ASP:OD1	1:A:1369:ASP:N	2.45	0.49
3:C:133:THR:HG23	3:C:135:ILE:HG22	1.94	0.49
15:M:33:ARG:HB3	15:M:38:THR:HB	1.93	0.49
15:M:50:LYS:HD3	15:M:55:LYS:HB2	1.94	0.49
1:A:544:ASP:HA	1:A:547:THR:HG22	1.94	0.49
2:B:768:ARG:NH2	6:L:58:ARG:O	2.44	0.49
7:P:286:PRO:HG2	7:P:313:TRP:CD2	2.47	0.49
12:O:410:PRO:HB3	12:O:422:TYR:CD1	2.47	0.49
12:O:414:ASP:OD1	12:O:414:ASP:N	2.44	0.49
19:Y:12:DG:H1'	19:Y:13:DA:H5'	1.94	0.49
2:B:593:CYS:HG	2:B:632:TYR:HD2	1.60	0.49
2:B:771:VAL:HG13	2:B:887:GLN:HB3	1.95	0.49
2:B:993:ILE:HG23	5:K:49:HIS:CG	2.48	0.49
3:C:170:THR:HB	3:C:192:PRO:HG2	1.88	0.49
16:N:355:SER:O	16:N:356:PHE:HB2	2.11	0.49
1:A:43:SER:HB3	1:A:51:LEU:HD12	1.93	0.49
1:A:1092:ASP:HB2	1:A:1223:TYR:H	1.78	0.49
1:A:1185:MET:HA	17:I:16:GLU:OE2	2.11	0.49
3:C:283:PHE:HE1	3:C:299:LEU:HD12	1.77	0.49
10:H:118:TYR:HB2	10:H:121:LEU:HB2	1.94	0.49
2:B:567:TYR:N	2:B:567:TYR:CD1	2.80	0.49
3:C:162:LEU:HD11	3:C:203:ARG:CD	2.38	0.49
5:K:45:HIS:O	5:K:47:GLU:HG3	2.12	0.49
7:P:219:TYR:HD2	7:P:271:ARG:HB3	1.78	0.49
2:B:733:LEU:N	2:B:733:LEU:CD2	2.75	0.49
2:B:1053:ASP:HA	2:B:1056:ILE:HD12	1.94	0.49
3:C:104:GLU:O	3:C:108:HIS:N	2.44	0.49
15:M:34:PRO:HB3	16:N:357:LEU:O	2.13	0.49
3:C:174:THR:OG1	3:C:175:TRP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:80:PHE:HZ	14:D:85:GLN:HG2	1.77	0.49
6:L:23:HIS:NE2	11:J:64:PRO:CG	2.76	0.49
12:O:84:ARG:NH2	12:O:524:GLU:OE1	2.46	0.49
17:I:19:ARG:HE	17:I:33:ASN:HA	1.77	0.49
1:A:258:PRO:HD2	1:A:283:LEU:HD11	1.95	0.49
1:A:554:LEU:HD23	1:A:556:ASP:H	1.77	0.49
2:B:274:LYS:HD2	17:I:13:ILE:HD11	1.95	0.49
3:C:24:VAL:O	3:C:303:ARG:NH1	2.42	0.49
3:C:180:ASN:O	3:C:181:GLN:C	2.51	0.49
1:A:372:ASP:HB2	1:A:487:ARG:HB3	1.95	0.49
2:B:245:VAL:CG2	2:B:250:GLU:CG	2.89	0.49
2:B:593:CYS:SG	2:B:594:ARG:N	2.86	0.49
12:O:60:HIS:NE2	12:O:112:LEU:O	2.44	0.49
12:O:405:SER:HB3	12:O:425:THR:O	2.12	0.49
17:I:33:ASN:C	17:I:35:THR:N	2.65	0.49
1:A:131:ARG:HD3	1:A:132:PRO:HD2	1.95	0.49
2:B:1039:ARG:NH2	19:Y:19:DT:H4'	2.27	0.49
7:P:286:PRO:HA	13:Q:38:PHE:CD2	2.48	0.49
12:O:416:ALA:HA	12:O:422:TYR:OH	2.13	0.49
2:B:608:ASN:C	2:B:608:ASN:HD22	2.15	0.48
12:O:378:LYS:HD2	12:O:379:GLN:HE21	1.77	0.48
15:M:48:LYS:N	15:M:57:GLU:O	2.44	0.48
1:A:659:SER:O	1:A:662:ASN:ND2	2.46	0.48
6:L:19:CYS:HG	6:L:24:THR:HG1	1.61	0.48
10:H:32:SER:HB3	10:H:37:MET:H	1.78	0.48
11:J:21:TYR:OH	11:J:31:GLU:OE1	2.23	0.48
14:D:61:GLN:HA	14:D:61:GLN:NE2	2.28	0.48
1:A:1297:LYS:HB3	1:A:1301:LEU:HD11	1.96	0.48
4:G:151:ARG:NH1	4:G:152:VAL:HG12	2.29	0.48
17:I:2:LEU:O	17:I:2:LEU:HG	2.13	0.48
17:I:31:VAL:O	17:I:31:VAL:HG12	2.13	0.48
1:A:583:LEU:HD23	5:K:67:PHE:HD1	1.78	0.48
2:B:526:LEU:N	2:B:526:LEU:CD2	2.73	0.48
3:C:116:HIS:CG	3:C:190:ILE:CG1	2.97	0.48
12:O:409:ILE:HD12	12:O:423:LEU:CD1	2.32	0.48
17:I:29:PRO:HG2	17:I:29:PRO:O	2.14	0.48
2:B:372:LEU:HD22	2:B:424:TRP:HZ3	1.78	0.48
2:B:514:LEU:HD13	2:B:568:ILE:HD11	1.96	0.48
3:C:309:SER:O	3:C:309:SER:OG	2.29	0.48
4:G:83:GLU:CA	14:D:85:GLN:NE2	2.69	0.48
15:M:203:GLU:O	15:M:205:TRP:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:GLU:HB2	17:I:39:THR:HB	1.95	0.48
2:B:514:LEU:HD11	2:B:562:MET:HG3	1.94	0.48
2:B:814:ILE:HD11	2:B:881:ILE:HD13	1.96	0.48
3:C:145:ARG:HH11	3:C:207:GLU:HG3	1.79	0.48
8:E:12:LYS:NZ	8:E:136:LEU:O	2.42	0.48
1:A:448:ASP:N	1:A:448:ASP:OD1	2.47	0.48
4:G:3:VAL:CA	14:D:11:LEU:HD21	2.37	0.48
15:M:30:TYR:O	16:N:358:GLN:HB2	2.13	0.48
2:B:42:GLN:HA	2:B:45:ASP:OD1	2.14	0.48
2:B:891:PRO:HB3	2:B:1011:LYS:HZ2	1.79	0.48
2:B:1080:CYS:HA	2:B:1101:VAL:HA	1.96	0.48
4:G:94:PRO:HA	4:G:121:ASP:HB2	1.96	0.48
7:P:220:ILE:CD1	7:P:271:ARG:HD2	2.43	0.48
13:Q:72:PRO:HA	13:Q:75:ILE:HG22	1.95	0.48
14:D:1:MET:HE3	14:D:1:MET:HB2	1.55	0.48
15:M:49:ILE:HG12	15:M:56:VAL:HG23	1.95	0.48
1:A:1369:ASP:OD1	4:G:23:ASN:ND2	2.47	0.48
2:B:900:ARG:HD2	2:B:1008:TYR:HB3	1.95	0.48
3:C:133:THR:O	3:C:133:THR:OG1	2.29	0.48
3:C:185:PHE:HB2	3:C:186:PRO:CD	2.42	0.48
10:H:96:VAL:HG12	10:H:116:VAL:HG22	1.95	0.48
14:D:58:CYS:CA	14:D:61:GLN:HB2	2.39	0.48
1:A:224:LEU:HD23	1:A:228:LYS:HD2	1.96	0.48
1:A:949:THR:HG21	1:A:973:ILE:HG21	1.95	0.48
1:A:1295:THR:O	1:A:1295:THR:OG1	2.27	0.48
2:B:280:GLN:HG2	15:M:142:LEU:HB3	1.96	0.48
2:B:480:CYS:SG	2:B:666:GLY:N	2.84	0.48
12:O:400:SER:OG	12:O:401:GLU:OE1	2.31	0.48
14:D:42:LEU:HD13	14:D:42:LEU:C	2.35	0.48
15:M:68:ASN:O	15:M:70:CYS:N	2.39	0.48
15:M:197:GLN:C	15:M:199:LYS:N	2.66	0.48
1:A:86:ILE:HD12	1:A:287:ILE:HG12	1.95	0.47
2:B:729:GLU:HG2	2:B:732:LYS:HE2	1.96	0.47
5:K:30:VAL:CG1	5:K:35:THR:HA	2.44	0.47
6:L:23:HIS:CE1	11:J:64:PRO:HG2	2.49	0.47
11:J:7:CYS:HB3	11:J:11:GLY:H	1.79	0.47
15:M:140:SER:HA	15:M:143:ASP:HB2	1.96	0.47
1:A:1269:ASN:O	1:A:1273:TYR:N	2.43	0.47
4:G:161:SER:HB2	4:G:162:PRO:CD	2.43	0.47
12:O:22:GLU:O	12:O:26:VAL:N	2.40	0.47
17:I:34:ILE:O	17:I:35:THR:C	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:863:ASP:OD1	2:B:863:ASP:N	2.47	0.47
2:B:1098:SER:O	2:B:1098:SER:OG	2.30	0.47
3:C:162:LEU:HD11	3:C:204:PRO:HD3	1.96	0.47
6:L:19:CYS:HB2	6:L:23:HIS:H	1.78	0.47
8:E:19:GLN:OE1	8:E:138:ASN:ND2	2.48	0.47
12:O:412:THR:CG2	12:O:413:PRO:HD2	2.45	0.47
15:M:17:LEU:H	15:M:17:LEU:HD23	1.79	0.47
19:Y:16:DA:H4'	19:Y:16:DA:OP1	2.14	0.47
4:G:103:PHE:CG	14:D:48:GLU:CD	2.88	0.47
1:A:585:PRO:O	1:A:599:GLN:NE2	2.45	0.47
2:B:251:ILE:HD13	2:B:251:ILE:N	2.29	0.47
14:D:4:LYS:HA	14:D:4:LYS:CE	2.35	0.47
1:A:30:GLN:NE2	2:B:1094:TYR:HE1	2.12	0.47
1:A:1323:LYS:HG3	19:Y:12:DG:H5"	1.97	0.47
3:C:78:ARG:HD2	5:K:50:THR:HA	1.97	0.47
7:P:289:LEU:CD1	12:O:357:ARG:HA	2.44	0.47
13:Q:78:PRO:HG3	14:D:7:ASN:ND2	2.29	0.47
15:M:46:SER:HB2	15:M:59:GLU:HB2	1.95	0.47
15:M:146:ASP:HA	15:M:149:HIS:CD2	2.49	0.47
2:B:516:SER:HA	2:B:520:VAL:HG22	1.96	0.47
2:B:530:GLU:H	2:B:530:GLU:CD	2.12	0.47
2:B:747:SER:O	2:B:747:SER:OG	2.31	0.47
2:B:1082:GLN:NE2	2:B:1095:CYS:SG	2.88	0.47
3:C:134:GLU:OE2	3:C:181:GLN:HG2	2.13	0.47
3:C:253:LEU:HD12	3:C:293:LEU:HD13	1.96	0.47
3:C:335:ARG:NH2	5:K:47:GLU:OE2	2.44	0.47
4:G:160:THR:O	4:G:160:THR:CG2	2.63	0.47
7:P:308:ILE:HD13	13:Q:31:VAL:CG1	2.45	0.47
8:E:82:VAL:HG23	8:E:86:THR:HB	1.96	0.47
12:O:20:ILE:HD11	13:Q:68:MET:HG3	1.95	0.47
14:D:32:LYS:HD3	14:D:32:LYS:H	1.80	0.47
14:D:74:LYS:HB3	14:D:74:LYS:HE3	1.64	0.47
15:M:76:GLN:HE21	15:M:76:GLN:CA	2.25	0.47
1:A:884:SER:O	1:A:1030:GLY:N	2.38	0.47
2:B:250:GLU:HA	2:B:250:GLU:OE1	2.13	0.47
2:B:801:LYS:HE2	2:B:801:LYS:N	2.19	0.47
12:O:170:ASP:O	12:O:173:PRO:HD2	2.15	0.47
15:M:38:THR:O	16:N:359:GLU:HG3	2.14	0.47
1:A:519:ALA:HA	1:A:523:MET:HE2	1.97	0.47
2:B:259:GLU:HB2	2:B:263:ALA:HB2	1.97	0.47
2:B:469:ARG:NH2	2:B:488:GLU:O	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:853:ASP:OD1	2:B:853:ASP:N	2.43	0.47
8:E:56:THR:OG1	8:E:78:GLU:OE1	2.31	0.47
15:M:115:ALA:HB1	15:M:128:PRO:CA	2.30	0.47
1:A:481:LYS:CB	1:A:487:ARG:NH2	2.63	0.47
2:B:286:TYR:OH	15:M:150:ARG:NH2	2.48	0.47
14:D:1:MET:HA	14:D:1:MET:HE2	1.96	0.47
15:M:50:LYS:O	15:M:54:GLN:HA	2.15	0.47
15:M:207:HIS:HB2	16:N:372:GLU:HG2	1.95	0.47
1:A:383:PRO:HG2	1:A:386:VAL:HB	1.97	0.46
7:P:283:VAL:O	7:P:283:VAL:CG1	2.62	0.46
1:A:397:ASN:HD21	1:A:400:ASN:HD21	1.64	0.46
2:B:40:VAL:HG22	2:B:452:MET:HB3	1.95	0.46
14:D:1:MET:O	14:D:1:MET:HG3	2.15	0.46
1:A:376:ARG:CZ	1:A:376:ARG:CB	2.93	0.46
1:A:572:LEU:CD1	5:K:83:ARG:HD2	2.44	0.46
1:A:1140:LEU:HD21	17:I:47:LYS:CA	2.45	0.46
5:K:90:LEU:N	5:K:90:LEU:CD1	2.77	0.46
14:D:52:TYR:O	14:D:55:LYS:HB2	2.14	0.46
1:A:97:TYR:HE2	2:B:1121:ASN:HB3	1.80	0.46
1:A:439:LYS:HA	1:A:439:LYS:HD3	1.79	0.46
1:A:483:HIS:CE1	2:B:893:ILE:CD1	2.93	0.46
2:B:156:ALA:HA	11:J:62:TYR:HE1	1.76	0.46
2:B:657:LEU:CG	2:B:658:GLU:H	2.26	0.46
12:O:156:PHE:HA	12:O:241:ARG:HG2	1.96	0.46
1:A:102:ILE:HD13	1:A:168:LYS:HB2	1.98	0.46
3:C:162:LEU:HD11	3:C:204:PRO:CD	2.45	0.46
13:Q:57:MET:O	13:Q:61:LYS:N	2.38	0.46
15:M:70:CYS:O	15:M:73:LYS:HB2	2.15	0.46
1:A:381:ALA:HB1	1:A:481:LYS:HB2	1.97	0.46
1:A:631:LEU:HD13	10:H:124:ARG:HD3	1.97	0.46
1:A:897:ILE:CD1	8:E:165:LEU:HD21	2.44	0.46
1:A:1118:GLU:CB	17:I:39:THR:C	2.83	0.46
1:A:1122:LEU:HA	17:I:36:ARG:HH22	1.80	0.46
1:A:1137:ILE:HG13	1:A:1144:VAL:CG2	2.45	0.46
2:B:657:LEU:CG	2:B:658:GLU:N	2.78	0.46
4:G:4:LEU:HD22	14:D:11:LEU:HD22	1.96	0.46
3:C:96:ASN:OD1	3:C:96:ASN:N	2.49	0.46
4:G:79:PRO:HG2	4:G:150:PHE:CD2	2.51	0.46
5:K:51:LEU:O	5:K:54:SER:N	2.43	0.46
5:K:64:GLU:HB3	5:K:90:LEU:CD2	2.37	0.46
8:E:74:VAL:HA	8:E:103:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:147:THR:HA	12:O:150:ARG:HB2	1.98	0.46
12:O:406:LEU:N	12:O:406:LEU:CD2	2.79	0.46
16:N:340:LEU:HD23	16:N:340:LEU:N	2.31	0.46
16:N:359:GLU:OE1	16:N:359:GLU:HA	2.16	0.46
19:Y:3:DC:H2"	19:Y:4:DC:C5	2.51	0.46
1:A:941:SER:HB3	1:A:980:ILE:HD13	1.98	0.46
2:B:809:LEU:O	2:B:810:ASP:HB3	2.15	0.46
7:P:288:GLY:O	12:O:357:ARG:HD2	2.16	0.46
14:D:117:LEU:HA	14:D:120:VAL:HG12	1.98	0.46
1:A:465:GLN:NE2	2:B:1051:GLU:OE2	2.49	0.46
2:B:531:LEU:HD13	2:B:531:LEU:HA	1.73	0.46
2:B:538:LEU:HD12	2:B:538:LEU:O	2.15	0.46
2:B:801:LYS:HB3	2:B:802:PRO:HD2	1.98	0.46
5:K:67:PHE:HB3	5:K:85:GLN:HB2	1.98	0.46
11:J:43:TYR:HA	11:J:46:ARG:HB2	1.98	0.46
12:O:407:GLN:N	12:O:407:GLN:CD	2.69	0.46
14:D:84:LEU:O	14:D:84:LEU:HD12	2.16	0.46
19:Y:1:DT:OP2	19:Y:1:DT:H72	2.15	0.46
2:B:423:ASN:OD1	2:B:434:GLN:NE2	2.49	0.46
2:B:538:LEU:HA	2:B:548:VAL:HA	1.98	0.46
3:C:193:VAL:HG11	3:C:314:GLY:HA3	1.98	0.46
4:G:103:PHE:HB3	14:D:48:GLU:OE1	2.15	0.46
4:G:160:THR:O	4:G:160:THR:HG22	2.15	0.46
4:G:161:SER:HB2	4:G:162:PRO:HD3	1.97	0.46
12:O:26:VAL:HA	12:O:29:ILE:HD12	1.97	0.46
17:I:30:TYR:C	17:I:30:TYR:CD2	2.90	0.46
5:K:29:MET:HB2	5:K:41:THR:HB	1.97	0.45
