



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 08:19 AM JST

PDB ID : 7FJJ / pdb_00007fjj
EMDB ID : EMD-31622
Title : human Pol III pre-termination complex
Authors : Hou, H.; Xu, Y.
Deposited on : 2021-08-04
Resolution : 3.60 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

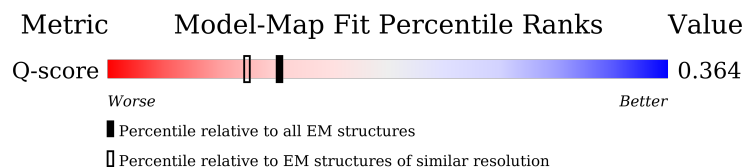
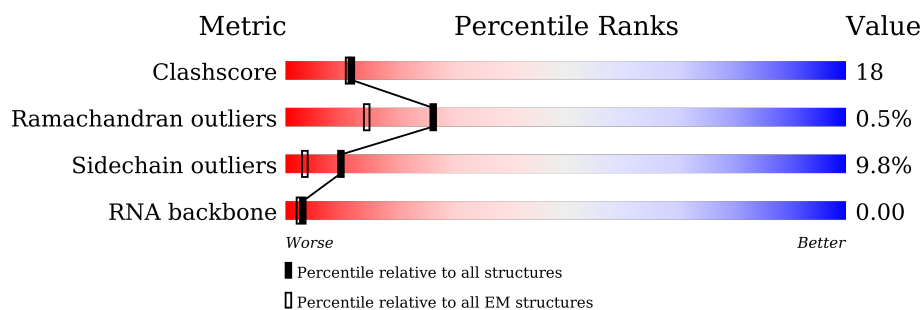
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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.



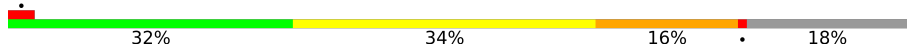
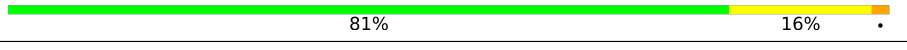
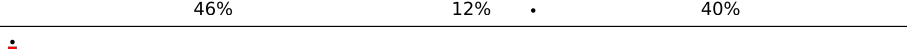
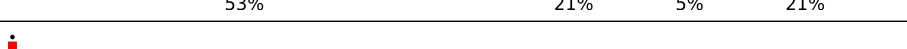
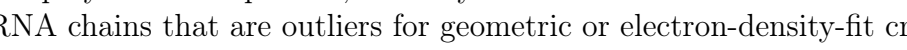
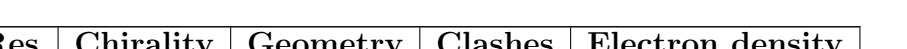
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	D	148	
5	E	210	
6	F	127	
7	G	204	
8	H	150	
9	I	108	
10	J	67	
11	K	133	
12	L	58	
13	M	708	
14	N	398	
15	O	534	
16	P	316	
17	Q	223	
18	R	10	
19	X	54	
20	Y	54	

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
22	ZN	J	2000	-	-	X	-
23	SF4	P	401	-	-	X	-

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 39474 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
1	A	1360	Total	C	N	O	S	0	0
			10675	6763	1865	1974	73		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1095	Total	C	N	O	S	0	0
			8644	5473	1512	1591	68		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	343	Total	C	N	O	S	0	0
			2736	1723	488	514	11		

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1715	1083	300	324	8		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	107	Total	C	N	O	S	0	0
			848	525	157	153	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	24	ALA	SER	variant	UNP Q9Y2Y1

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			512	331	87	88	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	202	Total	C	N	O	S	0	0
			1612	1012	274	316	10		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	146	Total	C	N	O	S	0	0
			1128	710	191	221	6		

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

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

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

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

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

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

- Molecule 18 is a RNA chain called RNA (5'-R(*CP*CP*GP*GP*GP*UP*GP*CP*UP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	4	Total	C	N	O	P	0	0
			86	38	15	29	4		

- Molecule 19 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	22	Total	C	N	O	P	0	0
			449	215	76	136	22		

- Molecule 20 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	22	Total	C	N	O	P	0	0
			447	212	79	134	22		

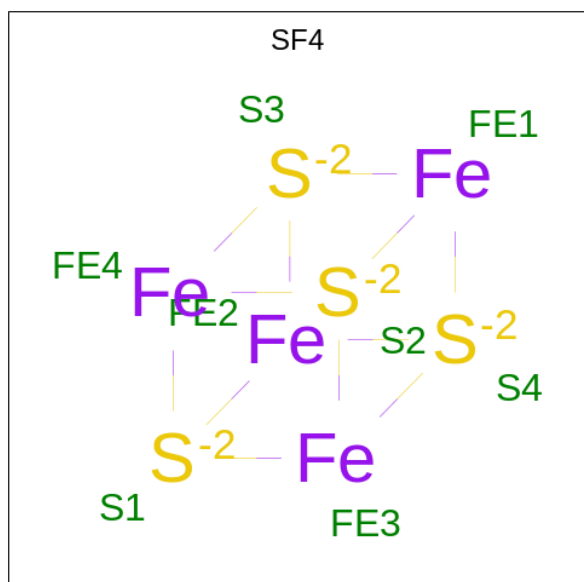
- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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

