



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 11:17 AM UTC

PDB ID : 7DN3 / pdb_00007dn3
EMDB ID : EMD-30779
Title : Structure of Human RNA Polymerase III elongation complex
Authors : Li, L.; Yu, Z.; Zhao, D.; Ren, Y.; Hou, H.; Xu, Y.
Deposited on : 2020-12-08
Resolution : 3.50 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

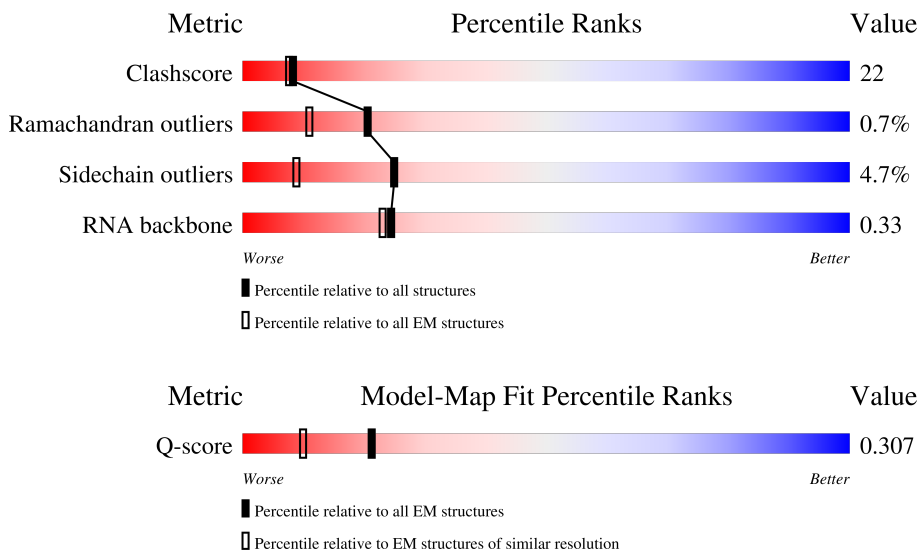
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.50 Å.

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



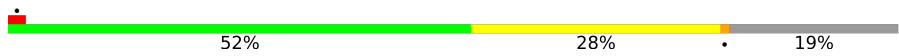
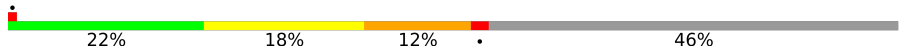
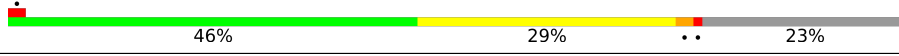





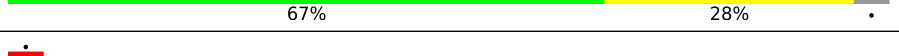
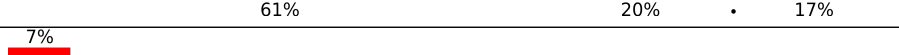
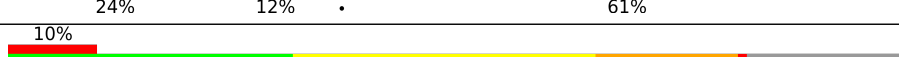
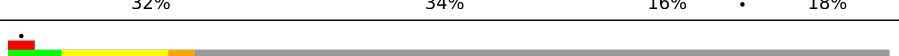

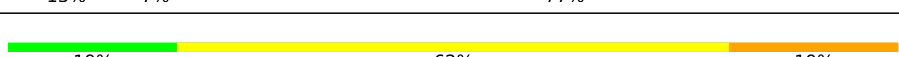
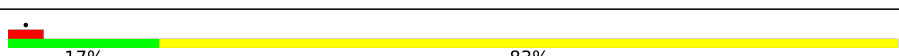
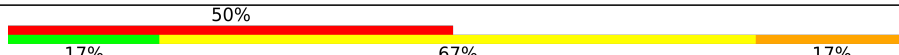

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	A	1390	
2	B	1133	
3	C	346	

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Mol	Chain	Length	Quality of chain
4	G	204	
5	I	108	
6	K	133	
7	L	58	
8	P	316	
9	E	210	
10	F	127	
11	H	150	
12	J	67	
13	O	534	
14	Q	223	
15	D	148	
16	M	708	
17	N	398	
18	X	16	
19	Y	23	
20	R	6	

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 i

There are 23 unique types of molecules in this entry. The entry contains 36856 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 polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	58	393	241	76	71	5	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

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

- Molecule 7 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		
7	L	44	372	231	72	63	6	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerase III subunit RPC6.

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

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC3.

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

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC7.

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

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC9.

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

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC5.

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

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC4.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
18	X	16	327	156	57	98	16	0	0

- Molecule 19 is a DNA chain called DNA (5'-D(P*TP*TP*CP*CP*GP*AP*GP*AP*TP*C P*AP*GP*AP*CP*GP*AP*GP*AP*TP*CP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
19	Y	23	477	225	93	136	23	0	0

- Molecule 20 is a RNA chain called RNA (5'-R(P*CP*CP*CP*GP*AP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
20	R	6	125	56	21	42	6	0	0

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of

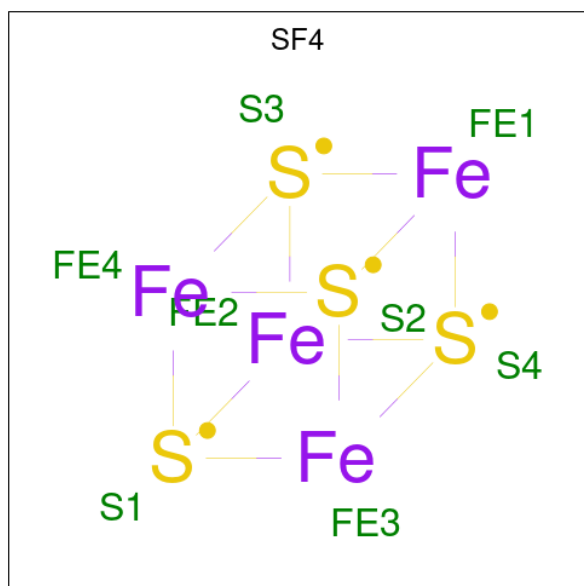
Interest" by depositor).

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

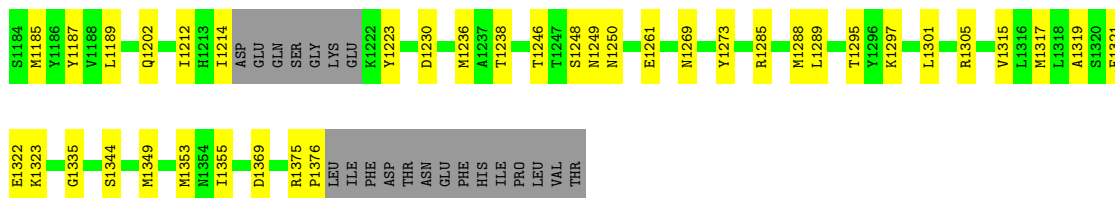
- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

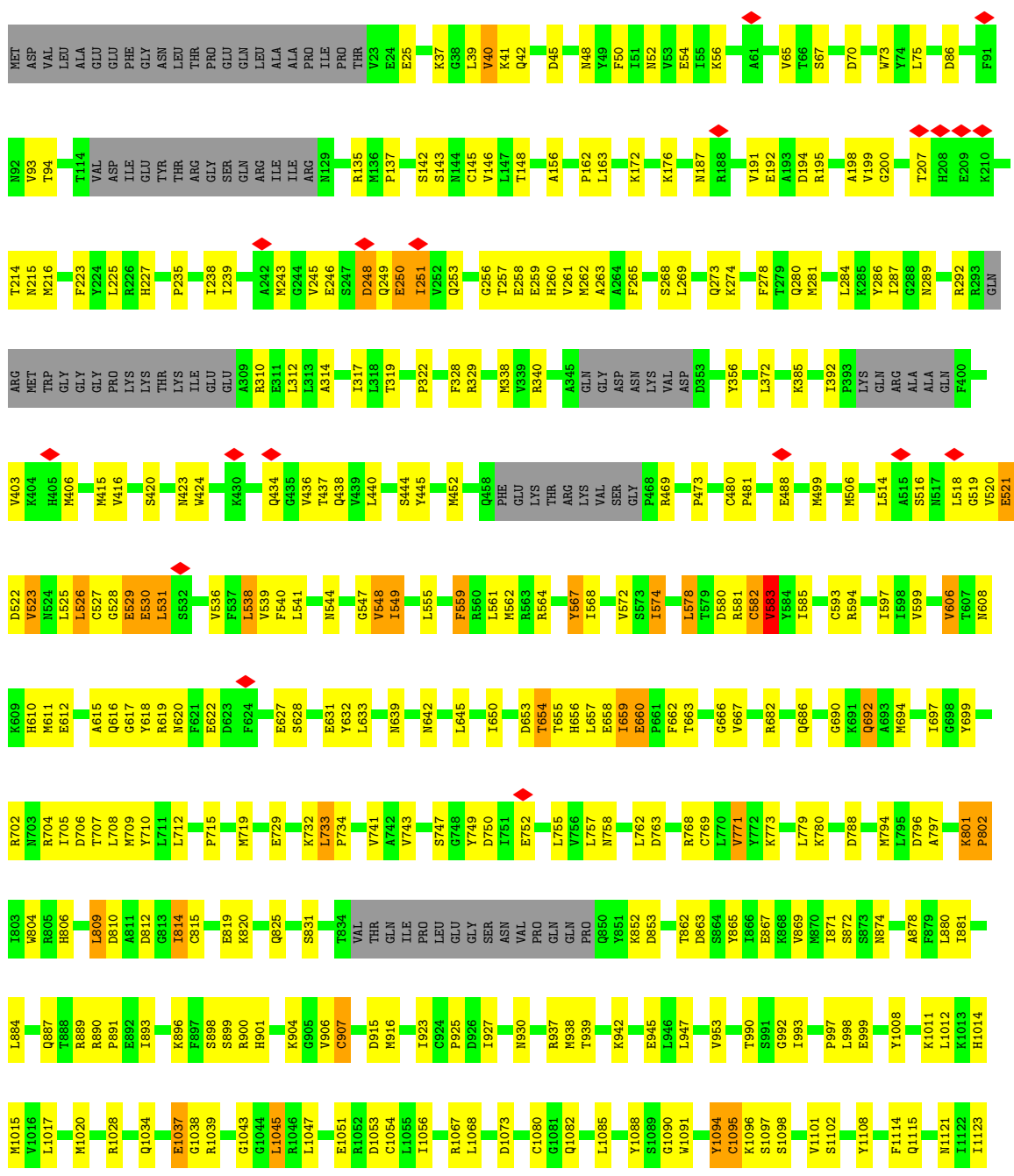
- Molecule 23 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



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



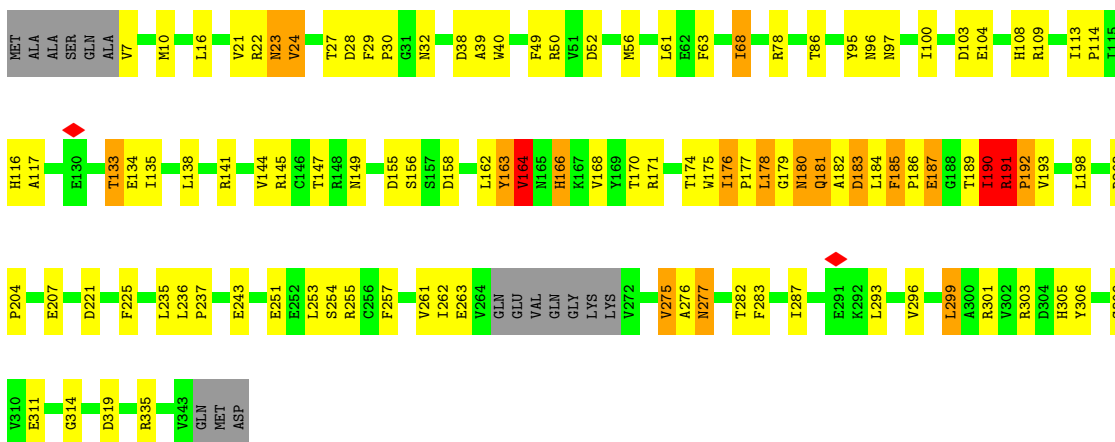
● Molecule 2: DNA-directed RNA polymerase III subunit RPC2





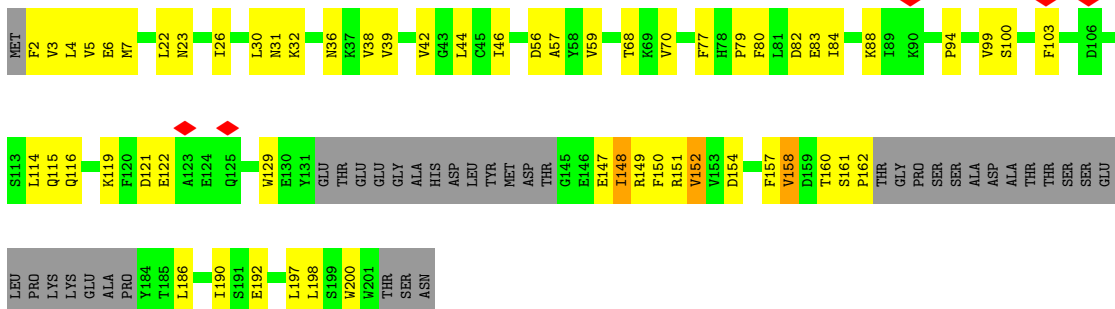
- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 64% 26% 5% 5%



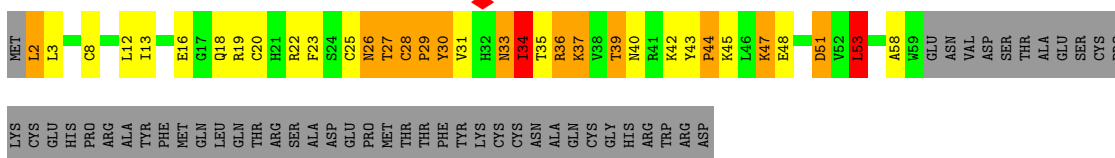
- Molecule 4: DNA-directed RNA polymerase III subunit RPC8

Chain G: 52% 28% 19%



- Molecule 5: DNA-directed RNA polymerase III subunit RPC10

Chain I: 22% 18% 12% 46%

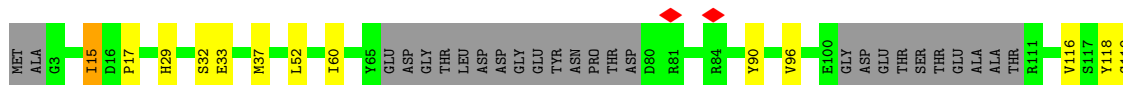


- Molecule 6: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K: 46% 29% 23%



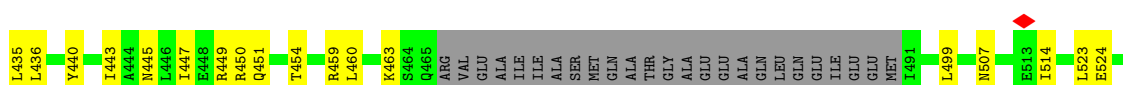
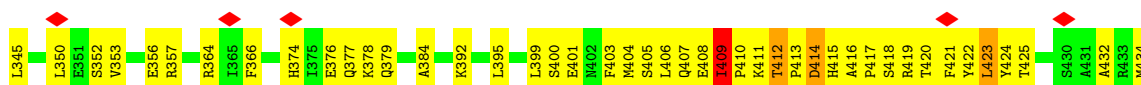
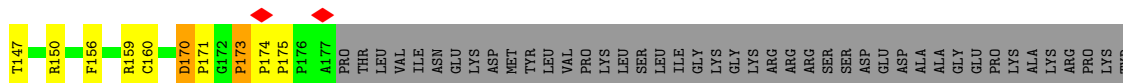
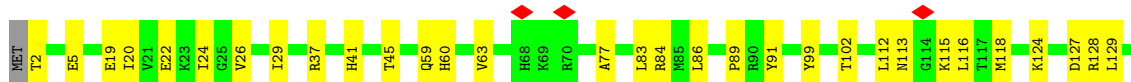
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC5



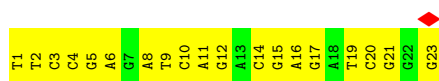
- Molecule 13: DNA-directed RNA polymerase III subunit RPC3



- Molecule 14: DNA-directed RNA polymerase III subunit RPC7

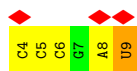


Chain Y:  17% 83%



- Molecule 20: RNA (5'-R(P*CP*CP*CP*GP*AP*U)-3')

Chain R:  17% 50% 67% 17%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98293	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.594	Depositor
Minimum map value	-0.377	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	339.2, 339.2, 339.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0600001, 1.0600001, 1.0600001	Depositor

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.54	0/10329	0.81	8/13920 (0.1%)
2	B	0.64	1/8410 (0.0%)	0.90	11/11338 (0.1%)
3	C	0.64	0/2694	0.93	8/3653 (0.2%)
4	G	0.54	0/1374	0.97	3/1868 (0.2%)
5	I	0.83	1/399 (0.3%)	1.51	9/542 (1.7%)
6	K	0.66	0/837	0.89	1/1129 (0.1%)
7	L	0.56	0/377	0.77	0/500
8	P	0.53	0/1028	0.95	2/1391 (0.1%)
9	E	0.53	0/1616	0.78	2/2180 (0.1%)
10	F	0.56	0/620	0.74	1/839 (0.1%)
11	H	0.57	0/1019	0.81	0/1366
12	J	0.75	0/516	0.86	0/696
13	O	0.41	0/3604	0.75	3/4872 (0.1%)
14	Q	0.61	0/742	0.94	1/996 (0.1%)
15	D	0.85	0/997	1.42	6/1343 (0.4%)
16	M	0.91	1/1301 (0.1%)	1.44	16/1754 (0.9%)
17	N	0.87	0/703	1.46	4/946 (0.4%)
18	X	0.38	0/365	1.09	4/561 (0.7%)
19	Y	0.43	0/536	0.58	0/826
20	R	0.36	0/138	0.68	0/212
All	All	0.60	3/37605 (0.0%)	0.92	79/50932 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	29	PRO	C-O	-6.48	1.18	1.24
2	B	692	GLN	CA-C	-5.53	1.45	1.52
16	M	45	LEU	N-CA	5.31	1.49	1.46

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ARG	N-CA-C	-11.12	99.70	113.38
1	A	55	VAL	N-CA-C	-9.49	104.09	113.20
5	I	58	ALA	N-CA-C	9.15	121.25	111.28
16	M	141	TYR	N-CA-C	-8.76	99.42	112.04
18	X	27	DT	C2'-C3'-O3'	-8.26	99.12	111.50
5	I	29	PRO	CB-CA-C	-8.12	105.05	111.87
16	M	66	ASN	N-CA-C	-7.82	99.71	109.64
18	X	34	DA	C2'-C3'-O3'	-7.71	99.94	111.50
13	O	412	THR	CB-CA-C	7.41	120.23	109.11
16	M	112	SER	N-CA-C	-7.41	103.19	114.16
2	B	41	LYS	N-CA-C	-7.38	104.52	113.97
15	D	58	CYS	N-CA-C	-7.33	104.08	112.87
15	D	10	LEU	N-CA-C	-7.21	101.79	113.19
5	I	44	PRO	N-CA-CB	7.05	110.65	103.25
4	G	148	ILE	CA-C-N	-6.97	113.20	123.11
4	G	148	ILE	C-N-CA	-6.97	113.20	123.11
16	M	137	PRO	N-CA-C	6.96	121.32	110.80
16	M	110	ASN	CA-C-N	-6.95	113.71	123.03
16	M	110	ASN	C-N-CA	-6.95	113.71	123.03
2	B	1039	ARG	N-CA-C	-6.91	103.85	112.90
2	B	317	ILE	N-CA-C	-6.87	105.80	111.91
4	G	158	VAL	N-CA-C	6.81	117.59	110.72
18	X	27	DT	C4'-C3'-O3'	6.72	120.08	110.00
5	I	53	LEU	N-CA-C	6.40	124.44	110.80
17	N	357	LEU	N-CA-C	-6.40	105.46	113.20
16	M	66	ASN	CB-CA-C	6.36	119.56	109.52
2	B	809	LEU	N-CA-C	6.33	118.99	111.71
3	C	182	ALA	N-CA-C	-6.33	105.50	113.72
9	E	8	TYR	N-CA-C	-6.24	105.52	113.01
5	I	47	LYS	N-CA-C	6.16	119.53	107.57
18	X	28	DC	C4'-C3'-O3'	-6.12	100.82	110.00
16	M	135	LEU	N-CA-C	6.11	117.91	109.54
17	N	352	THR	CB-CA-C	-6.02	98.44	110.42
16	M	198	LYS	N-CA-C	-5.99	105.05	112.47
13	O	173	PRO	N-CA-C	5.91	117.91	110.70
2	B	583	VAL	N-CA-C	-5.88	103.64	110.05
2	B	1090	GLY	N-CA-C	5.87	121.26	114.16
10	F	81	VAL	CB-CA-C	-5.83	104.53	111.65
8	P	303	SER	CA-C-N	5.83	125.94	119.87
8	P	303	SER	C-N-CA	5.83	125.94	119.87
16	M	108	THR	CB-CA-C	-5.80	100.91	110.72
17	N	258	LEU	N-CA-C	-5.79	104.97	111.28
17	N	369	ARG	N-CA-C	-5.78	104.98	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	LYS	N-CA-C	-5.75	107.51	114.75
6	K	50	THR	CB-CA-C	-5.75	101.25	110.79
2	B	812	ASP	N-CA-C	-5.73	105.02	113.61
2	B	250	GLU	CB-CA-C	-5.72	101.30	110.79
1	A	307	MET	N-CA-C	-5.69	106.39	113.38
13	O	403	PHE	N-CA-C	-5.66	106.05	113.12
1	A	1135	GLU	N-CA-C	-5.64	105.21	111.36
3	C	191	ARG	CA-C-N	5.61	126.85	119.84
3	C	191	ARG	C-N-CA	5.61	126.85	119.84
1	A	298	ILE	N-CA-C	-5.59	106.86	112.17
14	Q	78	PRO	N-CA-C	-5.59	107.53	114.68
2	B	567	TYR	CB-CA-C	5.59	120.06	110.79
15	D	85	GLN	N-CA-C	-5.56	105.22	111.28
16	M	64	THR	N-CA-C	-5.56	105.11	113.89
15	D	59	ARG	N-CA-C	-5.54	101.65	109.96
16	M	70	CYS	N-CA-C	5.51	117.87	108.67
5	I	26	ASN	CA-CB-CG	-5.46	107.14	112.60
16	M	141	TYR	CA-C-N	-5.42	112.08	120.31
16	M	141	TYR	C-N-CA	-5.42	112.08	120.31
5	I	51	ASP	N-CA-C	5.41	119.62	113.19
15	D	9	ALA	N-CA-C	5.39	117.42	108.20
3	C	177	PRO	N-CA-C	-5.38	102.23	110.95
15	D	19	LEU	N-CA-C	-5.37	105.43	111.28
1	A	1099	ARG	N-CA-C	-5.35	105.11	111.69
2	B	580	ASP	N-CA-C	-5.29	100.27	108.90
2	B	1094	TYR	N-CA-C	-5.29	102.03	109.96
9	E	127	LEU	N-CA-C	5.27	117.61	111.02
16	M	139	PHE	N-CA-C	-5.27	99.58	110.80
3	C	164	VAL	N-CA-C	-5.20	105.65	110.53
3	C	27	THR	CB-CA-C	-5.12	104.32	111.80
1	A	1110	LEU	N-CA-C	-5.11	105.15	111.33
3	C	163	TYR	CA-C-N	-5.09	114.05	120.56
3	C	163	TYR	C-N-CA	-5.09	114.05	120.56
16	M	77	ILE	CB-CA-C	5.04	119.55	111.29
5	I	34	ILE	CA-C-N	-5.00	113.89	121.05
5	I	34	ILE	C-N-CA	-5.00	113.89	121.05

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	345	0
2	B	8254	0	8364	335	0
3	C	2641	0	2615	153	0
4	G	1337	0	1306	112	0
5	I	393	0	339	69	0
6	K	822	0	810	64	0
7	L	372	0	382	20	0
8	P	1008	0	998	67	0
9	E	1590	0	1630	68	0
10	F	610	0	642	3	0
11	H	1002	0	999	11	0
12	J	507	0	524	25	0
13	O	3546	0	3585	148	0
14	Q	724	0	734	47	0
15	D	985	0	1006	126	0
16	M	1272	0	1264	157	0
17	N	697	0	742	70	0
18	X	327	0	182	37	0
19	Y	477	0	258	58	0
20	R	125	0	65	11	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	36856	0	36827	1590	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 22.