14:D:105:GLU:CD	14:D:105:GLU:H	2.19	0.45
1:A:396:VAL:HG21	1:A:444:LEU:HD21	1.98	0.45
1:A:404:LEU:HD12	1:A:407:LEU:HD21	1.98	0.45
1:A:845:THR:HG23	2:B:645:LEU:HD11	1.98	0.45
3:C:162:LEU:HD12	3:C:204:PRO:HD3	1.93	0.45
16:N:363:VAL:HG22	16:N:375:VAL:HA	1.99	0.45
1:A:767:CYS:HB2	1:A:797:ALA:HB2	1.99	0.45
2:B:385:LYS:HE2	2:B:385:LYS:HB3	1.80	0.45
3:C:30:PRO:HG3	3:C:39:ALA:HA	1.97	0.45
12:O:409:ILE:HG22	12:O:409:ILE:O	2.16	0.45
1:A:1116:TYR:O	1:A:1131:LYS:NZ	2.35	0.45
2:B:619:ARG:HH21	2:B:627:GLU:HG3	1.80	0.45
7:P:256:LYS:HE2	7:P:278:PRO:HA	1.99	0.45
15:M:66:ASN:CB	15:M:69:TYR:HE2	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:121:GLN:NE2	16:N:259:SER:O	2.49	0.45
1:A:307:MET:CA	1:A:307:MET:HE3	2.47	0.45
2:B:1095:CYS:O	2:B:1097:SER:N	2.48	0.45
4:G:80:PHE:CE2	4:G:82:ASP:HB2	2.51	0.45
7:P:304:PRO:CG	12:O:445:ASN:HD22	2.26	0.45
11:J:60:LEU:HA	11:J:60:LEU:HD23	1.56	0.45
12:O:59:GLN:NE2	12:O:113:ASN:O	2.42	0.45
13:Q:81:ARG:HE	13:Q:84:ILE:HD11	1.81	0.45
17:I:18:GLN:O	17:I:19:ARG:CG	2.58	0.45
1:A:925:LEU:HD11	1:A:1006:ILE:HD11	1.99	0.45
2:B:642:ASN:O	2:B:654:THR:O	2.34	0.45
12:O:19:GLU:OE2	13:Q:70:ARG:NE	2.47	0.45
15:M:56:VAL:HG13	15:M:102:PHE:HD2	1.82	0.45
1:A:55:VAL:HG22	1:A:55:VAL:O	2.16	0.45
1:A:307:MET:HE2	1:A:307:MET:HB3	1.66	0.45
2:B:216:MET:HB2	2:B:216:MET:HE3	1.76	0.45
12:O:412:THR:HG22	12:O:413:PRO:HD2	1.98	0.45
12:O:416:ALA:HB3	12:O:417:PRO:HD3	1.98	0.45
13:Q:86:ARG:HB2	13:Q:86:ARG:HH11	1.81	0.45
17:I:25:CYS:SG	17:I:26:ASN:N	2.90	0.45
1:A:483:HIS:NE2	2:B:893:ILE:HB	2.25	0.45
1:A:762:HIS:O	1:A:766:ALA:N	2.47	0.45
2:B:192:GLU:HG2	2:B:198:ALA:O	2.17	0.45
3:C:100:ILE:CG2	11:J:60:LEU:HD21	2.47	0.45
10:H:60:ILE:HG23	10:H:141:VAL:HG13	1.99	0.45
12:O:406:LEU:N	12:O:406:LEU:HD23	2.30	0.45
17:I:30:TYR:C	17:I:30:TYR:HD2	2.20	0.45
1:A:48:HIS:O	1:A:48:HIS:CD2	2.69	0.45
1:A:1305:ARG:HD2	1:A:1323:LYS:HE3	1.99	0.45
2:B:530:GLU:HA	2:B:536:VAL:CG2	2.36	0.45
2:B:561:LEU:HD13	2:B:561:LEU:HA	1.80	0.45
2:B:599:VAL:HG11	2:B:654:THR:CG2	2.46	0.45
3:C:147:THR:H	3:C:164:VAL:HB	1.81	0.45
3:C:162:LEU:CD1	3:C:203:ARG:HD2	2.41	0.45
6:L:34:ILE:O	6:L:44:MET:SD	2.75	0.45
8:E:7:THR:C	8:E:9:ARG:N	2.69	0.45
12:O:459:ARG:HG2	12:O:460:LEU:HD23	1.99	0.45
2:B:769:CYS:SG	2:B:1011:LYS:NZ	2.71	0.45
4:G:151:ARG:CZ	4:G:152:VAL:HG12	2.47	0.45
10:H:17:PRO:HG3	10:H:29:HIS:NE2	2.32	0.45
1:A:225:ASN:OD1	1:A:225:ASN:N	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:LEU:HD22	1:A:1046:THR:HG21	1.99	0.44
1:A:483:HIS:CB	1:A:487:ARG:NH1	2.79	0.44
1:A:1094:ASP:OD1	1:A:1094:ASP:N	2.49	0.44
1:A:1110:LEU:C	1:A:1110:LEU:CD1	2.85	0.44
1:A:1113:ILE:HG13	1:A:1113:ILE:O	2.16	0.44
2:B:618:TYR:CG	2:B:618:TYR:O	2.70	0.44
2:B:631:GLU:OE1	2:B:656:HIS:NE2	2.46	0.44
2:B:915:ASP:OD1	3:C:78:ARG:NH1	2.49	0.44
4:G:103:PHE:O	14:D:48:GLU:HB2	2.17	0.44
5:K:38:HIS:CE1	5:K:89:THR:HA	2.52	0.44
1:A:171:LEU:HD23	1:A:171:LEU:N	2.16	0.44
1:A:460:VAL:HG12	1:A:509:LEU:HD13	1.99	0.44
1:A:713:LYS:HG2	1:A:717:LEU:HD23	1.98	0.44
3:C:299:LEU:CD2	3:C:299:LEU:N	2.77	0.44
4:G:161:SER:CB	4:G:162:PRO:CD	2.95	0.44
15:M:111:THR:CG2	15:M:131:GLY:HA2	2.47	0.44
1:A:591:PRO:HG3	10:H:90:TYR:HD1	1.82	0.44
2:B:653:ASP:CG	2:B:653:ASP:O	2.53	0.44
3:C:311:GLU:OE2	11:J:42:ARG:NH2	2.45	0.44
5:K:42:PHE:N	5:K:82:LEU:O	2.50	0.44
7:P:293:PHE:CD2	23:P:401:SF4:S1	3.10	0.44
8:E:9:ARG:C	8:E:11:TRP:N	2.70	0.44
8:E:27:LEU:CD2	8:E:27:LEU:N	2.79	0.44
15:M:120:ARG:NH2	15:M:123:GLU:OE1	2.50	0.44
1:A:78:ASP:OD1	1:A:78:ASP:N	2.50	0.44
4:G:26:ILE:HG21	4:G:70:VAL:HG21	1.98	0.44
12:O:415:HIS:HB2	12:O:418:SER:O	2.17	0.44
1:A:417:GLY:H	1:A:453:HIS:HD1	1.65	0.44
1:A:1020:ASP:OD2	1:A:1024:ARG:NH2	2.50	0.44
8:E:7:THR:C	8:E:9:ARG:H	2.21	0.44
12:O:124:LYS:HA	12:O:124:LYS:HD3	1.76	0.44
12:O:416:ALA:N	12:O:417:PRO:CD	2.81	0.44
2:B:618:TYR:O	2:B:618:TYR:CD2	2.70	0.44
3:C:170:THR:CB	3:C:192:PRO:CG	2.85	0.44
5:K:41:THR:OG1	5:K:83:ARG:NH1	2.51	0.44
14:D:59:ARG:HB3	14:D:59:ARG:NH2	2.32	0.44
15:M:69:TYR:CD1	15:M:73:LYS:HE3	2.52	0.44
1:A:13:LYS:HD3	2:B:1102:SER:HB2	2.00	0.44
1:A:87:ASP:O	1:A:290:ASN:ND2	2.42	0.44
1:A:1183:SER:HB2	1:A:1187:TYR:HD2	1.83	0.44
2:B:617:GLY:C	2:B:619:ARG:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:762:LEU:HD22	2:B:891:PRO:HG2	1.99	0.44
2:B:806:HIS:HA	2:B:809:LEU:HD13	2.00	0.44
3:C:191:ARG:CG	3:C:192:PRO:HD2	2.03	0.44
3:C:235:LEU:HA	3:C:306:TYR:HA	2.00	0.44
12:O:423:LEU:HD23	12:O:423:LEU:N	2.32	0.44
1:A:423:GLN:HB2	1:A:427:GLN:HB2	2.00	0.44
1:A:1121:PHE:CG	17:I:37:LYS:HB2	2.52	0.44
2:B:235:PRO:HD2	2:B:238:ILE:HD12	2.00	0.44
2:B:599:VAL:CB	2:B:655:THR:O	2.50	0.44
2:B:611:MET:CA	2:B:611:MET:HE2	2.47	0.44
10:H:15:ILE:HG12	10:H:52:LEU:HG	2.00	0.44
12:O:406:LEU:HD23	12:O:406:LEU:H	1.83	0.44
14:D:114:GLU:N	14:D:114:GLU:OE2	2.51	0.44
15:M:194:GLU:CD	15:M:194:GLU:H	2.21	0.44
16:N:360:LEU:HB3	16:N:379:VAL:CB	2.47	0.44
20:R:8:A:C4	20:R:9:U:C5	3.06	0.44
1:A:1113:ILE:HB	1:A:1137:ILE:HD11	2.00	0.44
1:A:1144:VAL:HG12	1:A:1202:GLN:HG2	2.00	0.44
2:B:506:MET:SD	2:B:506:MET:N	2.91	0.44
14:D:95:VAL:HA	14:D:98:GLN:HB2	2.00	0.44
1:A:6:PHE:CE1	4:G:158:VAL:HB	2.53	0.43
1:A:874:ARG:HG2	1:A:1321:PHE:HZ	1.83	0.43
3:C:68:ILE:HD13	3:C:306:TYR:OH	2.19	0.43
3:C:275:VAL:HG13	3:C:275:VAL:O	2.17	0.43
4:G:115:GLN:HG3	4:G:116:GLN:HG3	2.00	0.43
12:O:399:LEU:HD12	12:O:404:MET:HB3	2.00	0.43
15:M:15:VAL:HG22	15:M:124:LEU:HD13	2.00	0.43
15:M:72:SER:HA	15:M:75:GLU:HB2	2.00	0.43
1:A:360:ARG:NH1	19:Y:18:DA:OP2	2.45	0.43
1:A:383:PRO:CA	1:A:483:HIS:O	2.66	0.43
1:A:384:VAL:HG23	1:A:481:LYS:O	2.18	0.43
1:A:876:VAL:HG21	2:B:1053:ASP:HB3	1.99	0.43
2:B:616:GLN:CD	2:B:618:TYR:CB	2.87	0.43
2:B:708:LEU:HD13	2:B:773:LYS:HD3	2.00	0.43
2:B:1091:TRP:CD1	4:G:162:PRO:CA	3.01	0.43
2:B:1091:TRP:HD1	4:G:162:PRO:HA	1.82	0.43
12:O:170:ASP:OD1	12:O:170:ASP:N	2.48	0.43
15:M:73:LYS:O	15:M:76:GLN:HB2	2.19	0.43
1:A:817:SER:OG	1:A:830:ALA:O	2.32	0.43
2:B:1073:ASP:HB3	2:B:1108:TYR:H	1.82	0.43
8:E:84:ILE:HA	8:E:87:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:159:ARG:NH1	13:Q:112:PRO:O	2.51	0.43
14:D:17:PHE:CD2	14:D:18:GLN:NE2	2.87	0.43
15:M:199:LYS:HB2	15:M:199:LYS:HZ3	1.77	0.43
16:N:360:LEU:O	16:N:379:VAL:HB	2.19	0.43
1:A:93:PHE:H	1:A:314:GLN:HE22	1.66	0.43
1:A:705:PRO:HB3	1:A:709:LEU:HD13	2.01	0.43
1:A:1080:ILE:HG12	1:A:1250:ASN:HD22	1.83	0.43
2:B:780:LYS:HA	2:B:878:ALA:HB1	2.00	0.43
4:G:147:GLU:OE2	14:D:100:MET:SD	2.76	0.43
12:O:413:PRO:O	12:O:415:HIS:HD2	2.01	0.43
17:I:2:LEU:N	17:I:2:LEU:CD2	2.82	0.43
17:I:33:ASN:N	17:I:33:ASN:HD22	2.16	0.43
1:A:259:PRO:HG2	2:B:1115:GLN:HE21	1.82	0.43
1:A:1061:MET:SD	1:A:1061:MET:N	2.92	0.43
1:A:1105:ILE:HG22	1:A:1238:THR:HG21	2.01	0.43
2:B:172:LYS:HE2	2:B:416:VAL:HG11	2.00	0.43
2:B:541:LEU:HA	2:B:585:ILE:O	2.18	0.43
3:C:96:ASN:ND2	3:C:207:GLU:OE1	2.51	0.43
3:C:116:HIS:NE2	3:C:190:ILE:HD11	2.28	0.43
4:G:6:GLU:CG	14:D:5:ASP:HB2	2.49	0.43
12:O:89:PRO:HG2	13:Q:54:GLU:HG2	2.00	0.43
15:M:17:LEU:O	15:M:19:LYS:HD3	2.18	0.43
15:M:76:GLN:HA	15:M:76:GLN:NE2	2.29	0.43
1:A:82:HIS:ND1	2:B:1088:TYR:CD2	2.86	0.43
1:A:252:LEU:HD13	1:A:255:LEU:HD12	1.99	0.43
1:A:670:ASP:OD1	1:A:670:ASP:N	2.50	0.43
1:A:1121:PHE:O	17:I:36:ARG:CZ	2.66	0.43
1:A:1317:MET:HG3	1:A:1344:SER:HB2	1.99	0.43
2:B:238:ILE:HD13	2:B:287:ILE:HD13	2.00	0.43
4:G:32:LYS:HE2	14:D:39:GLN:CG	2.48	0.43
4:G:80:PHE:CE2	14:D:81:ALA:HB1	2.54	0.43
14:D:87:LEU:N	14:D:87:LEU:HD23	2.32	0.43
15:M:196:LEU:O	15:M:198:LYS:N	2.47	0.43
2:B:538:LEU:HD13	2:B:540:PHE:CE1	2.53	0.43
2:B:564:ARG:NE	2:B:631:GLU:OE2	2.48	0.43
2:B:1085:LEU:HD23	2:B:1085:LEU:HA	1.80	0.43
13:Q:34:PRO:HG2	13:Q:37:LEU:CD2	2.49	0.43
20:R:8:A:H2'	20:R:9:U:C6	2.54	0.43
1:A:29:ARG:NH2	7:P:302:ILE:HD12	2.30	0.43
1:A:822:GLU:HG2	1:A:825:SER:HB2	2.00	0.43
2:B:48:ASN:O	2:B:52:ASN:ND2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:436:VAL:HG23	2:B:437:THR:HG23	2.00	0.43
1:A:596:THR:HG21	10:H:119:GLY:HA3	2.01	0.43
2:B:521:GLU:HG3	2:B:525:LEU:HD21	2.01	0.43
3:C:236:LEU:HD13	3:C:305:HIS:CE1	2.54	0.43
9:F:102:ILE:HG22	9:F:104:ILE:HB	2.00	0.43
14:D:69:PHE:HD2	14:D:69:PHE:O	2.02	0.43
19:Y:18:DA:N3	19:Y:18:DA:H2'	2.32	0.43
1:A:698:ILE:HG13	1:A:776:SER:HB2	2.01	0.43
1:A:720:GLY:HA3	1:A:759:ILE:HD11	2.00	0.43
2:B:740:THR:O	2:B:740:THR:OG1	2.32	0.43
23:P:401:SF4:S2	12:O:445:ASN:CG	2.97	0.43
10:H:15:ILE:HD13	10:H:15:ILE:HA	1.78	0.43
12:O:174:PRO:N	12:O:175:PRO:HD2	2.34	0.43
15:M:25:LEU:HB3	15:M:129:LEU:HD22	2.00	0.43
17:I:2:LEU:O	17:I:2:LEU:CD2	2.66	0.43
20:R:8:A:C5	20:R:9:U:C4	3.06	0.43
1:A:171:LEU:HG	1:A:171:LEU:O	2.19	0.42
1:A:484:ARG:H	1:A:484:ARG:HG2	1.54	0.42
1:A:1033:VAL:HG12	1:A:1289:LEU:HD22	2.01	0.42
2:B:194:ASP:O	2:B:195:ARG:NH1	2.52	0.42
2:B:243:MET:HG3	2:B:328:PHE:HB3	2.01	0.42
3:C:49:PHE:CZ	5:K:110:VAL:HG23	2.54	0.42
4:G:57:ALA:HA	4:G:68:THR:HG22	2.00	0.42
5:K:34:GLY:O	5:K:35:THR:CB	2.67	0.42
12:O:374:HIS:CE1	12:O:425:THR:HG1	2.32	0.42
14:D:17:PHE:CE1	14:D:21:THR:CG2	3.02	0.42
15:M:76:GLN:O	15:M:77:ILE:HG12	2.18	0.42
15:M:79:LEU:HD23	15:M:79:LEU:HA	1.91	0.42
17:I:2:LEU:HD23	17:I:2:LEU:N	2.33	0.42
2:B:292:ARG:NH1	2:B:314:ALA:O	2.45	0.42
12:O:63:VAL:HG22	12:O:77:ALA:HB2	1.99	0.42
14:D:59:ARG:HB3	14:D:59:ARG:HH21	1.83	0.42
17:I:13:ILE:HD12	17:I:23:PHE:HA	2.01	0.42
19:Y:1:DT:C6	19:Y:1:DT:OP1	2.71	0.42
1:A:87:ASP:OD2	1:A:254:ARG:NH2	2.52	0.42
1:A:117:LEU:HD12	1:A:237:LEU:HD21	2.01	0.42
1:A:571:ILE:HD13	1:A:682:ARG:HA	2.00	0.42
1:A:935:PRO:HA	1:A:1005:ARG:HH22	1.82	0.42
1:A:966:LEU:HD12	1:A:966:LEU:HA	1.80	0.42
4:G:4:LEU:HD22	14:D:11:LEU:HD13	2.01	0.42