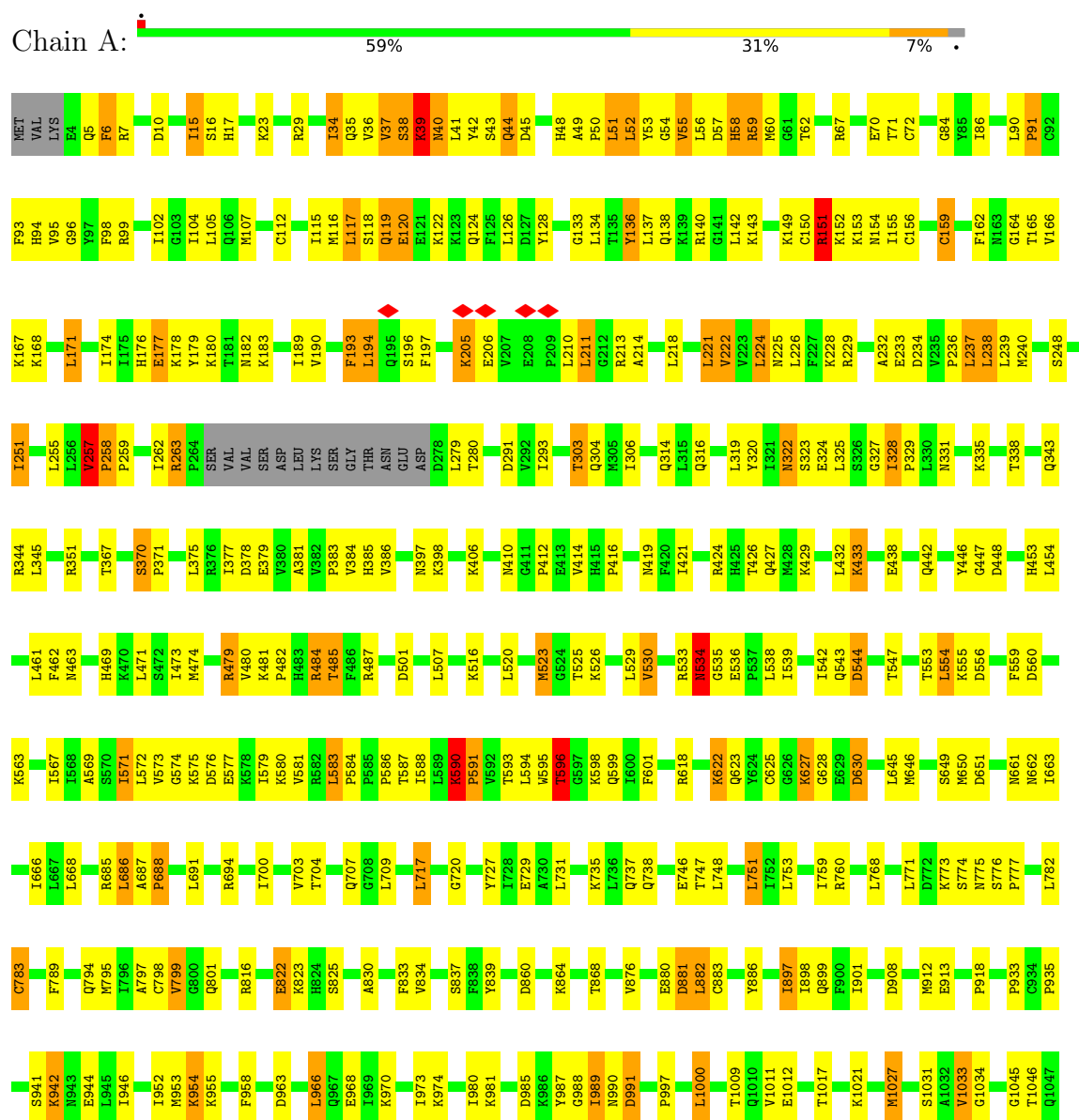


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
23	P	1	8	4	4	0

3 Residue-property plots

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

- Molecule 1: DNA-directed RNA polymerase III subunit RPC1

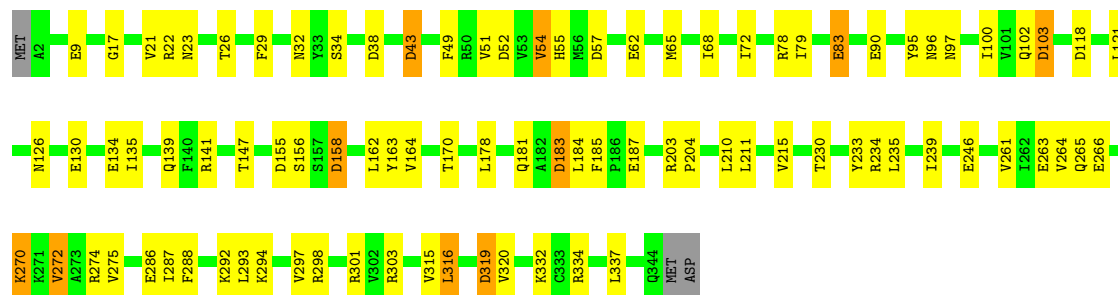






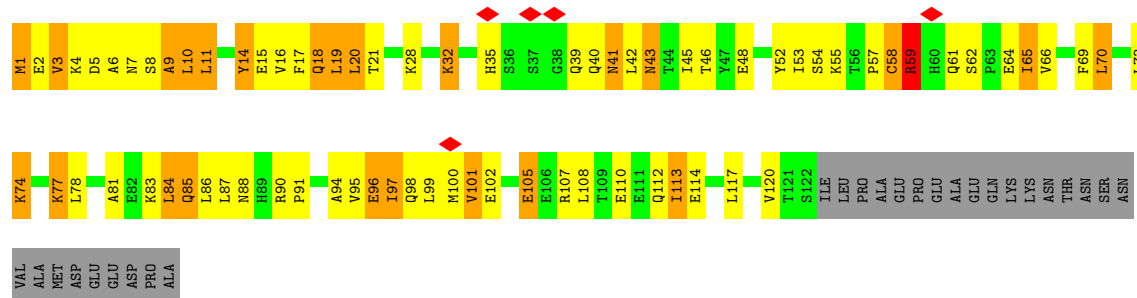
- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C:



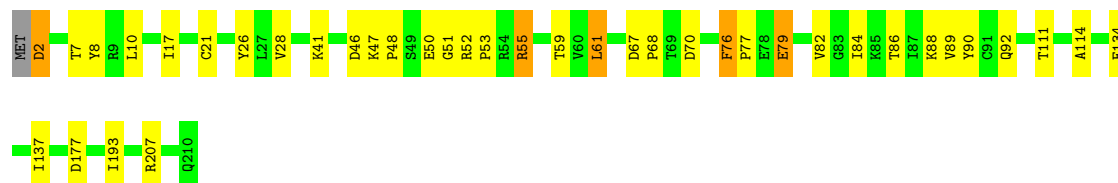
- Molecule 4: DNA-directed RNA polymerase III subunit RPC9

Chain D:



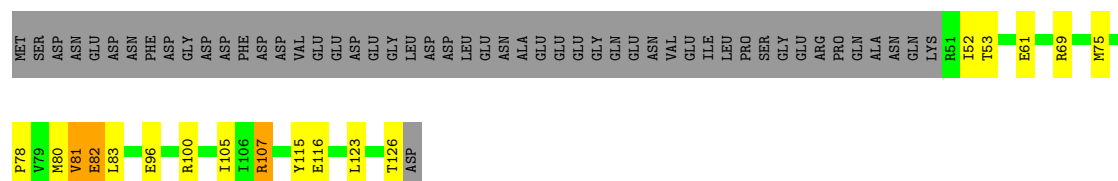
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:

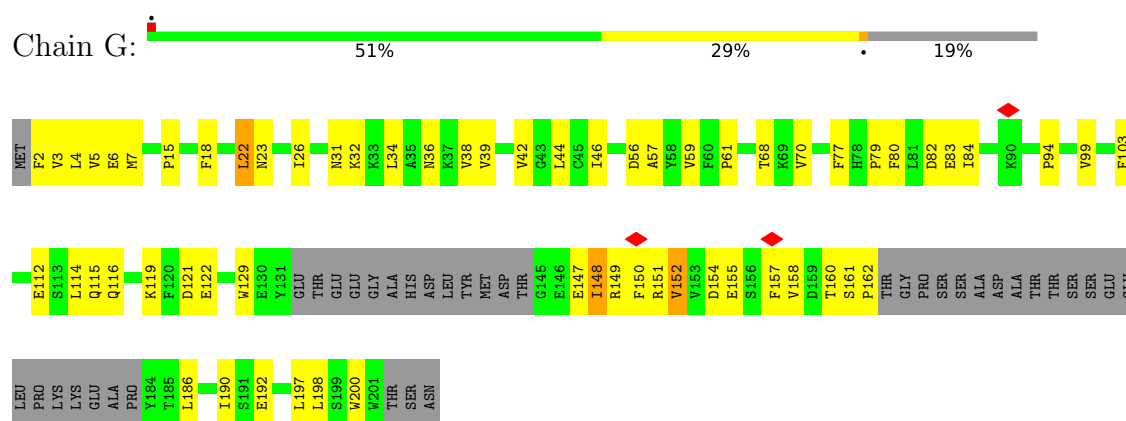


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

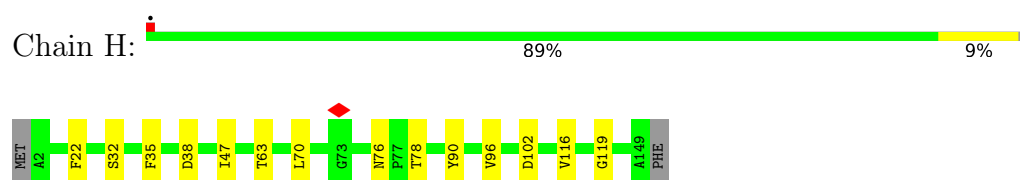
Chain F:



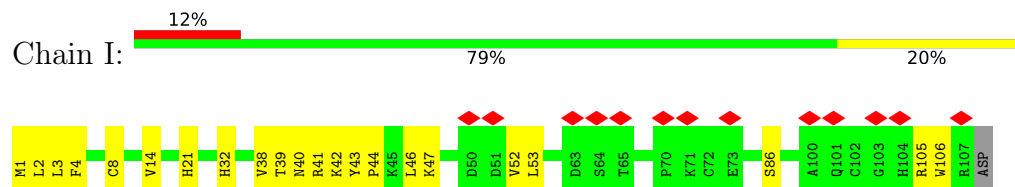
- Molecule 7: DNA-directed RNA polymerase III subunit RPC8



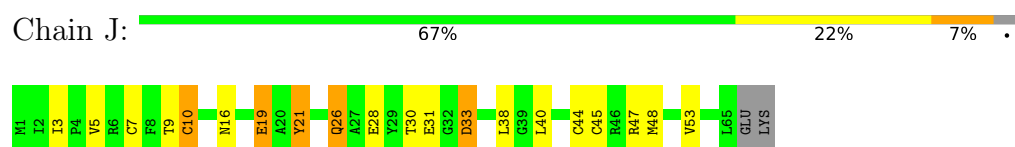
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



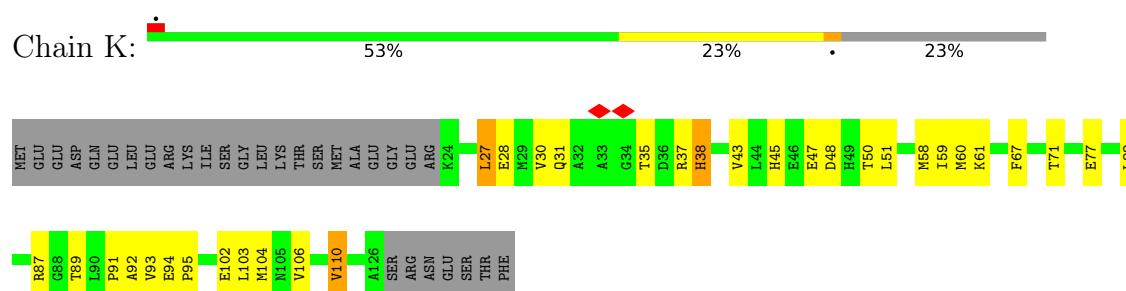
- Molecule 9: DNA-directed RNA polymerase III subunit RPC10



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

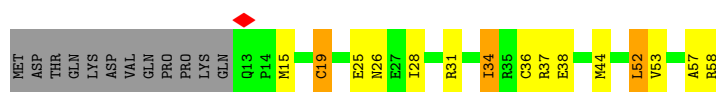


- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

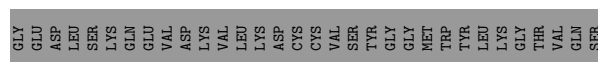
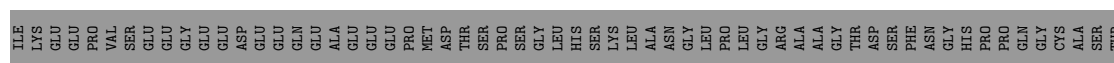
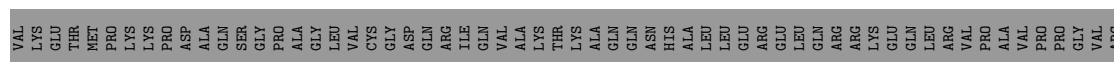
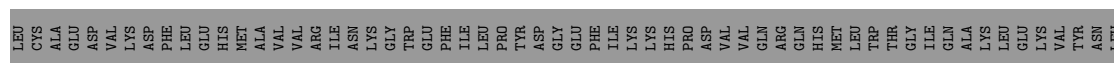
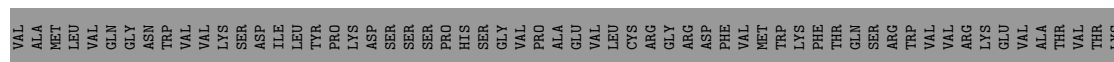
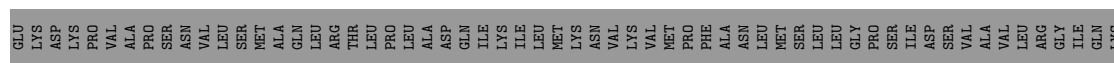