All (1590) 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)
18:X:31:DC:C6	18:X:32:DT:H72	1.37	1.55
16:M:31:PRO:HG2	16:M:136:ARG:CD	1.57	1.34
17:N:357:LEU:HD23	17:N:358:GLN:NE2	1.43	1.30
13:O:356:GLU:OE1	14:Q:39:PRO:HD3	1.33	1.29
6:K:40:VAL:CG2	6:K:92:ALA:HB1	1.64	1.27
1:A:484:ARG:HH21	2:B:1017:LEU:CD2	1.48	1.26
3:C:191:ARG:CB	3:C:192:PRO:HD3	1.61	1.25
6:K:40:VAL:HG22	6:K:92:ALA:CB	1.65	1.25
13:O:409:ILE:CG1	13:O:423:LEU:HD11	1.67	1.24
9:E:112:PRO:HB2	19:Y:6:DA:C5'	1.68	1.23
13:O:409:ILE:CD1	13:O:423:LEU:HD11	1.68	1.22
13:O:374:HIS:HB3	13:O:423:LEU:CD1	1.70	1.21
13:O:409:ILE:CG2	13:O:423:LEU:HD21	1.72	1.19
13:O:409:ILE:N	13:O:410:PRO:HD2	1.58	1.18
13:O:410:PRO:HB2	13:O:419:ARG:NH2	1.59	1.16
1:A:483:HIS:CD2	2:B:893:ILE:HB	1.80	1.16
1:A:484:ARG:HH21	2:B:1017:LEU:HD23	0.99	1.15
14:Q:106:LEU:HD12	14:Q:107:PRO:HD2	1.25	1.15
1:A:571:ILE:HD11	1:A:682:ARG:HG2	1.28	1.15
13:O:409:ILE:HG13	13:O:423:LEU:CD1	1.76	1.15
3:C:191:ARG:HG3	3:C:192:PRO:CD	1.76	1.14
13:O:409:ILE:H	13:O:410:PRO:CD	1.60	1.12
18:X:31:DC:C6	18:X:32:DT:C7	2.32	1.13
18:X:31:DC:C5	18:X:32:DT:H72	1.83	1.12
9:E:84:ILE:CD1	18:X:41:DA:H4'	1.78	1.12
4:G:103:PHE:HB3	15:D:48:GLU:HB3	1.25	1.11
9:E:84:ILE:HD12	18:X:41:DA:H4'	1.14	1.11
1:A:29:ARG:HH12	8:P:302:ILE:CD1	1.64	1.10
3:C:191:ARG:HB2	3:C:192:PRO:HD3	1.14	1.10
13:O:410:PRO:CB	13:O:419:ARG:HH21	1.62	1.10
3:C:191:ARG:CG	3:C:192:PRO:HD3	1.81	1.10
13:O:374:HIS:HB3	13:O:423:LEU:HD12	1.18	1.10
17:N:357:LEU:CD2	17:N:358:GLN:NE2	2.14	1.10
1:A:29:ARG:HH12	8:P:302:ILE:HD11	1.04	1.10
1:A:383:PRO:HB3	1:A:483:HIS:O	1.50	1.10
3:C:181:GLN:HE21	3:C:181:GLN:HA	1.03	1.09
2:B:518:LEU:HD21	2:B:555:LEU:HA	1.29	1.09
3:C:116:HIS:CD2	3:C:190:ILE:HD11	1.87	1.09
2:B:692:GLN:HE22	20:R:8:A:H5'	1.15	1.08
3:C:191:ARG:CG	3:C:192:PRO:CD	2.31	1.08
7:L:34:ILE:HD12	7:L:34:ILE:H	1.16	1.08
4:G:148:ILE:HG23	4:G:190:ILE:CG2	1.83	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:11:LEU:HD23	15:D:11:LEU:H	1.19	1.08
16:M:31:PRO:CG	16:M:136:ARG:HD2	1.83	1.08
13:O:352:SER:O	13:O:356:GLU:HG2	1.51	1.07
13:O:410:PRO:HB2	13:O:419:ARG:HH21	0.93	1.07
13:O:409:ILE:CB	13:O:423:LEU:HD21	1.83	1.07
3:C:191:ARG:HG3	3:C:192:PRO:HD2	1.17	1.07
4:G:32:LYS:HZ3	15:D:39:GLN:HG3	1.16	1.06
8:P:284:ARG:HB2	13:O:356:GLU:HG3	1.32	1.06
16:M:32:VAL:HG11	16:M:137:PRO:HD3	1.35	1.06
16:M:140:SER:O	16:M:144:LYS:HG3	1.56	1.06
3:C:170:THR:HB	3:C:192:PRO:HG3	1.36	1.04
8:P:299:GLY:HA2	8:P:303:SER:CB	1.89	1.03
1:A:484:ARG:NH2	2:B:1017:LEU:CD2	2.22	1.02
1:A:481:LYS:HB3	1:A:487:ARG:HH21	1.20	1.02
3:C:191:ARG:CB	3:C:192:PRO:CD	2.36	1.02
9:E:83:GLY:HA3	18:X:41:DA:OP1	1.58	1.01
4:G:148:ILE:HG23	4:G:190:ILE:HG23	1.41	1.01
16:M:116:ALA:HB2	17:N:269:LEU:HB2	1.04	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
4:G:32:LYS:CB	15:D:39:GLN:HG3	1.90	1.00
13:O:409:ILE:HG21	13:O:423:LEU:HD21	1.39	1.00
3:C:116:HIS:CB	3:C:190:ILE:HG13	1.91	0.99
16:M:31:PRO:CG	16:M:136:ARG:CD	2.37	0.99
8:P:304:PRO:HG3	13:O:445:ASN:ND2	1.75	0.99
9:E:84:ILE:HD12	18:X:41:DA:C4'	1.90	0.99
13:O:407:GLN:HB3	13:O:422:TYR:HB3	1.41	0.99
18:X:31:DC:H42	19:Y:12:DG:H1	1.07	0.99
13:O:377:GLN:HB3	13:O:421:PHE:HZ	1.26	0.99
16:M:31:PRO:HG2	16:M:136:ARG:HD2	1.00	0.99
17:N:357:LEU:CD2	17:N:358:GLN:HE22	1.70	0.99
13:O:409:ILE:HG13	13:O:423:LEU:HD11	1.28	0.99
16:M:115:ALA:HB1	16:M:128:PRO:HA	1.44	0.98
1:A:1116:TYR:HB3	5:I:40:ASN:CB	1.92	0.98
4:G:32:LYS:HB3	15:D:39:GLN:CG	1.92	0.98
2:B:599:VAL:HB	2:B:655:THR:O	1.63	0.98
7:L:23:HIS:NE2	12:J:64:PRO:HB2	1.78	0.97
14:Q:27:LEU:HD22	14:Q:27:LEU:H	1.27	0.97
9:E:112:PRO:CB	19:Y:6:DA:H4'	1.94	0.97
19:Y:15:DG:H8	19:Y:15:DG:H5''	1.29	0.97
8:P:300:GLY:H	8:P:303:SER:HB3	1.30	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1099:ARG:CG	1:A:1141:ARG:HB2	1.96	0.96
5:I:20:CYS:SG	5:I:22:ARG:NH1	2.39	0.96
3:C:116:HIS:HB3	3:C:190:ILE:HG13	1.45	0.95
16:M:31:PRO:HG2	16:M:136:ARG:NE	1.81	0.95
4:G:32:LYS:HB3	15:D:39:GLN:HG3	0.99	0.95
13:O:409:ILE:H	13:O:410:PRO:HD2	0.79	0.95
2:B:692:GLN:HE22	20:R:8:A:C5'	1.79	0.95
1:A:1099:ARG:HG2	1:A:1141:ARG:CG	1.95	0.95
3:C:117:ALA:HB2	3:C:189:THR:HG22	1.47	0.95
16:M:116:ALA:HB2	17:N:269:LEU:CB	1.96	0.94
17:N:357:LEU:HD23	17:N:358:GLN:HE22	1.06	0.94
4:G:84:ILE:H	15:D:85:GLN:HE22	1.06	0.94
2:B:312:LEU:HD22	16:M:188:ARG:HG2	1.49	0.94
3:C:299:LEU:H	3:C:299:LEU:HD23	1.30	0.93
8:P:284:ARG:HA	8:P:284:ARG:NE	1.80	0.93
18:X:31:DC:N4	19:Y:12:DG:H1	1.66	0.93
13:O:409:ILE:HD12	13:O:423:LEU:HD11	1.48	0.93
1:A:428:MET:HE3	1:A:428:MET:HA	1.47	0.93
1:A:484:ARG:NH2	2:B:1017:LEU:HD23	1.82	0.93
4:G:32:LYS:HZ3	15:D:39:GLN:CG	1.79	0.93
1:A:456:ASP:HA	1:A:478:ALA:O	1.67	0.93
9:E:112:PRO:HB2	19:Y:6:DA:H5''	1.51	0.92
13:O:409:ILE:HB	13:O:423:LEU:HD21	1.49	0.92
4:G:83:GLU:HA	15:D:85:GLN:NE2	1.83	0.92
2:B:530:GLU:HA	2:B:536:VAL:HG21	1.51	0.92
1:A:481:LYS:HB3	1:A:487:ARG:NH2	1.84	0.92
3:C:170:THR:HB	3:C:192:PRO:CG	1.99	0.92
19:Y:17:DG:C8	19:Y:17:DG:H5''	2.05	0.92
14:Q:106:LEU:HD12	14:Q:107:PRO:CD	2.00	0.91
2:B:802:PRO:HG2	2:B:806:HIS:HD2	1.35	0.91
3:C:134:GLU:HG3	3:C:179:GLY:N	1.86	0.91
19:Y:17:DG:H5''	19:Y:17:DG:H8	1.32	0.91
1:A:481:LYS:HD2	1:A:482:PRO:HD3	1.50	0.91
1:A:1099:ARG:HG2	1:A:1141:ARG:HG2	1.50	0.91
5:I:28:CYS:O	5:I:28:CYS:SG	2.27	0.91
15:D:11:LEU:H	15:D:11:LEU:CD2	1.84	0.91
2:B:692:GLN:NE2	20:R:8:A:H5'	1.84	0.91
2:B:1014:HIS:NE2	20:R:8:A:H4'	1.85	0.90
1:A:1099:ARG:NH1	1:A:1099:ARG:HB2	1.86	0.90
8:P:299:GLY:HA2	8:P:303:SER:HB3	1.51	0.90
15:D:97:ILE:HA	15:D:101:VAL:HB	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:412:THR:HB	13:O:419:ARG:HA	1.50	0.90
15:D:4:LYS:HE2	15:D:4:LYS:HA	1.52	0.89
8:P:284:ARG:HA	8:P:284:ARG:HE	1.34	0.89
15:D:17:PHE:HB2	15:D:53:ILE:HG21	1.53	0.89
16:M:136:ARG:H	16:M:136:ARG:HH21	1.19	0.89
2:B:660:GLU:OE1	2:B:660:GLU:HA	1.70	0.89
2:B:156:ALA:HA	12:J:62:TYR:CE1	2.07	0.88
3:C:181:GLN:HA	3:C:181:GLN:NE2	1.87	0.88
16:M:71:ARG:CZ	16:M:71:ARG:HA	2.03	0.88
1:A:1117:ILE:O	5:I:40:ASN:HA	1.74	0.88
9:E:27:LEU:CD2	9:E:63:ALA:O	2.21	0.88
2:B:801:LYS:HE2	2:B:801:LYS:H	1.39	0.88
1:A:29:ARG:NH1	8:P:302:ILE:HD11	1.88	0.88
4:G:103:PHE:HB3	15:D:48:GLU:CB	2.04	0.87
5:I:27:THR:HB	16:M:69:TYR:HB3	1.56	0.87
14:Q:27:LEU:H	14:Q:27:LEU:CD2	1.87	0.87
5:I:27:THR:HG22	5:I:29:PRO:HD3	1.55	0.87
13:O:407:GLN:O	13:O:410:PRO:HD2	1.73	0.87
1:A:484:ARG:NH2	2:B:1017:LEU:HD21	1.88	0.87
1:A:1099:ARG:HG2	1:A:1141:ARG:HB2	1.55	0.87
1:A:483:HIS:HD2	2:B:893:ILE:HB	1.31	0.87
2:B:801:LYS:H	2:B:801:LYS:CE	1.88	0.86
3:C:113:ILE:CG2	3:C:192:PRO:HB3	2.06	0.86
9:E:27:LEU:HD23	9:E:27:LEU:H	1.40	0.86
5:I:22:ARG:HG2	5:I:29:PRO:HB3	1.58	0.86
3:C:183:ASP:OD1	3:C:183:ASP:N	2.07	0.86
4:G:103:PHE:O	15:D:48:GLU:HB3	1.74	0.86
13:O:407:GLN:O	13:O:410:PRO:CD	2.24	0.86
6:K:40:VAL:HG22	6:K:92:ALA:HB1	0.86	0.86
16:M:31:PRO:CG	16:M:136:ARG:NE	2.39	0.86
1:A:171:LEU:H	1:A:171:LEU:HD23	1.39	0.85
13:O:409:ILE:HG13	13:O:423:LEU:CG	2.06	0.85
15:D:11:LEU:HD23	15:D:11:LEU:N	1.91	0.85
4:G:3:VAL:HA	15:D:11:LEU:HD21	1.58	0.85
13:O:377:GLN:HB3	13:O:421:PHE:CZ	2.10	0.85
16:M:49:ILE:HG23	16:M:54:GLN:HG3	1.56	0.85
18:X:31:DC:N1	18:X:32:DT:H72	1.91	0.85
9:E:112:PRO:HB2	19:Y:6:DA:H5'	1.57	0.85
13:O:374:HIS:CB	13:O:423:LEU:HD12	2.06	0.84
1:A:1099:ARG:HG2	1:A:1141:ARG:CB	2.06	0.84
13:O:415:HIS:O	13:O:419:ARG:HG3	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:58:CYS:HA	15:D:61:GLN:HB2	1.60	0.84
7:L:34:ILE:HD12	7:L:34:ILE:N	1.92	0.83
6:K:86:THR:HG21	6:K:90:LEU:HB2	1.58	0.83
9:E:112:PRO:HB2	19:Y:6:DA:C4'	2.06	0.83
4:G:84:ILE:N	15:D:85:GLN:HE22	1.77	0.83
6:K:64:GLU:HB3	6:K:90:LEU:HD21	1.59	0.83
3:C:181:GLN:HE21	3:C:181:GLN:CA	1.86	0.83
3:C:191:ARG:HB2	3:C:192:PRO:CD	2.00	0.83
2:B:814:ILE:HD13	2:B:814:ILE:N	1.94	0.82
1:A:483:HIS:NE2	2:B:893:ILE:HD12	1.94	0.82
2:B:25:GLU:O	2:B:611:MET:HG2	1.78	0.82
4:G:32:LYS:NZ	15:D:39:GLN:CG	2.43	0.82
4:G:148:ILE:HG23	4:G:190:ILE:HG21	1.60	0.82
3:C:113:ILE:HG21	3:C:192:PRO:HB3	1.61	0.82
9:E:84:ILE:HG13	18:X:41:DA:H5''	1.62	0.82
1:A:568:ILE:O	1:A:571:ILE:HG22	1.79	0.82
1:A:1137:ILE:HD12	1:A:1142:LEU:HD21	1.58	0.82
1:A:383:PRO:CB	1:A:483:HIS:O	2.27	0.82
15:D:43:ASN:H	15:D:43:ASN:HD22	1.25	0.82
1:A:481:LYS:CB	1:A:487:ARG:HH21	1.93	0.81
1:A:785:SER:O	1:A:786:LYS:HD2	1.81	0.81
13:O:409:ILE:HB	13:O:423:LEU:CD2	2.09	0.81
13:O:407:GLN:CB	13:O:422:TYR:HB3	2.11	0.81
2:B:904:LYS:HE3	20:R:9:U:OP1	1.81	0.81
2:B:1091:TRP:HE1	4:G:162:PRO:CD	1.94	0.81
8:P:299:GLY:HA2	8:P:303:SER:HB2	1.61	0.81
6:K:86:THR:HG21	6:K:90:LEU:CB	2.11	0.80
16:M:199:LYS:HB2	16:M:199:LYS:NZ	1.96	0.80
3:C:162:LEU:CD1	3:C:204:PRO:HD3	2.12	0.80
1:A:483:HIS:CE1	2:B:893:ILE:HD12	2.16	0.80
1:A:1099:ARG:HB2	1:A:1099:ARG:CZ	2.07	0.80
4:G:32:LYS:NZ	15:D:39:GLN:HG3	1.97	0.79
1:A:383:PRO:HB3	1:A:484:ARG:HA	1.64	0.79
16:M:116:ALA:CB	17:N:269:LEU:HB2	2.00	0.79
18:X:31:DC:C5	18:X:32:DT:C7	2.63	0.79
5:I:18:GLN:O	5:I:19:ARG:HG2	1.82	0.79
8:P:284:ARG:HB2	13:O:356:GLU:CG	2.13	0.79
16:M:48:LYS:HB2	16:M:57:GLU:HB2	1.65	0.79
19:Y:3:DC:H2''	19:Y:4:DC:C5	2.17	0.79
1:A:500:PHE:CD2	2:B:752:GLU:HB2	2.18	0.79
2:B:256:GLY:HA2	2:B:531:LEU:HD11	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:300:GLY:N	8:P:303:SER:HB3	1.97	0.79
1:A:1099:ARG:HG3	1:A:1141:ARG:HB2	1.63	0.79
3:C:162:LEU:HD11	3:C:203:ARG:HD2	1.65	0.78
4:G:103:PHE:CG	15:D:48:GLU:OE1	2.36	0.78
15:D:10:LEU:HD23	15:D:10:LEU:O	1.84	0.78
2:B:245:VAL:CG2	2:B:250:GLU:HG2	2.14	0.78
1:A:483:HIS:NE2	2:B:893:ILE:CG1	2.47	0.77
5:I:34:ILE:HG13	5:I:36:ARG:HE	1.49	0.77
16:M:136:ARG:HH21	16:M:136:ARG:N	1.80	0.77
2:B:650:ILE:HG23	2:B:654:THR:HG21	1.65	0.77
3:C:185:PHE:HB3	3:C:186:PRO:HD3	1.65	0.77
2:B:1038:GLY:O	2:B:1043:GLY:HA2	1.84	0.77
23:P:401:SF4:S2	13:O:445:ASN:OD1	2.43	0.77
3:C:185:PHE:CB	3:C:186:PRO:CD	2.62	0.77
16:M:115:ALA:CB	16:M:128:PRO:HA	2.15	0.77
2:B:802:PRO:HG2	2:B:806:HIS:CD2	2.19	0.76
16:M:32:VAL:HG11	16:M:137:PRO:CD	2.14	0.76
4:G:32:LYS:HZ3	4:G:32:LYS:HB3	1.49	0.76
4:G:151:ARG:HD2	4:G:151:ARG:O	1.85	0.76
14:Q:82:GLN:CD	15:D:107:ARG:HH21	1.93	0.76
2:B:253:GLN:HB3	2:B:527:CYS:HB2	1.68	0.76
8:P:293:PHE:HE2	8:P:307:CYS:HB2	1.51	0.76
15:D:54:SER:HA	15:D:59:ARG:NH1	2.00	0.75
1:A:483:HIS:CD2	2:B:893:ILE:CB	2.67	0.75
2:B:1091:TRP:HE1	4:G:162:PRO:N	1.84	0.75
9:E:112:PRO:HB2	19:Y:6:DA:H4'	1.64	0.75
18:X:31:DC:N3	19:Y:12:DG:N2	2.32	0.75
1:A:456:ASP:HB2	1:A:479:ARG:HD3	1.69	0.75
2:B:156:ALA:HA	12:J:62:TYR:CD1	2.20	0.75
2:B:530:GLU:HG3	2:B:548:VAL:HG21	1.68	0.75
1:A:465:GLN:HG2	19:Y:19:DT:H2''	1.69	0.75
4:G:103:PHE:O	15:D:48:GLU:CB	2.35	0.75
7:L:35:ARG:HE	7:L:42:ARG:HH21	1.33	0.75
17:N:368:SER:HA	17:N:371:GLY:C	2.12	0.75
17:N:357:LEU:HD23	17:N:358:GLN:HE21	1.52	0.75
1:A:1110:LEU:HD12	1:A:1110:LEU:O	1.87	0.74
9:E:27:LEU:HD23	9:E:63:ALA:O	1.86	0.74
14:Q:27:LEU:HD22	14:Q:27:LEU:N	2.00	0.74
1:A:366:ARG:NH2	19:Y:20:DC:O4'	2.20	0.74
4:G:36:ASN:OD1	15:D:45:ILE:HB	1.85	0.74
6:K:40:VAL:CG2	6:K:92:ALA:CB	2.41	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:PRO:HB3	1:A:419:ASN:HB3	1.70	0.74
4:G:79:PRO:HG2	4:G:150:PHE:CE2	2.23	0.73
2:B:620:ASN:HB3	2:B:622:GLU:OE1	1.88	0.73
17:N:352:THR:HG21	17:N:382:LYS:HB2	1.68	0.73
6:K:86:THR:HB	6:K:90:LEU:HD22	1.69	0.73
1:A:29:ARG:NH1	8:P:302:ILE:CD1	2.46	0.73
3:C:68:ILE:N	3:C:68:ILE:HD12	2.05	0.72
13:O:409:ILE:CG1	13:O:423:LEU:CD1	2.47	0.72
4:G:99:VAL:HG21	4:G:148:ILE:HD11	1.70	0.72
13:O:356:GLU:OE1	14:Q:39:PRO:CD	2.26	0.72
1:A:428:MET:HA	1:A:428:MET:CE	2.19	0.72
1:A:1112:GLU:O	5:I:45:LYS:HA	1.89	0.72
5:I:34:ILE:HG13	5:I:34:ILE:O	1.88	0.72
16:M:56:VAL:HG12	16:M:135:LEU:HD22	1.69	0.72
2:B:526:LEU:HG	17:N:358:GLN:HE21	1.52	0.72
2:B:1091:TRP:HE1	4:G:162:PRO:CG	2.02	0.72
8:P:288:GLY:O	13:O:357:ARG:NH1	2.23	0.72
16:M:136:ARG:NH2	16:M:136:ARG:HB2	2.05	0.72
1:A:1118:GLU:HB3	5:I:39:THR:C	2.14	0.72
16:M:136:ARG:H	16:M:136:ARG:NH2	1.88	0.72
1:A:415:HIS:NE2	1:A:480:VAL:HG21	2.04	0.72
15:D:1:MET:HA	15:D:1:MET:HE2	1.72	0.72
16:M:118:LEU:HD23	16:M:118:LEU:O	1.89	0.72
6:K:86:THR:CG2	6:K:90:LEU:HB2	2.19	0.72
6:K:42:PHE:CZ	6:K:92:ALA:O	2.43	0.71
6:K:42:PHE:HZ	6:K:92:ALA:O	1.73	0.71
1:A:385:HIS:CD2	1:A:484:ARG:NH1	2.57	0.71
19:Y:15:DG:H8	19:Y:15:DG:C5'	2.02	0.71
5:I:3:LEU:HB2	5:I:12:LEU:HD12	1.72	0.71
6:K:86:THR:CB	6:K:90:LEU:HB2	2.20	0.71
2:B:539:VAL:HA	2:B:583:VAL:HG22	1.70	0.71
2:B:608:ASN:ND2	2:B:612:GLU:OE2	2.24	0.71
16:M:15:VAL:HA	16:M:124:LEU:HB2	1.71	0.71
2:B:522:ASP:HB2	2:B:547:GLY:HA2	1.72	0.71
1:A:483:HIS:NE2	2:B:893:ILE:CD1	2.53	0.71
1:A:1133:SER:HB3	1:A:1136:ARG:HG2	1.73	0.70
4:G:151:ARG:HD2	4:G:151:ARG:C	2.16	0.70
13:O:409:ILE:HG21	13:O:423:LEU:CD2	2.18	0.70
15:D:77:LYS:O	15:D:77:LYS:HG3	1.90	0.70
2:B:526:LEU:N	2:B:526:LEU:HD22	2.06	0.70
3:C:116:HIS:CG	3:C:190:ILE:HD11	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:519:GLY:O	2:B:549:ILE:HG23	1.90	0.70
1:A:1323:LYS:N	19:Y:15:DG:OP1	2.24	0.70
7:L:34:ILE:H	7:L:34:ILE:CD1	1.97	0.70
2:B:191:VAL:HA	2:B:199:VAL:HG22	1.74	0.70
16:M:76:GLN:HE21	16:M:76:GLN:HA	1.57	0.70
2:B:801:LYS:CD	2:B:801:LYS:N	2.55	0.69
19:Y:15:DG:H5 ⁺	19:Y:15:DG:C8	2.20	0.69
2:B:594:ARG:NH1	2:B:658:GLU:OE2	2.25	0.69
2:B:801:LYS:N	2:B:801:LYS:HD3	2.07	0.69
16:M:118:LEU:HD23	16:M:118:LEU:C	2.16	0.69
1:A:483:HIS:NE2	2:B:893:ILE:HG13	2.08	0.69
8:P:284:ARG:CB	13:O:356:GLU:HG3	2.18	0.69
15:D:1:MET:O	15:D:1:MET:SD	2.51	0.69
17:N:357:LEU:CD2	17:N:358:GLN:HE21	2.05	0.69
2:B:257:THR:H	2:B:531:LEU:HG	1.57	0.69
2:B:526:LEU:HD22	2:B:526:LEU:H	1.56	0.69
2:B:802:PRO:HD2	2:B:806:HIS:HB2	1.75	0.69
17:N:365:LEU:HD22	17:N:373:MET:HG3	1.75	0.69
3:C:170:THR:O	3:C:191:ARG:CD	2.37	0.69
14:Q:106:LEU:CD1	14:Q:107:PRO:HD2	2.14	0.69
17:N:271:LEU:HG	17:N:272:PRO:HD2	1.75	0.69
2:B:163:LEU:HD11	2:B:732:LYS:HD2	1.74	0.69
2:B:245:VAL:HG23	2:B:250:GLU:HG2	1.75	0.69
2:B:289:ASN:HD21	2:B:310:ARG:HE	1.39	0.69
1:A:464:ARG:NH1	1:A:503:ASP:OD1	2.26	0.68
7:L:23:HIS:NE2	12:J:64:PRO:CB	2.55	0.68
4:G:32:LYS:NZ	15:D:39:GLN:HG2	2.07	0.68
5:I:34:ILE:O	5:I:36:ARG:NE	2.26	0.68
2:B:733:LEU:N	2:B:733:LEU:HD23	2.09	0.68
16:M:30:TYR:HB2	17:N:359:GLU:O	1.93	0.68
1:A:29:ARG:HH22	8:P:302:ILE:HD12	1.58	0.68
1:A:1137:ILE:HG13	1:A:1144:VAL:HG22	1.74	0.68
9:E:41:LYS:HA	9:E:44:SER:HB3	1.76	0.68
9:E:168:ASN:O	9:E:169:GLN:HB3	1.92	0.68
1:A:897:ILE:HD11	9:E:165:LEU:HD11	1.76	0.68
1:A:1214:ILE:HG22	5:I:53:LEU:HA	1.74	0.68
2:B:1038:GLY:O	2:B:1043:GLY:N	2.27	0.68
6:K:90:LEU:HD12	6:K:90:LEU:H	1.59	0.68
2:B:438:GLN:HE22	20:R:6:C:H5 ⁺	1.60	0.67
17:N:368:SER:OG	17:N:373:MET:SD	2.52	0.67
1:A:171:LEU:H	1:A:171:LEU:CD2	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1096:ASP:O	1:A:1099:ARG:HB3	1.93	0.67
2:B:278:PHE:HB3	2:B:284:LEU:HD21	1.77	0.67
13:O:409:ILE:HG13	13:O:423:LEU:HG	1.76	0.67
1:A:1121:PHE:CD2	5:I:37:LYS:HB2	2.29	0.67
1:A:415:HIS:HE2	1:A:480:VAL:HG21	1.59	0.67
1:A:897:ILE:HD12	9:E:165:LEU:HD21	1.76	0.67
3:C:114:PRO:O	3:C:192:PRO:HA	1.94	0.67
13:O:409:ILE:CB	13:O:423:LEU:CD2	2.67	0.67
9:E:197:SER:H	9:E:201:GLY:HA2	1.60	0.67
1:A:785:SER:O	1:A:786:LYS:CD	2.42	0.67
1:A:1121:PHE:O	5:I:36:ARG:NH2	2.28	0.67
2:B:901:HIS:NE2	2:B:945:GLU:OE2	2.27	0.66
2:B:1038:GLY:O	2:B:1043:GLY:CA	2.42	0.66
16:M:71:ARG:HA	16:M:71:ARG:NH1	2.09	0.66
5:I:33:ASN:O	5:I:35:THR:N	2.28	0.66
3:C:21:VAL:HG23	3:C:24:VAL:HG13	1.77	0.66
3:C:185:PHE:CB	3:C:186:PRO:HD3	2.25	0.66
3:C:263:GLU:HB2	3:C:276:ALA:HB2	1.78	0.66
2:B:39:LEU:HD21	2:B:667:VAL:HG11	1.78	0.66
2:B:200:GLY:HA2	2:B:215:ASN:HA	1.77	0.66
17:N:365:LEU:N	17:N:365:LEU:HD23	2.11	0.66
3:C:187:GLU:HG3	3:C:187:GLU:O	1.95	0.66
7:L:35:ARG:HE	7:L:42:ARG:NH2	1.93	0.66
1:A:896:ASP:HA	9:E:169:GLN:HG3	1.77	0.66
8:P:289:LEU:HA	13:O:357:ARG:HG2	1.76	0.66
2:B:1091:TRP:NE1	4:G:162:PRO:N	2.44	0.65
3:C:162:LEU:CD1	3:C:204:PRO:CD	2.75	0.65
8:P:304:PRO:HG3	13:O:445:ASN:HD22	1.59	0.65
16:M:56:VAL:HG11	16:M:135:LEU:HD13	1.77	0.65
1:A:572:LEU:HD13	6:K:83:ARG:HD2	1.79	0.65
4:G:103:PHE:CB	15:D:48:GLU:HB3	2.15	0.65
17:N:346:LEU:HD12	17:N:346:LEU:N	2.12	0.65
16:M:106:GLN:HG3	16:M:133:LEU:HG	1.78	0.65
1:A:43:SER:HB2	1:A:54:GLY:HA3	1.78	0.65
1:A:625:CYS:CB	1:A:632:CYS:SG	2.85	0.65
2:B:574:ILE:HG23	2:B:585:ILE:HG13	1.79	0.65
3:C:299:LEU:H	3:C:299:LEU:CD2	2.06	0.65
2:B:258:GLU:HG3	2:B:260:HIS:HD2	1.62	0.65
2:B:916:MET:HG2	2:B:925:PRO:HD2	1.79	0.65
16:M:206:VAL:HA	17:N:368:SER:HB2	1.79	0.65
5:I:22:ARG:CG	5:I:29:PRO:HB3	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:299:GLY:CA	8:P:303:SER:HB3	2.24	0.65
16:M:27:LEU:HB2	16:M:132:ILE:HG12	1.78	0.65
1:A:1141:ARG:HE	1:A:1141:ARG:HA	1.62	0.65
3:C:277:ASN:N	3:C:277:ASN:OD1	2.30	0.65
1:A:1110:LEU:HD12	1:A:1110:LEU:C	2.20	0.64
16:M:16:TYR:N	16:M:124:LEU:O	2.25	0.64
1:A:33:HIS:CE1	2:B:1088:TYR:HE2	2.15	0.64
1:A:1141:ARG:HA	1:A:1141:ARG:NE	2.10	0.64
2:B:692:GLN:NE2	20:R:8:A:C5'	2.54	0.64
3:C:78:ARG:HD3	6:K:50:THR:HG22	1.80	0.64
15:D:73:LEU:HD13	15:D:83:LYS:HB2	1.78	0.64
1:A:38:SER:HA	14:Q:24:GLY:HA2	1.80	0.64
1:A:869:GLY:HA3	19:Y:17:DG:H1'	1.80	0.64
2:B:499:MET:HE3	2:B:663:THR:HG21	1.80	0.64
14:Q:86:ARG:NH1	14:Q:86:ARG:HB2	2.12	0.64
1:A:474:MET:HE1	1:A:539:ILE:HD11	1.80	0.64
2:B:611:MET:CA	2:B:611:MET:HE2	2.27	0.64
2:B:617:GLY:C	2:B:619:ARG:H	2.05	0.64
14:Q:82:GLN:HG2	15:D:107:ARG:NH2	2.13	0.64
16:M:136:ARG:HH21	16:M:136:ARG:HB2	1.63	0.64
3:C:78:ARG:CD	6:K:50:THR:HG22	2.29	0.63
15:D:43:ASN:H	15:D:43:ASN:ND2	1.96	0.63
16:M:199:LYS:HB2	16:M:199:LYS:HZ2	1.62	0.63
16:M:37:MET:H	16:M:37:MET:HE2	1.62	0.63
16:M:42:ILE:HD12	16:M:42:ILE:O	1.98	0.63
16:M:147:ALA:O	16:M:150:ARG:HB2	1.97	0.63
16:M:205:TRP:O	17:N:368:SER:HB2	1.97	0.63
1:A:45:ASP:HB2	1:A:50:PRO:HD2	1.79	0.63
9:E:84:ILE:HD12	18:X:41:DA:C3'	2.28	0.63
16:M:71:ARG:HH12	16:M:74:GLY:HA3	1.63	0.63
15:D:14:TYR:HD2	15:D:18:GLN:HE21	1.47	0.63
6:K:90:LEU:HD12	6:K:90:LEU:N	2.12	0.63
2:B:214:THR:HG21	2:B:319:THR:H	1.63	0.63
2:B:896:LYS:HD2	2:B:1012:LEU:HD11	1.80	0.63
1:A:1214:ILE:CG2	5:I:53:LEU:HA	2.29	0.63
8:P:293:PHE:CE1	14:Q:31:VAL:HG12	2.33	0.63
6:K:48:ASP:OD2	6:K:48:ASP:N	2.31	0.63
7:L:29:LYS:O	7:L:32:ASP:HB2	1.99	0.63
13:O:412:THR:CB	13:O:419:ARG:HA	2.24	0.63
1:A:1114:SER:HA	1:A:1133:SER:H	1.63	0.62
8:P:199:LYS:NZ	8:P:245:ASP:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:159:ARG:HA	13:O:235:TRP:HB3	1.80	0.62
15:D:2:GLU:H	15:D:2:GLU:CD	2.07	0.62
18:X:27:DT:H6	18:X:27:DT:H3'	1.65	0.62
2:B:521:GLU:HG2	2:B:525:LEU:HD11	1.80	0.62
4:G:79:PRO:CG	4:G:150:PHE:CE2	2.82	0.62
13:O:407:GLN:CG	13:O:422:TYR:HB3	2.29	0.62
2:B:657:LEU:HG	2:B:658:GLU:N	2.14	0.62
1:A:1322:GLU:HG2	19:Y:15:DG:H4'	1.80	0.62
2:B:801:LYS:H	2:B:801:LYS:CD	2.12	0.62
8:P:302:ILE:HG22	8:P:302:ILE:O	2.00	0.62
1:A:467:SER:HG	2:B:1054:CYS:HG	1.47	0.62
1:A:913:GLU:HB2	1:A:917:GLU:O	1.99	0.62
4:G:32:LYS:HZ3	4:G:32:LYS:CB	2.12	0.62
6:K:89:THR:HG22	6:K:89:THR:O	2.00	0.62
8:P:220:ILE:HD11	8:P:271:ARG:HD2	1.80	0.62
8:P:304:PRO:HG3	13:O:445:ASN:HD21	1.64	0.62
16:M:107:THR:O	16:M:107:THR:OG1	2.13	0.62
2:B:245:VAL:HG21	2:B:250:GLU:HG2	1.80	0.62
3:C:116:HIS:CG	3:C:190:ILE:CD1	2.83	0.62
16:M:147:ALA:O	16:M:150:ARG:N	2.32	0.62
3:C:109:ARG:NH2	3:C:198:LEU:O	2.33	0.62
16:M:32:VAL:HG23	16:M:33:ARG:HG2	1.81	0.62
16:M:102:PHE:HD1	16:M:137:PRO:HA	1.64	0.62
2:B:657:LEU:HG	2:B:658:GLU:H	1.65	0.61
3:C:254:SER:HA	3:C:262:ILE:HG21	1.81	0.61
5:I:33:ASN:C	5:I:35:THR:H	2.07	0.61
16:M:33:ARG:HD2	16:M:38:THR:HG21	1.80	0.61
17:N:329:LEU:C	17:N:329:LEU:HD23	2.25	0.61
1:A:353:ARG:NH1	19:Y:16:DA:OP1	2.30	0.61
1:A:303:THR:H	13:O:377:GLN:HE22	1.47	0.61
1:A:465:GLN:OE1	1:A:506:ASN:ND2	2.33	0.61
9:E:27:LEU:HD23	9:E:27:LEU:N	2.14	0.61
9:E:151:MET:HE2	9:E:155:GLU:HB3	1.82	0.61
9:E:83:GLY:CA	18:X:41:DA:OP1	2.43	0.61
16:M:50:LYS:HE2	16:M:55:LYS:HE3	1.81	0.61
16:M:117:ALA:HB2	16:M:127:THR:OG1	2.01	0.61
2:B:526:LEU:H	2:B:526:LEU:CD2	2.14	0.61