12:O:233:ILE:HD12	12:O:233:ILE:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:34:PRO:HG2	13:Q:37:LEU:HD23	2.01	0.42
1:A:691:LEU:HD12	1:A:691:LEU:HA	1.91	0.42
1:A:865:THR:HA	1:A:868:THR:HG22	2.01	0.42
5:K:86:THR:CB	5:K:90:LEU:HD22	2.42	0.42
15:M:99:LYS:HB3	15:M:101:THR:HG23	2.01	0.42
16:N:269:LEU:HA	16:N:383:LEU:O	2.20	0.42
19:Y:11:DA:H2'	19:Y:12:DG:C8	2.54	0.42
1:A:38:SER:OG	1:A:54:GLY:O	2.35	0.42
2:B:529:GLU:HG3	16:N:353:ALA:HB1	2.01	0.42
7:P:222:GLU:HA	7:P:225:ILE:HG22	2.02	0.42
8:E:27:LEU:HD22	8:E:63:ALA:O	2.13	0.42
15:M:54:GLN:HB3	15:M:104:SER:HB3	2.01	0.42
1:A:303:THR:HA	1:A:306:ILE:HG22	2.00	0.42
1:A:385:HIS:CD2	1:A:484:ARG:HH11	2.35	0.42
1:A:663:ILE:H	1:A:663:ILE:HG13	1.57	0.42
2:B:94:THR:O	2:B:94:THR:HG23	2.19	0.42
2:B:702:ARG:NH1	3:C:100:ILE:O	2.39	0.42
8:E:49:SER:O	8:E:49:SER:OG	2.35	0.42
15:M:58:LEU:H	15:M:101:THR:HG22	1.84	0.42
2:B:340:ARG:HH12	2:B:581:ARG:NH2	2.18	0.42
2:B:606:VAL:O	2:B:610:HIS:HB2	2.20	0.42
3:C:134:GLU:HG3	3:C:178:LEU:HB3	2.01	0.42
3:C:181:GLN:NE2	3:C:181:GLN:CA	2.60	0.42
3:C:283:PHE:CE1	3:C:299:LEU:HD12	2.55	0.42
4:G:197:LEU:HD13	4:G:200:TRP:CH2	2.54	0.42
7:P:294:ASP:C	7:P:294:ASP:OD2	2.58	0.42
11:J:9:THR:OG1	11:J:10:CYS:N	2.53	0.42
12:O:459:ARG:H	12:O:459:ARG:HD3	1.85	0.42
14:D:11:LEU:CD2	14:D:11:LEU:N	2.57	0.42
15:M:32:VAL:C	15:M:34:PRO:HD3	2.40	0.42
16:N:356:PHE:CE2	16:N:380:LYS:HA	2.53	0.42
19:Y:6:DA:H2"	19:Y:7:DG:C8	2.54	0.42
1:A:941:SER:HB2	1:A:980:ILE:HG21	2.01	0.42
1:A:1140:LEU:HB2	1:A:1142:LEU:HD22	2.01	0.42
2:B:594:ARG:NH2	2:B:663:THR:OG1	2.52	0.42
3:C:86:THR:OG1	3:C:225:PHE:O	2.36	0.42
3:C:257:PHE:CZ	3:C:287:ILE:HD11	2.54	0.42
4:G:38:VAL:HG11	4:G:186:LEU:HB2	2.01	0.42
5:K:40:VAL:HG13	5:K:92:ALA:HB3	2.00	0.42
7:P:206:ARG:CZ	7:P:217:TRP:HE1	2.33	0.42
9:F:109:TYR:HD1	9:F:109:TYR:HA	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:2:THR:O	12:O:2:THR:OG1	2.34	0.42
15:M:32:VAL:CG1	15:M:137:PRO:HD3	2.26	0.42
15:M:50:LYS:HG3	15:M:201:ALA:HA	2.02	0.42
15:M:68:ASN:C	15:M:70:CYS:N	2.73	0.42
16:N:264:GLU:H	16:N:264:GLU:HG3	1.62	0.42
1:A:1315:VAL:O	1:A:1319:ALA:N	2.47	0.42
2:B:257:THR:CG2	2:B:528:GLY:HA2	2.50	0.42
2:B:899:SER:HB2	2:B:942:LYS:HZ1	1.85	0.42
4:G:103:PHE:HB3	14:D:48:GLU:CG	2.49	0.42
8:E:6:GLU:C	8:E:8:TYR:N	2.73	0.42
15:M:118:LEU:C	15:M:118:LEU:CD2	2.85	0.42
15:M:194:GLU:OE1	15:M:194:GLU:N	2.52	0.42
1:A:24:SER:HA	1:A:249:ASP:HB3	2.02	0.42
1:A:801:GLN:NE2	1:A:802:GLN:O	2.52	0.42
2:B:214:THR:HG22	2:B:227:HIS:CE1	2.55	0.42
2:B:538:LEU:HD12	2:B:582:CYS:HA	2.02	0.42
3:C:251:GLU:O	3:C:255:ARG:NE	2.53	0.42
5:K:40:VAL:HG21	5:K:92:ALA:CB	2.44	0.42
12:O:459:ARG:NH1	12:O:460:LEU:HB2	2.34	0.42
15:M:56:VAL:HG12	15:M:135:LEU:CD2	2.45	0.42
2:B:257:THR:HG21	2:B:528:GLY:HA2	2.01	0.41
2:B:633:LEU:HD11	2:B:656:HIS:CD2	2.55	0.41
2:B:947:LEU:HD12	2:B:947:LEU:HA	1.87	0.41
3:C:78:ARG:HE	3:C:78:ARG:HB2	1.55	0.41
3:C:185:PHE:HB2	3:C:186:PRO:HD2	2.01	0.41
3:C:237:PRO:HB3	3:C:283:PHE:CE2	2.53	0.41
6:L:26:ASN:HB2	6:L:44:MET:HE1	2.01	0.41
7:P:269:LEU:HD23	7:P:269:LEU:HA	1.78	0.41
8:E:159:LEU:HD11	8:E:206:TYR:CG	2.54	0.41
12:O:432:ALA:HB1	12:O:523:LEU:HD21	2.02	0.41
1:A:34:ILE:HD11	1:A:59:ARG:HH11	1.85	0.41
1:A:42:TYR:HD2	1:A:44:GLN:HE21	1.68	0.41
1:A:136:TYR:HE1	1:A:140:ARG:HE	1.68	0.41
1:A:286:ILE:O	1:A:290:ASN:N	2.52	0.41
1:A:420:PHE:HB2	1:A:451:GLU:HB2	2.01	0.41
1:A:593:THR:HG23	3:C:32:ASN:HA	2.02	0.41
1:A:1092:ASP:OD1	1:A:1092:ASP:N	2.43	0.41
2:B:376:LEU:HD23	2:B:376:LEU:HA	1.85	0.41
2:B:820:LYS:HB3	2:B:865:TYR:CE2	2.55	0.41
5:K:76:SER:OG	5:K:77:GLU:N	2.53	0.41
12:O:34:GLN:HA	12:O:35:PRO:HD3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:353:VAL:HG21	12:O:435:LEU:HD21	2.02	0.41
14:D:2:GLU:HG2	14:D:2:GLU:O	2.19	0.41
14:D:66:VAL:O	14:D:70:LEU:HB2	2.20	0.41
15:M:50:LYS:HD3	15:M:54:GLN:O	2.20	0.41
1:A:1140:LEU:CD2	17:I:47:LYS:CB	2.96	0.41
2:B:260:HIS:ND1	2:B:261:VAL:HG23	2.35	0.41
2:B:597:ILE:HG13	2:B:659:ILE:HG12	2.02	0.41
2:B:998:LEU:O	3:C:21:VAL:HG21	2.21	0.41
5:K:40:VAL:CG1	5:K:92:ALA:HB3	2.51	0.41
7:P:200:GLN:NE2	7:P:257:GLU:OE2	2.54	0.41
7:P:227:LYS:HD2	7:P:240:ASN:HB3	2.03	0.41
12:O:269:THR:HG21	12:O:298:PRO:HD3	2.01	0.41
15:M:20:SER:OG	15:M:214:ARG:NH1	2.53	0.41
15:M:69:TYR:HB2	15:M:73:LYS:HD2	2.02	0.41
1:A:563:LYS:HE3	1:A:567:ILE:HD11	2.01	0.41
1:A:1328:LEU:HD23	1:A:1328:LEU:HA	1.83	0.41
2:B:262:MET:SD	2:B:262:MET:N	2.93	0.41
2:B:682:ARG:HD3	2:B:682:ARG:HA	1.83	0.41
2:B:1095:CYS:SG	2:B:1095:CYS:O	2.78	0.41
4:G:79:PRO:HG3	4:G:150:PHE:CE2	2.55	0.41
8:E:9:ARG:C	8:E:11:TRP:H	2.22	0.41
12:O:459:ARG:O	12:O:463:LYS:NZ	2.41	0.41
1:A:579:ILE:HA	5:K:31:GLN:HE22	1.85	0.41
1:A:630:ASP:HB3	1:A:637:TYR:CD2	2.55	0.41
1:A:643:SER:O	1:A:643:SER:OG	2.38	0.41
2:B:619:ARG:NH2	2:B:627:GLU:HG3	2.36	0.41
3:C:61:LEU:HG	3:C:63:PHE:HD1	1.85	0.41
3:C:155:ASP:N	3:C:155:ASP:OD1	2.52	0.41
7:P:220:ILE:O	7:P:224:GLY:N	2.51	0.41
8:E:168:ASN:HB2	8:E:172:ARG:HH21	1.86	0.41
14:D:3:VAL:O	14:D:3:VAL:CG2	2.68	0.41
15:M:195:PHE:H	15:M:195:PHE:HD1	1.69	0.41
1:A:1297:LYS:HE2	1:A:1297:LYS:HB2	1.87	0.41
2:B:137:PRO:HD2	2:B:415:MET:HG2	2.01	0.41
2:B:1091:TRP:NE1	4:G:162:PRO:CD	2.75	0.41
3:C:116:HIS:CB	3:C:190:ILE:CG1	2.82	0.41
4:G:5:VAL:HG12	4:G:7:MET:HG3	2.03	0.41
6:L:23:HIS:NE2	11:J:64:PRO:HG2	2.36	0.41
14:D:14:TYR:OH	14:D:63:PRO:HB3	2.21	0.41
15:M:116:ALA:HB3	16:N:269:LEU:N	2.36	0.41
1:A:99:ARG:HD2	1:A:99:ARG:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1127:PHE:HA	1:A:1177:PRO:HA	2.01	0.41
2:B:796:ASP:O	2:B:797:ALA:HB3	2.21	0.41
3:C:21:VAL:CG2	3:C:24:VAL:CG1	2.99	0.41
4:G:42:VAL:HG21	14:D:3:VAL:HG11	2.02	0.41
12:O:115:LYS:HD3	12:O:115:LYS:HA	1.86	0.41
15:M:76:GLN:CA	15:M:76:GLN:NE2	2.83	0.41
16:N:333:LYS:H	16:N:333:LYS:CD	2.34	0.41
1:A:18:ILE:HD11	1:A:1349:MET:HE1	2.02	0.41
2:B:40:VAL:HG22	2:B:452:MET:CB	2.50	0.41
2:B:608:ASN:ND2	2:B:608:ASN:C	2.73	0.41
2:B:758:ASN:HB3	2:B:916:MET:SD	2.61	0.41
2:B:779:LEU:HB3	2:B:788:ASP:HB2	2.01	0.41
3:C:178:LEU:HD23	3:C:178:LEU:HA	1.71	0.41
12:O:376:GLU:HB3	12:O:424:TYR:HD1	1.85	0.41
15:M:71:ARG:O	15:M:75:GLU:N	2.46	0.41
1:A:464:ARG:HB2	1:A:505:MET:HE3	2.03	0.41
1:A:516:LYS:NZ	9:F:88:ASP:OD1	2.52	0.41
2:B:265:PHE:O	2:B:268:SER:OG	2.28	0.41
3:C:149:ASN:OD1	3:C:149:ASN:N	2.53	0.41
7:P:286:PRO:CB	13:Q:38:PHE:CD2	3.04	0.41
8:E:116:GLN:HA	8:E:119:VAL:HG22	2.02	0.41
8:E:186:LYS:HB2	8:E:186:LYS:HE2	1.91	0.41
14:D:50:LEU:HD22	14:D:50:LEU:HA	1.97	0.41
15:M:42:ILE:HB	15:M:210:TYR:CE1	2.55	0.41
15:M:119:TYR:HD1	15:M:124:LEU:HA	1.85	0.41
15:M:213:LEU:HB3	15:M:214:ARG:HH21	1.86	0.41
1:A:222:VAL:HG11	12:O:406:LEU:HD13	2.03	0.41
1:A:974:LYS:HA	1:A:977:SER:HB3	2.02	0.41
2:B:819:GLU:OE2	6:L:51:ARG:NH1	2.54	0.41
3:C:321:LEU:HA	3:C:321:LEU:HD23	1.85	0.41
4:G:80:PHE:CD2	4:G:82:ASP:HB2	2.56	0.41
7:P:232:MET:SD	7:P:232:MET:N	2.94	0.41
12:O:503:LYS:HB2	12:O:503:LYS:HE2	1.88	0.41
15:M:121:GLN:HG3	16:N:258:LEU:HD22	2.02	0.41
15:M:145:ALA:O	15:M:148:LYS:HB2	2.21	0.41
1:A:848:PHE:HE2	2:B:473:PRO:HA	1.86	0.40
1:A:1176:THR:HA	1:A:1177:PRO:HD3	1.93	0.40
2:B:37:LYS:HD3	2:B:632:TYR:OH	2.22	0.40
4:G:46:ILE:HG23	14:D:45:ILE:HG13	2.01	0.40
5:K:77:GLU:H	5:K:77:GLU:HG2	1.63	0.40
7:P:287:CYS:O	7:P:287:CYS:SG	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:49:LEU:HD23	11:J:49:LEU:HA	1.89	0.40
12:O:138:THR:HG21	13:Q:104:ARG:HB2	2.03	0.40
1:A:134:LEU:HD23	1:A:134:LEU:HA	1.90	0.40
1:A:289:LEU:HD12	1:A:289:LEU:HA	1.84	0.40
1:A:407:LEU:HD12	1:A:408:VAL:N	2.36	0.40
2:B:171:VAL:HG13	2:B:416:VAL:HG13	2.03	0.40
2:B:810:ASP:HB2	2:B:816:SER:HB3	2.03	0.40
2:B:814:ILE:HG13	2:B:881:ILE:HD13	2.04	0.40
3:C:317:PRO:HA	3:C:318:PRO:HD3	1.96	0.40
4:G:192:GLU:OE2	4:G:197:LEU:HD11	2.21	0.40
12:O:399:LEU:CD1	12:O:404:MET:HB3	2.50	0.40
14:D:94:ALA:HA	14:D:117:LEU:HD22	2.03	0.40
1:A:562:ALA:HB2	3:C:29:PHE:HE2	1.86	0.40
2:B:526:LEU:HG	16:N:358:GLN:NE2	2.28	0.40
2:B:587:SER:O	2:B:587:SER:OG	2.34	0.40
5:K:48:ASP:HB2	5:K:49:HIS:H	1.78	0.40
10:H:124:ARG:NH2	10:H:126:GLN:OE1	2.49	0.40
15:M:51:PRO:HD3	15:M:203:GLU:HB2	2.03	0.40
1:A:579:ILE:O	5:K:83:ARG:NH2	2.54	0.40
1:A:620:LYS:HD3	1:A:637:TYR:HE1	1.87	0.40
1:A:773:LYS:HE3	1:A:773:LYS:HB2	1.82	0.40
2:B:523:VAL:HG12	15:M:107:THR:HB	2.03	0.40
8:E:116:GLN:O	8:E:120:ASP:N	2.51	0.40
12:O:106:ILE:HD13	12:O:125:VAL:HG11	2.03	0.40
15:M:56:VAL:HG13	15:M:56:VAL:O	2.22	0.40
1:A:291:ASP:O	1:A:295:LYS:N	2.52	0.40
1:A:382:VAL:HG11	1:A:454:LEU:HD23	2.04	0.40
1:A:1121:PHE:CD2	17:I:37:LYS:CB	3.01	0.40
2:B:257:THR:HG21	2:B:528:GLY:CA	2.52	0.40
2:B:1091:TRP:CD1	4:G:162:PRO:N	2.90	0.40
3:C:26:THR:OG1	3:C:27:THR:N	2.54	0.40
15:M:17:LEU:O	15:M:17:LEU:HG	2.22	0.40
15:M:28:PHE:CD2	16:N:363:VAL:HG21	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1281/1390 (92%)	1154 (90%)	124 (10%)	3 (0%)	47 78
2	B	1030/1133 (91%)	925 (90%)	100 (10%)	5 (0%)	29 63
3	C	326/346 (94%)	293 (90%)	30 (9%)	3 (1%)	17 51
4	G	160/204 (78%)	137 (86%)	23 (14%)	0	100 100
5	K	101/133 (76%)	91 (90%)	8 (8%)	2 (2%)	7 33
6	L	42/58 (72%)	40 (95%)	1 (2%)	1 (2%)	6 30
7	P	128/316 (40%)	102 (80%)	25 (20%)	1 (1%)	19 53
8	E	188/210 (90%)	172 (92%)	15 (8%)	1 (0%)	29 63
9	F	74/127 (58%)	68 (92%)	6 (8%)	0	100 100
10	H	116/150 (77%)	101 (87%)	15 (13%)	0	100 100
11	J	62/67 (92%)	58 (94%)	4 (6%)	0	100 100
12	O	435/534 (82%)	416 (96%)	18 (4%)	1 (0%)	47 78
13	Q	82/223 (37%)	72 (88%)	9 (11%)	1 (1%)	13 44
14	D	120/148 (81%)	109 (91%)	10 (8%)	1 (1%)	19 53
15	M	148/708 (21%)	110 (74%)	33 (22%)	5 (3%)	3 23
16	N	88/398 (22%)	80 (91%)	6 (7%)	2 (2%)	6 31
17	I	45/108 (42%)	33 (73%)	9 (20%)	3 (7%)	1 9
All	All	4426/6253 (71%)	3961 (90%)	436 (10%)	29 (1%)	26 56