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

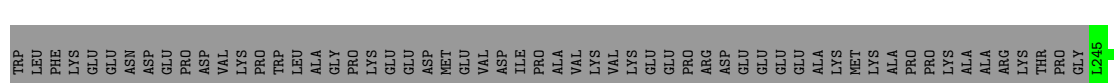


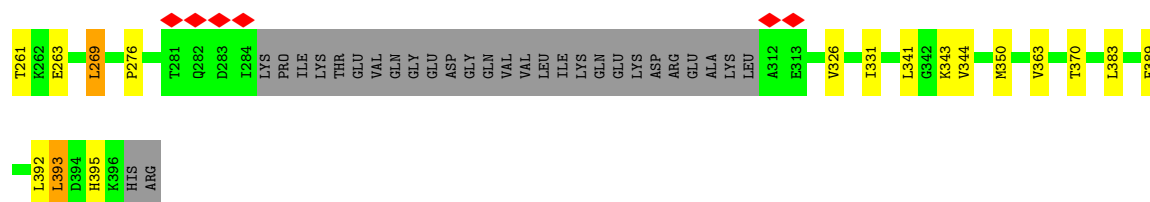


• Molecule 13: DNA-directed RNA polymerase III subunit RPC5

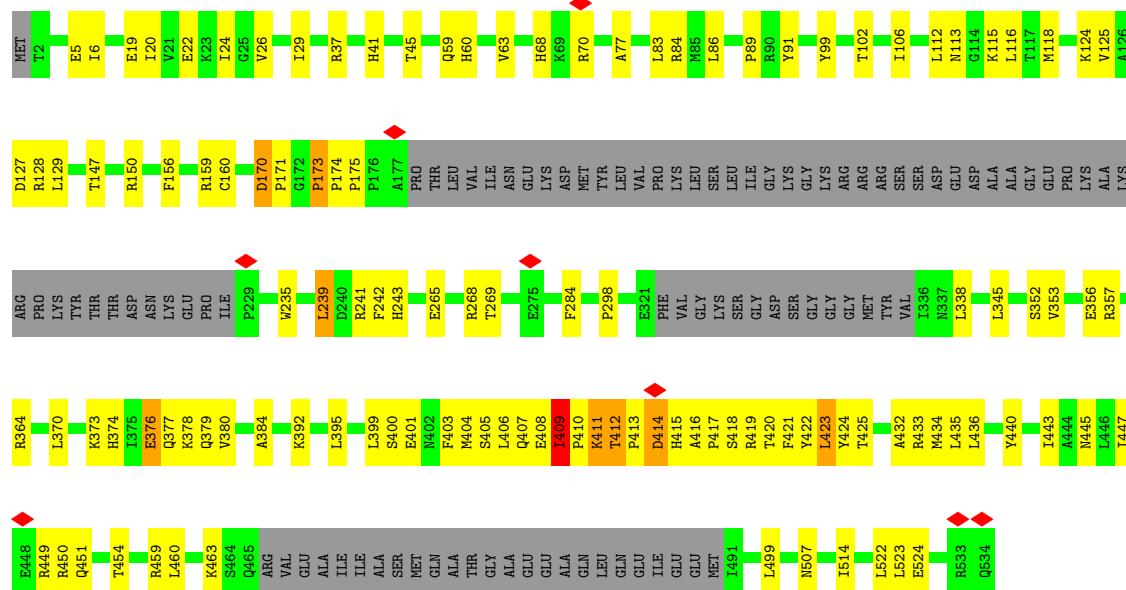


• Molecule 14: DNA-directed RNA polymerase III subunit RPC4

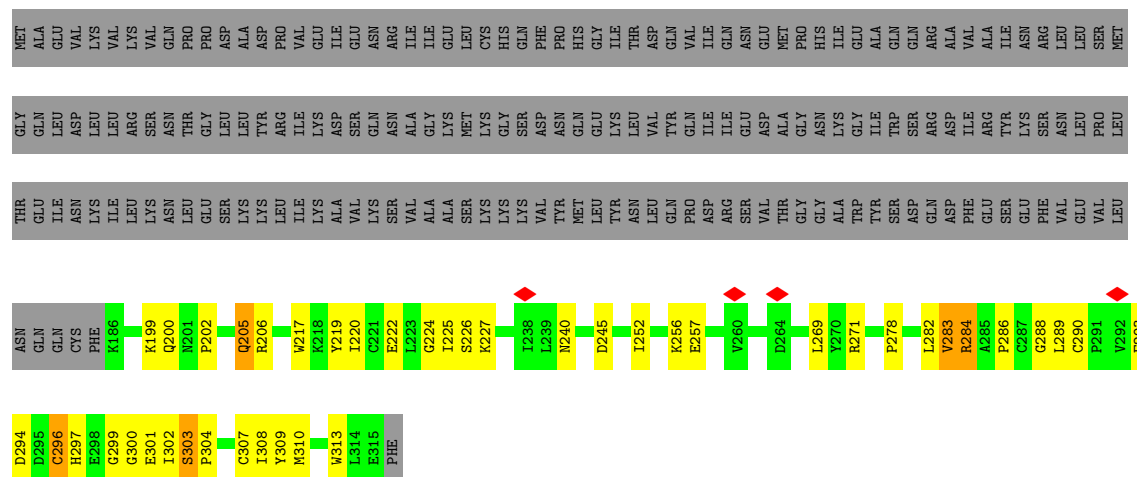




• Molecule 15: DNA-directed RNA polymerase III subunit RPC3

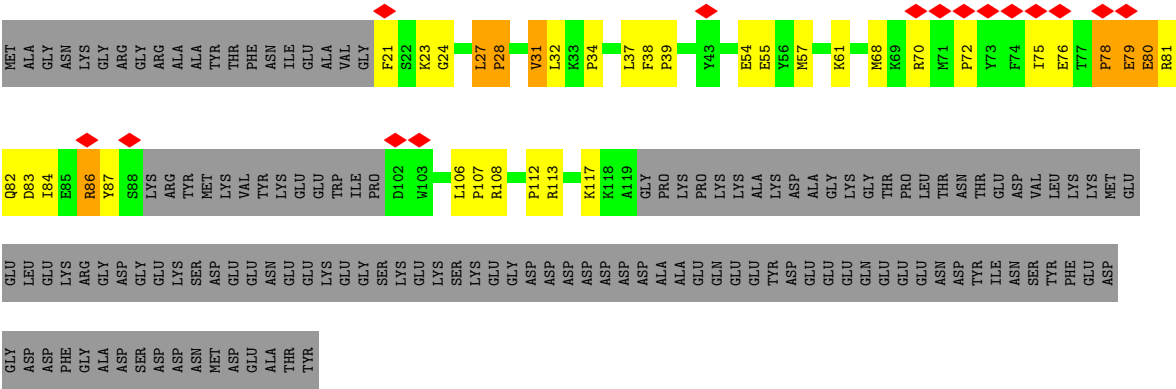


• Molecule 16: DNA-directed RNA polymerase III subunit RPC6



• Molecule 17: DNA-directed RNA polymerase III subunit RPC7

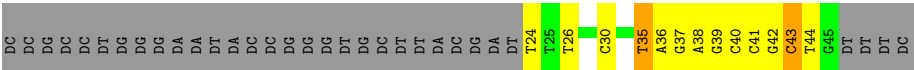




● Molecule 18: RNA (5'-R(*CP*CP*GP*GP*GP*UP*GP*CP*UP*G)-3')



● Molecule 19: non-template DNA



● Molecule 20: template DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48593	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.080	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size ($\text{\AA}$)	379.44, 379.44, 379.44	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.054, 1.054, 1.054	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, ZN, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.95	6/10866 (0.1%)	1.35	39/14648 (0.3%)
2	B	0.95	1/8807 (0.0%)	1.33	28/11875 (0.2%)
3	C	0.90	0/2790	1.20	3/3782 (0.1%)
4	D	0.86	0/997	1.42	6/1343 (0.4%)
5	E	0.59	0/1745	0.95	4/2358 (0.2%)
6	F	0.89	0/620	1.20	0/839
7	G	0.54	0/1374	0.97	3/1868 (0.2%)
8	H	0.33	0/1207	0.63	0/1628
9	I	0.27	0/869	0.63	0/1174
10	J	0.85	0/521	1.30	1/703 (0.1%)
11	K	0.84	0/837	1.24	1/1129 (0.1%)
12	L	0.87	0/394	1.14	0/524
13	M	0.72	0/1648	0.88	0/2232
14	N	0.77	0/1137	0.97	2/1530 (0.1%)
15	O	0.42	0/3604	0.75	5/4872 (0.1%)
16	P	0.54	0/1028	0.95	2/1391 (0.1%)
17	Q	0.61	0/742	0.93	1/996 (0.1%)
18	R	0.73	0/95	0.95	0/146
19	X	0.45	0/501	0.96	2/771 (0.3%)
20	Y	0.47	0/499	1.19	5/767 (0.7%)
All	All	0.82	7/40281 (0.0%)	1.18	102/54576 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1082	GLN	C-N	-7.88	1.23	1.33
1	A	258	PRO	C-O	-6.11	1.19	1.25
1	A	694	ARG	C-O	-5.72	1.17	1.24
1	A	559	PHE	C-O	-5.68	1.17	1.23
1	A	91	PRO	C-O	-5.24	1.17	1.23
1	A	584	PRO	C-O	-5.24	1.20	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	688	PRO	C-O	-5.11	1.17	1.24