4:G:151:ARG:HG3	4:G:152:VAL:HG13	1.82	0.61
14:Q:82:GLN:CG	15:D:107:ARG:HH21	2.12	0.61
15:D:20:LEU:HD11	15:D:46:THR:HB	1.82	0.61
2:B:733:LEU:HG	2:B:733:LEU:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:8:CYS:HG	5:I:25:CYS:HG	1.48	0.61
2:B:804:TRP:HB2	2:B:825:GLN:HE21	1.64	0.61
13:O:91:TYR:OH	13:O:243:HIS:NE2	2.33	0.61
17:N:329:LEU:HD23	17:N:329:LEU:O	2.00	0.60
1:A:385:HIS:CD2	1:A:484:ARG:HH12	2.19	0.60
2:B:862:THR:OG1	2:B:887:GLN:NE2	2.34	0.60
9:E:7:THR:HG22	9:E:7:THR:O	2.01	0.60
1:A:366:ARG:NH2	19:Y:20:DC:C4'	2.64	0.60
1:A:1116:TYR:CD1	5:I:42:LYS:CB	2.84	0.60
2:B:616:GLN:CD	2:B:618:TYR:HB2	2.27	0.60
6:K:64:GLU:CB	6:K:90:LEU:HD21	2.32	0.60
13:O:284:PHE:HA	13:O:338:LEU:HB2	1.83	0.60
15:D:18:GLN:OE1	15:D:18:GLN:HA	2.02	0.60
3:C:185:PHE:HB3	3:C:186:PRO:CD	2.28	0.60
13:O:507:ASN:ND2	14:Q:55:GLU:OE2	2.34	0.60
16:M:75:GLU:HA	16:M:75:GLU:OE2	2.00	0.60
2:B:1037:GLU:O	2:B:1037:GLU:HG2	1.94	0.60
16:M:102:PHE:HA	16:M:138:SER:H	1.66	0.60
17:N:271:LEU:HA	17:N:385:CYS:HB2	1.83	0.60
16:M:31:PRO:CD	16:M:136:ARG:CD	2.79	0.60
17:N:357:LEU:HD21	17:N:358:GLN:NE2	2.14	0.60
13:O:410:PRO:CB	13:O:419:ARG:NH2	2.40	0.60
19:Y:23:DG:C8	19:Y:23:DG:O5'	2.55	0.60
3:C:109:ARG:NH1	12:J:3:ILE:O	2.34	0.60
15:D:110:GLU:OE2	15:D:110:GLU:HA	2.01	0.60
2:B:312:LEU:HD22	16:M:188:ARG:N	2.17	0.59
2:B:899:SER:HB2	2:B:942:LYS:HZ1	1.67	0.59
12:J:56:ILE:O	12:J:60:LEU:HG	2.02	0.59
2:B:526:LEU:HD23	17:N:357:LEU:HD21	1.83	0.59
3:C:97:ASN:ND2	3:C:103:ASP:OD1	2.35	0.59
6:K:90:LEU:H	6:K:90:LEU:CD1	2.15	0.59
14:Q:80:GLU:HA	14:Q:86:ARG:CD	2.33	0.59
16:M:60:MET:HB2	16:M:100:GLN:HB3	1.85	0.59
2:B:704:ARG:NH1	2:B:706:ASP:OD2	2.35	0.59
3:C:116:HIS:CD2	3:C:190:ILE:CD1	2.75	0.59
8:P:304:PRO:CG	13:O:445:ASN:ND2	2.59	0.59
14:Q:113:ARG:HH21	14:Q:117:LYS:HA	1.67	0.59
16:M:69:TYR:HD1	16:M:73:LYS:HE3	1.67	0.59
3:C:262:ILE:HD12	3:C:275:VAL:HA	1.84	0.59
9:E:112:PRO:CB	19:Y:6:DA:C5'	2.62	0.59
14:Q:78:PRO:HG3	15:D:7:ASN:HD22	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1140:LEU:CD2	5:I:48:GLU:H	2.15	0.59
8:P:293:PHE:CE2	8:P:307:CYS:HB2	2.34	0.59
3:C:23:ASN:OD1	3:C:23:ASN:N	2.34	0.59
14:Q:82:GLN:HG2	15:D:107:ARG:HH21	1.66	0.59
15:D:1:MET:O	15:D:1:MET:CG	2.51	0.59
18:X:27:DT:C3'	18:X:27:DT:C6	2.86	0.59
19:Y:23:DG:O5'	19:Y:23:DG:H8	1.86	0.59
1:A:301:ALA:O	13:O:392:LYS:NZ	2.36	0.59
16:M:208:LEU:HA	17:N:373:MET:O	2.03	0.59
1:A:1116:TYR:CE1	5:I:42:LYS:CB	2.86	0.59
2:B:65:VAL:HB	2:B:75:LEU:HB3	1.85	0.59
1:A:1122:LEU:HG	1:A:1123:PRO:HD2	1.85	0.59
2:B:593:CYS:SG	2:B:632:TYR:HB3	2.42	0.59
3:C:162:LEU:HD23	3:C:162:LEU:O	2.03	0.59
2:B:620:ASN:HB3	2:B:622:GLU:CD	2.28	0.59
3:C:50:ARG:NH2	3:C:52:ASP:OD2	2.36	0.59
5:I:18:GLN:C	5:I:19:ARG:HG2	2.28	0.59
15:D:1:MET:HE2	15:D:1:MET:CA	2.32	0.59
3:C:171:ARG:HA	3:C:191:ARG:NE	2.18	0.58
15:D:108:LEU:O	15:D:113:ILE:HG22	2.02	0.58
1:A:742:CYS:SG	1:A:743:THR:N	2.70	0.58
2:B:145:CYS:SG	2:B:146:VAL:N	2.76	0.58
4:G:79:PRO:CG	4:G:150:PHE:CD2	2.86	0.58
8:P:282:LEU:HD22	13:O:356:GLU:OE2	2.03	0.58
1:A:421:ILE:HG13	1:A:432:LEU:HD11	1.84	0.58
2:B:526:LEU:HD11	17:N:358:GLN:HG3	1.83	0.58
3:C:116:HIS:CG	3:C:190:ILE:HG13	2.38	0.58
4:G:3:VAL:HG23	15:D:9:ALA:HB2	1.84	0.58
17:N:268:PHE:HB3	17:N:382:LYS:HA	1.85	0.58
4:G:5:VAL:HG22	15:D:6:ALA:O	2.03	0.58
6:K:83:ARG:HE	6:K:85:GLN:HE21	1.50	0.58
16:M:77:ILE:HD11	16:M:145:ALA:HA	1.85	0.58
1:A:562:ALA:HB2	3:C:29:PHE:CE2	2.38	0.58
1:A:905:ASP:OD2	1:A:1285:ARG:NH2	2.36	0.58
4:G:122:GLU:OE2	4:G:129:TRP:NE1	2.37	0.58
17:N:344:VAL:HG12	17:N:344:VAL:O	2.03	0.58
1:A:23:LYS:HG3	2:B:1123:ILE:HG13	1.86	0.58
15:D:96:GLU:O	15:D:101:VAL:N	2.36	0.58
15:D:102:GLU:N	15:D:102:GLU:CD	2.62	0.58
2:B:616:GLN:HG3	2:B:618:TYR:H	1.67	0.58
9:E:84:ILE:H	18:X:41:DA:H5''	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:17:PHE:HB2	15:D:53:ILE:CG2	2.28	0.58
16:M:65:LEU:C	16:M:65:LEU:HD23	2.28	0.58
1:A:404:LEU:HA	1:A:407:LEU:HG	1.85	0.58
2:B:223:PHE:H	2:B:269:LEU:HD11	1.68	0.58
3:C:162:LEU:HG	3:C:204:PRO:HD3	1.85	0.57
4:G:112:GLU:OE1	4:G:119:LYS:NZ	2.37	0.57
6:K:66:GLU:HG2	6:K:87:ARG:HG2	1.86	0.57
17:N:357:LEU:CD2	17:N:357:LEU:H	2.17	0.57
2:B:750:ASP:OD1	2:B:750:ASP:N	2.36	0.57
2:B:814:ILE:HD13	2:B:814:ILE:H	1.69	0.57
15:D:54:SER:HA	15:D:59:ARG:CZ	2.34	0.57
2:B:530:GLU:H	2:B:530:GLU:CD	2.12	0.57
2:B:810:ASP:CG	2:B:810:ASP:O	2.47	0.57
6:K:86:THR:OG1	6:K:90:LEU:HB2	2.05	0.57
15:D:43:ASN:HD22	15:D:43:ASN:N	2.01	0.57
1:A:419:ASN:N	1:A:419:ASN:OD1	2.37	0.57
2:B:757:LEU:HD23	2:B:762:LEU:HD21	1.85	0.57
16:M:28:PHE:CZ	17:N:365:LEU:HD21	2.39	0.57
1:A:386:VAL:HG23	2:B:1020:MET:HE2	1.85	0.57
2:B:999:GLU:HA	3:C:21:VAL:HG22	1.87	0.57
1:A:483:HIS:CD2	2:B:893:ILE:HD12	2.40	0.57
13:O:364:ARG:NH2	13:O:384:ALA:O	2.35	0.57
13:O:409:ILE:CD1	13:O:423:LEU:CD1	2.63	0.57
1:A:407:LEU:C	1:A:407:LEU:HD12	2.30	0.57
5:I:20:CYS:SG	5:I:22:ARG:HG3	2.44	0.57
13:O:113:ASN:HB2	13:O:116:LEU:HD21	1.86	0.57
4:G:114:LEU:HD21	4:G:192:GLU:H	1.68	0.57
16:M:119:TYR:HD2	17:N:267:LEU:HD12	1.68	0.57
7:L:34:ILE:HG22	7:L:44:MET:SD	2.45	0.57
9:E:112:PRO:CG	19:Y:6:DA:H4'	2.34	0.57
16:M:31:PRO:HD2	16:M:136:ARG:HD3	1.85	0.57
2:B:329:ARG:CG	2:B:523:VAL:HG13	2.35	0.57
2:B:831:SER:HA	2:B:853:ASP:HA	1.86	0.57
9:E:6:GLU:C	9:E:8:TYR:H	2.13	0.57
11:H:32:SER:OG	11:H:33:GLU:N	2.37	0.57
17:N:357:LEU:HD23	17:N:357:LEU:H	1.69	0.57
1:A:407:LEU:O	1:A:417:GLY:HA2	2.04	0.56
1:A:544:ASP:OD2	1:A:544:ASP:C	2.47	0.56
7:L:23:HIS:CD2	12:J:64:PRO:HB2	2.39	0.56
2:B:259:GLU:O	2:B:263:ALA:N	2.31	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)
1:A:899:GLN:NE2	1:A:1288:MET:O	2.38	0.56
1:A:1121:PHE:CG	5:I:37:LYS:CB	2.88	0.56
4:G:99:VAL:CG2	4:G:148:ILE:HD11	2.34	0.56
5:I:2:LEU:O	5:I:2:LEU:HD23	2.05	0.56
13:O:419:ARG:HD2	13:O:422:TYR:CE1	2.39	0.56
16:M:68:ASN:O	16:M:68:ASN:ND2	2.23	0.56
19:Y:23:DG:H1	20:R:4:C:H42	1.54	0.56
1:A:1008:PRO:HA	1:A:1011:VAL:HG12	1.86	0.56
1:A:1138:ARG:O	1:A:1138:ARG:HG2	2.05	0.56
2:B:536:VAL:HG22	2:B:536:VAL:O	2.05	0.56
3:C:16:LEU:O	3:C:299:LEU:HD21	2.05	0.56
1:A:883:CYS:HB3	1:A:1355:ILE:HG23	1.87	0.56
2:B:526:LEU:HG	17:N:358:GLN:HB3	1.85	0.56
4:G:31:ASN:HB3	15:D:42:LEU:HG	1.87	0.56
8:P:309:TYR:OH	14:Q:32:LEU:O	2.24	0.56
1:A:731:LEU:HD13	1:A:748:LEU:HD22	1.86	0.56
1:A:1119:GLU:HA	1:A:1128:ILE:HA	1.87	0.56
2:B:528:GLY:O	2:B:531:LEU:HB2	2.06	0.56
2:B:1091:TRP:CD1	4:G:162:PRO:HA	2.41	0.56
3:C:171:ARG:HA	3:C:191:ARG:CZ	2.36	0.56
3:C:179:GLY:H	3:C:181:GLN:HG2	1.71	0.56
6:K:34:GLY:O	6:K:35:THR:HB	2.06	0.56
8:P:296:CYS:SG	8:P:297:HIS:N	2.79	0.56
17:N:333:LYS:N	17:N:333:LYS:HD3	2.20	0.56
1:A:367:THR:HG22	2:B:1020:MET:HA	1.87	0.56
3:C:162:LEU:HD12	3:C:204:PRO:CD	2.35	0.56
16:M:31:PRO:HD2	16:M:136:ARG:CD	2.35	0.56
3:C:49:PHE:CE1	3:C:68:ILE:HD11	2.41	0.56
3:C:184:LEU:HD12	3:C:184:LEU:N	2.20	0.56
9:E:13:ILE:HD11	9:E:132:GLN:HG3	1.87	0.56
1:A:851:THR:HG21	2:B:481:PRO:HB2	1.88	0.56
1:A:855:ARG:NH2	2:B:481:PRO:O	2.39	0.56
2:B:733:LEU:HD23	2:B:733:LEU:H	1.69	0.56
9:E:112:PRO:HB3	19:Y:6:DA:H4'	1.85	0.56
16:M:22:ALA:HB2	16:M:127:THR:HB	1.87	0.56
16:M:69:TYR:CD2	16:M:69:TYR:N	2.70	0.56
1:A:659:SER:OG	1:A:661:ASN:OD1	2.24	0.55
1:A:1123:PRO:HD3	5:I:34:ILE:HD12	1.87	0.55
1:A:1230:ASP:OD1	1:A:1230:ASP:N	2.40	0.55
4:G:147:GLU:OE1	15:D:100:MET:SD	2.64	0.55
8:P:290:CYS:SG	23:P:401:SF4:S4	3.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:73:LYS:HE2	16:M:98:ASP:OD2	2.05	0.55
19:Y:19:DT:H4'	19:Y:19:DT:OP1	2.06	0.55
15:D:78:LEU:HD13	15:D:86:LEU:HD11	1.86	0.55
16:M:136:ARG:HH21	16:M:136:ARG:CB	2.19	0.55
13:O:410:PRO:HB3	13:O:422:TYR:CE1	2.42	0.55
18:X:27:DT:C6	18:X:27:DT:H5'	2.41	0.55
1:A:791:ASN:ND2	2:B:938:MET:SD	2.73	0.55
1:A:1135:GLU:OE1	1:A:1135:GLU:N	2.39	0.55
2:B:70:ASP:HB2	2:B:392:ILE:HG21	1.89	0.55
6:K:44:LEU:HD12	6:K:80:ILE:HD11	1.87	0.55
1:A:30:GLN:NE2	2:B:1094:TYR:CE1	2.75	0.55
1:A:303:THR:O	1:A:307:MET:HB2	2.06	0.55
2:B:86:ASP:O	2:B:135:ARG:NH2	2.40	0.55
2:B:253:GLN:HB3	2:B:527:CYS:CB	2.36	0.55
3:C:237:PRO:HA	3:C:301:ARG:HA	1.89	0.55
1:A:415:HIS:O	1:A:453:HIS:ND1	2.38	0.55
1:A:1136:ARG:O	1:A:1139:LEU:N	2.39	0.55
1:A:560:ASP:OD2	3:C:32:ASN:ND2	2.40	0.55
2:B:187:ASN:HD21	2:B:322:PRO:HD3	1.70	0.55
3:C:100:ILE:HG21	12:J:60:LEU:HD21	1.89	0.55
3:C:170:THR:CB	3:C:192:PRO:HG3	2.23	0.55
13:O:265:GLU:OE1	13:O:268:ARG:NH1	2.40	0.55
16:M:144:LYS:NZ	16:M:144:LYS:HB3	2.21	0.55
2:B:444:SER:OG	2:B:445:TYR:N	2.40	0.55
2:B:660:GLU:HG3	2:B:662:PHE:CE2	2.41	0.55
3:C:162:LEU:CG	3:C:204:PRO:HD3	2.37	0.55
1:A:351:ARG:HA	1:A:355:ASN:HB2	1.89	0.55
1:A:537:PRO:HG3	1:A:665:TYR:HB2	1.89	0.55
1:A:1140:LEU:HD23	5:I:48:GLU:HA	1.88	0.55
2:B:273:GLN:NE2	2:B:278:PHE:O	2.40	0.55
4:G:154:ASP:OD1	4:G:154:ASP:N	2.39	0.55
8:P:283:VAL:O	8:P:283:VAL:HG13	2.07	0.55
16:M:68:ASN:HD22	16:M:68:ASN:C	2.09	0.55
16:M:111:THR:HG21	16:M:131:GLY:HA2	1.88	0.55
2:B:518:LEU:HD21	2:B:555:LEU:CA	2.21	0.55
2:B:654:THR:O	2:B:655:THR:OG1	2.18	0.55
16:M:108:THR:OG1	16:M:108:THR:O	2.21	0.55
6:K:95:PRO:O	6:K:99:GLY:N	2.40	0.54
15:D:112:GLN:O	15:D:112:GLN:NE2	2.40	0.54
16:M:31:PRO:HG3	16:M:136:ARG:NE	2.20	0.54
1:A:408:VAL:HG21	1:A:421:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:612:GLU:OE1	2:B:612:GLU:HA	2.07	0.54
2:B:656:HIS:ND1	2:B:656:HIS:N	2.55	0.54
16:M:28:PHE:HZ	17:N:365:LEU:HD21	1.72	0.54
16:M:31:PRO:CG	16:M:136:ARG:HE	2.16	0.54
16:M:59:GLU:O	16:M:61:ALA:N	2.39	0.54
1:A:383:PRO:CB	1:A:484:ARG:HA	2.36	0.54
1:A:991:ASP:OD1	1:A:991:ASP:N	2.38	0.54
1:A:1133:SER:HB3	1:A:1136:ARG:CG	2.36	0.54
2:B:578:LEU:N	2:B:578:LEU:HD23	2.23	0.54
2:B:999:GLU:OE1	3:C:24:VAL:HG21	2.07	0.54
3:C:38:ASP:N	3:C:38:ASP:OD1	2.37	0.54
13:O:99:TYR:OH	13:O:150:ARG:NH1	2.40	0.54
17:N:273:ASP:N	17:N:273:ASP:OD1	2.40	0.54
18:X:27:DT:H6	18:X:27:DT:C3'	2.20	0.54
1:A:571:ILE:HG23	1:A:571:ILE:O	2.08	0.54
1:A:630:ASP:N	1:A:630:ASP:OD1	2.40	0.54
1:A:1153:ILE:O	1:A:1156:SER:OG	2.26	0.54
1:A:1212:ILE:CG2	5:I:51:ASP:HA	2.38	0.54
2:B:750:ASP:O	2:B:930:ASN:ND2	2.40	0.54
8:P:290:CYS:HB2	8:P:293:PHE:HB2	1.90	0.54
15:D:4:LYS:HE2	15:D:4:LYS:CA	2.31	0.54
1:A:1121:PHE:CG	5:I:37:LYS:HB3	2.42	0.54
13:O:239:LEU:HA	13:O:242:PHE:HD2	1.73	0.54
16:M:50:LYS:HD2	16:M:204:PRO:HG3	1.89	0.54
1:A:483:HIS:HB2	1:A:487:ARG:NH1	2.22	0.54
1:A:1164:ASP:OD1	1:A:1164:ASP:N	2.40	0.54
8:P:289:LEU:HD13	13:O:357:ARG:HA	1.89	0.54
2:B:356:TYR:OH	2:B:639:ASN:ND2	2.41	0.54
3:C:95:TYR:HE1	7:L:52:LEU:HD12	1.73	0.54
4:G:32:LYS:HE2	15:D:39:GLN:HG2	1.90	0.54
19:Y:15:DG:C5'	19:Y:15:DG:C8	2.85	0.54
1:A:37:VAL:HG11	14:Q:28:PRO:HD3	1.90	0.54
2:B:660:GLU:HG3	2:B:662:PHE:CD2	2.43	0.54
3:C:141:ARG:HB2	3:C:176:ILE:HD11	1.90	0.54
3:C:180:ASN:O	3:C:181:GLN:C	2.51	0.54
3:C:191:ARG:CD	3:C:192:PRO:HD3	2.38	0.54
8:P:227:LYS:O	8:P:240:ASN:ND2	2.41	0.54
16:M:49:ILE:N	16:M:206:VAL:HG21	2.23	0.54
1:A:362:ASP:OD2	2:B:1028:ARG:NH2	2.41	0.54
4:G:32:LYS:CE	15:D:39:GLN:HG2	2.38	0.54
4:G:44:LEU:HB3	4:G:77:PHE:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:268:PHE:HD2	17:N:382:LYS:HG2	1.73	0.54
2:B:1080:CYS:HB3	2:B:1101:VAL:HG22	1.90	0.54
13:O:115:LYS:HE2	13:O:160:CYS:HB2	1.89	0.54
15:D:11:LEU:CD2	15:D:11:LEU:N	2.57	0.54
15:D:14:TYR:CE2	15:D:18:GLN:HG2	2.43	0.54
1:A:760:ARG:HD2	1:A:800:GLY:HA3	1.91	0.53
2:B:523:VAL:HG12	2:B:523:VAL:O	2.09	0.53
15:D:2:GLU:OE1	15:D:2:GLU:N	2.27	0.53
16:M:70:CYS:SG	16:M:71:ARG:N	2.77	0.53
17:N:360:LEU:HB3	17:N:379:VAL:HB	1.90	0.53
2:B:715:PRO:HB2	2:B:734:PRO:HG2	1.89	0.53
3:C:184:LEU:HD12	3:C:184:LEU:H	1.73	0.53
13:O:171:PRO:O	13:O:174:PRO:HD2	2.07	0.53
13:O:374:HIS:HB3	13:O:423:LEU:HD13	1.79	0.53
13:O:412:THR:OG1	13:O:420:THR:HG23	2.08	0.53
14:Q:27:LEU:O	14:Q:28:PRO:C	2.49	0.53
15:D:62:SER:HB2	15:D:65:ILE:HG23	1.89	0.53
1:A:315:LEU:O	1:A:319:LEU:N	2.40	0.53
1:A:482:PRO:CG	6:K:76:SER:HB2	2.38	0.53
2:B:142:SER:OG	2:B:143:SER:N	2.41	0.53
2:B:814:ILE:CD1	2:B:881:ILE:HD13	2.39	0.53
6:K:50:THR:OG1	6:K:51:LEU:N	2.40	0.53
13:O:86:LEU:HD21	13:O:443:ILE:HD13	1.89	0.53
13:O:409:ILE:CG1	13:O:423:LEU:CG	2.84	0.53
1:A:1248:SER:OG	1:A:1249:ASN:N	2.41	0.53
3:C:116:HIS:HB3	3:C:190:ILE:CG1	2.28	0.53
5:I:36:ARG:HA	5:I:36:ARG:CZ	2.38	0.53
16:M:71:ARG:HA	16:M:71:ARG:NE	2.21	0.53
3:C:134:GLU:HG3	3:C:179:GLY:CA	2.38	0.53
9:E:163:TYR:HB3	9:E:165:LEU:HD13	1.91	0.53
16:M:52:LYS:HG3	16:M:53:GLN:OE1	2.08	0.53
19:Y:23:DG:H8	19:Y:23:DG:P	2.31	0.53
1:A:374:ASN:ND2	2:B:749:TYR:OH	2.42	0.53
4:G:32:LYS:HE3	15:D:35:HIS:HD2	1.73	0.53
9:E:116:GLN:NE2	19:Y:6:DA:OP1	2.42	0.53
10:F:107:ARG:NE	10:F:117:ASP:OD1	2.42	0.53
1:A:788:SER:OG	1:A:789:PHE:N	2.38	0.53
2:B:176:LYS:HE3	2:B:420:SER:HA	1.89	0.53
2:B:769:CYS:SG	2:B:1011:LYS:NZ	2.71	0.53
4:G:103:PHE:CB	15:D:48:GLU:OE1	2.57	0.53
5:I:34:ILE:HG13	5:I:36:ARG:NE	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:419:ARG:HD2	13:O:422:TYR:CZ	2.44	0.53
2:B:990:THR:HA	2:B:997:PRO:HA	1.90	0.53
4:G:56:ASP:OD1	4:G:56:ASP:N	2.41	0.53
2:B:872:SER:O	2:B:880:LEU:N	2.42	0.53
6:K:107:CYS:HA	6:K:110:VAL:HG12	1.90	0.53
8:P:286:PRO:HG3	14:Q:38:PHE:CD2	2.44	0.53
1:A:5:GLN:HG3	4:G:36:ASN:O	2.09	0.53
2:B:530:GLU:OE2	2:B:530:GLU:N	2.28	0.53
2:B:794:MET:O	2:B:802:PRO:HD3	2.09	0.53
2:B:1091:TRP:HE1	4:G:162:PRO:HG3	1.74	0.53
3:C:243:GLU:HB3	3:C:296:VAL:HG13	1.91	0.53
6:K:68:CYS:SG	6:K:69:GLY:N	2.81	0.53
8:P:286:PRO:HG2	8:P:313:TRP:CG	2.44	0.53
13:O:376:GLU:HG3	13:O:424:TYR:HB2	1.91	0.53
2:B:245:VAL:HG21	2:B:250:GLU:CG	2.39	0.52
3:C:235:LEU:HD23	3:C:306:TYR:HB3	1.90	0.52
12:J:9:THR:OG1	12:J:44:CYS:SG	2.67	0.52
13:O:407:GLN:O	13:O:410:PRO:CG	2.56	0.52
17:N:333:LYS:HD3	17:N:333:LYS:H	1.74	0.52
19:Y:14:DC:H1'	19:Y:15:DG:C8	2.44	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:852:LYS:NZ	2:B:853:ASP:O	2.39	0.52
2:B:874:ASN:OD1	2:B:874:ASN:N	2.38	0.52
4:G:32:LYS:CB	4:G:32:LYS:NZ	2.72	0.52
5:I:19:ARG:O	5:I:19:ARG:HG3	2.08	0.52
9:E:17:ILE:HA	9:E:20:LEU:HB3	1.90	0.52
13:O:24:ILE:HD11	13:O:45:THR:HG21	1.90	0.52
9:E:112:PRO:CB	19:Y:6:DA:H5''	2.31	0.52
17:N:367:ASP:O	17:N:371:GLY:N	2.43	0.52
1:A:241:ASN:HB3	1:A:1335:GLY:HA3	1.91	0.52
4:G:103:PHE:CG	15:D:48:GLU:CD	2.88	0.52
1:A:415:HIS:CE1	1:A:480:VAL:HG21	2.44	0.52
2:B:162:PRO:HD2	2:B:699:TYR:HD2	1.75	0.52
14:Q:82:GLN:OE1	15:D:107:ARG:NH2	2.39	0.52
17:N:269:LEU:HD22	17:N:385:CYS:SG	2.50	0.52
1:A:7:ARG:NH1	1:A:8:GLU:O	2.43	0.52
3:C:68:ILE:HD12	3:C:68:ILE:H	1.75	0.52
9:E:84:ILE:CG1	18:X:41:DA:H5''	2.38	0.52
10:F:73:ILE:HD11	10:F:79:VAL:HG13	1.92	0.52
16:M:79:LEU:HD22	16:M:98:ASP:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:PRO:HG2	6:K:76:SER:HB2	1.90	0.52
1:A:874:ARG:NH1	1:A:1075:ASN:OD1	2.40	0.52
1:A:897:ILE:HD12	9:E:165:LEU:CD2	2.39	0.52
3:C:117:ALA:CB	3:C:189:THR:HG22	2.29	0.52
3:C:134:GLU:CG	3:C:178:LEU:HB3	2.39	0.52
3:C:237:PRO:HB3	3:C:283:PHE:HE2	1.75	0.52
9:E:168:ASN:O	9:E:169:GLN:CB	2.58	0.52
12:J:33:ASP:OD1	12:J:33:ASP:N	2.41	0.52
15:D:43:ASN:ND2	15:D:43:ASN:N	2.57	0.52
17:N:349:THR:O	17:N:349:THR:OG1	2.27	0.52
2:B:1091:TRP:HA	2:B:1101:VAL:HG21	1.92	0.52
1:A:109:CYS:SG	1:A:111:THR:OG1	2.61	0.52
1:A:10:ASP:OD1	1:A:10:ASP:N	2.41	0.52
2:B:612:GLU:O	2:B:615:ALA:HB3	2.09	0.52
2:B:1045:LEU:HB2	19:Y:20:DC:OP1	2.10	0.52
9:E:15:LYS:HE3	9:E:34:ASP:HA	1.92	0.52
15:D:57:PRO:C	15:D:59:ARG:N	2.64	0.52
16:M:16:TYR:HA	17:N:326:VAL:HG22	1.92	0.52
1:A:1185:MET:HA	5:I:16:GLU:OE2	2.10	0.51
2:B:526:LEU:N	2:B:526:LEU:CD2	2.73	0.51
2:B:898:SER:HA	2:B:904:LYS:HA	1.92	0.51
14:Q:80:GLU:HA	14:Q:86:ARG:HD3	1.92	0.51
17:N:266:LEU:O	17:N:380:LYS:HB2	2.10	0.51
1:A:1118:GLU:CB	5:I:39:THR:C	2.83	0.51
2:B:608:ASN:C	2:B:608:ASN:HD22	2.15	0.51
2:B:992:GLY:O	3:C:78:ARG:NH2	2.42	0.51
3:C:39:ALA:HB1	6:K:63:PRO:HG3	1.91	0.51
4:G:32:LYS:CE	15:D:39:GLN:CG	2.87	0.51
13:O:440:TYR:OH	13:O:524:GLU:OE2	2.28	0.51
18:X:34:DA:H2 ⁺	18:X:35:DT:H72	1.92	0.51
2:B:705:ILE:HG23	2:B:884:LEU:HD13	1.92	0.51
2:B:937:ARG:HB3	2:B:939:THR:HG23	1.93	0.51
13:O:118:MET:SD	14:Q:108:ARG:NH2	2.74	0.51
15:D:59:ARG:NE	15:D:59:ARG:H	2.07	0.51
16:M:65:LEU:HD23	16:M:65:LEU:O	2.10	0.51
1:A:340:GLY:N	1:A:343:GLN:OE1	2.41	0.51
1:A:1170:GLU:H	1:A:1172:VAL:HG12	1.75	0.51
2:B:741:VAL:HG12	2:B:927:ILE:HB	1.93	0.51
3:C:24:VAL:O	3:C:303:ARG:NH1	2.42	0.51
4:G:7:MET:HE3	15:D:1:MET:SD	2.51	0.51
13:O:450:ARG:O	13:O:454:THR:OG1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:460:LEU:HB3	13:O:499:LEU:HD11	1.92	0.51
16:M:15:VAL:O	17:N:327:GLY:N	2.43	0.51
1:A:6:PHE:HE2	4:G:157:PHE:CD2	2.28	0.51
1:A:22:MET:O	2:B:1125:ARG:NH2	2.42	0.51
2:B:516:SER:O	16:M:113:ARG:NH1	2.43	0.51
2:B:871:ILE:HG12	2:B:881:ILE:HG12	1.91	0.51
6:K:64:GLU:HB3	6:K:90:LEU:CD2	2.37	0.51
8:P:202:PRO:O	8:P:205:GLN:NE2	2.37	0.51
16:M:31:PRO:CD	16:M:136:ARG:HD2	2.36	0.51
1:A:307:MET:HE2	1:A:307:MET:O	2.11	0.51
1:A:543:GLN:HG2	1:A:786:LYS:HD3	1.93	0.51
2:B:538:LEU:HB3	2:B:548:VAL:HG22	1.93	0.51
1:A:1118:GLU:HG3	5:I:39:THR:H	1.76	0.51
1:A:1121:PHE:O	5:I:36:ARG:NH1	2.43	0.51
1:A:1261:GLU:OE1	9:E:195:ARG:NH1	2.40	0.51
1:A:1375:ARG:NH1	1:A:1376:PRO:O	2.43	0.51
2:B:1034:GLN:NE2	2:B:1073:ASP:OD2	2.44	0.51
9:E:6:GLU:O	9:E:9:ARG:HG3	2.10	0.51
12:J:44:CYS:SG	12:J:45:CYS:N	2.84	0.51
13:O:37:ARG:O	13:O:41:HIS:ND1	2.39	0.51
15:D:42:LEU:HD13	15:D:42:LEU:C	2.35	0.51
18:X:27:DT:H3'	18:X:27:DT:C6	2.46	0.51
1:A:456:ASP:HB2	1:A:479:ARG:CD	2.39	0.51
1:A:571:ILE:O	1:A:571:ILE:HG13	2.10	0.51
2:B:1014:HIS:NE2	20:R:8:A:C4'	2.67	0.51
4:G:32:LYS:HG2	15:D:39:GLN:HB2	1.93	0.51
4:G:99:VAL:HG11	4:G:148:ILE:HG12	1.91	0.51
6:K:86:THR:HG21	6:K:90:LEU:HB3	1.91	0.51
8:P:286:PRO:HA	14:Q:38:PHE:HD2	1.75	0.51
18:X:37:DT:H2''	18:X:38:DC:C5	2.45	0.51
1:A:43:SER:HB3	1:A:51:LEU:HD12	1.93	0.51
1:A:469:HIS:CD2	1:A:471:LEU:HB2	2.46	0.51
2:B:889:ARG:NH1	2:B:1015:MET:SD	2.81	0.51
3:C:40:TRP:HB2	6:K:61:LYS:HB3	1.93	0.51
3:C:163:TYR:CD1	3:C:166:HIS:HB3	2.45	0.51
13:O:407:GLN:N	13:O:407:GLN:CD	2.69	0.51
2:B:763:ASP:OD1	2:B:890:ARG:NH1	2.40	0.51
1:A:1140:LEU:HD21	5:I:48:GLU:H	1.75	0.50
2:B:694:MET:HE3	2:B:710:TYR:HB3	1.92	0.50
3:C:113:ILE:CG2	3:C:192:PRO:CB	2.85	0.50
3:C:221:ASP:OD2	7:L:58:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:308:ILE:HD13	14:Q:31:VAL:HG11	1.93	0.50
9:E:80:PRO:HA	9:E:107:GLN:HB2	1.92	0.50
13:O:127:ASP:HB3	13:O:128:ARG:HH11	1.75	0.50
1:A:385:HIS:HD2	1:A:484:ARG:NH1	2.08	0.50
1:A:465:GLN:HG2	19:Y:19:DT:C2'	2.40	0.50
1:A:811:ASP:OD1	1:A:811:ASP:N	2.44	0.50
1:A:1181:SER:OG	1:A:1182:LYS:N	2.42	0.50
2:B:40:VAL:HG12	2:B:40:VAL:O	2.11	0.50
2:B:853:ASP:N	2:B:853:ASP:OD1	2.43	0.50
4:G:103:PHE:CD2	15:D:48:GLU:OE1	2.63	0.50
5:I:33:ASN:C	5:I:35:THR:N	2.65	0.50
8:P:252:ILE:HG23	8:P:257:GLU:HB3	1.93	0.50
13:O:436:LEU:HB2	13:O:523:LEU:HD22	1.93	0.50
3:C:144:VAL:HG21	3:C:168:VAL:HG13	1.93	0.50
16:M:110:ASN:OD1	16:M:110:ASN:N	2.45	0.50
1:A:812:GLY:HA3	2:B:473:PRO:HG2	1.93	0.50
2:B:246:GLU:OE1	2:B:281:MET:N	2.42	0.50
2:B:768:ARG:NH2	7:L:58:ARG:O	2.44	0.50
8:P:286:PRO:HG2	8:P:313:TRP:CD2	2.47	0.50
1:A:466:PRO:HB3	19:Y:17:DG:N2	2.26	0.50
1:A:625:CYS:HB3	1:A:632:CYS:SG	2.51	0.50
2:B:559:PHE:HB3	2:B:574:ILE:HG13	1.93	0.50
3:C:309:SER:O	3:C:309:SER:OG	2.29	0.50
5:I:2:LEU:O	5:I:2:LEU:CG	2.59	0.50
5:I:30:TYR:C	5:I:30:TYR:CD2	2.90	0.50
9:E:84:ILE:HD11	18:X:41:DA:H4'	1.86	0.50
15:D:41:ASN:OD1	15:D:41:ASN:N	2.30	0.50
2:B:686:GLN:O	2:B:690:GLY:N	2.37	0.50
5:I:34:ILE:O	5:I:35:THR:C	2.51	0.50
6:K:45:HIS:O	6:K:47:GLU:HG3	2.12	0.50
13:O:5:GLU:HG3	13:O:83:LEU:HD11	1.92	0.50
16:M:121:GLN:HG2	17:N:259:SER:HA	1.93	0.50
1:A:554:LEU:HD23	1:A:556:ASP:H	1.77	0.50
1:A:914:GLY:O	1:A:915:LYS:HB3	2.12	0.50
2:B:258:GLU:HG3	2:B:260:HIS:CD2	2.44	0.50
2:B:329:ARG:HG2	2:B:523:VAL:HG13	1.93	0.50
13:O:410:PRO:HB3	13:O:422:TYR:CD1	2.47	0.50
13:O:460:LEU:HA	13:O:463:LYS:HG2	1.94	0.50
1:A:894:THR:OG1	1:A:896:ASP:OD1	2.27	0.50
3:C:170:THR:HB	3:C:192:PRO:HG2	1.89	0.50