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	523	VAL
2	B	802	PRO
3	C	190	ILE
3	C	191	ARG
6	L	35	ARG

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Mol	Chain	Res	Type
7	P	296	CYS
12	O	409	ILE
14	D	8	SER
17	I	34	ILE
17	I	43	TYR
2	B	530	GLU
2	B	1096	LYS
5	K	35	THR
5	K	92	ALA
15	M	77	ILE
15	M	199	LYS
1	A	482	PRO
17	I	44	PRO
8	E	7	THR
15	M	41	ASP
16	N	352	THR
13	Q	28	PRO
15	M	109	SER
15	M	204	PRO
1	A	942	LYS
2	B	40	VAL
3	C	192	PRO
16	N	344	VAL
1	A	1177	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1124/1212 (93%)	1095 (97%)	29 (3%)	46	73
2	B	912/988 (92%)	880 (96%)	32 (4%)	36	66
3	C	290/302 (96%)	274 (94%)	16 (6%)	21	53
4	G	149/181 (82%)	146 (98%)	3 (2%)	55	78
5	K	92/119 (77%)	91 (99%)	1 (1%)	73	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	L	41/55 (74%)	39 (95%)	2 (5%)	25 57
7	P	114/280 (41%)	110 (96%)	4 (4%)	36 66
8	E	177/192 (92%)	174 (98%)	3 (2%)	60 80
9	F	66/111 (60%)	66 (100%)	0	100 100
10	H	110/131 (84%)	110 (100%)	0	100 100
11	J	53/56 (95%)	53 (100%)	0	100 100
12	O	400/476 (84%)	390 (98%)	10 (2%)	47 73
13	Q	81/195 (42%)	72 (89%)	9 (11%)	6 24
14	D	114/136 (84%)	88 (77%)	26 (23%)	1 3
15	M	138/622 (22%)	115 (83%)	23 (17%)	2 9
16	N	81/347 (23%)	67 (83%)	14 (17%)	2 8
17	I	34/94 (36%)	26 (76%)	8 (24%)	1 2
All	All	3976/5497 (72%)	3796 (96%)	180 (4%)	31 59