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1083	CYS	CB-CA-C	17.40	137.92	110.95
2	B	1083	CYS	N-CA-CB	-11.68	93.05	109.98
2	B	1095	CYS	N-CA-C	-11.11	84.97	107.41
1	A	37	VAL	N-CA-C	-9.90	102.99	112.29
1	A	40	ASN	N-CA-C	-9.36	101.78	113.01
20	Y	1	DG	C2'-C3'-O3'	-9.30	97.55	111.50
2	B	1095	CYS	N-CA-CB	-8.80	94.19	110.56
2	B	1042	ASP	CB-CA-C	8.52	118.27	109.83
2	B	1084	GLY	N-CA-C	-8.26	103.32	115.63
2	B	1082	GLN	CA-C-N	7.92	131.40	120.63
2	B	1082	GLN	C-N-CA	7.92	131.40	120.63
1	A	258	PRO	N-CA-CB	-7.81	98.82	103.19
1	A	59	ARG	N-CA-C	-7.76	103.95	113.50
1	A	238	LEU	N-CA-C	-7.54	103.81	113.16
4	D	58	CYS	N-CA-C	-7.42	103.97	112.87
15	O	412	THR	CB-CA-C	7.39	120.19	109.11
20	Y	0	DA	C2'-C3'-O3'	-7.32	100.52	111.50
2	B	1122	ILE	CA-C-N	-7.25	117.67	122.60
2	B	1122	ILE	C-N-CA	-7.25	117.67	122.60
4	D	10	LEU	N-CA-C	-7.16	101.87	113.19
20	Y	5	DC	C2'-C3'-O3'	-7.13	100.80	111.50
7	G	148	ILE	CA-C-N	-6.91	113.30	123.11
7	G	148	ILE	C-N-CA	-6.91	113.30	123.11
20	Y	4	DG	C2'-C3'-O3'	-6.83	101.26	111.50
1	A	591	PRO	N-CA-C	-6.82	103.72	113.47
7	G	158	VAL	N-CA-C	6.78	117.56	110.72
1	A	830	ALA	N-CA-C	-6.71	105.13	113.38
1	A	44	GLN	N-CA-C	-6.71	99.90	109.96
19	X	43	DC	C2'-C3'-O3'	6.58	121.37	111.50
10	J	10	CYS	CB-CA-C	6.48	121.86	110.85
1	A	746	GLU	N-CA-C	-6.46	105.29	113.43
1	A	258	PRO	N-CA-C	6.45	116.67	110.47
1	A	918	PRO	N-CA-C	6.43	122.47	113.53
1	A	933	PRO	N-CA-C	-6.29	99.51	112.47
1	A	622	LYS	CA-C-O	-6.11	114.90	121.56
1	A	1049	THR	N-CA-C	-6.10	105.60	113.16
15	O	173	PRO	N-CA-C	6.07	118.11	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	817	PRO	N-CA-CB	-6.05	97.74	103.19
1	A	167	LYS	N-CA-C	6.04	119.89	111.56
2	B	380	PHE	CA-CB-CG	5.99	119.79	113.80
1	A	783	CYS	N-CA-C	-5.88	101.24	110.36
2	B	514	LEU	N-CA-C	-5.88	104.88	111.28
1	A	935	PRO	N-CA-C	-5.87	102.65	111.57
5	E	59	THR	N-CA-C	-5.86	104.68	112.94
16	P	303	SER	CA-C-N	5.84	125.94	119.87
16	P	303	SER	C-N-CA	5.84	125.94	119.87
1	A	560	ASP	N-CA-CB	-5.81	102.13	110.44
1	A	1203	GLY	CA-C-O	-5.80	118.23	122.23
2	B	246	GLU	CA-C-O	-5.78	115.26	121.56
2	B	301	PRO	N-CA-CB	5.76	109.30	103.25
1	A	151	ARG	N-CA-C	-5.74	105.38	112.38
1	A	661	ASN	N-CA-C	-5.71	106.21	112.72
15	O	403	PHE	N-CA-C	-5.71	105.98	113.12
14	N	326	VAL	N-CA-C	-5.68	107.97	113.53
4	D	85	GLN	N-CA-C	-5.66	105.11	111.28
1	A	1228	GLU	CB-CA-C	-5.66	101.73	110.78
19	X	35	DT	C2'-C3'-O3'	-5.62	103.07	111.50
1	A	344	ARG	N-CA-C	-5.60	107.08	114.31
2	B	748	GLY	N-CA-C	-5.58	107.41	115.27
1	A	543	GLN	CB-CA-C	-5.57	109.66	117.23
14	N	146	GLU	N-CA-C	5.56	117.14	111.14
17	Q	78	PRO	N-CA-C	-5.52	107.61	114.68
4	D	59	ARG	N-CA-C	-5.51	101.70	109.96
4	D	19	LEU	N-CA-C	-5.43	105.36	111.28
2	B	507	GLU	N-CA-C	5.43	117.27	111.36
1	A	128	TYR	N-CA-C	-5.41	105.28	111.07
1	A	534	ASN	N-CA-C	-5.37	107.74	114.56
1	A	371	PRO	N-CA-C	5.37	119.92	111.38
1	A	419	ASN	CB-CA-C	5.36	118.08	109.07
1	A	482	PRO	N-CA-CB	5.32	109.18	103.33
4	D	9	ALA	N-CA-C	5.32	117.29	108.20
1	A	1187	TYR	CB-CA-C	5.30	120.97	110.42
2	B	354	ARG	N-CA-C	-5.29	106.41	112.92
2	B	507	GLU	CA-C-O	-5.27	114.84	120.42
2	B	397	ALA	N-CA-C	-5.26	105.72	111.82
1	A	39	LYS	N-CA-C	5.23	118.02	110.28
1	A	622	LYS	N-CA-C	-5.22	103.14	110.50
1	A	1176	THR	CB-CA-C	5.20	115.32	110.17
5	E	68	PRO	N-CA-C	-5.19	106.32	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	596	THR	CB-CA-C	5.14	119.64	109.66
1	A	257	VAL	N-CA-CB	5.14	114.86	110.08
3	C	83	GLU	CA-C-N	-5.13	118.89	122.59
3	C	83	GLU	C-N-CA	-5.13	118.89	122.59
11	K	93	VAL	N-CA-C	-5.13	105.54	110.72
5	E	2	ASP	CA-C-N	5.13	131.33	121.54
5	E	2	ASP	C-N-CA	5.13	131.33	121.54
2	B	749	TYR	N-CA-C	-5.12	106.88	113.02
20	Y	2	DC	C5'-C4'-O4'	-5.11	101.73	109.40
2	B	551	ASP	CB-CA-C	-5.11	102.73	111.31
1	A	1208	SER	CA-C-O	-5.10	114.41	120.89
1	A	576	ASP	N-CA-C	-5.09	107.07	113.28
3	C	170	THR	CB-CA-C	5.09	120.55	110.17
2	B	587	SER	N-CA-C	-5.08	105.40	112.30
1	A	590	LYS	N-CA-CB	5.05	119.36	110.37
2	B	94	THR	CB-CA-C	5.03	119.03	111.89
15	O	376	GLU	CA-C-N	5.03	131.14	121.54
15	O	376	GLU	C-N-CA	5.03	131.14	121.54
2	B	742	ALA	CA-C-N	-5.02	116.20	122.48
2	B	742	ALA	C-N-CA	-5.02	116.20	122.48
2	B	553	LYS	CB-CA-C	5.01	119.12	110.79
1	A	775	ASN	N-CA-C	-5.01	101.80	109.76
2	B	267	PRO	CB-CA-C	-5.01	104.36	112.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10675	0	10918	469	0
2	B	8644	0	8749	245	0
3	C	2736	0	2712	83	0
4	D	985	0	1006	126	0
5	E	1715	0	1733	45	0
6	F	610	0	642	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1337	0	1306	113	0
8	H	1186	0	1147	31	0
9	I	848	0	812	55	0
10	J	512	0	526	20	0
11	K	822	0	810	49	0
12	L	388	0	395	16	0
13	M	1612	0	1572	36	0
14	N	1128	0	1181	37	0
15	O	3546	0	3585	157	0
16	P	1008	0	998	60	0
17	Q	724	0	734	54	0
18	R	86	0	44	11	0
19	X	449	0	251	26	0
20	Y	447	0	248	31	0
21	A	1	0	0	0	0
22	A	2	0	0	1	0
22	B	1	0	0	0	0
22	I	2	0	0	0	0
22	J	1	0	0	2	0
22	L	1	0	0	0	0
23	P	8	0	0	4	0
All	All	39474	0	39369	1384	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 18.