4:G:115:GLN:NE2	4:G:192:GLU:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:30:TYR:C	5:I:30:TYR:HD2	2.20	0.50
11:H:118:TYR:HB2	11:H:121:LEU:HB2	1.94	0.50
15:D:105:GLU:CD	15:D:105:GLU:H	2.19	0.50
3:C:299:LEU:HD23	3:C:299:LEU:N	2.11	0.49
16:M:33:ARG:HB3	16:M:38:THR:HB	1.93	0.49
16:M:199:LYS:HB2	16:M:199:LYS:HZ3	1.75	0.49
1:A:360:ARG:NH1	19:Y:20:DC:OP2	2.44	0.49
1:A:410:ASN:HB3	1:A:414:VAL:HB	1.93	0.49
1:A:1092:ASP:HB2	1:A:1223:TYR:H	1.78	0.49
2:B:567:TYR:N	2:B:567:TYR:CD1	2.80	0.49
2:B:1098:SER:O	2:B:1098:SER:OG	2.30	0.49
4:G:84:ILE:HD11	4:G:149:ARG:HH21	1.77	0.49
5:I:19:ARG:HE	5:I:33:ASN:HA	1.77	0.49
13:O:405:SER:HB3	13:O:425:THR:O	2.12	0.49
1:A:1369:ASP:OD1	1:A:1369:ASP:N	2.45	0.49
2:B:372:LEU:HD22	2:B:424:TRP:HZ3	1.78	0.49
3:C:283:PHE:HE1	3:C:299:LEU:HD12	1.78	0.49
4:G:3:VAL:CA	15:D:11:LEU:HD21	2.37	0.49
8:P:219:TYR:HD2	8:P:271:ARG:HB3	1.78	0.49
13:O:84:ARG:NH2	13:O:524:GLU:OE1	2.46	0.49
2:B:697:ILE:HD12	2:B:709:MET:HG3	1.93	0.49
4:G:39:VAL:HB	4:G:42:VAL:HB	1.94	0.49
15:D:58:CYS:CA	15:D:61:GLN:HB2	2.39	0.49
1:A:87:ASP:O	1:A:290:ASN:ND2	2.42	0.49
2:B:907:CYS:O	2:B:907:CYS:SG	2.70	0.49
3:C:104:GLU:O	3:C:108:HIS:N	2.44	0.49
3:C:133:THR:HG23	3:C:135:ILE:HG22	1.94	0.49
4:G:80:PHE:HZ	15:D:85:GLN:HG2	1.77	0.49
8:P:220:ILE:CD1	8:P:271:ARG:HD2	2.43	0.49
16:M:105:SER:HB2	16:M:136:ARG:HH12	1.76	0.49
17:N:355:SER:O	17:N:356:PHE:HB2	2.11	0.49
1:A:1349:MET:HE1	2:B:1114:PHE:HZ	1.78	0.49
2:B:67:SER:OG	2:B:73:TRP:NE1	2.39	0.49
13:O:409:ILE:HD12	13:O:423:LEU:CD1	2.32	0.49
16:M:49:ILE:HG12	16:M:56:VAL:HG23	1.95	0.49
2:B:993:ILE:HG23	6:K:49:HIS:CG	2.48	0.49
13:O:414:ASP:OD1	13:O:414:ASP:N	2.44	0.49
13:O:416:ALA:HA	13:O:422:TYR:OH	2.13	0.49
14:Q:72:PRO:HA	14:Q:75:ILE:HG22	1.95	0.49
18:X:33:DG:N2	19:Y:11:DA:C2	2.81	0.49
1:A:544:ASP:HA	1:A:547:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:733:LEU:N	2:B:733:LEU:CD2	2.75	0.49
3:C:189:THR:O	3:C:191:ARG:N	2.45	0.49
5:I:2:LEU:O	5:I:2:LEU:HG	2.13	0.49
13:O:60:HIS:NE2	13:O:112:LEU:O	2.45	0.49
19:Y:17:DG:C8	19:Y:17:DG:C5'	2.88	0.49
2:B:514:LEU:HD11	2:B:562:MET:HG3	1.95	0.49
3:C:185:PHE:HB2	3:C:186:PRO:CD	2.42	0.49
16:M:76:GLN:HE21	16:M:76:GLN:CA	2.25	0.49
17:N:357:LEU:HD23	17:N:357:LEU:N	2.27	0.49
1:A:884:SER:O	1:A:1030:GLY:N	2.38	0.48
2:B:245:VAL:CG2	2:B:250:GLU:CG	2.89	0.48
2:B:292:ARG:NH1	2:B:314:ALA:O	2.45	0.48
2:B:593:CYS:SG	2:B:594:ARG:N	2.86	0.48
2:B:1053:ASP:HA	2:B:1056:ILE:HD12	1.94	0.48
3:C:133:THR:O	3:C:133:THR:OG1	2.30	0.48
6:K:86:THR:CB	6:K:90:LEU:HD22	2.42	0.48
9:E:9:ARG:C	9:E:11:TRP:N	2.70	0.48
2:B:611:MET:HE2	2:B:611:MET:N	2.28	0.48
2:B:900:ARG:HD2	2:B:1008:TYR:HB3	1.95	0.48
3:C:253:LEU:HD12	3:C:293:LEU:HD13	1.96	0.48
3:C:335:ARG:NH2	6:K:47:GLU:OE2	2.44	0.48
7:L:23:HIS:NE2	12:J:64:PRO:CG	2.76	0.48
8:P:286:PRO:HA	14:Q:38:PHE:CD2	2.48	0.48
13:O:378:LYS:HD2	13:O:379:GLN:HE21	1.77	0.48
16:M:207:HIS:HB2	17:N:372:GLU:HG2	1.95	0.48
1:A:481:LYS:CB	1:A:487:ARG:NH2	2.63	0.48
1:A:949:THR:HG21	1:A:973:ILE:HG21	1.95	0.48
2:B:269:LEU:O	2:B:273:GLN:N	2.35	0.48
2:B:747:SER:O	2:B:747:SER:OG	2.31	0.48
2:B:771:VAL:HG13	2:B:887:GLN:HB3	1.94	0.48
2:B:156:ALA:CA	12:J:62:TYR:CE1	2.88	0.48
13:O:22:GLU:O	13:O:26:VAL:N	2.40	0.48
14:Q:57:MET:O	14:Q:61:LYS:N	2.38	0.48
16:M:68:ASN:O	16:M:70:CYS:N	2.39	0.48
16:M:203:GLU:O	16:M:205:TRP:N	2.47	0.48
1:A:258:PRO:HD2	1:A:283:LEU:HD11	1.95	0.48
1:A:372:ASP:HB2	1:A:487:ARG:HB3	1.95	0.48
1:A:1136:ARG:NH1	5:I:47:LYS:HA	2.28	0.48
2:B:40:VAL:HG22	2:B:452:MET:HB3	1.95	0.48
2:B:469:ARG:NH2	2:B:488:GLU:O	2.39	0.48
3:C:134:GLU:OE2	3:C:181:GLN:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:115:ALA:HB1	16:M:128:PRO:CA	2.30	0.48
16:M:194:GLU:CD	16:M:194:GLU:H	2.21	0.48
1:A:131:ARG:HD3	1:A:132:PRO:HD2	1.95	0.48
1:A:1353:MET:HE1	2:B:1056:ILE:HG12	1.96	0.48
2:B:42:GLN:HA	2:B:45:ASP:OD1	2.14	0.48
2:B:250:GLU:HA	2:B:250:GLU:OE1	2.13	0.48
2:B:403:VAL:HA	2:B:406:MET:HE1	1.96	0.48
23:P:401:SF4:S2	13:O:445:ASN:CG	2.97	0.48
12:J:7:CYS:HB3	12:J:11:GLY:H	1.78	0.48
13:O:156:PHE:HA	13:O:241:ARG:HG2	1.96	0.48
14:Q:78:PRO:HG3	15:D:7:ASN:ND2	2.29	0.48
15:D:61:GLN:NE2	15:D:61:GLN:HA	2.28	0.48
19:Y:17:DG:H8	19:Y:17:DG:C5'	2.15	0.48
2:B:480:CYS:SG	2:B:666:GLY:N	2.84	0.48
2:B:1080:CYS:HA	2:B:1101:VAL:HA	1.96	0.48
4:G:7:MET:HE3	15:D:1:MET:HE1	1.96	0.48
4:G:161:SER:HB2	4:G:162:PRO:CD	2.43	0.48
5:I:18:GLN:O	5:I:19:ARG:CG	2.58	0.48
9:E:7:THR:C	9:E:9:ARG:H	2.21	0.48
13:O:531:MET:HE3	13:O:531:MET:HB2	1.76	0.48
1:A:224:LEU:HD23	1:A:228:LYS:HD2	1.96	0.48
2:B:611:MET:CA	2:B:611:MET:CE	2.84	0.48
16:M:46:SER:HB2	16:M:59:GLU:HB2	1.95	0.48
16:M:146:ASP:HA	16:M:149:HIS:CD2	2.49	0.48
1:A:1369:ASP:OD1	4:G:23:ASN:ND2	2.47	0.48
5:I:31:VAL:O	5:I:31:VAL:HG12	2.13	0.48
11:H:32:SER:HB3	11:H:37:MET:H	1.79	0.48
1:A:572:LEU:CD1	6:K:83:ARG:HD2	2.44	0.48
1:A:583:LEU:HD23	6:K:67:PHE:HD1	1.78	0.48
1:A:1212:ILE:HG21	5:I:51:ASP:HA	1.95	0.48
4:G:151:ARG:NH1	4:G:152:VAL:HG12	2.29	0.48
9:E:82:VAL:HG23	9:E:86:THR:HB	1.96	0.48
16:M:34:PRO:HB3	17:N:357:LEU:O	2.13	0.48
16:M:37:MET:HE2	16:M:37:MET:N	2.28	0.48
1:A:30:GLN:NE2	2:B:1094:TYR:HE1	2.12	0.47
2:B:616:GLN:CD	2:B:618:TYR:CB	2.87	0.47
3:C:180:ASN:OD1	3:C:180:ASN:N	2.37	0.47
7:L:19:CYS:HB2	7:L:23:HIS:H	1.78	0.47
13:O:400:SER:OG	13:O:401:GLU:OE1	2.31	0.47
1:A:86:ILE:HD12	1:A:287:ILE:HG12	1.95	0.47
1:A:1145:ASN:H	1:A:1148:THR:HG1	1.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:59:GLN:NE2	13:O:113:ASN:O	2.42	0.47
16:M:17:LEU:H	16:M:17:LEU:HD23	1.79	0.47
16:M:38:THR:O	17:N:359:GLU:HG3	2.14	0.47
16:M:50:LYS:HD3	16:M:55:LYS:HB2	1.94	0.47
1:A:383:PRO:HG2	1:A:386:VAL:HB	1.97	0.47
3:C:116:HIS:HB2	3:C:190:ILE:HG13	1.89	0.47
15:D:32:LYS:HD3	15:D:32:LYS:H	1.80	0.47
15:D:52:TYR:O	15:D:55:LYS:HB2	2.15	0.47
2:B:280:GLN:HG2	16:M:142:LEU:HB3	1.96	0.47
2:B:617:GLY:C	2:B:619:ARG:N	2.70	0.47
2:B:653:ASP:CG	2:B:653:ASP:O	2.53	0.47
2:B:729:GLU:HG2	2:B:732:LYS:HE2	1.96	0.47
3:C:116:HIS:CG	3:C:190:ILE:CG1	2.97	0.47
13:O:20:ILE:HD11	14:Q:68:MET:HG3	1.95	0.47
16:M:48:LYS:N	16:M:57:GLU:O	2.44	0.47
19:Y:21:DG:O5'	19:Y:21:DG:H8	1.96	0.47
3:C:162:LEU:HD11	3:C:203:ARG:CD	2.38	0.47
4:G:161:SER:HB2	4:G:162:PRO:HD3	1.97	0.47
9:E:7:THR:C	9:E:9:ARG:N	2.69	0.47
15:D:102:GLU:N	15:D:102:GLU:OE2	2.40	0.47
16:M:32:VAL:C	16:M:34:PRO:HD3	2.40	0.47
1:A:585:PRO:O	1:A:599:GLN:NE2	2.45	0.47
1:A:897:ILE:CD1	9:E:165:LEU:HD21	2.44	0.47
1:A:1116:TYR:O	1:A:1131:LYS:NZ	2.35	0.47
2:B:516:SER:HA	2:B:520:VAL:HG22	1.96	0.47
3:C:162:LEU:HD11	3:C:204:PRO:HD3	1.96	0.47
5:I:29:PRO:HG2	5:I:29:PRO:O	2.14	0.47
11:H:96:VAL:HG12	11:H:116:VAL:HG22	1.95	0.47
18:X:36:DC:H2'	18:X:37:DT:H71	1.96	0.47
1:A:171:LEU:HD23	1:A:171:LEU:N	2.17	0.47
1:A:631:LEU:HD13	11:H:124:ARG:HD3	1.97	0.47
1:A:1118:GLU:HB2	5:I:39:THR:HB	1.96	0.47
2:B:274:LYS:HD2	5:I:13:ILE:HD11	1.95	0.47
2:B:438:GLN:NE2	20:R:6:C:H5'	2.27	0.47
2:B:809:LEU:O	2:B:810:ASP:HB3	2.15	0.47
4:G:4:LEU:HD22	15:D:11:LEU:HD22	1.96	0.47
7:L:23:HIS:CE1	12:J:64:PRO:HG2	2.49	0.47
9:E:12:LYS:NZ	9:E:136:LEU:O	2.42	0.47
13:O:170:ASP:O	13:O:173:PRO:HD2	2.15	0.47
16:M:197:GLN:C	16:M:199:LYS:N	2.67	0.47
1:A:659:SER:O	1:A:662:ASN:ND2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1297:LYS:HB3	1:A:1301:LEU:HD11	1.96	0.47
3:C:30:PRO:HG3	3:C:39:ALA:HA	1.97	0.47
9:E:19:GLN:OE1	9:E:138:ASN:ND2	2.48	0.47
9:E:27:LEU:HD22	9:E:63:ALA:O	2.13	0.47
9:E:84:ILE:HD12	18:X:41:DA:O3'	2.15	0.47
3:C:145:ARG:HH11	3:C:207:GLU:HG3	1.79	0.47
4:G:160:THR:CG2	4:G:160:THR:O	2.63	0.47
8:P:289:LEU:CD1	13:O:357:ARG:HA	2.44	0.47
8:P:308:ILE:HD13	14:Q:31:VAL:CG1	2.45	0.47
9:E:6:GLU:C	9:E:8:TYR:N	2.73	0.47
2:B:514:LEU:HD13	2:B:568:ILE:HD11	1.96	0.47
6:K:30:VAL:CG1	6:K:35:THR:HA	2.44	0.47
16:M:30:TYR:O	17:N:358:GLN:HB2	2.13	0.47
16:M:68:ASN:C	16:M:70:CYS:N	2.73	0.47
18:X:40:DG:H2''	18:X:41:DA:C8	2.50	0.47
1:A:225:ASN:OD1	1:A:225:ASN:N	2.34	0.46
2:B:251:ILE:HD13	2:B:251:ILE:N	2.29	0.46
2:B:286:TYR:OH	16:M:150:ARG:NH2	2.48	0.46
1:A:1122:LEU:HA	5:I:36:ARG:HH22	1.80	0.46
2:B:657:LEU:CG	2:B:658:GLU:H	2.26	0.46
2:B:814:ILE:HD11	2:B:881:ILE:HD13	1.96	0.46
2:B:863:ASP:OD1	2:B:863:ASP:N	2.47	0.46
2:B:1082:GLN:NE2	2:B:1095:CYS:SG	2.88	0.46
6:K:67:PHE:HB3	6:K:85:GLN:HB2	1.98	0.46
9:E:14:ARG:HG2	9:E:18:MET:HE2	1.97	0.46
13:O:412:THR:CG2	13:O:413:PRO:HD2	2.45	0.46
16:M:140:SER:HA	16:M:143:ASP:HB2	1.96	0.46
3:C:162:LEU:HD11	3:C:204:PRO:CD	2.45	0.46
3:C:174:THR:OG1	3:C:175:TRP:N	2.45	0.46
4:G:26:ILE:HG21	4:G:70:VAL:HG21	1.98	0.46
13:O:406:LEU:N	13:O:406:LEU:HD23	2.30	0.46
16:M:70:CYS:O	16:M:73:LYS:HB2	2.15	0.46
1:A:48:HIS:O	1:A:48:HIS:CD2	2.69	0.46
1:A:625:CYS:SG	1:A:632:CYS:SG	3.07	0.46
1:A:941:SER:HB3	1:A:980:ILE:HD13	1.98	0.46
3:C:299:LEU:CD2	3:C:299:LEU:N	2.77	0.46
14:Q:81:ARG:HE	14:Q:84:ILE:HD11	1.81	0.46
2:B:619:ARG:HH21	2:B:627:GLU:HG3	1.80	0.46
2:B:657:LEU:CG	2:B:658:GLU:N	2.78	0.46
3:C:96:ASN:OD1	3:C:96:ASN:N	2.49	0.46
4:G:80:PHE:CE2	4:G:82:ASP:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:222:GLU:O	8:P:226:SER:OG	2.27	0.46
1:A:465:GLN:NE2	2:B:1051:GLU:OE2	2.49	0.46
1:A:1269:ASN:O	1:A:1273:TYR:N	2.43	0.46
2:B:538:LEU:HD12	2:B:538:LEU:O	2.15	0.46
12:J:43:TYR:HA	12:J:46:ARG:HB2	1.98	0.46
16:M:66:ASN:CB	16:M:69:TYR:HE2	2.29	0.46
1:A:845:THR:HG23	2:B:645:LEU:HD11	1.98	0.46
1:A:1113:ILE:HG13	1:A:1113:ILE:O	2.16	0.46
2:B:608:ASN:ND2	2:B:608:ASN:C	2.73	0.46
4:G:94:PRO:HA	4:G:121:ASP:HB2	1.96	0.46
4:G:103:PHE:HB3	15:D:48:GLU:OE1	2.15	0.46
13:O:26:VAL:HA	13:O:29:ILE:HD12	1.97	0.46
13:O:170:ASP:OD1	13:O:170:ASP:N	2.48	0.46
16:M:50:LYS:O	16:M:54:GLN:HA	2.15	0.46
1:A:376:ARG:CZ	1:A:376:ARG:CB	2.93	0.46
1:A:966:LEU:HD12	1:A:966:LEU:HA	1.80	0.46
2:B:259:GLU:HB2	2:B:263:ALA:HB2	1.97	0.46
2:B:338:MET:HE2	2:B:338:MET:HB3	1.81	0.46
13:O:147:THR:HA	13:O:150:ARG:HB2	1.98	0.46
16:M:118:LEU:C	16:M:118:LEU:CD2	2.85	0.46
1:A:474:MET:HE2	1:A:525:THR:HG22	1.97	0.46
1:A:713:LYS:HG2	1:A:717:LEU:HD23	1.98	0.46
2:B:702:ARG:NH2	2:B:867:GLU:OE2	2.36	0.46
4:G:160:THR:O	4:G:160:THR:HG22	2.15	0.46
13:O:406:LEU:N	13:O:406:LEU:CD2	2.79	0.46
13:O:416:ALA:HB3	13:O:417:PRO:HD3	1.98	0.46
15:D:84:LEU:O	15:D:84:LEU:HD12	2.16	0.46
16:M:56:VAL:HG12	16:M:135:LEU:CD2	2.45	0.46
1:A:483:HIS:NE2	2:B:893:ILE:HB	2.25	0.46
2:B:801:LYS:HE2	2:B:801:LYS:N	2.19	0.46
3:C:162:LEU:CD1	3:C:203:ARG:HD2	2.41	0.46
8:P:283:VAL:O	8:P:283:VAL:CG1	2.62	0.46
13:O:374:HIS:ND1	13:O:425:THR:OG1	2.42	0.46
15:D:4:LYS:HA	15:D:4:LYS:CE	2.34	0.46
17:N:268:PHE:O	17:N:383:LEU:N	2.39	0.46
17:N:359:GLU:OE1	17:N:359:GLU:HA	2.16	0.46
1:A:461:LEU:HD22	1:A:523:MET:HE1	1.98	0.45
1:A:481:LYS:CD	1:A:482:PRO:HD3	2.35	0.45
2:B:801:LYS:HB3	2:B:802:PRO:HD2	1.98	0.45
2:B:915:ASP:OD1	3:C:78:ARG:NH1	2.49	0.45
9:E:74:VAL:HA	9:E:103:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:121:GLN:NE2	17:N:259:SER:O	2.49	0.45
18:X:39:DG:N2	19:Y:5:DG:C2	2.84	0.45
1:A:102:ILE:HD13	1:A:168:LYS:HB2	1.98	0.45
1:A:1137:ILE:HG13	1:A:1144:VAL:CG2	2.45	0.45
2:B:423:ASN:OD1	2:B:434:GLN:NE2	2.49	0.45
9:E:9:ARG:C	9:E:11:TRP:H	2.22	0.45
13:O:412:THR:HG22	13:O:413:PRO:HD2	1.99	0.45
1:A:483:HIS:CB	1:A:487:ARG:NH1	2.79	0.45
2:B:707:THR:HG21	19:Y:23:DG:H5'	1.98	0.45
4:G:151:ARG:C	4:G:151:ARG:CD	2.85	0.45
5:I:25:CYS:SG	5:I:26:ASN:N	2.90	0.45
8:P:288:GLY:O	13:O:357:ARG:HD2	2.16	0.45
15:D:96:GLU:H	15:D:96:GLU:HG2	1.44	0.45
1:A:55:VAL:HG22	1:A:55:VAL:O	2.16	0.45
1:A:381:ALA:HB1	1:A:481:LYS:HB2	1.97	0.45
2:B:599:VAL:HG11	2:B:654:THR:CG2	2.46	0.45
3:C:156:SER:O	3:C:156:SER:OG	2.33	0.45
6:K:77:GLU:H	6:K:77:GLU:HG2	1.63	0.45
6:K:90:LEU:N	6:K:90:LEU:CD1	2.77	0.45
14:Q:86:ARG:HB2	14:Q:86:ARG:HH11	1.81	0.45
17:N:340:LEU:HD23	17:N:340:LEU:N	2.31	0.45
1:A:448:ASP:N	1:A:448:ASP:OD1	2.47	0.45
1:A:925:LEU:HD11	1:A:1006:ILE:HD11	1.99	0.45
2:B:538:LEU:HA	2:B:548:VAL:HA	1.98	0.45
2:B:1045:LEU:CB	19:Y:20:DC:OP1	2.65	0.45
6:K:90:LEU:HA	6:K:91:PRO:HD3	1.79	0.45
8:P:294:ASP:C	8:P:294:ASP:OD2	2.58	0.45
13:O:409:ILE:HG22	13:O:409:ILE:O	2.16	0.45
1:A:876:VAL:HG21	2:B:1053:ASP:HB3	1.99	0.45
1:A:1305:ARG:HD2	1:A:1323:LYS:HE3	1.99	0.45
2:B:642:ASN:O	2:B:654:THR:O	2.34	0.45
2:B:814:ILE:H	2:B:814:ILE:CD1	2.29	0.45
3:C:56:MET:HE1	6:K:122:LYS:HE3	1.99	0.45
3:C:78:ARG:HD2	6:K:50:THR:HA	1.97	0.45
3:C:193:VAL:HG11	3:C:314:GLY:HA3	1.98	0.45
19:Y:10:DC:H5''	19:Y:10:DC:H6	1.82	0.45
1:A:1094:ASP:OD1	1:A:1094:ASP:N	2.49	0.45
1:A:1140:LEU:CD2	5:I:48:GLU:N	2.79	0.45
13:O:409:ILE:N	13:O:410:PRO:CD	2.34	0.45
14:Q:27:LEU:CD2	14:Q:27:LEU:N	2.63	0.45
16:M:71:ARG:O	16:M:75:GLU:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:1:DT:H1'	19:Y:2:DT:H5'	1.99	0.45
1:A:97:TYR:HE2	2:B:1121:ASN:HB3	1.80	0.45
1:A:1121:PHE:CG	5:I:37:LYS:HB2	2.52	0.45
2:B:1095:CYS:O	2:B:1097:SER:N	2.48	0.45
4:G:83:GLU:CA	15:D:85:GLN:NE2	2.69	0.45
7:L:34:ILE:O	7:L:44:MET:SD	2.75	0.45
13:O:447:ILE:O	13:O:451:GLN:N	2.47	0.45
18:X:31:DC:N3	19:Y:12:DG:C2	2.85	0.45
3:C:147:THR:H	3:C:164:VAL:HB	1.81	0.45
3:C:275:VAL:HG13	3:C:275:VAL:O	2.17	0.45
5:I:33:ASN:C	5:I:33:ASN:HD22	2.25	0.45
6:K:29:MET:HB2	6:K:41:THR:HB	1.97	0.45
1:A:404:LEU:HD12	1:A:407:LEU:HD21	1.98	0.45
1:A:822:GLU:HG2	1:A:825:SER:HB2	2.00	0.45
9:E:27:LEU:CD2	9:E:27:LEU:N	2.79	0.45
18:X:31:DC:C2	19:Y:12:DG:N2	2.81	0.45
1:A:307:MET:HE2	1:A:307:MET:HB3	1.51	0.44
1:A:468:LEU:HD22	1:A:1046:THR:HG21	1.99	0.44
1:A:670:ASP:OD1	1:A:670:ASP:N	2.50	0.44
2:B:762:LEU:HD22	2:B:891:PRO:HG2	1.99	0.44
4:G:79:PRO:HG2	4:G:150:PHE:CD2	2.51	0.44
8:P:256:LYS:HE2	8:P:278:PRO:HA	1.99	0.44
9:E:112:PRO:CB	19:Y:6:DA:C4'	2.68	0.44
15:D:117:LEU:HA	15:D:120:VAL:HG12	1.98	0.44
17:N:363:VAL:HG22	17:N:375:VAL:HA	1.98	0.44
1:A:417:GLY:H	1:A:453:HIS:HD1	1.65	0.44
6:K:38:HIS:CE1	6:K:89:THR:HA	2.52	0.44
8:P:293:PHE:CD2	23:P:401:SF4:S1	3.10	0.44
13:O:415:HIS:HB2	13:O:418:SER:O	2.17	0.44
13:O:434:MET:HB3	13:O:434:MET:HE2	1.86	0.44
15:D:1:MET:HE3	15:D:1:MET:HB2	1.87	0.44
1:A:397:ASN:HD21	1:A:400:ASN:HD21	1.64	0.44
1:A:1082:THR:O	1:A:1082:THR:OG1	2.34	0.44
1:A:1183:SER:HB2	1:A:1187:TYR:HD2	1.83	0.44
1:A:1317:MET:HG3	1:A:1344:SER:HB2	1.99	0.44
2:B:56:LYS:HE2	2:B:56:LYS:HB3	1.86	0.44
2:B:618:TYR:O	2:B:618:TYR:CD2	2.70	0.44
3:C:100:ILE:CG2	12:J:60:LEU:HD21	2.47	0.44
15:D:57:PRO:C	15:D:59:ARG:H	2.25	0.44
1:A:762:HIS:O	1:A:766:ALA:N	2.47	0.44
2:B:1073:ASP:HB3	2:B:1108:TYR:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:319:ASP:OD2	6:K:122:LYS:NZ	2.39	0.44
4:G:88:LYS:O	4:G:100:SER:N	2.40	0.44
13:O:63:VAL:HG22	13:O:77:ALA:HB2	1.99	0.44
14:Q:78:PRO:HD2	14:Q:79:GLU:CD	2.43	0.44
15:D:59:ARG:HB3	15:D:59:ARG:NH2	2.33	0.44
16:M:31:PRO:HG2	16:M:136:ARG:HE	1.68	0.44
16:M:120:ARG:NH2	16:M:123:GLU:OE1	2.50	0.44
1:A:484:ARG:H	1:A:484:ARG:HG2	1.54	0.44
2:B:259:GLU:H	2:B:259:GLU:HG3	1.65	0.44
2:B:526:LEU:HG	17:N:358:GLN:NE2	2.28	0.44
6:K:51:LEU:O	6:K:52:GLY:C	2.60	0.44
13:O:423:LEU:HD23	13:O:423:LEU:N	2.32	0.44
1:A:252:LEU:HD13	1:A:255:LEU:HD12	1.99	0.44
1:A:1113:ILE:HB	1:A:1137:ILE:HD11	2.00	0.44
3:C:235:LEU:HA	3:C:306:TYR:HA	2.00	0.44
6:K:42:PHE:N	6:K:82:LEU:O	2.50	0.44
8:P:269:LEU:HD23	8:P:269:LEU:HA	1.78	0.44
9:E:84:ILE:HG13	18:X:41:DA:C5'	2.41	0.44
13:O:406:LEU:HD23	13:O:406:LEU:H	1.83	0.44
1:A:396:VAL:HG21	1:A:444:LEU:HD21	1.98	0.44
1:A:591:PRO:HG3	11:H:90:TYR:HD1	1.82	0.44
1:A:817:SER:OG	1:A:830:ALA:O	2.32	0.44
1:A:869:GLY:HA3	19:Y:17:DG:C1'	2.45	0.44
1:A:928:ILE:HD13	1:A:928:ILE:HA	1.85	0.44
2:B:618:TYR:O	2:B:618:TYR:CG	2.70	0.44
2:B:806:HIS:HA	2:B:809:LEU:HD13	2.00	0.44
3:C:96:ASN:ND2	3:C:207:GLU:OE1	2.51	0.44
5:I:2:LEU:HD23	5:I:2:LEU:N	2.33	0.44
11:H:15:ILE:HD13	11:H:15:ILE:HA	1.78	0.44
13:O:459:ARG:HG2	13:O:460:LEU:HD23	1.99	0.44
16:M:56:VAL:HG13	16:M:102:PHE:HD2	1.82	0.44
16:M:76:GLN:O	16:M:77:ILE:HG12	2.18	0.44
1:A:460:VAL:HG12	1:A:509:LEU:HD13	1.99	0.44
2:B:172:LYS:HE2	2:B:416:VAL:HG11	2.00	0.44
2:B:1085:LEU:HD23	2:B:1085:LEU:HA	1.80	0.44
4:G:32:LYS:HE2	15:D:39:GLN:CG	2.48	0.44
4:G:147:GLU:OE2	15:D:100:MET:SD	2.76	0.44
9:E:27:LEU:CD2	9:E:27:LEU:H	2.21	0.44
2:B:192:GLU:HG2	2:B:198:ALA:O	2.17	0.44
3:C:170:THR:CB	3:C:192:PRO:CG	2.84	0.44
4:G:161:SER:CB	4:G:162:PRO:CD	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:25:LEU:HB3	16:M:129:LEU:HD22	2.00	0.44
16:M:72:SER:HA	16:M:75:GLU:HB2	2.00	0.44
16:M:196:LEU:O	16:M:198:LYS:N	2.47	0.44
17:N:356:PHE:CE2	17:N:380:LYS:HA	2.53	0.44
1:A:78:ASP:OD1	1:A:78:ASP:N	2.50	0.43
1:A:483:HIS:CE1	2:B:893:ILE:CD1	2.93	0.43
1:A:767:CYS:HB2	1:A:797:ALA:HB2	1.99	0.43
2:B:216:MET:HE3	2:B:216:MET:HB2	1.81	0.43
2:B:628:SER:O	2:B:628:SER:OG	2.36	0.43
11:H:15:ILE:HG12	11:H:52:LEU:HG	2.00	0.43
11:H:17:PRO:HG3	11:H:29:HIS:NE2	2.32	0.43
13:O:159:ARG:NH1	14:Q:112:PRO:O	2.51	0.43
13:O:399:LEU:HD12	13:O:404:MET:HB3	2.00	0.43
15:D:95:VAL:HA	15:D:98:GLN:HB2	2.00	0.43
17:N:360:LEU:HB3	17:N:379:VAL:CB	2.47	0.43
1:A:6:PHE:CE1	4:G:158:VAL:HB	2.53	0.43
1:A:93:PHE:H	1:A:314:GLN:HE22	1.67	0.43
1:A:935:PRO:HA	1:A:1005:ARG:HH22	1.82	0.43
1:A:956:SER:O	1:A:956:SER:OG	2.35	0.43
1:A:1020:ASP:OD2	1:A:1024:ARG:NH2	2.50	0.43
2:B:436:VAL:HG23	2:B:437:THR:HG23	2.00	0.43
2:B:506:MET:SD	2:B:506:MET:N	2.91	0.43
2:B:541:LEU:HA	2:B:585:ILE:O	2.18	0.43
2:B:780:LYS:HA	2:B:878:ALA:HB1	2.00	0.43
8:P:220:ILE:O	8:P:224:GLY:N	2.51	0.43
1:A:82:HIS:ND1	2:B:1088:TYR:CD2	2.86	0.43
1:A:259:PRO:HG2	2:B:1115:GLN:HE21	1.82	0.43
1:A:303:THR:HA	1:A:306:ILE:HG22	2.01	0.43
1:A:423:GLN:HB2	1:A:427:GLN:HB2	2.00	0.43
1:A:874:ARG:HG2	1:A:1321:PHE:HZ	1.83	0.43
1:A:1121:PHE:O	5:I:36:ARG:CZ	2.66	0.43
2:B:599:VAL:CB	2:B:655:THR:O	2.50	0.43
2:B:682:ARG:HA	2:B:682:ARG:HD3	1.82	0.43
3:C:86:THR:OG1	3:C:225:PHE:O	2.36	0.43
4:G:103:PHE:O	15:D:48:GLU:HB2	2.16	0.43
13:O:2:THR:O	13:O:2:THR:OG1	2.34	0.43
1:A:571:ILE:HD13	1:A:682:ARG:HA	2.00	0.43
1:A:1061:MET:SD	1:A:1061:MET:N	2.92	0.43
1:A:1144:VAL:HG12	1:A:1202:GLN:HG2	1.99	0.43
2:B:243:MET:HG3	2:B:328:PHE:HB3	2.01	0.43
3:C:68:ILE:HD13	3:C:306:TYR:OH	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:33:ASN:HD22	5:I:33:ASN:N	2.16	0.43
10:F:102:ILE:HG22	10:F:104:ILE:HB	2.00	0.43
14:Q:34:PRO:HG2	14:Q:37:LEU:CD2	2.49	0.43
15:D:87:LEU:N	15:D:87:LEU:HD23	2.32	0.43
1:A:383:PRO:CA	1:A:483:HIS:O	2.66	0.43
1:A:640:ILE:HD11	1:A:650:MET:HE1	2.01	0.43
1:A:1080:ILE:HG12	1:A:1250:ASN:HD22	1.83	0.43
2:B:194:ASP:O	2:B:195:ARG:NH1	2.52	0.43
2:B:235:PRO:HD2	2:B:238:ILE:HD12	2.00	0.43
5:I:2:LEU:O	5:I:2:LEU:CD2	2.66	0.43
11:H:60:ILE:HG23	11:H:141:VAL:HG13	1.99	0.43
13:O:89:PRO:HG2	14:Q:54:GLU:HG2	2.00	0.43
16:M:73:LYS:O	16:M:76:GLN:HB2	2.19	0.43
16:M:76:GLN:HA	16:M:76:GLN:NE2	2.29	0.43
1:A:171:LEU:HG	1:A:171:LEU:O	2.19	0.43
2:B:1091:TRP:CD1	4:G:162:PRO:CA	3.01	0.43
3:C:10:MET:HE2	3:C:10:MET:HB3	1.91	0.43
4:G:30:LEU:HD23	4:G:30:LEU:HA	1.90	0.43
4:G:151:ARG:CZ	4:G:152:VAL:HG12	2.47	0.43
6:K:41:THR:OG1	6:K:83:ARG:NH1	2.51	0.43
15:D:1:MET:O	15:D:1:MET:HG3	2.15	0.43
15:D:17:PHE:CD2	15:D:18:GLN:NE2	2.87	0.43
15:D:114:GLU:N	15:D:114:GLU:OE2	2.51	0.43
16:M:111:THR:CG2	16:M:131:GLY:HA2	2.47	0.43
1:A:720:GLY:HA3	1:A:759:ILE:HD11	2.00	0.43
1:A:1027:MET:SD	1:A:1031:SER:OG	2.75	0.43
2:B:529:GLU:HG3	17:N:353:ALA:HB1	2.01	0.43
2:B:708:LEU:HD13	2:B:773:LYS:HD3	2.00	0.43
4:G:6:GLU:CG	15:D:5:ASP:HB2	2.49	0.43
9:E:84:ILE:HA	9:E:87:ILE:HD12	2.00	0.43
15:D:74:LYS:HB3	15:D:74:LYS:HE3	1.64	0.43
16:M:17:LEU:O	16:M:19:LYS:HD3	2.18	0.43
1:A:384:VAL:HG23	1:A:481:LYS:O	2.18	0.43
3:C:134:GLU:HG3	3:C:178:LEU:C	2.40	0.43
3:C:178:LEU:HD23	3:C:178:LEU:HA	1.71	0.43
6:K:40:VAL:HG13	6:K:92:ALA:HB3	2.00	0.43
13:O:413:PRO:O	13:O:415:HIS:HD2	2.01	0.43
16:M:54:GLN:HB3	16:M:104:SER:HB3	2.01	0.43
17:N:360:LEU:O	17:N:379:VAL:HB	2.19	0.43
1:A:87:ASP:OD2	1:A:254:ARG:NH2	2.52	0.43
1:A:1033:VAL:HG12	1:A:1289:LEU:HD22	2.01	0.43