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	6	PHE
1	A	7	ARG
1	A	48	HIS
1	A	307	MET
1	A	428	MET
1	A	464	ARG
1	A	481	LYS
1	A	483	HIS
1	A	484	ARG
1	A	493	CYS
1	A	503	ASP
1	A	542	ILE
1	A	593	THR
1	A	631	LEU
1	A	663	ILE
1	A	974	LYS
1	A	1099	ARG
1	A	1107	LYS
1	A	1110	LEU
1	A	1113	ILE

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Mol	Chain	Res	Type
1	A	1115	GLU
1	A	1124	ASP
1	A	1135	GLU
1	A	1137	ILE
1	A	1167	VAL
1	A	1185	MET
1	A	1209	ARG
1	A	1224	LYS
2	B	27	TRP
2	B	93	VAL
2	B	207	THR
2	B	249	GLN
2	B	251	ILE
2	B	310	ARG
2	B	529	GLU
2	B	531	LEU
2	B	538	LEU
2	B	544	ASN
2	B	549	ILE
2	B	559	PHE
2	B	574	ILE
2	B	578	LEU
2	B	582	CYS
2	B	606	VAL
2	B	608	ASN
2	B	654	THR
2	B	656	HIS
2	B	733	LEU
2	B	764	ARG
2	B	801	LYS
2	B	815	CYS
2	B	863	ASP
2	B	869	VAL
2	B	907	CYS
2	B	1004	PHE
2	B	1013	LYS
2	B	1037	GLU
2	B	1045	LEU
2	B	1095	CYS
2	B	1111	LYS
3	C	23	ASN
3	C	24	VAL

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Mol	Chain	Res	Type
3	C	68	ILE
3	C	120	ARG
3	C	133	THR
3	C	166	HIS
3	C	178	LEU
3	C	180	ASN
3	C	181	GLN
3	C	183	ASP
3	C	185	PHE
3	C	187	GLU
3	C	190	ILE
3	C	261	VAL
3	C	277	ASN
3	C	282	THR
4	G	22	LEU
4	G	83	GLU
4	G	198	LEU
5	K	50	THR
6	L	34	ILE
6	L	43	ILE
7	P	205	GLN
7	P	247	LYS
7	P	284	ARG
7	P	307	CYS
8	E	9	ARG
8	E	127	LEU
8	E	165	LEU
12	O	170	ASP
12	O	361	ARG
12	O	378	LYS
12	O	406	LEU
12	O	408	GLU
12	O	409	ILE
12	O	411	LYS
12	O	414	ASP
12	O	423	LEU
12	O	459	ARG
13	Q	27	LEU
13	Q	31	VAL
13	Q	48	LEU
13	Q	79	GLU
13	Q	80	GLU