All (1384) 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)
1:A:1116:TYR:CE1	9:I:43:TYR:HE1	1.36	1.43
8:H:76:ASN:HD21	11:K:87:ARG:CZ	1.29	1.42
8:H:78:THR:CB	11:K:87:ARG:HH22	1.34	1.39
1:A:1116:TYR:CE1	9:I:43:TYR:CE1	2.14	1.35
1:A:1116:TYR:CD1	9:I:43:TYR:CE1	2.12	1.35
1:A:1140:LEU:CD2	9:I:52:VAL:HG11	1.61	1.31
1:A:1117:ILE:CG2	9:I:42:LYS:HB3	1.59	1.31
1:A:1112:GLU:OE1	9:I:47:LYS:CD	1.84	1.26
2:B:721:LYS:CE	2:B:731:GLU:OE2	1.84	1.26
10:J:7:CYS:SG	10:J:10:CYS:SG	2.34	1.26
3:C:263:GLU:OE2	3:C:274:ARG:HD3	1.26	1.25
2:B:721:LYS:HE2	2:B:731:GLU:OE2	1.10	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1119:GLU:OE1	9:I:40:ASN:HB3	1.37	1.24
15:O:409:ILE:CD1	15:O:423:LEU:HD11	1.68	1.23
15:O:356:GLU:OE1	17:Q:39:PRO:HD3	1.33	1.22
15:O:374:HIS:HB3	15:O:423:LEU:CD1	1.70	1.22
1:A:1118:GLU:CG	9:I:41:ARG:HG2	1.68	1.21
15:O:409:ILE:CG1	15:O:423:LEU:HD11	1.68	1.21
15:O:409:ILE:CG2	15:O:423:LEU:HD21	1.72	1.18
15:O:410:PRO:HB2	15:O:419:ARG:NH2	1.59	1.18
1:A:1140:LEU:HD23	9:I:52:VAL:HG11	1.17	1.17
1:A:1118:GLU:HG2	9:I:41:ARG:CG	1.76	1.16
15:O:409:ILE:HG13	15:O:423:LEU:CD1	1.76	1.16
8:H:78:THR:OG1	11:K:87:ARG:NH2	1.79	1.15
3:C:287:ILE:HD11	3:C:293:LEU:HB3	1.26	1.15
15:O:409:ILE:H	15:O:410:PRO:CD	1.60	1.13
15:O:409:ILE:HG13	15:O:423:LEU:HD11	1.28	1.13
10:J:26:GLN:HA	10:J:26:GLN:HE21	1.00	1.13
4:D:48:GLU:HB3	7:G:103:PHE:HB3	1.24	1.12
8:H:78:THR:CB	11:K:87:ARG:NH2	2.10	1.12
8:H:76:ASN:HD21	11:K:87:ARG:NH2	1.48	1.11
17:Q:106:LEU:HD12	17:Q:107:PRO:HD2	1.25	1.11
15:O:356:GLU:HG3	16:P:284:ARG:HB2	1.32	1.11
15:O:409:ILE:N	15:O:410:PRO:HD2	1.58	1.11
15:O:374:HIS:HB3	15:O:423:LEU:HD12	1.18	1.11
15:O:410:PRO:CB	15:O:419:ARG:HH21	1.62	1.10
1:A:1117:ILE:HG23	9:I:42:LYS:HB3	1.33	1.10
8:H:76:ASN:ND2	11:K:87:ARG:CZ	2.15	1.10
15:O:409:ILE:CB	15:O:423:LEU:HD21	1.83	1.09
15:O:352:SER:O	15:O:356:GLU:HG2	1.51	1.08
7:G:148:ILE:HG23	7:G:190:ILE:CG2	1.83	1.08
10:J:10:CYS:SG	22:J:2000:ZN:ZN	1.42	1.08
1:A:1112:GLU:OE1	9:I:47:LYS:HD3	0.92	1.07
1:A:1117:ILE:HG23	9:I:42:LYS:CB	1.84	1.07
8:H:78:THR:HB	11:K:87:ARG:NH1	1.69	1.07
15:O:410:PRO:HB2	15:O:419:ARG:HH21	0.93	1.07
4:D:39:GLN:HG3	7:G:32:LYS:HZ3	1.14	1.06
8:H:78:THR:HB	11:K:87:ARG:HH12	1.19	1.06
1:A:596:THR:HG21	8:H:119:GLY:O	1.54	1.05
18:R:11:G:N2	20:Y:17:DC:C5	2.27	1.03
4:D:11:LEU:HD23	4:D:11:LEU:H	1.18	1.02
4:D:85:GLN:HE22	7:G:84:ILE:H	1.06	1.02
16:P:299:GLY:HA2	16:P:303:SER:CB	1.89	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:407:GLN:HB3	15:O:422:TYR:HB3	1.41	1.01
1:A:51:LEU:HD22	1:A:51:LEU:H	1.24	1.00
15:O:445:ASN:ND2	16:P:304:PRO:HG3	1.75	1.00
4:D:39:GLN:HG3	7:G:32:LYS:CB	1.90	1.00
15:O:409:ILE:HG21	15:O:423:LEU:HD21	1.39	1.00
1:A:1117:ILE:CG2	9:I:42:LYS:CB	2.39	1.00
8:H:78:THR:HB	11:K:87:ARG:NH2	1.75	1.00
1:A:159:CYS:SG	22:A:1903:ZN:ZN	1.49	0.99
4:D:39:GLN:CG	7:G:32:LYS:HB3	1.92	0.99
1:A:1117:ILE:HG22	9:I:42:LYS:HB3	1.41	0.99
4:D:39:GLN:HG3	7:G:32:LYS:HB3	0.99	0.99
1:A:37:VAL:HG11	17:Q:28:PRO:HD3	1.44	0.98
7:G:148:ILE:HG23	7:G:190:ILE:HG23	1.41	0.98
8:H:78:THR:HB	11:K:87:ARG:CZ	1.93	0.98
2:B:276:GLN:HA	2:B:276:GLN:HE21	1.25	0.98
1:A:1116:TYR:HD1	9:I:43:TYR:CE1	1.73	0.98
4:D:39:GLN:CG	7:G:32:LYS:HZ3	1.75	0.98
1:A:180:LYS:NZ	1:A:182:ASN:OD1	1.96	0.98
15:O:377:GLN:HB3	15:O:421:PHE:HZ	1.27	0.97
1:A:258:PRO:HB3	1:A:262:ILE:HD11	1.47	0.97
10:J:26:GLN:HA	10:J:26:GLN:NE2	1.71	0.97
17:Q:27:LEU:HD22	17:Q:27:LEU:H	1.26	0.96
18:R:11:G:H1	20:Y:17:DC:H41	1.13	0.96
15:O:409:ILE:HD12	15:O:423:LEU:HD11	1.48	0.96
16:P:300:GLY:H	16:P:303:SER:HB3	1.30	0.96
20:Y:5:DC:H2''	20:Y:6:DT:H5'	1.48	0.96
1:A:1140:LEU:HD23	9:I:52:VAL:CG1	1.95	0.96
19:X:43:DC:C6	19:X:44:DT:H72	2.01	0.95
1:A:1116:TYR:HD1	9:I:43:TYR:CD1	1.83	0.95
1:A:1125:ASP:H	9:I:21:HIS:CE1	1.85	0.95
15:O:409:ILE:H	15:O:410:PRO:HD2	0.79	0.93
16:P:284:ARG:HA	16:P:284:ARG:NE	1.80	0.93
1:A:587:THR:HG21	8:H:119:GLY:HA3	1.45	0.93
12:L:34:ILE:HD12	12:L:34:ILE:H	1.34	0.93
1:A:1140:LEU:CD2	9:I:52:VAL:CG1	2.47	0.92
8:H:76:ASN:ND2	11:K:87:ARG:NH2	2.14	0.92
16:P:299:GLY:HA2	16:P:303:SER:HB3	1.51	0.92
15:O:412:THR:HB	15:O:419:ARG:HA	1.50	0.92
3:C:288:PHE:HA	3:C:294:LYS:HG2	1.53	0.91
4:D:85:GLN:NE2	7:G:83:GLU:HA	1.84	0.91
2:B:306:ILE:HD13	2:B:306:ILE:H	1.36	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:78:THR:HB	11:K:87:ARG:HH22	1.28	0.91
2:B:249:GLN:HE22	14:N:144:LYS:HE3	1.35	0.91
15:O:409:ILE:HB	15:O:423:LEU:HD21	1.49	0.91
18:R:11:G:H22	20:Y:17:DC:H5	1.19	0.91
4:D:17:PHE:HB2	4:D:53:ILE:HG21	1.53	0.91
1:A:1116:TYR:CD1	9:I:43:TYR:CD1	2.58	0.90
2:B:282:GLN:NE2	13:M:146:ASP:OD2	2.04	0.90
4:D:11:LEU:H	4:D:11:LEU:CD2	1.84	0.90
4:D:4:LYS:HE2	4:D:4:LYS:HA	1.52	0.90
5:E:61:LEU:H	5:E:61:LEU:HD22	1.35	0.90
16:P:284:ARG:HA	16:P:284:ARG:HE	1.33	0.90
3:C:9:GLU:OE2	3:C:298:ARG:NH1	2.05	0.90
4:D:97:ILE:HA	4:D:101:VAL:HB	1.54	0.89