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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	0.43
4:G:80:PHE:CE2	15:D:81:ALA:HB1	2.54	0.43
6:K:34:GLY:O	6:K:35:THR:CB	2.67	0.43
8:P:304:PRO:CG	13:O:445:ASN:HD22	2.26	0.43
15:D:59:ARG:HB3	15:D:59:ARG:HH21	1.83	0.43
1:A:1236:MET:HE2	1:A:1246:THR:HG23	2.00	0.43
2:B:440:LEU:HD23	2:B:440:LEU:HA	1.90	0.43
2:B:702:ARG:NH1	3:C:100:ILE:O	2.39	0.43
2:B:719:MET:HE2	2:B:953:VAL:HG22	2.01	0.43
3:C:155:ASP:N	3:C:155:ASP:OD1	2.52	0.43
4:G:197:LEU:HD13	4:G:200:TRP:CH2	2.54	0.43
13:O:174:PRO:N	13:O:175:PRO:HD2	2.34	0.43
13:O:416:ALA:N	13:O:417:PRO:CD	2.81	0.43
1:A:1007:THR:HA	1:A:1008:PRO:HD3	1.89	0.42
2:B:1095:CYS:C	2:B:1097:SER:H	2.27	0.42
7:L:26:ASN:HB2	7:L:44:MET:HE1	2.00	0.42
14:Q:34:PRO:HG2	14:Q:37:LEU:HD23	2.01	0.42
16:M:45:LEU:O	16:M:46:SER:C	2.60	0.42
1:A:13:LYS:HD3	2:B:1102:SER:HB2	2.00	0.42
1:A:117:LEU:HD12	1:A:237:LEU:HD21	2.01	0.42
1:A:286:ILE:O	1:A:290:ASN:N	2.52	0.42
1:A:698:ILE:HG13	1:A:776:SER:HB2	2.01	0.42
1:A:1140:LEU:HB2	1:A:1142:LEU:HD22	2.01	0.42
2:B:257:THR:HG21	2:B:528:GLY:HA2	2.01	0.42
2:B:564:ARG:NE	2:B:631:GLU:OE2	2.47	0.42
3:C:236:LEU:HD13	3:C:305:HIS:CE1	2.54	0.42
3:C:237:PRO:HB3	3:C:283:PHE:CE2	2.53	0.42
6:K:51:LEU:O	6:K:54:SER:N	2.43	0.42
1:A:801:GLN:NE2	1:A:802:GLN:O	2.52	0.42
2:B:48:ASN:O	2:B:52:ASN:ND2	2.52	0.42
2:B:94:THR:O	2:B:94:THR:HG23	2.19	0.42
3:C:61:LEU:HG	3:C:63:PHE:HD1	1.85	0.42
5:I:2:LEU:N	5:I:2:LEU:CD2	2.82	0.42
13:O:345:LEU:HD23	13:O:345:LEU:HA	1.89	0.42
1:A:596:THR:HG21	11:H:119:GLY:HA3	2.01	0.42
1:A:865:THR:HA	1:A:868:THR:HG22	2.01	0.42
2:B:137:PRO:HD2	2:B:415:MET:HG2	2.01	0.42
2:B:530:GLU:CD	2:B:530:GLU:N	2.77	0.42
2:B:538:LEU:HD13	2:B:540:PHE:CE1	2.53	0.42
2:B:801:LYS:CE	2:B:801:LYS:N	2.68	0.42
4:G:46:ILE:HG23	15:D:45:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:222:GLU:HA	8:P:225:ILE:HG22	2.02	0.42
13:O:124:LYS:HA	13:O:124:LYS:HD3	1.76	0.42
1:A:42:TYR:HD2	1:A:44:GLN:HE21	1.68	0.42
1:A:563:LYS:HE3	1:A:567:ILE:HD11	2.01	0.42
1:A:1121:PHE:CD2	5:I:37:LYS:CB	3.00	0.42
1:A:1323:LYS:CA	19:Y:15:DG:OP1	2.68	0.42
2:B:238:ILE:HD13	2:B:287:ILE:HD13	2.00	0.42
2:B:1091:TRP:HD1	4:G:162:PRO:HA	1.82	0.42
9:E:159:LEU:HD11	9:E:206:TYR:CG	2.54	0.42
13:O:409:ILE:HB	13:O:423:LEU:CG	2.49	0.42
18:X:27:DT:H2'	18:X:28:DC:C6	2.55	0.42
1:A:667:LEU:HD23	1:A:667:LEU:HA	1.87	0.42
1:A:742:CYS:HG	1:A:743:THR:H	1.61	0.42
1:A:1105:ILE:HG22	1:A:1238:THR:HG21	2.01	0.42
1:A:1315:VAL:O	1:A:1319:ALA:N	2.47	0.42
2:B:594:ARG:NH2	2:B:663:THR:OG1	2.52	0.42
3:C:162:LEU:HD12	3:C:204:PRO:HD3	1.93	0.42
4:G:115:GLN:HG3	4:G:116:GLN:HG3	2.01	0.42
19:Y:3:DC:H2''	19:Y:4:DC:H5	1.76	0.42
1:A:1099:ARG:NH1	1:A:1099:ARG:CB	2.72	0.42
2:B:796:ASP:O	2:B:796:ASP:CG	2.62	0.42
14:Q:49:LYS:HA	14:Q:49:LYS:HD2	1.94	0.42
15:D:69:PHE:HD2	15:D:69:PHE:O	2.02	0.42
16:M:15:VAL:HG22	16:M:124:LEU:HD13	2.00	0.42
16:M:50:LYS:HD3	16:M:54:GLN:O	2.20	0.42
17:N:357:LEU:CD2	17:N:357:LEU:N	2.83	0.42
19:Y:21:DG:N2	20:R:6:C:C2	2.88	0.42
1:A:99:ARG:HA	1:A:99:ARG:HD2	1.84	0.42
1:A:366:ARG:HH21	19:Y:20:DC:H4'	1.84	0.42
1:A:385:HIS:CD2	1:A:484:ARG:HH11	2.35	0.42
1:A:1295:THR:O	1:A:1295:THR:OG1	2.27	0.42
2:B:260:HIS:ND1	2:B:261:VAL:HG23	2.35	0.42
2:B:1095:CYS:SG	2:B:1095:CYS:O	2.78	0.42
3:C:49:PHE:CZ	6:K:110:VAL:HG23	2.54	0.42
13:O:19:GLU:OE2	14:Q:70:ARG:NE	2.47	0.42
13:O:269:THR:HG21	13:O:298:PRO:HD3	2.01	0.42
15:D:65:ILE:C	15:D:65:ILE:HD12	2.44	0.42
16:M:20:SER:OG	16:M:214:ARG:NH1	2.53	0.42
16:M:76:GLN:CA	16:M:76:GLN:NE2	2.83	0.42
1:A:136:TYR:HE1	1:A:140:ARG:HE	1.68	0.42
1:A:941:SER:C	1:A:943:ASN:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:941:SER:HB2	1:A:980:ILE:HG21	2.01	0.42
3:C:251:GLU:O	3:C:255:ARG:NE	2.53	0.42
3:C:311:GLU:OE2	12:J:42:ARG:NH2	2.45	0.42
4:G:4:LEU:HD22	15:D:11:LEU:HD13	2.01	0.42
4:G:38:VAL:HG11	4:G:186:LEU:HB2	2.02	0.42
4:G:57:ALA:HA	4:G:68:THR:HG22	2.01	0.42
4:G:148:ILE:CG2	4:G:190:ILE:HG23	2.29	0.42
5:I:13:ILE:HD12	5:I:23:PHE:HA	2.01	0.42
12:J:60:LEU:HD23	12:J:60:LEU:HA	1.56	0.42
13:O:459:ARG:NH1	13:O:460:LEU:HB2	2.34	0.42
15:D:3:VAL:O	15:D:3:VAL:CG2	2.68	0.42
16:M:50:LYS:HG3	16:M:201:ALA:HA	2.01	0.42
16:M:194:GLU:OE1	16:M:194:GLU:N	2.53	0.42
1:A:974:LYS:HA	1:A:977:SER:HB3	2.02	0.42
2:B:597:ILE:HG13	2:B:659:ILE:HG12	2.02	0.42
2:B:779:LEU:HB3	2:B:788:ASP:HB2	2.01	0.42
3:C:138:LEU:HD12	3:C:138:LEU:HA	1.91	0.42
8:P:310:MET:HE1	13:O:449:ARG:HB2	2.01	0.42
13:O:170:ASP:CG	13:O:173:PRO:HG2	2.45	0.42
1:A:1140:LEU:HD23	5:I:48:GLU:N	2.35	0.41
2:B:521:GLU:HG3	2:B:525:LEU:HD21	2.01	0.41
2:B:891:PRO:HB3	2:B:1011:LYS:HZ2	1.85	0.41
3:C:134:GLU:HG3	3:C:178:LEU:HB3	2.01	0.41
3:C:257:PHE:CZ	3:C:287:ILE:HD11	2.54	0.41
1:A:593:THR:HG23	3:C:32:ASN:HA	2.02	0.41
2:B:262:MET:SD	2:B:262:MET:N	2.93	0.41
2:B:265:PHE:O	2:B:268:SER:OG	2.28	0.41
2:B:796:ASP:O	2:B:797:ALA:HB3	2.21	0.41
2:B:998:LEU:O	3:C:21:VAL:HG21	2.21	0.41
3:C:78:ARG:HE	3:C:78:ARG:HB2	1.55	0.41
3:C:116:HIS:NE2	3:C:190:ILE:HD11	2.28	0.41
3:C:149:ASN:OD1	3:C:149:ASN:N	2.53	0.41
8:P:227:LYS:HD2	8:P:240:ASN:HB3	2.03	0.41
15:D:66:VAL:O	15:D:70:LEU:HB2	2.20	0.41
16:M:28:PHE:CD2	17:N:363:VAL:HG21	2.55	0.41
16:M:42:ILE:HB	16:M:210:TYR:CE1	2.55	0.41
16:M:58:LEU:H	16:M:101:THR:HG22	1.84	0.41
16:M:99:LYS:HB3	16:M:101:THR:HG23	2.01	0.41
1:A:579:ILE:HA	6:K:31:GLN:HE22	1.85	0.41
8:P:200:GLN:NE2	8:P:257:GLU:OE2	2.54	0.41
13:O:376:GLU:O	13:O:421:PHE:HE2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:269:LEU:HA	17:N:383:LEU:O	2.19	0.41
2:B:340:ARG:HH12	2:B:581:ARG:NH2	2.17	0.41
2:B:606:VAL:O	2:B:610:HIS:HB2	2.20	0.41
2:B:1017:LEU:HD23	2:B:1017:LEU:HA	1.89	0.41
3:C:283:PHE:CE1	3:C:299:LEU:HD12	2.55	0.41
6:K:40:VAL:CG1	6:K:92:ALA:HB3	2.51	0.41
9:E:116:GLN:HA	9:E:119:VAL:HG22	2.02	0.41
13:O:399:LEU:CD1	13:O:404:MET:HB3	2.50	0.41
15:D:17:PHE:CE1	15:D:21:THR:CG2	3.03	0.41
16:M:69:TYR:HB2	16:M:73:LYS:HD2	2.02	0.41
16:M:69:TYR:CD1	16:M:73:LYS:HE3	2.51	0.41
16:M:119:TYR:HD1	16:M:124:LEU:HA	1.85	0.41
16:M:135:LEU:HA	16:M:135:LEU:HD23	1.85	0.41
1:A:24:SER:HA	1:A:249:ASP:HB3	2.02	0.41
1:A:420:PHE:HB2	1:A:451:GLU:HB2	2.01	0.41
1:A:705:PRO:HB3	1:A:709:LEU:HD13	2.01	0.41
2:B:248:ASP:N	2:B:248:ASP:OD1	2.53	0.41
6:K:40:VAL:HG21	6:K:92:ALA:CB	2.44	0.41
8:P:286:PRO:CB	14:Q:38:PHE:CD2	3.04	0.41
16:M:49:ILE:HG23	16:M:54:GLN:CG	2.40	0.41
16:M:79:LEU:HD23	16:M:79:LEU:HA	1.91	0.41
2:B:611:MET:CE	2:B:611:MET:HA	2.41	0.41
3:C:21:VAL:CG2	3:C:24:VAL:CG1	2.99	0.41
4:G:42:VAL:HG21	15:D:3:VAL:HG11	2.02	0.41
4:G:79:PRO:HG3	4:G:150:PHE:CE2	2.55	0.41
4:G:80:PHE:CD2	4:G:82:ASP:HB2	2.56	0.41
12:J:8:PHE:H	12:J:48:MET:HE3	1.85	0.41
12:J:49:LEU:HA	12:J:49:LEU:HD23	1.89	0.41
2:B:523:VAL:HG12	16:M:107:THR:HB	2.03	0.41
2:B:758:ASN:HB3	2:B:916:MET:SD	2.61	0.41
3:C:185:PHE:HB2	3:C:186:PRO:HD2	2.01	0.41
4:G:103:PHE:HB3	15:D:48:GLU:CG	2.49	0.41
4:G:147:GLU:CD	15:D:100:MET:SD	3.04	0.41
6:K:40:VAL:HG21	6:K:92:ALA:HB1	1.84	0.41
9:E:56:THR:OG1	9:E:78:GLU:OE1	2.31	0.41
12:J:9:THR:OG1	12:J:10:CYS:N	2.53	0.41
13:O:102:THR:HA	13:O:129:LEU:HD11	2.02	0.41
13:O:115:LYS:HD3	13:O:115:LYS:HA	1.86	0.41
13:O:376:GLU:HB3	13:O:424:TYR:HD1	1.85	0.41
16:M:121:GLN:HG3	17:N:258:LEU:HD22	2.02	0.41
18:X:31:DC:H2''	18:X:32:DT:H5'	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1140:LEU:HD23	5:I:48:GLU:H	1.82	0.41
1:A:1178:ARG:HA	1:A:1189:LEU:HD21	2.03	0.41
2:B:820:LYS:HB3	2:B:865:TYR:CE2	2.55	0.41
2:B:947:LEU:HD12	2:B:947:LEU:HA	1.87	0.41
4:G:192:GLU:OE2	4:G:197:LEU:HD11	2.21	0.41
13:O:350:LEU:HD13	13:O:366:PHE:HZ	1.86	0.41
16:M:68:ASN:C	16:M:70:CYS:H	2.26	0.41
18:X:33:DG:C2	19:Y:11:DA:N1	2.89	0.41
1:A:29:ARG:NH2	8:P:302:ILE:HD12	2.30	0.41
1:A:106:GLN:HG3	1:A:166:VAL:HB	2.03	0.41
2:B:40:VAL:HG22	2:B:452:MET:CB	2.50	0.41
2:B:214:THR:HG22	2:B:227:HIS:CE1	2.55	0.41
2:B:257:THR:CG2	2:B:528:GLY:HA2	2.50	0.41
2:B:538:LEU:HD12	2:B:582:CYS:HA	2.02	0.41
2:B:633:LEU:HD11	2:B:656:HIS:CD2	2.55	0.41
4:G:5:VAL:HG12	4:G:7:MET:HG3	2.03	0.41
4:G:83:GLU:HA	15:D:85:GLN:HE21	1.80	0.41
4:G:103:PHE:CD1	15:D:48:GLU:CD	2.99	0.41
6:K:76:SER:OG	6:K:77:GLU:N	2.53	0.41
7:L:23:HIS:NE2	12:J:64:PRO:HG2	2.36	0.41
8:P:206:ARG:CZ	8:P:217:TRP:HE1	2.33	0.41
8:P:299:GLY:C	8:P:303:SER:HB3	2.46	0.41
13:O:459:ARG:O	13:O:463:LYS:NZ	2.40	0.41
16:M:32:VAL:CG1	16:M:137:PRO:HD3	2.26	0.41
16:M:51:PRO:HD3	16:M:203:GLU:HB2	2.03	0.41
18:X:31:DC:N1	18:X:32:DT:C7	2.72	0.41
1:A:848:PHE:HE2	2:B:473:PRO:HA	1.86	0.41
2:B:385:LYS:HB3	2:B:385:LYS:HE2	1.80	0.41
8:P:287:CYS:O	8:P:287:CYS:SG	2.79	0.41
9:E:114:ALA:O	9:E:117:SER:OG	2.32	0.41
13:O:353:VAL:HG21	13:O:435:LEU:HD21	2.02	0.41
15:D:14:TYR:OH	15:D:63:PRO:HB3	2.21	0.41
19:Y:8:DA:C8	19:Y:9:DT:H72	2.56	0.41
1:A:34:ILE:HD11	1:A:59:ARG:HH11	1.85	0.40
1:A:630:ASP:HB3	1:A:637:TYR:CD2	2.55	0.40
9:E:168:ASN:HB2	9:E:172:ARG:HH21	1.86	0.40
1:A:509:LEU:C	2:B:1067:ARG:HH12	2.29	0.40
2:B:619:ARG:NH2	2:B:627:GLU:HG3	2.36	0.40
2:B:707:THR:HG21	19:Y:23:DG:C5'	2.52	0.40
2:B:712:LEU:HD23	2:B:712:LEU:HA	1.84	0.40
2:B:819:GLU:OE2	7:L:51:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:923:ILE:HD11	12:J:42:ARG:HB2	2.04	0.40
2:B:1047:LEU:HD22	2:B:1068:LEU:HD21	2.03	0.40
15:D:2:GLU:HG2	15:D:2:GLU:O	2.19	0.40
1:A:407:LEU:HD12	1:A:408:VAL:N	2.35	0.40
1:A:476:HIS:NE2	1:A:496:TYR:OH	2.36	0.40
2:B:37:LYS:HD3	2:B:632:TYR:OH	2.21	0.40
2:B:50:PHE:HA	2:B:54:GLU:HB2	2.03	0.40
12:J:57:GLU:H	12:J:57:GLU:HG2	1.73	0.40
13:O:432:ALA:HB1	13:O:523:LEU:HD21	2.02	0.40
15:D:90:ARG:O	15:D:91:PRO:C	2.63	0.40
16:M:121:GLN:HG2	17:N:258:LEU:C	2.45	0.40
17:N:333:LYS:H	17:N:333:LYS:CD	2.34	0.40
1:A:171:LEU:CD2	1:A:171:LEU:N	2.80	0.40
1:A:620:LYS:HD3	1:A:637:TYR:HE1	1.87	0.40
1:A:1132:LEU:HD11	1:A:1149:VAL:HG21	2.03	0.40
1:A:1321:PHE:HD1	1:A:1321:PHE:HA	1.82	0.40
3:C:22:ARG:O	3:C:23:ASN:C	2.63	0.40
3:C:138:LEU:HD21	3:C:189:THR:HG21	2.03	0.40
8:P:289:LEU:HD11	13:O:356:GLU:O	2.22	0.40
9:E:185:ILE:HG21	9:E:209:VAL:HG11	2.03	0.40
1:A:382:VAL:HG11	1:A:454:LEU:HD23	2.04	0.40
1:A:481:LYS:CB	1:A:482:PRO:CD	2.99	0.40
1:A:818:LEU:HA	1:A:818:LEU:HD23	1.85	0.40
2:B:37:LYS:HB3	2:B:37:LYS:HE3	1.89	0.40
2:B:1091:TRP:CD1	4:G:161:SER:C	3.00	0.40
4:G:2:PHE:CD2	15:D:16:VAL:HG21	2.57	0.40
9:E:32:GLU:C	9:E:35:GLN:HE22	2.29	0.40
13:O:392:LYS:HD2	13:O:395:LEU:HD12	2.04	0.40
13:O:514:ILE:HD11	14:Q:54:GLU:HG3	2.03	0.40
14:Q:86:ARG:HB2	14:Q:86:ARG:CZ	2.52	0.40
16:M:116:ALA:HB3	17:N:269:LEU:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1281/1390 (92%)	1153 (90%)	125 (10%)	3 (0%)	43	74
2	B	1030/1133 (91%)	926 (90%)	99 (10%)	5 (0%)	24	57
3	C	326/346 (94%)	293 (90%)	30 (9%)	3 (1%)	14	47
4	G	160/204 (78%)	137 (86%)	23 (14%)	0	100	100
5	I	56/108 (52%)	40 (71%)	12 (21%)	4 (7%)	1	10
6	K	101/133 (76%)	91 (90%)	8 (8%)	2 (2%)	6	32
7	L	42/58 (72%)	40 (95%)	1 (2%)	1 (2%)	4	29
8	P	128/316 (40%)	102 (80%)	25 (20%)	1 (1%)	16	49
9	E	188/210 (90%)	172 (92%)	15 (8%)	1 (0%)	24	57
10	F	74/127 (58%)	68 (92%)	6 (8%)	0	100	100
11	H	116/150 (77%)	101 (87%)	15 (13%)	0	100	100
12	J	62/67 (92%)	58 (94%)	4 (6%)	0	100	100
13	O	435/534 (82%)	416 (96%)	18 (4%)	1 (0%)	43	74
14	Q	82/223 (37%)	72 (88%)	9 (11%)	1 (1%)	10	41
15	D	120/148 (81%)	109 (91%)	10 (8%)	1 (1%)	16	49
16	M	148/708 (21%)	110 (74%)	33 (22%)	5 (3%)	3	23
17	N	88/398 (22%)	80 (91%)	6 (7%)	2 (2%)	5	30
All	All	4437/6253 (71%)	3968 (89%)	439 (10%)	30 (1%)	20	51