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Mol	Chain	Res	Type
13	Q	81	ARG
13	Q	83	ASP
13	Q	86	ARG
13	Q	87	TYR
14	D	1	MET
14	D	3	VAL
14	D	11	LEU
14	D	14	TYR
14	D	15	GLU
14	D	17	PHE
14	D	18	GLN
14	D	19	LEU
14	D	20	LEU
14	D	32	LYS
14	D	40	GLN
14	D	41	ASN
14	D	43	ASN
14	D	59	ARG
14	D	64	GLU
14	D	69	PHE
14	D	70	LEU
14	D	74	LYS
14	D	77	LYS
14	D	84	LEU
14	D	88	ASN
14	D	96	GLU
14	D	97	ILE
14	D	101	VAL
14	D	105	GLU
14	D	113	ILE
15	M	42	ILE
15	M	66	ASN
15	M	68	ASN
15	M	69	TYR
15	M	71	ARG
15	M	75	GLU
15	M	76	GLN
15	M	77	ILE
15	M	107	THR
15	M	111	THR
15	M	114	TYR
15	M	120	ARG

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Mol	Chain	Res	Type
15	M	121	GLN
15	M	136	ARG
15	M	138	SER
15	M	142	LEU
15	M	144	LYS
15	M	188	ARG
15	M	193	TYR
15	M	194	GLU
15	M	195	PHE
15	M	199	LYS
15	M	214	ARG
16	N	255	LEU
16	N	258	LEU
16	N	271	LEU
16	N	273	ASP
16	N	328	LYS
16	N	329	LEU
16	N	330	LEU
16	N	343	LYS
16	N	352	THR
16	N	358	GLN
16	N	360	LEU
16	N	373	MET
16	N	379	VAL
16	N	382	LYS
17	I	2	LEU
17	I	27	THR
17	I	28	CYS
17	I	30	TYR
17	I	33	ASN
17	I	36	ARG
17	I	37	LYS
17	I	39	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	48	HIS
1	A	94	HIS
1	A	374	ASN
1	A	385	HIS

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Mol	Chain	Res	Type
1	A	397	ASN
1	A	465	GLN
1	A	506	ASN
1	A	511	GLN
1	A	543	GLN
1	A	693	ASN
1	A	738	GLN
2	B	52	ASN
2	B	129	ASN
2	B	187	ASN
2	B	227	HIS
2	B	260	HIS
2	B	289	ASN
2	B	413	ASN
2	B	417	ASN
2	B	434	GLN
2	B	542	ASN
2	B	639	ASN
2	B	703	ASN
2	B	806	HIS
2	B	825	GLN
2	B	887	GLN
2	B	1082	GLN
2	B	1100	HIS
3	C	42	GLN
3	C	59	ASN
3	C	181	GLN
5	K	38	HIS
5	K	85	GLN
6	L	26	ASN
7	P	200	GLN
7	P	240	ASN
7	P	274	ASN
7	P	306	ASN
8	E	35	GLN
8	E	129	GLN
8	E	138	ASN
12	O	14	GLN
12	O	49	GLN
12	O	113	ASN
12	O	337	ASN
12	O	377	GLN

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Mol	Chain	Res	Type
12	O	379	GLN
12	O	415	HIS
12	O	445	ASN
12	O	451	GLN
12	O	457	ASN
12	O	465	GLN
12	O	507	ASN
14	D	7	ASN
14	D	35	HIS
14	D	43	ASN
14	D	61	GLN
14	D	85	GLN
14	D	98	GLN
14	D	112	GLN
15	M	29	GLN
15	M	66	ASN
15	M	76	GLN
16	N	358	GLN
17	I	10	ASN
17	I	33	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	R	2/3 (66%)	2 (100%)	1 (50%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	R	9	U
20	R	10	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	R	9	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	SF4	P	401	7	0,12,12	-	-	-		

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
23	SF4	P	401	7	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

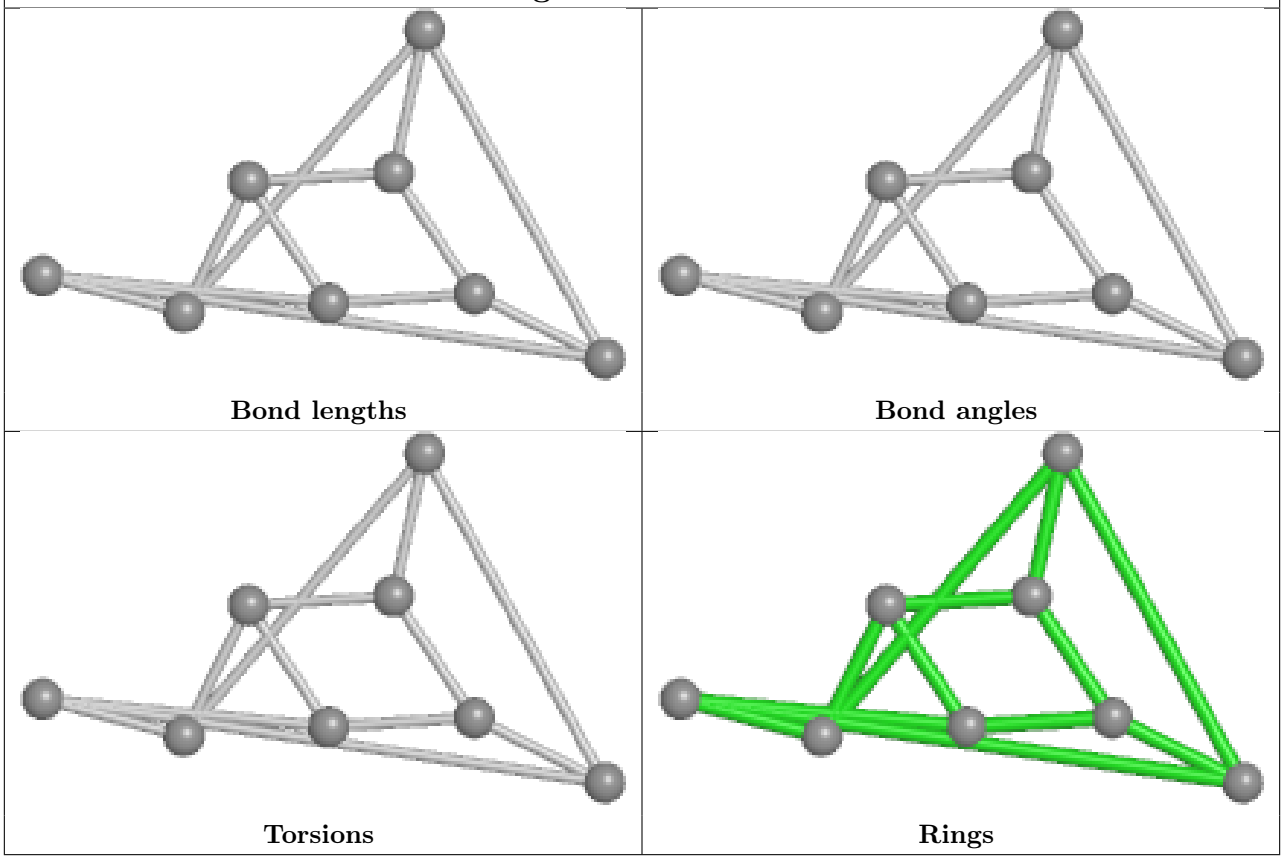
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	P	401	SF4	4	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 then 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.

Ligand SF4 P 401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

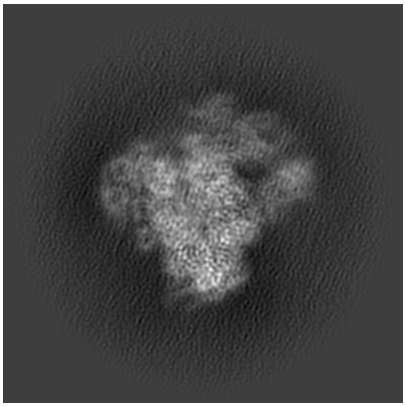
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30865. These allow visual inspection of the internal detail of the map and identification of artifacts.

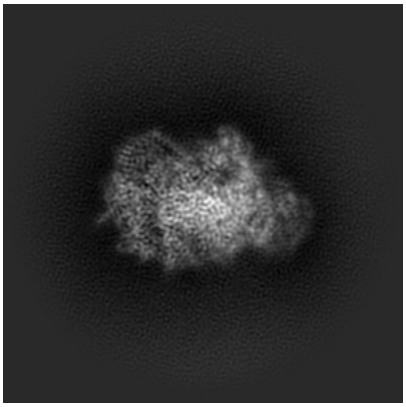
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

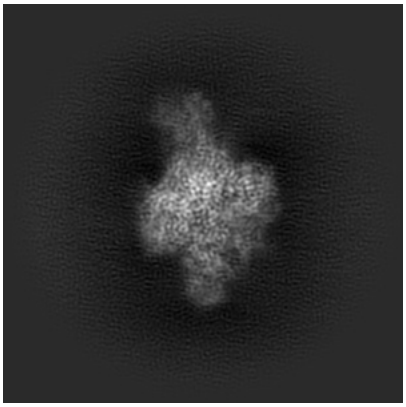
6.1.1 Primary map



X



Y

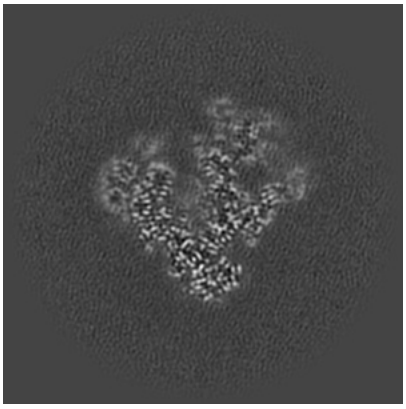


Z

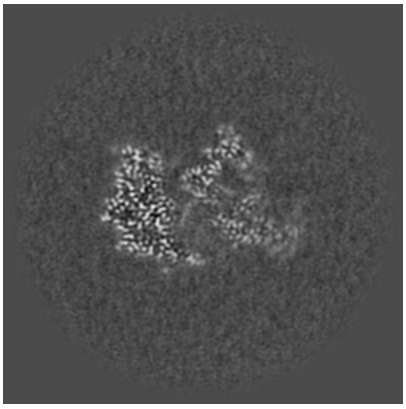
The images above show the map projected in three orthogonal directions.