17:Q:106:LEU:HD12	17:Q:107:PRO:CD	2.00	0.89
15:O:407:GLN:O	15:O:410:PRO:HD2	1.73	0.89
1:A:1116:TYR:HE1	9:I:43:TYR:HE1	0.88	0.88
4:D:48:GLU:CB	7:G:103:PHE:HB3	2.04	0.87
17:Q:27:LEU:H	17:Q:27:LEU:CD2	1.86	0.87
4:D:48:GLU:HB3	7:G:103:PHE:O	1.74	0.86
10:J:10:CYS:HG	22:J:2000:ZN:ZN	0.55	0.86
1:A:1143:GLU:OE2	5:E:2:ASP:OD1	1.91	0.86
1:A:1112:GLU:CD	9:I:47:LYS:HD3	2.00	0.85
1:A:461:LEU:HD21	2:B:1063:LEU:HD21	1.58	0.85
4:D:11:LEU:HD21	7:G:3:VAL:HA	1.58	0.85
15:O:377:GLN:HB3	15:O:421:PHE:CZ	2.10	0.85
15:O:407:GLN:O	15:O:410:PRO:CD	2.24	0.85
4:D:43:ASN:H	4:D:43:ASN:HD22	1.25	0.85
15:O:374:HIS:CB	15:O:423:LEU:HD12	2.06	0.85
1:A:1146:ALA:HB2	1:A:1171:ALA:HA	1.58	0.84
15:O:409:ILE:HG13	15:O:423:LEU:CG	2.06	0.84
2:B:276:GLN:HA	2:B:276:GLN:NE2	1.90	0.83
4:D:58:CYS:HA	4:D:61:GLN:HB2	1.60	0.83
18:R:11:G:N2	20:Y:17:DC:H5	1.72	0.83
1:A:1092:ASP:OD1	1:A:1092:ASP:N	2.11	0.83
4:D:11:LEU:HD23	4:D:11:LEU:N	1.91	0.83
2:B:25:GLU:OE2	2:B:25:GLU:HA	1.79	0.82
3:C:287:ILE:CD1	3:C:293:LEU:HB3	2.09	0.82
8:H:78:THR:CB	11:K:87:ARG:HH12	1.91	0.82
15:O:415:HIS:O	15:O:419:ARG:HG3	1.78	0.82
5:E:111:THR:HG21	19:X:44:DT:OP2	1.79	0.82
1:A:1116:TYR:HE1	9:I:43:TYR:CE1	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:SER:HB2	15:O:373:LYS:HE3	1.62	0.82
2:B:991:SER:HB2	2:B:998:LEU:HD21	1.61	0.81
7:G:148:ILE:HG23	7:G:190:ILE:HG21	1.60	0.81
15:O:409:ILE:HB	15:O:423:LEU:CD2	2.09	0.81
1:A:115:ILE:HD11	1:A:234:ASP:O	1.80	0.81
1:A:1051:LYS:HE3	1:A:1051:LYS:O	1.80	0.81
16:P:299:GLY:HA2	16:P:303:SER:HB2	1.61	0.81
19:X:37:DG:H2'	19:X:38:DA:C8	2.16	0.81
2:B:507:GLU:CD	2:B:507:GLU:H	1.87	0.81
15:O:407:GLN:CB	15:O:422:TYR:HB3	2.10	0.81
4:D:39:GLN:CG	7:G:32:LYS:NZ	2.43	0.80
4:D:85:GLN:HE22	7:G:84:ILE:N	1.77	0.80
3:C:263:GLU:OE2	3:C:274:ARG:CD	2.21	0.80
3:C:287:ILE:HD11	3:C:293:LEU:CB	2.10	0.80
1:A:1261:GLU:HG3	5:E:193:ILE:HD13	1.61	0.80
3:C:78:ARG:HE	11:K:50:THR:HG22	1.46	0.80
19:X:39:DG:H2''	19:X:40:DC:H5'	1.62	0.79
4:D:39:GLN:HG3	7:G:32:LYS:NZ	1.97	0.79
1:A:1121:PHE:HE2	9:I:14:VAL:HG21	1.46	0.79
1:A:1117:ILE:HG23	9:I:42:LYS:HB2	1.64	0.78
1:A:1118:GLU:HG2	9:I:41:ARG:HG2	0.85	0.78
4:D:48:GLU:OE1	7:G:103:PHE:CG	2.35	0.78
1:A:587:THR:CG2	8:H:119:GLY:HA3	2.13	0.78
15:O:356:GLU:CG	16:P:284:ARG:HB2	2.13	0.78
1:A:59:ARG:HG3	1:A:70:GLU:HB2	1.65	0.77
2:B:213:ARG:HB3	2:B:213:ARG:HH21	1.49	0.77
4:D:10:LEU:HD23	4:D:10:LEU:O	1.83	0.77
1:A:1112:GLU:O	9:I:46:LEU:CD2	2.32	0.77
16:P:300:GLY:N	16:P:303:SER:HB3	1.97	0.77
2:B:361:ARG:HD2	2:B:591:ARG:HG2	1.64	0.77
4:D:54:SER:HA	4:D:59:ARG:NH1	2.00	0.77
1:A:1055:PHE:HA	1:A:1062:ASN:HA	1.67	0.76
2:B:578:LEU:HD23	2:B:578:LEU:H	1.49	0.76
1:A:322:ASN:C	1:A:322:ASN:HD22	1.93	0.76
4:D:107:ARG:HH21	17:Q:82:GLN:CD	1.92	0.76
15:O:445:ASN:OD1	23:P:401:SF4:S2	2.43	0.76
5:E:79:GLU:H	5:E:79:GLU:CD	1.92	0.76
7:G:151:ARG:HD2	7:G:151:ARG:O	1.85	0.76
3:C:239:ILE:HD12	3:C:239:ILE:H	1.50	0.76
1:A:1233:ARG:HD3	5:E:134:GLU:HG2	1.67	0.76
2:B:721:LYS:NZ	2:B:731:GLU:OE2	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:45:ILE:HB	7:G:36:ASN:OD1	1.85	0.75
17:Q:106:LEU:CD1	17:Q:107:PRO:HD2	2.13	0.75
2:B:236:ILE:HA	2:B:239:ILE:HD12	1.68	0.75
17:Q:27:LEU:HD22	17:Q:27:LEU:N	2.00	0.75
19:X:24:DT:H2'	19:X:24:DT:O2	1.87	0.75
5:E:84:ILE:HD12	5:E:84:ILE:H	1.51	0.75
1:A:586:PRO:HG3	1:A:595:TRP:CZ2	2.21	0.75
1:A:1119:GLU:CD	1:A:1119:GLU:H	1.94	0.75
2:B:506:MET:HG3	2:B:587:SER:HB2	1.68	0.75
6:F:82:GLU:O	6:F:82:GLU:HG2	1.84	0.75
1:A:1112:GLU:O	9:I:46:LEU:HD23	1.87	0.75
3:C:65:MET:HE2	3:C:68:ILE:HG21	1.69	0.74
15:O:356:GLU:OE1	17:Q:39:PRO:CD	2.26	0.74
16:P:293:PHE:HE2	16:P:307:CYS:HB2	1.51	0.74
2:B:995:GLY:O	3:C:233:TYR:OH	2.04	0.74
3:C:288:PHE:O	3:C:294:LYS:HD3	1.87	0.74
7:G:99:VAL:HG21	7:G:148:ILE:HD11	1.70	0.74
2:B:619:ARG:CZ	2:B:619:ARG:HB3	2.17	0.74
12:L:25:GLU:H	12:L:25:GLU:CD	1.95	0.74
3:C:163:TYR:CE1	3:C:204:PRO:HD3	2.23	0.74
4:D:48:GLU:CB	7:G:103:PHE:O	2.35	0.74
7:G:32:LYS:HZ3	7:G:32:LYS:HB3	1.52	0.74
8:H:78:THR:HG1	11:K:87:ARG:NH2	1.83	0.74
1:A:45:ASP:HB2	1:A:50:PRO:HD2	1.68	0.73
7:G:79:PRO:HG2	7:G:150:PHE:CE2	2.24	0.73
1:A:98:PHE:HE2	1:A:168:LYS:HD3	1.53	0.73
1:A:1121:PHE:CE2	9:I:14:VAL:HG21	2.23	0.73
5:E:55:ARG:H	5:E:55:ARG:HD3	1.52	0.73
2:B:542:ASN:N	2:B:542:ASN:HD22	1.86	0.73
3:C:163:TYR:CD1	3:C:204:PRO:HD3	2.24	0.73
10:J:10:CYS:SG	10:J:44:CYS:SG	2.87	0.72
1:A:17:HIS:CD2	1:A:1337:LYS:HG3	2.24	0.72
1:A:544:ASP:HA	1:A:547:THR:HG22	1.70	0.72
4:D:77:LYS:O	4:D:77:LYS:HG3	1.90	0.72
3:C:135:ILE:H	3:C:135:ILE:HD12	1.54	0.72
12:L:26:ASN:HB2	12:L:44:MET:HE1	1.71	0.72
8:H:78:THR:CB	11:K:87:ARG:NH1	2.50	0.71
15:O:357:ARG:NH1	16:P:288:GLY:O	2.23	0.71
2:B:236:ILE:HD11	2:B:265:PHE:HE1	1.55	0.71
2:B:249:GLN:HE22	14:N:144:LYS:CE	2.02	0.71
1:A:941:SER:HB3	1:A:980:ILE:HG21	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:874:ASN:OD1	2:B:874:ASN:N	2.23	0.71