All (30) 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
5	I	34	ILE
5	I	43	TYR
7	L	35	ARG
8	P	296	CYS
15	D	8	SER
2	B	530	GLU
2	B	1096	LYS
6	K	35	THR

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Mol	Chain	Res	Type
6	K	92	ALA
13	O	409	ILE
16	M	77	ILE
16	M	199	LYS
1	A	482	PRO
5	I	53	LEU
9	E	7	THR
16	M	41	ASP
17	N	352	THR
14	Q	28	PRO
16	M	109	SER
16	M	204	PRO
1	A	942	LYS
2	B	40	VAL
3	C	192	PRO
5	I	44	PRO
17	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%)	1094 (97%)	30 (3%)	39 62
2	B	912/988 (92%)	872 (96%)	40 (4%)	25 51
3	C	290/302 (96%)	268 (92%)	22 (8%)	12 37
4	G	149/181 (82%)	145 (97%)	4 (3%)	39 62
5	I	34/94 (36%)	26 (76%)	8 (24%)	1 4
6	K	92/119 (77%)	90 (98%)	2 (2%)	45 65
7	L	41/55 (74%)	38 (93%)	3 (7%)	13 38
8	P	114/280 (41%)	112 (98%)	2 (2%)	51 69
9	E	177/192 (92%)	175 (99%)	2 (1%)	65 74
10	F	66/111 (60%)	66 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	H	110/131 (84%)	109 (99%)	1 (1%)	70	76
12	J	53/56 (95%)	53 (100%)	0	100	100
13	O	400/476 (84%)	393 (98%)	7 (2%)	51	69
14	Q	81/195 (42%)	74 (91%)	7 (9%)	10	33
15	D	114/136 (84%)	87 (76%)	27 (24%)	1	4
16	M	138/622 (22%)	120 (87%)	18 (13%)	4	21
17	N	81/347 (23%)	66 (82%)	15 (18%)	1	9
All	All	3976/5497 (72%)	3788 (95%)	188 (5%)	25	49