6.2 Central slices

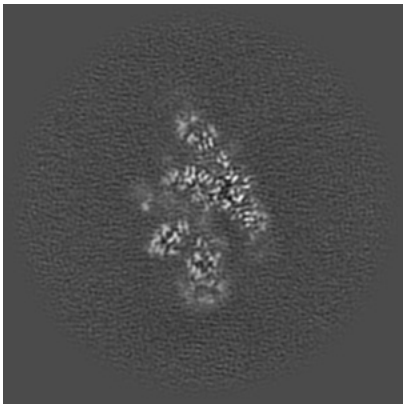
6.2.1 Primary map



X Index: 160



Y Index: 160

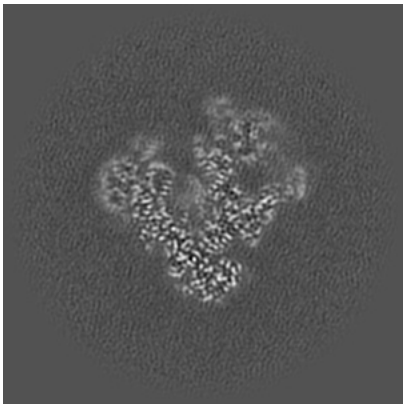


Z Index: 160

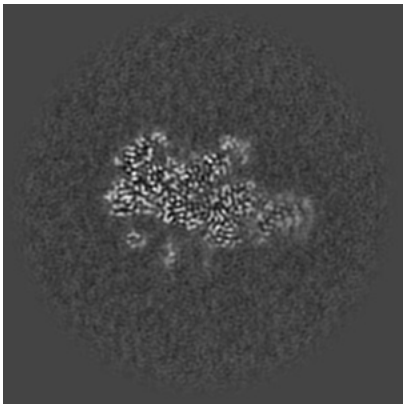
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

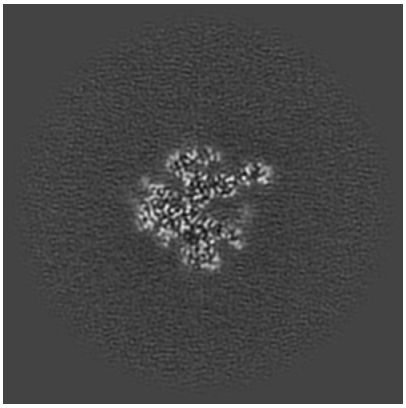
6.3.1 Primary map



X Index: 161



Y Index: 175

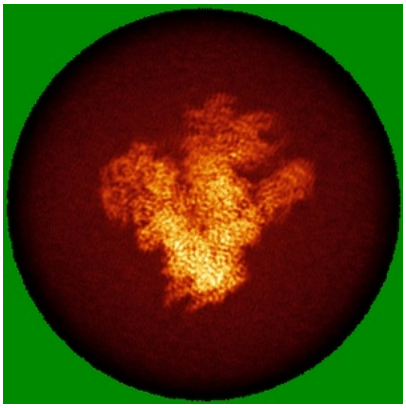


Z Index: 133

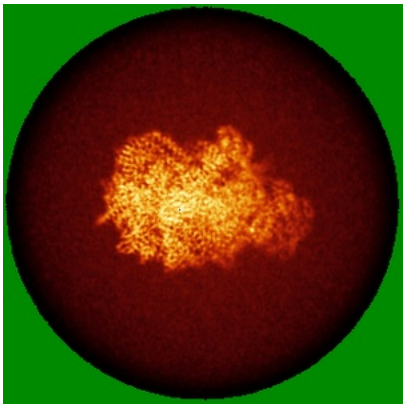
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

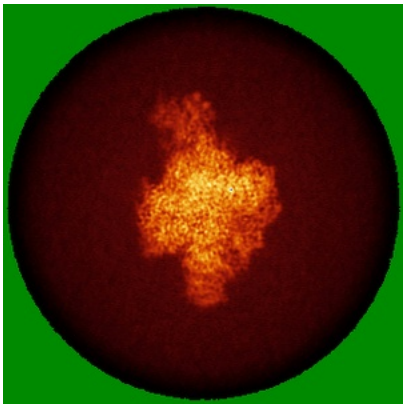
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

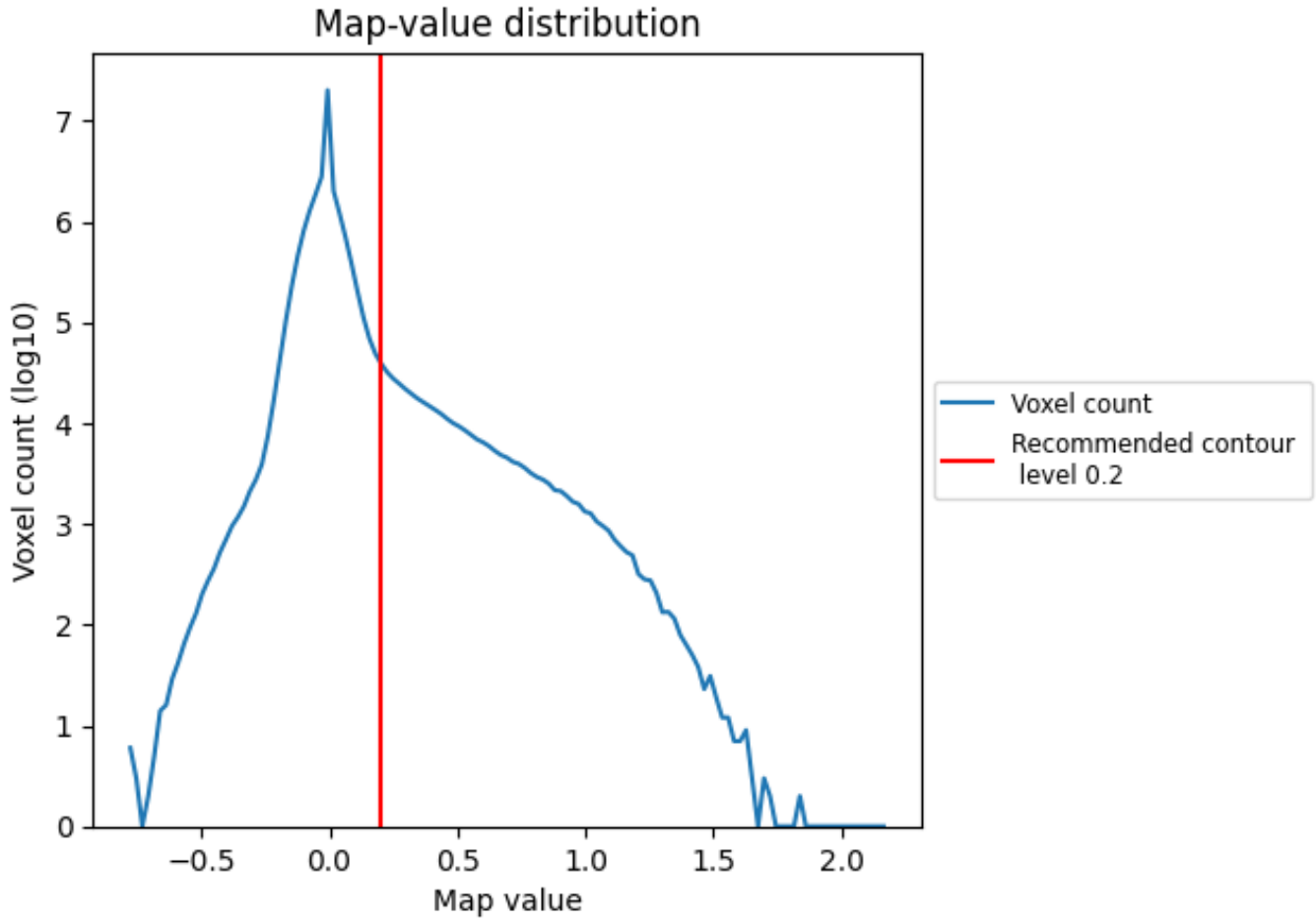
6.6 Mask visualisation (i)

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

7 Map analysis

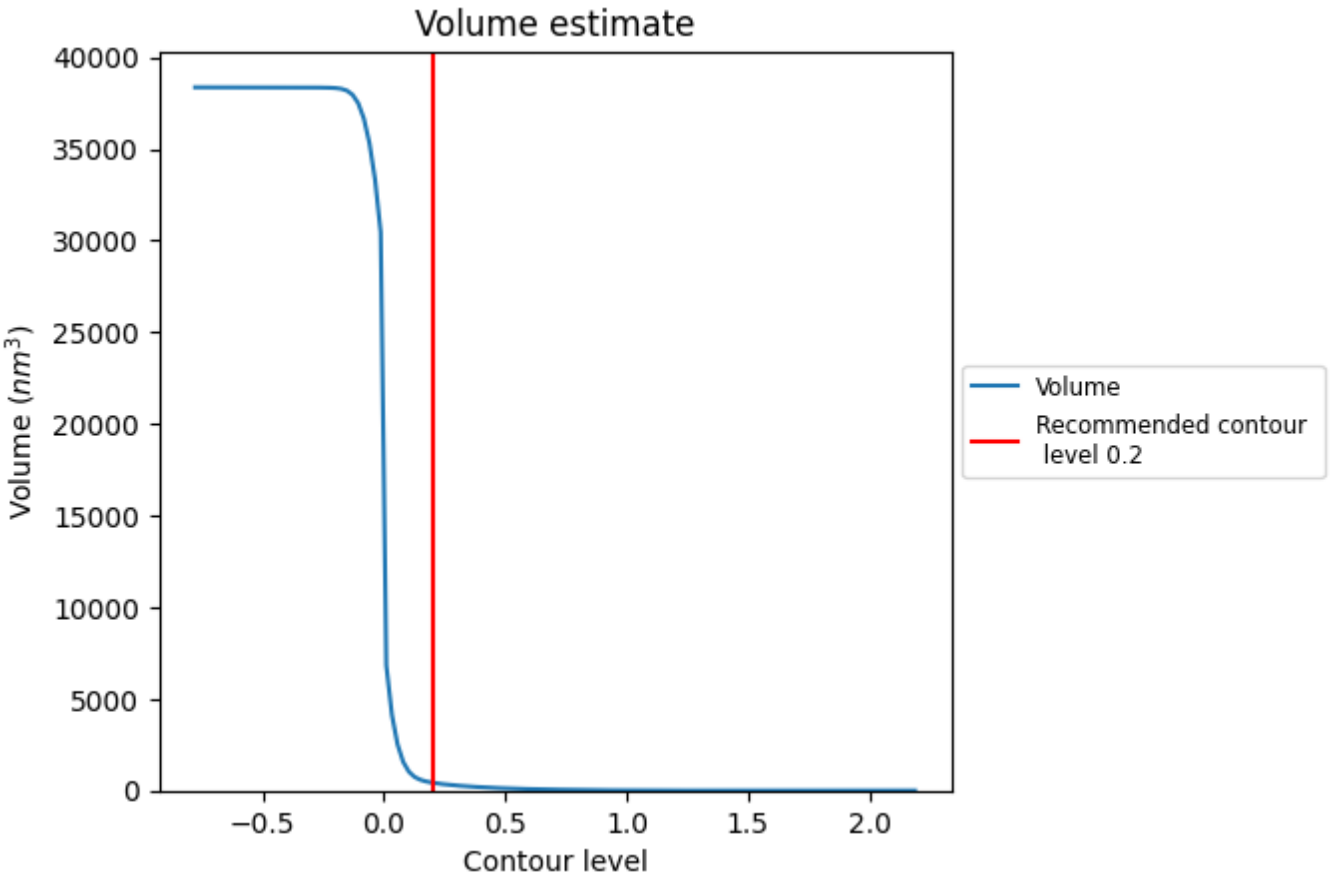
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