7:G:151:ARG:HD2	7:G:151:ARG:C	2.16	0.71
4:D:1:MET:HA	4:D:1:MET:HE2	1.71	0.70
1:A:115:ILE:HG13	1:A:234:ASP:HB3	1.71	0.70
1:A:303:THR:H	15:O:377:GLN:HE22	1.38	0.70
13:M:227:CYS:O	13:M:228:PRO:C	2.34	0.70
4:D:39:GLN:HG2	7:G:32:LYS:NZ	2.07	0.69
1:A:738:GLN:HA	1:A:747:THR:HG21	1.74	0.69
5:E:111:THR:CG2	19:X:44:DT:OP2	2.41	0.69
1:A:36:VAL:O	1:A:36:VAL:HG12	1.93	0.69
2:B:733:LEU:HD23	2:B:733:LEU:H	1.58	0.69
4:D:1:MET:O	4:D:1:MET:SD	2.51	0.69
20:Y:10:DG:H2''	20:Y:11:DT:H5'	1.73	0.69
15:O:356:GLU:HG3	16:P:284:ARG:CB	2.18	0.69
15:O:409:ILE:HG21	15:O:423:LEU:CD2	2.18	0.69
20:Y:11:DT:H2''	20:Y:12:DC:C5	2.28	0.69
1:A:51:LEU:HD13	1:A:51:LEU:N	2.08	0.68
1:A:1129:LEU:O	1:A:1129:LEU:HD23	1.93	0.68
8:H:76:ASN:HD21	11:K:87:ARG:NE	1.88	0.68
15:O:409:ILE:HG13	15:O:423:LEU:HG	1.75	0.68
1:A:119:GLN:OE1	1:A:119:GLN:N	2.26	0.68
4:D:48:GLU:HB3	7:G:103:PHE:CB	2.15	0.68
1:A:479:ARG:NH2	1:A:479:ARG:HB3	2.09	0.68
1:A:822:GLU:CD	1:A:822:GLU:H	2.01	0.68
2:B:236:ILE:HD11	2:B:265:PHE:CE1	2.28	0.68
1:A:816:ARG:HD3	1:A:823:LYS:HG2	1.75	0.68
1:A:1230:ASP:OD1	1:A:1230:ASP:N	2.25	0.68
5:E:47:LYS:N	5:E:48:PRO:HD2	2.09	0.68
5:E:55:ARG:HD3	5:E:55:ARG:N	2.09	0.68
1:A:102:ILE:HD13	1:A:168:LYS:HB2	1.75	0.67
2:B:119:TYR:HD1	2:B:119:TYR:H	1.40	0.67
1:A:213:ARG:H	1:A:213:ARG:HD2	1.59	0.67
16:P:299:GLY:CA	16:P:303:SER:HB3	2.24	0.67
2:B:30:LEU:HD13	2:B:499:MET:HG3	1.74	0.67
15:O:357:ARG:HG2	16:P:289:LEU:HA	1.76	0.67
15:O:412:THR:CB	15:O:419:ARG:HA	2.24	0.67
2:B:1080:CYS:SG	2:B:1083:CYS:SG	2.93	0.67
1:A:880:GLU:HG3	1:A:1343:VAL:HG22	1.75	0.67
15:O:445:ASN:HD22	16:P:304:PRO:HG3	1.59	0.67
19:X:43:DC:N3	20:Y:1:DG:N2	2.40	0.67
1:A:5:GLN:OE1	1:A:5:GLN:N	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:11:DT:H2'	20:Y:11:DT:O2	1.95	0.66
1:A:1128:ILE:HG23	1:A:1176:THR:HG23	1.76	0.66
13:M:238:LEU:HD13	14:N:341:LEU:HG	1.77	0.66
10:J:26:GLN:HE21	10:J:26:GLN:CA	1.82	0.66
20:Y:12:DC:H2'	20:Y:13:DT:H71	1.78	0.66
13:M:49:ILE:HD13	14:N:363:VAL:HG11	1.78	0.65
1:A:213:ARG:HD2	1:A:213:ARG:N	2.12	0.65
2:B:59:MET:HE2	2:B:80:ILE:HG13	1.78	0.65
1:A:154:ASN:HB3	1:A:162:PHE:HE1	1.61	0.65
1:A:942:LYS:HD3	1:A:981:LYS:HB2	1.79	0.65
1:A:224:LEU:HD22	1:A:228:LYS:HE3	1.78	0.65
2:B:259:GLU:H	2:B:259:GLU:CD	2.04	0.65
2:B:733:LEU:HD23	2:B:733:LEU:N	2.11	0.65
1:A:383:PRO:HB3	1:A:484:ARG:HA	1.79	0.65
1:A:479:ARG:HB3	1:A:479:ARG:HH21	1.60	0.65
2:B:364:LEU:HD21	2:B:502:ILE:HD12	1.78	0.65
2:B:242:ALA:HB1	2:B:284:LEU:HD23	1.78	0.65
17:Q:86:ARG:NH1	17:Q:86:ARG:HB2	2.12	0.65
5:E:84:ILE:HD13	19:X:44:DT:H3'	1.77	0.65
10:J:26:GLN:NE2	10:J:26:GLN:CA	2.49	0.65
1:A:1178:ARG:HG3	1:A:1189:LEU:HD21	1.78	0.64
1:A:438:GLU:OE1	1:A:438:GLU:N	2.27	0.64
2:B:23:VAL:O	2:B:23:VAL:HG23	1.97	0.64
3:C:139:GLN:HG2	3:C:211:LEU:HD11	1.79	0.64
1:A:193:PHE:CD1	1:A:193:PHE:C	2.76	0.64
1:A:997:PRO:HB2	1:A:1000:LEU:HD23	1.78	0.63
1:A:1094:ASP:OD1	1:A:1094:ASP:N	2.32	0.63
4:D:73:LEU:HD13	4:D:83:LYS:HB2	1.78	0.63
16:P:220:ILE:HD11	16:P:271:ARG:HD2	1.80	0.63
1:A:38:SER:HB2	1:A:54:GLY:HA2	1.78	0.63
1:A:386:VAL:HG23	2:B:1020:MET:HE2	1.80	0.63
3:C:288:PHE:HA	3:C:294:LYS:CG	2.27	0.63
4:D:41:ASN:OD1	4:D:41:ASN:N	2.30	0.63
16:P:293:PHE:CE1	17:Q:31:VAL:HG12	2.33	0.63
1:A:17:HIS:CD2	1:A:17:HIS:O	2.52	0.63
2:B:750:ASP:HA	2:B:754:ALA:HB3	1.80	0.63
4:D:107:ARG:NH2	17:Q:82:GLN:HG2	2.13	0.63
12:L:34:ILE:HG22	12:L:44:MET:HG3	1.80	0.63
1:A:17:HIS:HB2	1:A:1337:LYS:HE2	1.80	0.63
1:A:1048:MET:HA	1:A:1280:MET:CE	2.28	0.63
4:D:17:PHE:HB2	4:D:53:ILE:CG2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:407:GLN:CG	15:O:422:TYR:HB3	2.29	0.63
1:A:569:ALA:HA	1:A:572:LEU:HD12	1.80	0.63
3:C:270:LYS:NZ	3:C:270:LYS:HB3	2.13	0.63
1:A:864:LYS:HZ2	1:A:1048:MET:HB2	1.63	0.63
11:K:58:MET:HE3	11:K:58:MET:HA	1.81	0.63
1:A:193:PHE:C	1:A:193:PHE:HD1	2.07	0.62
2:B:204:THR:HG23	2:B:213:ARG:HG2	1.81	0.62
2:B:527:CYS:O	2:B:527:CYS:SG	2.57	0.62
3:C:54:VAL:CG1	3:C:62:GLU:HG2	2.29	0.62
1:A:53:TYR:O	1:A:53:TYR:HD1	1.81	0.62
1:A:136:TYR:HD1	1:A:136:TYR:O	1.81	0.62
1:A:171:LEU:HD22	1:A:327:GLY:O	1.99	0.62
3:C:102:GLN:OE1	3:C:102:GLN:N	2.32	0.62
4:D:2:GLU:H	4:D:2:GLU:CD	2.07	0.62
7:G:79:PRO:CG	7:G:150:PHE:CE2	2.82	0.62
4:D:107:ARG:HH21	17:Q:82:GLN:CG	2.12	0.62
13:M:248:MET:HE1	14:N:276:PRO:HA	1.81	0.62
15:O:159:ARG:HA	15:O:235:TRP:HB3	1.80	0.62
1:A:328:ILE:HD12	1:A:328:ILE:H	1.64	0.62
1:A:484:ARG:HH11	1:A:484:ARG:HB3	1.64	0.62
2:B:507:GLU:CD	2:B:507:GLU:N	2.58	0.62
2:B:1095:CYS:O	2:B:1097:SER:N	2.28	0.62
1:A:98:PHE:CE2	1:A:168:LYS:HD3	2.34	0.62
2:B:549:ILE:HD12	2:B:549:ILE:O	2.00	0.62
2:B:991:SER:HB2	2:B:998:LEU:CD2	2.29	0.62
3:C:134:GLU:HG2	3:C:181:GLN:HG3	1.82	0.62
1:A:197:PHE:HD1	1:A:197:PHE:O	1.82	0.62
1:A:1112:GLU:O	9:I:46:LEU:HD22	2.00	0.62
4:D:14:TYR:HD2	4:D:18:GLN:HE21	1.47	0.62
18:R:10:U:H3'	18:R:11:G:H8	1.65	0.62