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	6	PHE
1	A	48	HIS
1	A	225	ASN
1	A	287	ILE
1	A	307	MET
1	A	380	VAL
1	A	419	ASN
1	A	428	MET
1	A	481	LYS
1	A	483	HIS
1	A	484	ARG
1	A	503	ASP
1	A	542	ILE
1	A	593	THR
1	A	663	ILE
1	A	670	ASP
1	A	758	VAL
1	A	1099	ARG
1	A	1110	LEU
1	A	1113	ILE
1	A	1115	GLU
1	A	1124	ASP
1	A	1135	GLU
1	A	1137	ILE
1	A	1140	LEU
1	A	1144	VAL
1	A	1160	VAL

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Mol	Chain	Res	Type
1	A	1167	VAL
1	A	1173	VAL
2	B	93	VAL
2	B	148	THR
2	B	207	THR
2	B	225	LEU
2	B	239	ILE
2	B	248	ASP
2	B	249	GLN
2	B	251	ILE
2	B	521	GLU
2	B	526	LEU
2	B	529	GLU
2	B	531	LEU
2	B	538	LEU
2	B	544	ASN
2	B	548	VAL
2	B	549	ILE
2	B	559	PHE
2	B	561	LEU
2	B	572	VAL
2	B	574	ILE
2	B	578	LEU
2	B	582	CYS
2	B	583	VAL
2	B	606	VAL
2	B	654	THR
2	B	659	ILE
2	B	660	GLU
2	B	733	LEU
2	B	743	VAL
2	B	755	LEU
2	B	771	VAL
2	B	801	LYS
2	B	814	ILE
2	B	815	CYS
2	B	869	VAL
2	B	906	VAL
2	B	907	CYS
2	B	1037	GLU
2	B	1045	LEU
2	B	1095	CYS

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Mol	Chain	Res	Type
3	C	7	VAL
3	C	23	ASN
3	C	24	VAL
3	C	28	ASP
3	C	68	ILE
3	C	133	THR
3	C	158	ASP
3	C	164	VAL
3	C	166	HIS
3	C	176	ILE
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	275	VAL
3	C	277	ASN
3	C	282	THR
3	C	299	LEU
4	G	22	LEU
4	G	59	VAL
4	G	152	VAL
4	G	198	LEU
5	I	2	LEU
5	I	27	THR
5	I	28	CYS
5	I	30	TYR
5	I	33	ASN
5	I	36	ARG
5	I	37	LYS
5	I	39	THR
6	K	48	ASP
6	K	50	THR
7	L	24	THR
7	L	34	ILE
7	L	43	ILE
8	P	283	VAL
8	P	284	ARG
9	E	9	ARG

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Mol	Chain	Res	Type
9	E	165	LEU
11	H	15	ILE
13	O	170	ASP
13	O	239	LEU
13	O	408	GLU
13	O	409	ILE
13	O	411	LYS
13	O	414	ASP
13	O	423	LEU
14	Q	27	LEU
14	Q	31	VAL
14	Q	79	GLU
14	Q	80	GLU
14	Q	83	ASP
14	Q	86	ARG
14	Q	87	TYR
15	D	1	MET
15	D	3	VAL
15	D	11	LEU
15	D	14	TYR
15	D	15	GLU
15	D	18	GLN
15	D	19	LEU
15	D	20	LEU
15	D	32	LYS
15	D	40	GLN
15	D	41	ASN
15	D	43	ASN
15	D	44	THR
15	D	59	ARG
15	D	64	GLU
15	D	65	ILE
15	D	70	LEU
15	D	74	LYS
15	D	77	LYS
15	D	84	LEU
15	D	88	ASN
15	D	96	GLU
15	D	97	ILE
15	D	99	LEU
15	D	101	VAL
15	D	105	GLU

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Mol	Chain	Res	Type
15	D	113	ILE
16	M	42	ILE
16	M	69	TYR
16	M	71	ARG
16	M	75	GLU
16	M	76	GLN
16	M	77	ILE
16	M	107	THR
16	M	109	SER
16	M	111	THR
16	M	114	TYR
16	M	121	GLN
16	M	136	ARG
16	M	142	LEU
16	M	144	LYS
16	M	193	TYR
16	M	194	GLU
16	M	195	PHE
16	M	199	LYS
17	N	258	LEU
17	N	271	LEU
17	N	273	ASP
17	N	328	LYS
17	N	329	LEU
17	N	330	LEU
17	N	343	LYS
17	N	352	THR
17	N	358	GLN
17	N	360	LEU
17	N	365	LEU
17	N	373	MET
17	N	375	VAL
17	N	379	VAL
17	N	382	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	48	HIS
1	A	94	HIS
1	A	114	HIS

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Mol	Chain	Res	Type
1	A	163	ASN
1	A	374	ASN
1	A	385	HIS
1	A	397	ASN
1	A	465	GLN
1	A	506	ASN
1	A	543	GLN
1	A	662	ASN
1	A	707	GLN
1	A	738	GLN
1	A	872	GLN
1	A	885	GLN
1	A	1180	ASN
1	A	1202	GLN
1	A	1277	ASN
1	A	1327	HIS
2	B	43	HIS
2	B	52	ASN
2	B	92	ASN
2	B	129	ASN
2	B	187	ASN
2	B	227	HIS
2	B	289	ASN
2	B	410	GLN
2	B	434	GLN
2	B	438	GLN
2	B	542	ASN
2	B	639	ASN
2	B	642	ASN
2	B	692	GLN
2	B	703	ASN
2	B	716	GLN
2	B	774	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	116	HIS
3	C	127	GLN

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Mol	Chain	Res	Type
3	C	143	GLN
3	C	160	ASN
3	C	181	GLN
3	C	305	HIS
5	I	33	ASN
6	K	38	HIS
7	L	26	ASN
8	P	200	GLN
8	P	207	ASN
8	P	240	ASN
9	E	35	GLN
9	E	129	GLN
11	H	29	HIS
11	H	130	ASN
12	J	26	GLN
13	O	3	GLN
13	O	14	GLN
13	O	49	GLN
13	O	113	ASN
13	O	146	ASN
13	O	337	ASN
13	O	355	GLN
13	O	377	GLN
13	O	379	GLN
13	O	415	HIS
13	O	445	ASN
13	O	457	ASN
13	O	465	GLN
13	O	507	ASN
15	D	7	ASN
15	D	35	HIS
15	D	39	GLN
15	D	43	ASN
15	D	61	GLN
15	D	85	GLN
15	D	89	HIS
15	D	98	GLN
16	M	29	GLN
16	M	66	ASN
16	M	76	GLN
16	M	121	GLN
16	M	149	HIS

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Mol	Chain	Res	Type
17	N	358	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	R	5/6 (83%)	2 (40%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	R	5	C
20	R	9	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	SF4	P	401	8	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	8	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

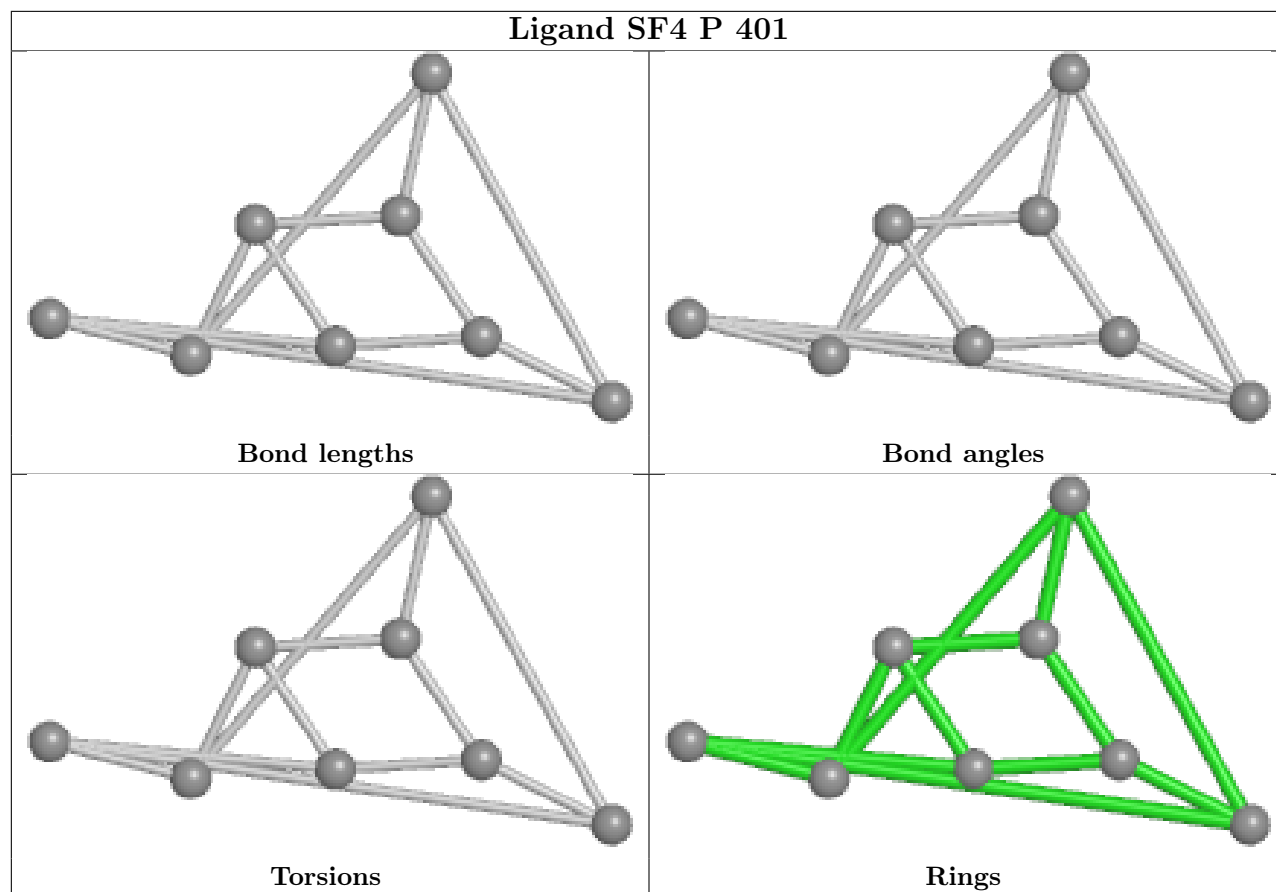
There are no torsion outliers.

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

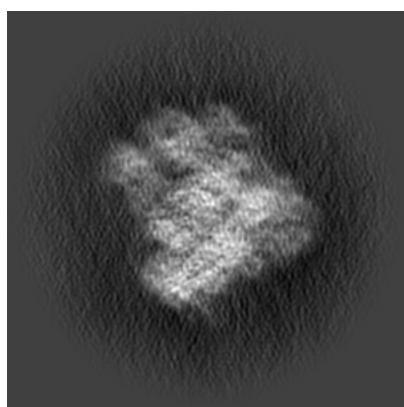
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30779. These allow visual inspection of the internal detail of the map and identification of artifacts.