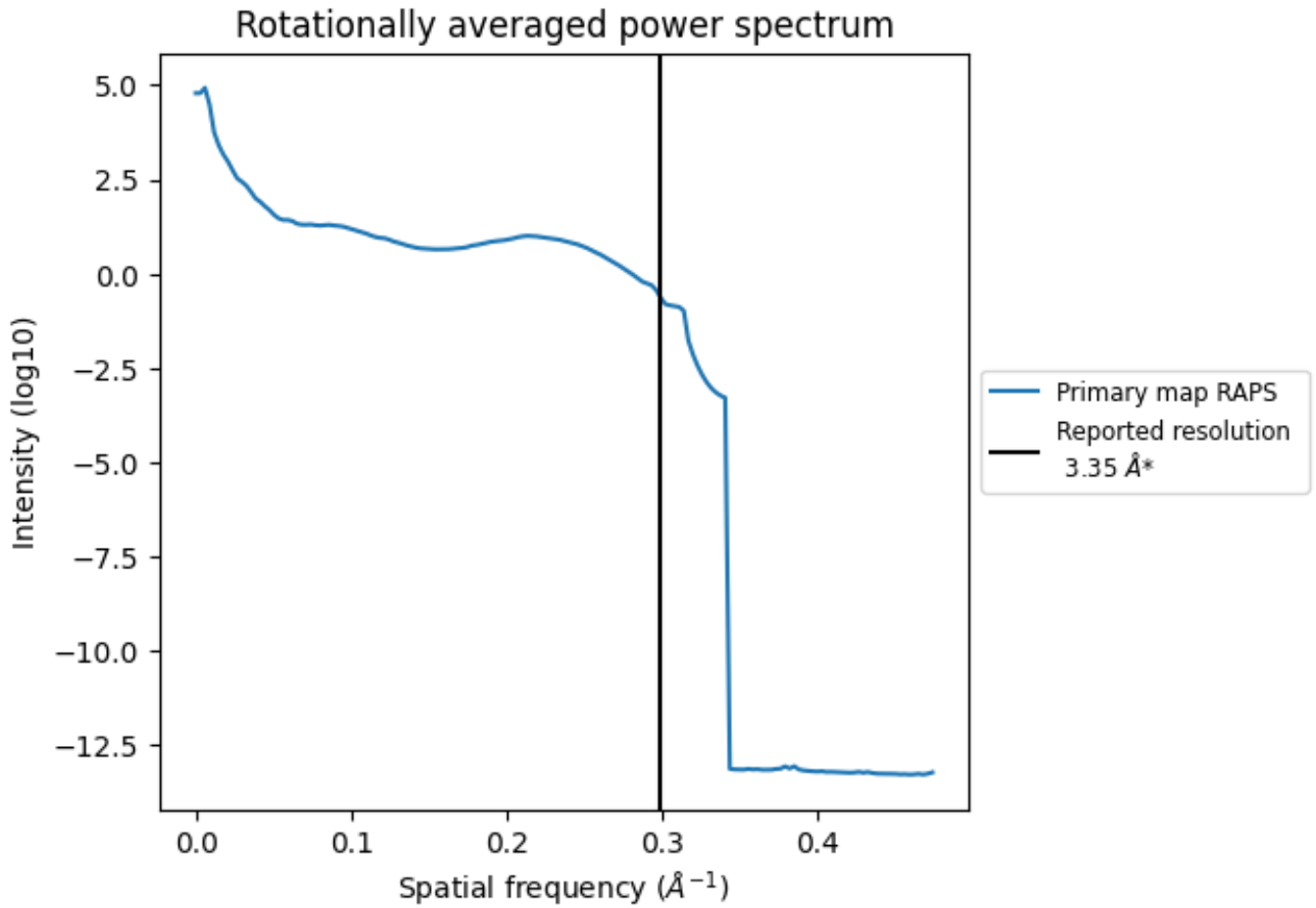
7.2 Volume estimate



The volume at the recommended contour level is 431 nm^3; this corresponds to an approximate mass of 389 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 (i)



*Reported resolution corresponds to spatial frequency of 0.299 $Å^{-1}$

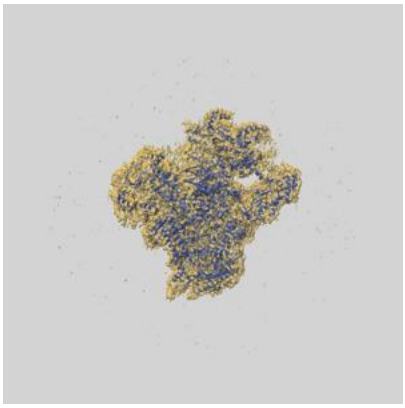
8 Fourier-Shell correlation

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

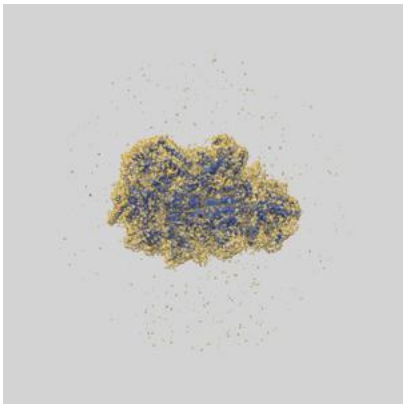
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30865 and PDB model 7DU2. Per-residue inclusion information can be found in section 3 on page 8.

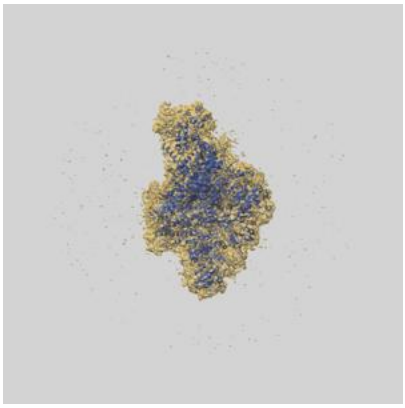
9.1 Map-model overlay



X



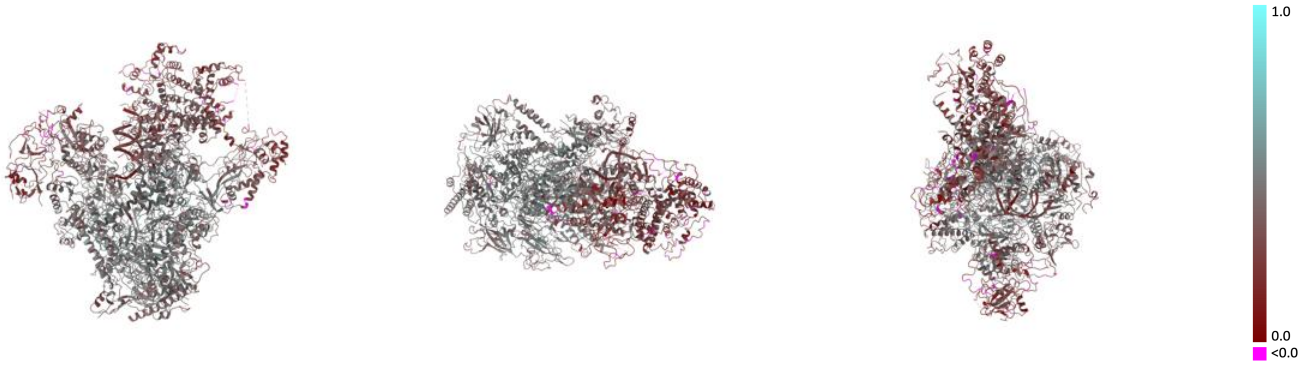
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

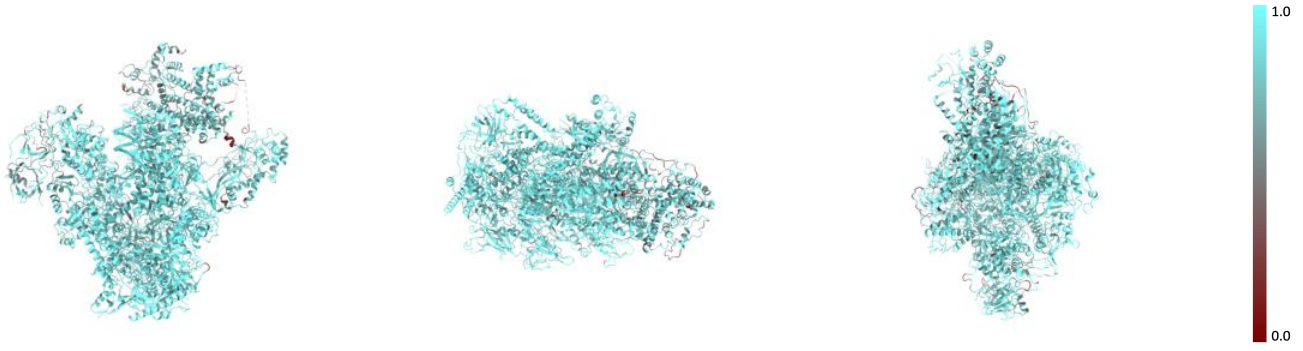
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

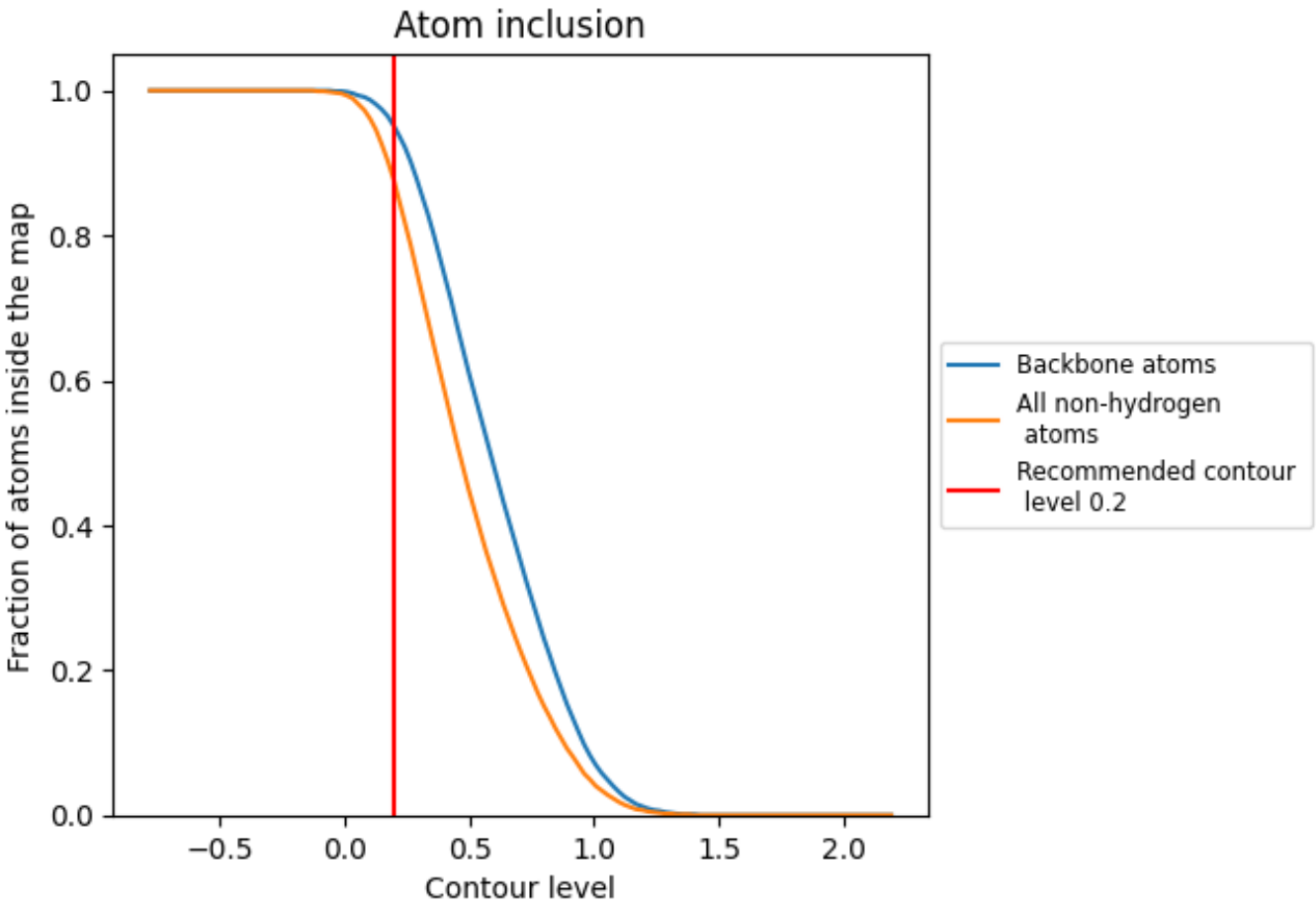
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 87% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8740	0.3890
A	0.9100	0.4470
B	0.9070	0.4500
C	0.9110	0.4230
D	0.8070	0.2150
E	0.9090	0.3820
F	0.9480	0.4800
G	0.8820	0.3320
H	0.9120	0.4300
I	0.8230	0.2920
J	0.9330	0.4620
K	0.9170	0.4210
L	0.9470	0.4200
M	0.7560	0.1990
N	0.7980	0.2740
O	0.7730	0.2850
P	0.6900	0.2070
Q	0.6460	0.2540
R	0.6130	0.2660
X	0.9200	0.2460
Y	0.9340	0.3170