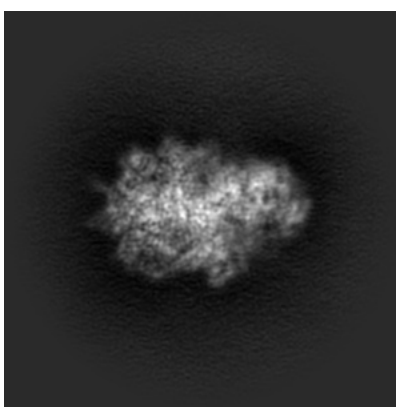
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

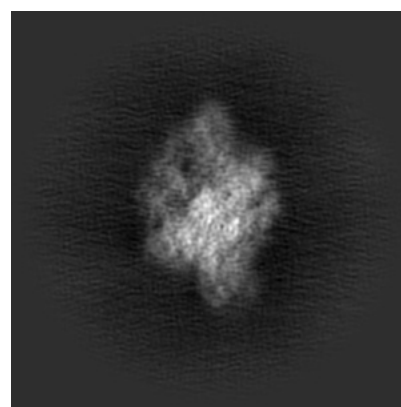
6.1.1 Primary map



X



Y

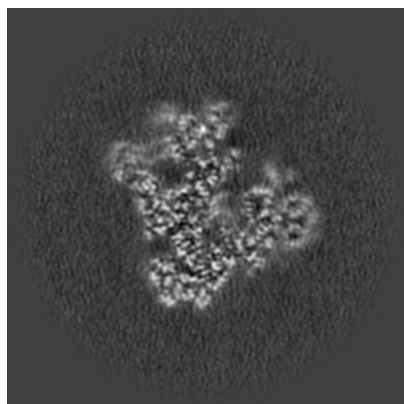


Z

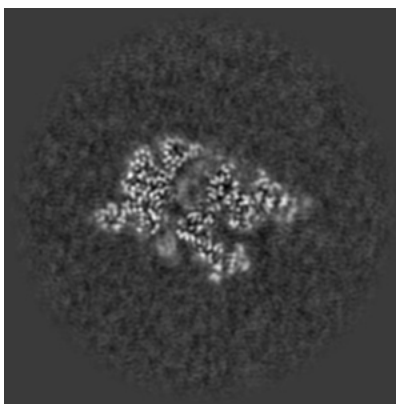
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

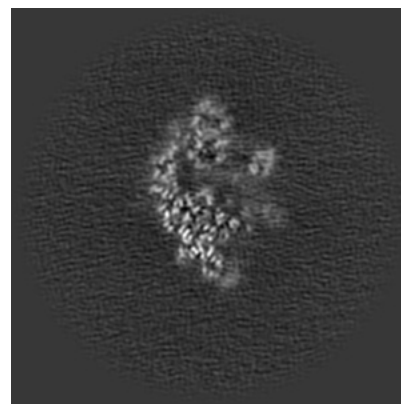
6.2.1 Primary map



X Index: 160



Y Index: 160

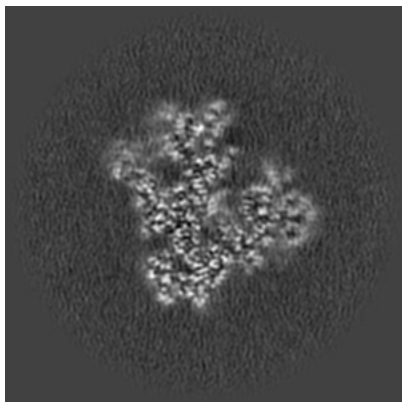


Z Index: 160

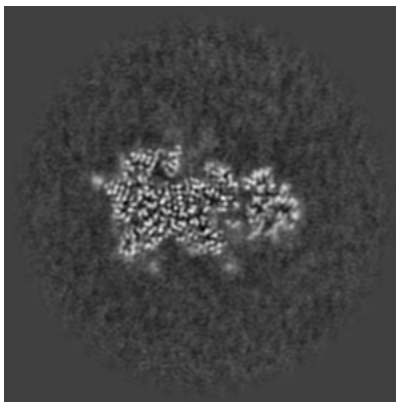
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

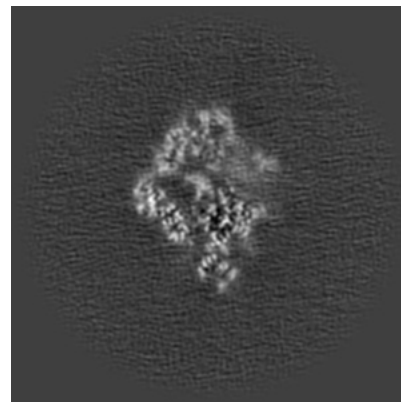
6.3.1 Primary map



X Index: 159



Y Index: 145

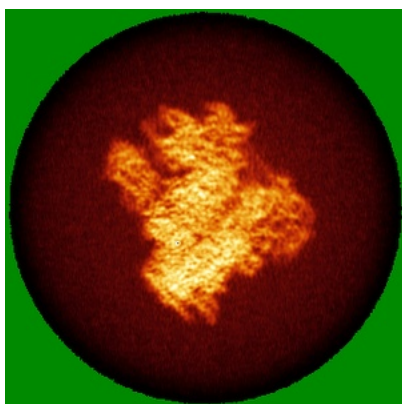


Z Index: 170

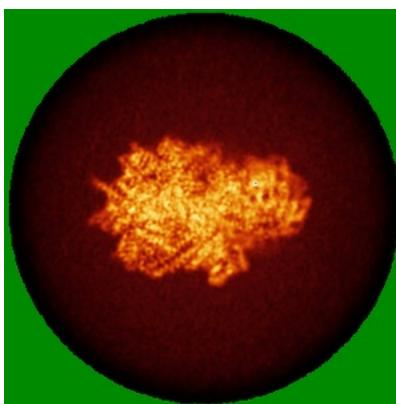
The images above show the largest variance slices of the map in three orthogonal directions.

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

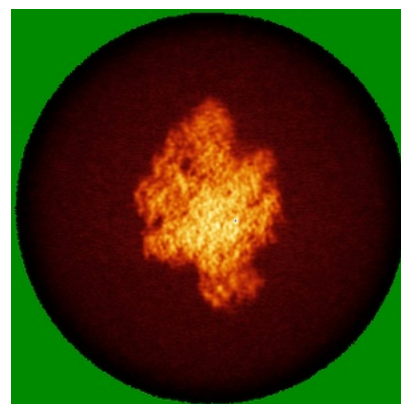
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

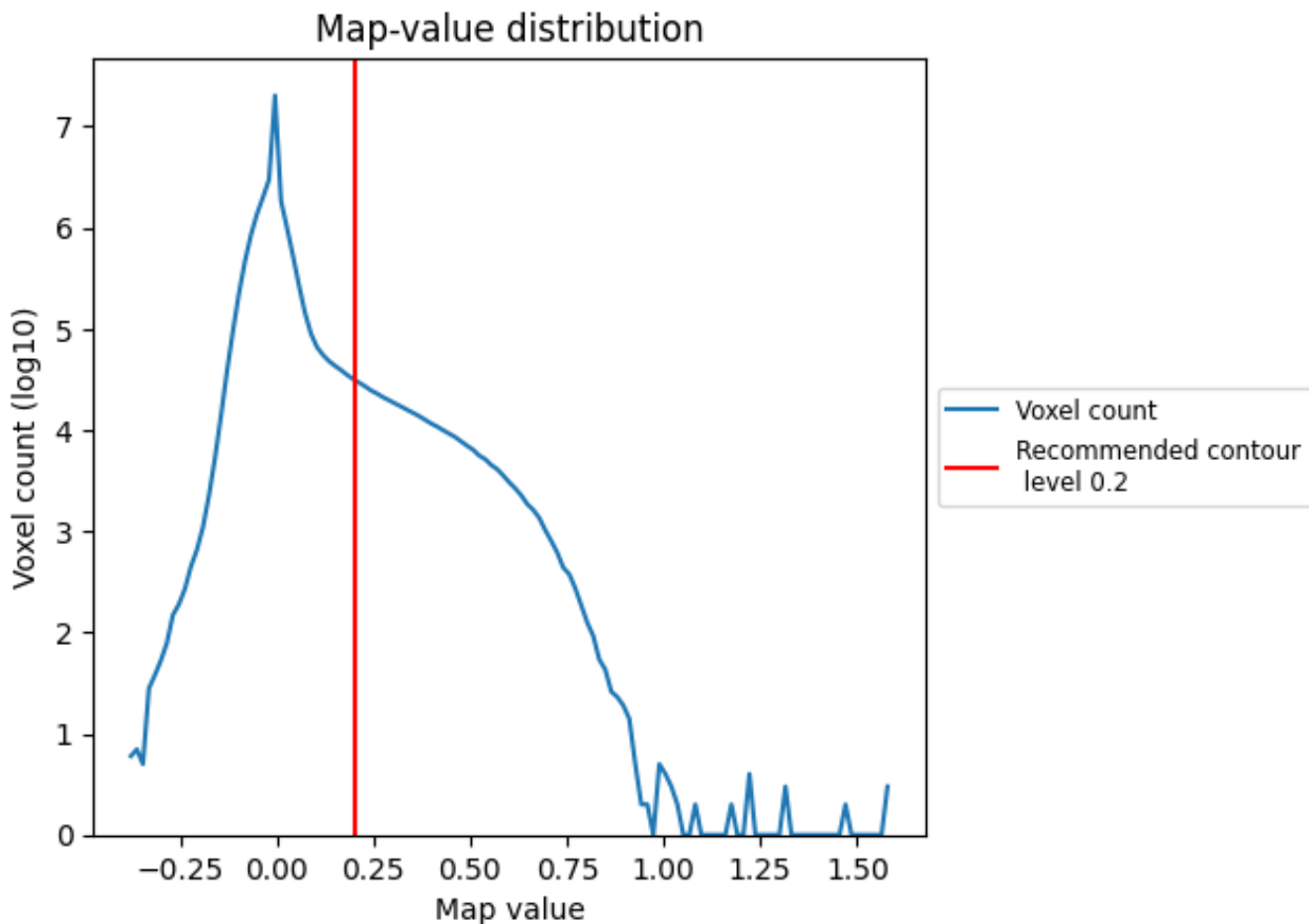
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

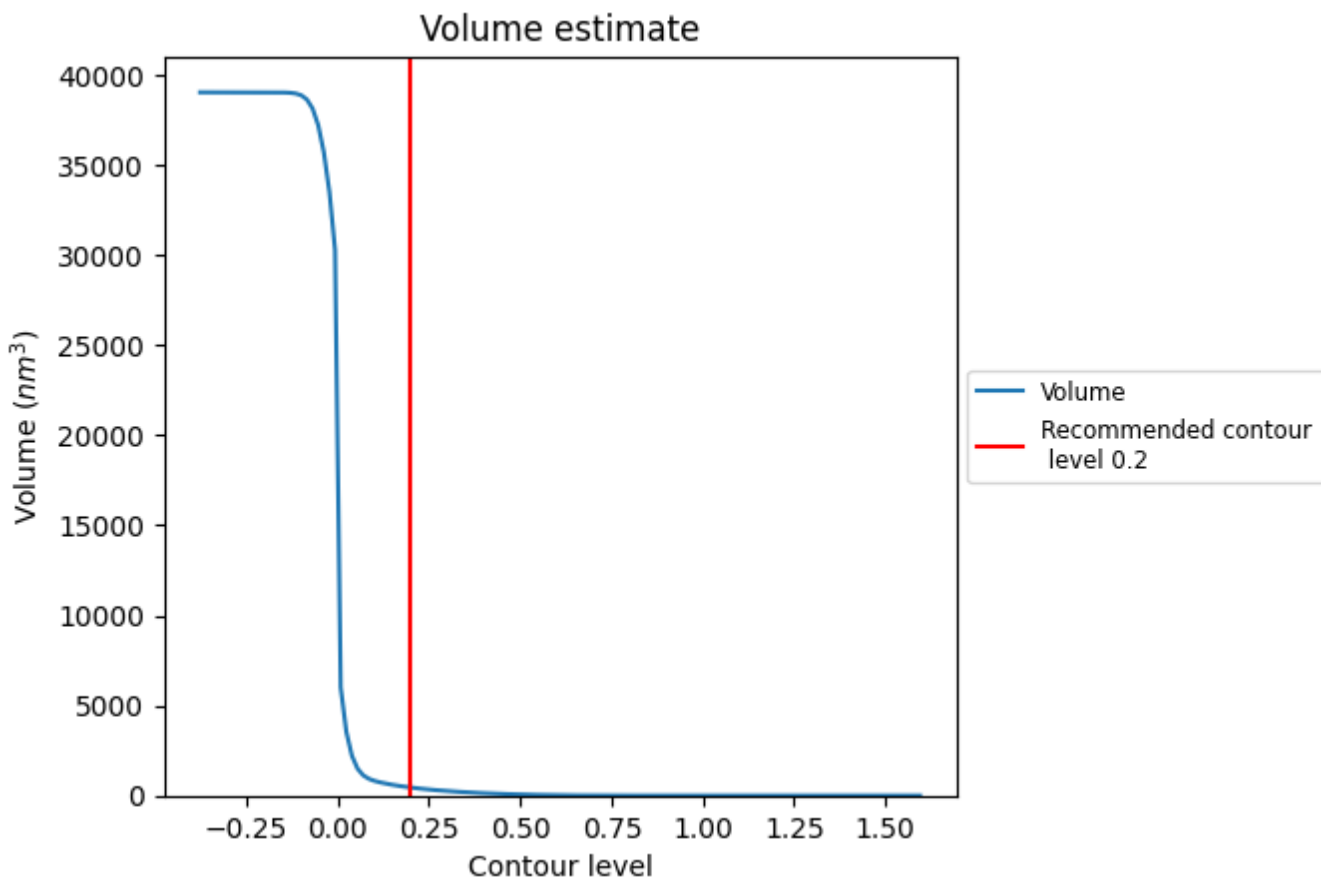
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

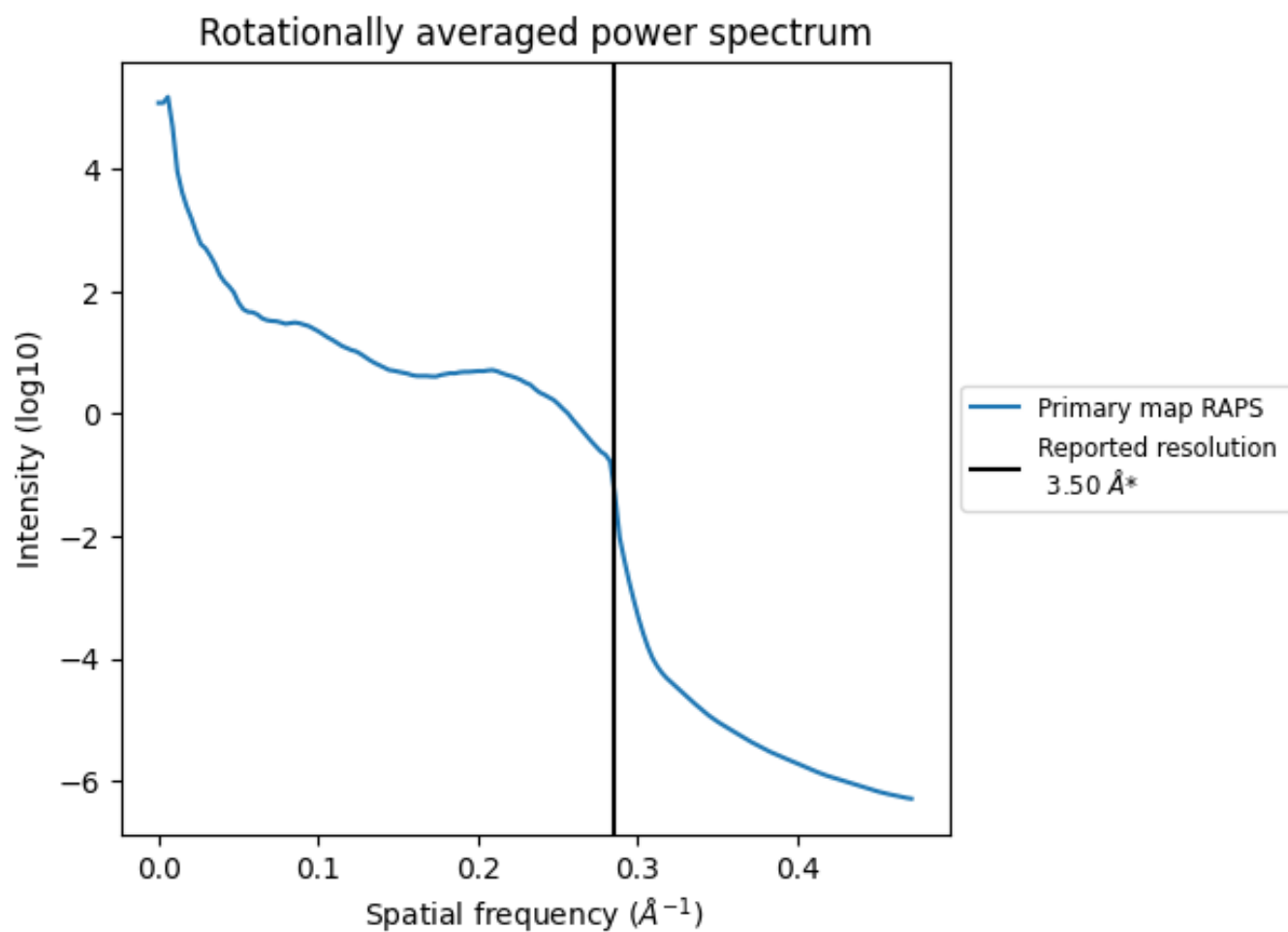
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 447 nm^3 ; this corresponds to an approximate mass of 404 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 0.286\AA^{-1}

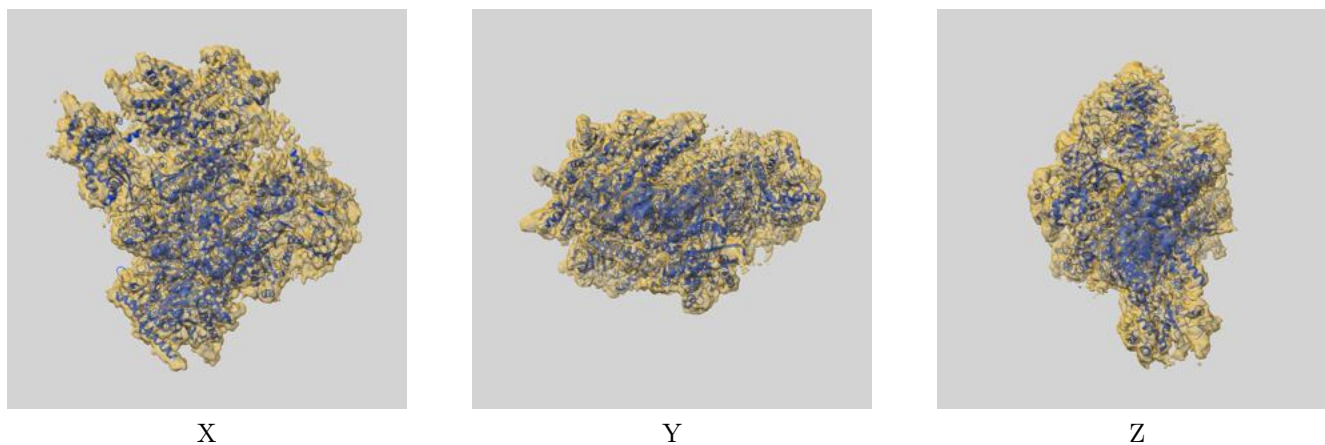
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

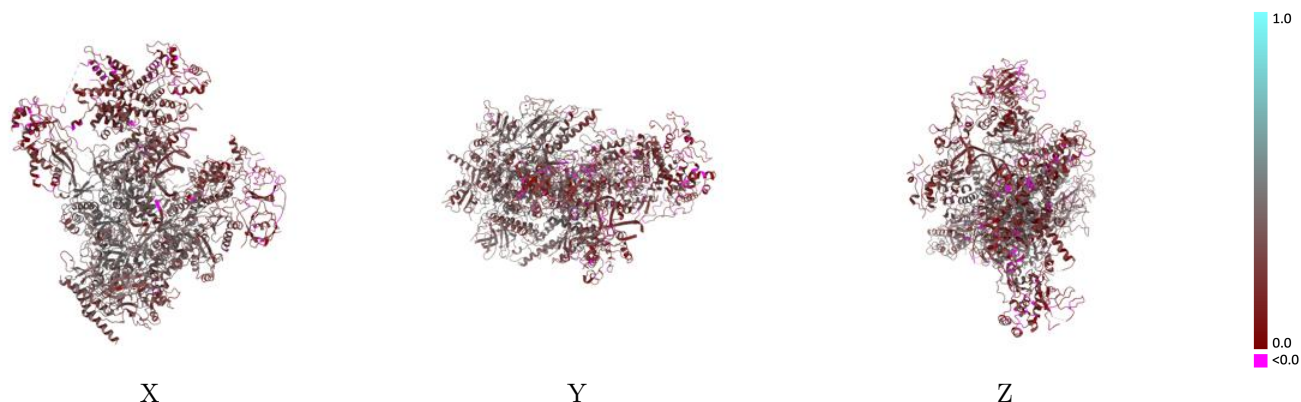
This section contains information regarding the fit between EMDB map EMD-30779 and PDB model 7DN3. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



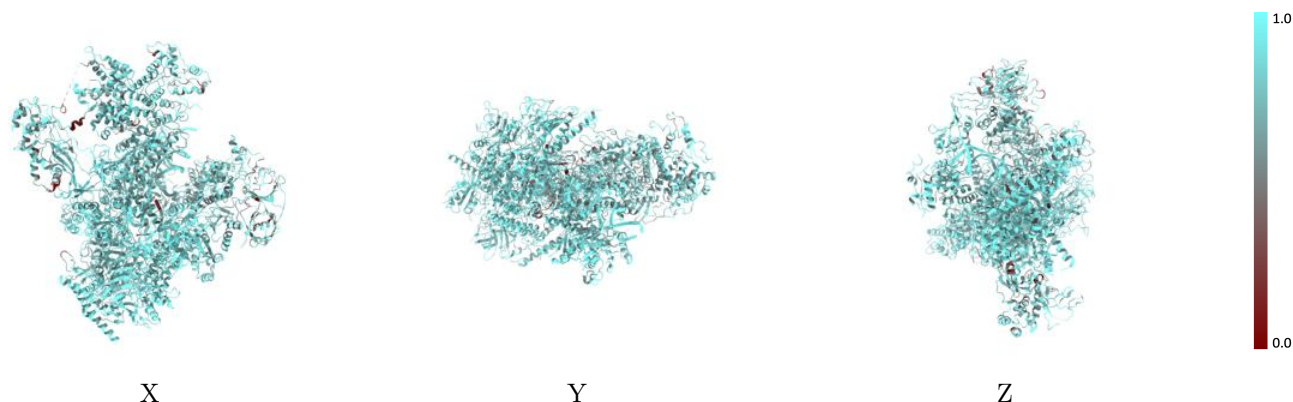
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



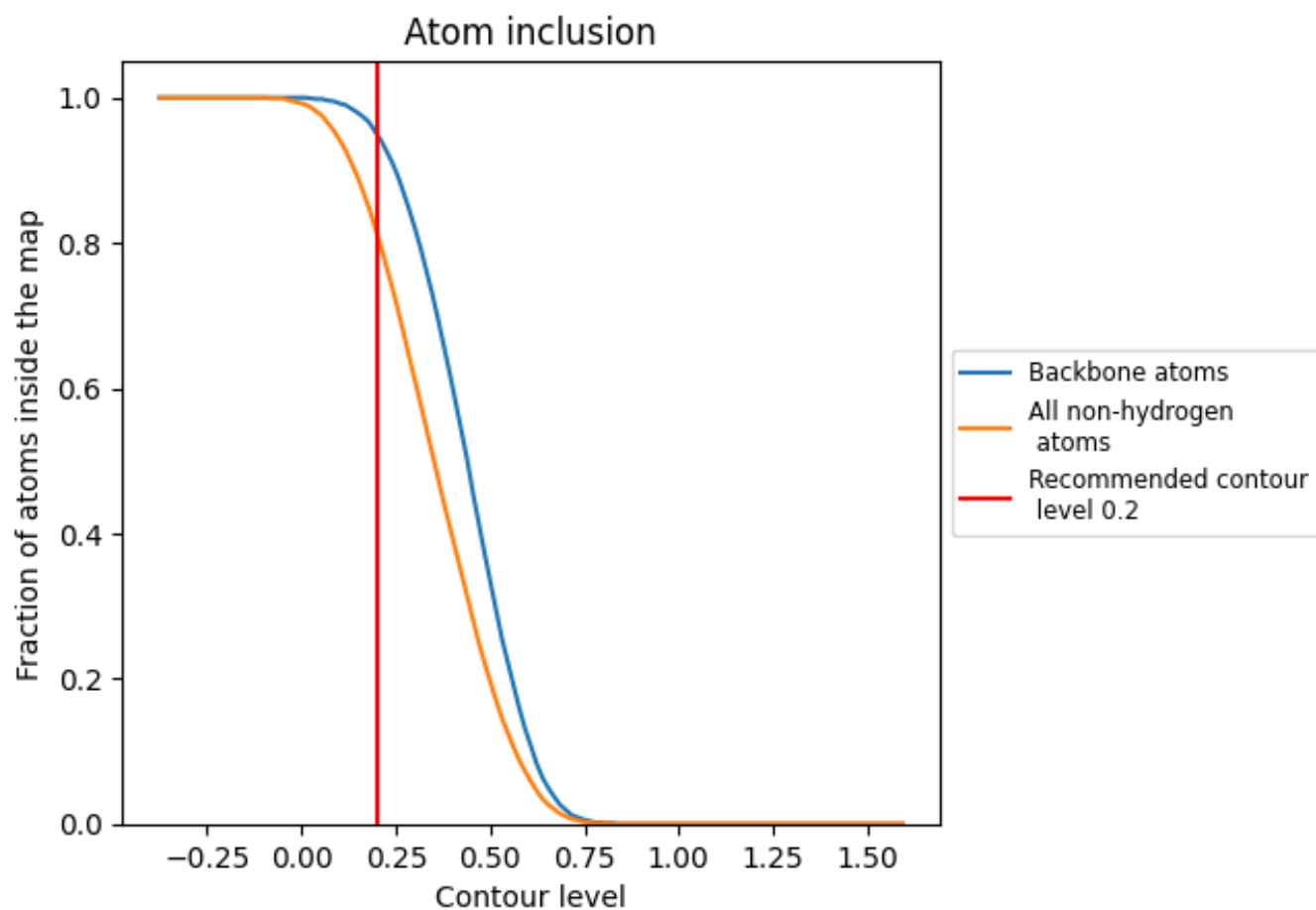
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 81% 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	 0.8130	 0.3070
A	 0.8410	 0.3690
B	 0.8200	 0.3550
C	 0.8500	 0.3290
D	 0.7100	 0.1770
E	 0.8110	 0.2710
F	 0.8730	 0.4090
G	 0.8160	 0.2350
H	 0.8330	 0.3350
I	 0.8530	 0.2630
J	 0.8530	 0.3450
K	 0.8580	 0.3530
L	 0.8600	 0.3590
M	 0.7250	 0.1520
N	 0.6680	 0.1450
O	 0.7780	 0.2020
P	 0.7720	 0.1600
Q	 0.6670	 0.1680
R	 0.4400	 0.2550
X	 0.8650	 0.2370
Y	 0.8800	 0.2880