1:A:1369:ASP:OD1	7:G:23:ASN:ND2	2.33	0.61
2:B:685:TYR:HB3	2:B:689:MET:HE3	1.81	0.61
1:A:322:ASN:C	1:A:322:ASN:ND2	2.58	0.61
16:P:199:LYS:NZ	16:P:245:ASP:O	2.32	0.61
1:A:107:MET:O	1:A:116:MET:HG2	1.99	0.61
1:A:474:MET:HE1	1:A:539:ILE:HD11	1.81	0.61
3:C:187:GLU:H	3:C:187:GLU:CD	2.09	0.61
4:D:20:LEU:HD11	4:D:46:THR:HB	1.82	0.61
8:H:78:THR:CB	11:K:87:ARG:CZ	2.66	0.61
16:P:293:PHE:CE2	16:P:307:CYS:HB2	2.34	0.61
1:A:1360:PHE:CZ	6:F:61:GLU:HA	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:GLU:HA	9:I:40:ASN:O	2.01	0.61
7:G:151:ARG:HG3	7:G:152:VAL:HG13	1.82	0.61
1:A:57:ASP:C	1:A:59:ARG:H	2.08	0.61
1:A:591:PRO:HG2	8:H:47:ILE:HD12	1.82	0.61
1:A:822:GLU:HG2	1:A:825:SER:HB2	1.82	0.61
15:O:91:TYR:OH	15:O:243:HIS:NE2	2.33	0.61
1:A:51:LEU:H	1:A:51:LEU:CD2	1.95	0.60
2:B:876:GLU:OE1	2:B:876:GLU:N	2.31	0.60
15:O:507:ASN:ND2	17:Q:55:GLU:OE2	2.34	0.60
1:A:7:ARG:HD3	1:A:7:ARG:C	2.27	0.60
1:A:149:LYS:O	1:A:153:LYS:HG3	2.01	0.60
2:B:758:ASN:HB3	2:B:916:MET:SD	2.40	0.60
16:P:302:ILE:HG22	16:P:302:ILE:O	2.00	0.60
1:A:48:HIS:CG	1:A:48:HIS:O	2.54	0.60
1:A:1120:VAL:HG22	9:I:39:THR:HG22	1.84	0.60
1:A:57:ASP:O	1:A:59:ARG:N	2.35	0.60
1:A:102:ILE:HG23	1:A:166:VAL:HG12	1.84	0.60
2:B:916:MET:HG2	2:B:925:PRO:HD2	1.84	0.60
2:B:348:ASP:OD1	2:B:348:ASP:N	2.32	0.60
1:A:120:GLU:CD	1:A:120:GLU:C	2.70	0.60
1:A:985:ASP:HA	1:A:989:ILE:HG12	1.83	0.60
1:A:1261:GLU:OE2	5:E:207:ARG:NH2	2.31	0.60
12:L:34:ILE:HD12	12:L:34:ILE:N	2.12	0.60
1:A:38:SER:C	17:Q:24:GLY:HA2	2.27	0.60
1:A:1073:ILE:HG21	1:A:1271:ILE:HG13	1.84	0.60
1:A:414:VAL:HG12	1:A:416:PRO:HD2	1.84	0.60
2:B:542:ASN:HD22	2:B:542:ASN:H	1.48	0.60
1:A:7:ARG:N	7:G:38:VAL:O	2.29	0.59
1:A:953:MET:HA	1:A:953:MET:HE2	1.85	0.59
1:A:1087:ALA:HB3	1:A:1225:LEU:HD12	1.84	0.59
1:A:1159:ARG:NH1	19:X:41:DC:OP1	2.35	0.59
1:A:1208:SER:O	1:A:1209:ARG:HB2	2.01	0.59
4:D:107:ARG:HH21	17:Q:82:GLN:HG2	1.66	0.59
1:A:1048:MET:CB	1:A:1280:MET:HE1	2.32	0.59
1:A:1128:ILE:HD13	1:A:1128:ILE:C	2.27	0.59
4:D:108:LEU:O	4:D:113:ILE:HG22	2.02	0.59
10:J:19:GLU:CD	10:J:19:GLU:H	2.09	0.59
1:A:136:TYR:CD1	1:A:136:TYR:C	2.81	0.59
1:A:1220:LYS:O	1:A:1220:LYS:HG2	2.02	0.59
2:B:59:MET:HE1	2:B:78:LEU:C	2.26	0.59
4:D:1:MET:O	4:D:1:MET:CG	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:9:ALA:HB2	7:G:3:VAL:HG23	1.85	0.59
17:Q:80:GLU:HA	17:Q:86:ARG:CD	2.33	0.59
1:A:1122:LEU:HG	1:A:1123:PRO:HD2	1.84	0.59
3:C:54:VAL:HG11	3:C:62:GLU:HG2	1.85	0.59
7:G:79:PRO:CG	7:G:150:PHE:CD2	2.86	0.59
1:A:84:GLY:O	1:A:257:VAL:N	2.33	0.59
15:O:445:ASN:HD21	16:P:304:PRO:HG3	1.64	0.59
1:A:586:PRO:HG3	1:A:595:TRP:CH2	2.37	0.59
1:A:1155:THR:HG23	1:A:1155:THR:O	2.02	0.59
2:B:1095:CYS:O	2:B:1095:CYS:SG	2.61	0.59
15:O:364:ARG:NH2	15:O:384:ALA:O	2.35	0.59
1:A:737:GLN:N	1:A:737:GLN:OE1	2.34	0.59
1:A:1140:LEU:HD21	9:I:52:VAL:HG11	1.75	0.59
1:A:53:TYR:O	1:A:53:TYR:CD1	2.56	0.58
3:C:163:TYR:CE1	3:C:204:PRO:CD	2.86	0.58
4:D:7:ASN:HD22	17:Q:78:PRO:HG3	1.67	0.58
4:D:110:GLU:OE2	4:D:110:GLU:HA	2.01	0.58
15:O:356:GLU:OE2	16:P:282:LEU:HD22	2.03	0.58
3:C:183:ASP:OD1	3:C:183:ASP:N	2.35	0.58
4:D:18:GLN:OE1	4:D:18:GLN:HA	2.02	0.58
2:B:24:GLU:OE1	2:B:24:GLU:HA	2.04	0.58
3:C:139:GLN:HB2	3:C:178:LEU:HD11	1.85	0.58
1:A:102:ILE:HG12	1:A:174:ILE:HG12	1.86	0.58
1:A:166:VAL:HG13	1:A:174:ILE:HG23	1.85	0.58
2:B:88:GLU:H	2:B:88:GLU:CD	2.11	0.58
2:B:259:GLU:OE1	2:B:259:GLU:N	2.27	0.58
1:A:17:HIS:CD2	1:A:1337:LYS:CG	2.87	0.58
3:C:316:LEU:N	3:C:316:LEU:HD23	2.18	0.58
1:A:136:TYR:HD1	1:A:136:TYR:C	2.12	0.58
15:O:284:PHE:HA	15:O:338:LEU:HB2	1.84	0.58
2:B:1051:GLU:OE1	2:B:1051:GLU:N	2.31	0.58
7:G:114:LEU:HD21	7:G:192:GLU:H	1.68	0.58
1:A:58:HIS:O	1:A:70:GLU:HG2	2.04	0.58
1:A:1076:ALA:HB3	1:A:1302:GLY:HA3	1.86	0.58
17:Q:113:ARG:HH21	17:Q:117:LYS:HA	1.67	0.58
1:A:331:ASN:O	1:A:331:ASN:ND2	2.37	0.58
4:D:43:ASN:H	4:D:43:ASN:ND2	1.96	0.58
4:D:54:SER:HA	4:D:59:ARG:CZ	2.34	0.58
7:G:112:GLU:OE1	7:G:119:LYS:NZ	2.37	0.58
8:H:78:THR:CG2	11:K:87:ARG:HH12	2.17	0.58
1:A:587:THR:HG23	1:A:599:GLN:CD	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:396:ARG:NH1	2:B:396:ARG:HB2	2.19	0.57
15:O:410:PRO:CB	15:O:419:ARG:NH2	2.40	0.57
20:Y:17:DC:H2'	20:Y:18:DA:O4'	2.03	0.57
1:A:137:LEU:HD21	1:A:1310:LYS:HA	1.85	0.57
1:A:1242:LYS:O	1:A:1242:LYS:HG3	2.01	0.57
2:B:721:LYS:NZ	2:B:731:GLU:CD	2.62	0.57
4:D:1:MET:HE2	4:D:1:MET:CA	2.31	0.57
4:D:6:ALA:O	7:G:5:VAL:HG22	2.03	0.57
7:G:99:VAL:CG2	7:G:148:ILE:HD11	2.34	0.57
13:M:249:LEU:HD13	14:N:389:PHE:CE1	2.38	0.57
2:B:542:ASN:HD21	2:B:587:SER:H	1.52	0.57
2:B:1047:LEU:HD13	2:B:1067:ARG:HG2	1.86	0.57
4:D:102:GLU:N	4:D:102:GLU:CD	2.62	0.57
13:M:227:CYS:O	13:M:229:GLY:N	2.37	0.57
7:G:32:LYS:HZ3	7:G:32:LYS:CB	2.17	0.57
2:B:118:GLU:HG3	2:B:127:ILE:HG12	1.87	0.57
7:G:122:GLU:OE2	7:G:129:TRP:NE1	2.37	0.57
15:O:419:ARG:HD2	15:O:422:TYR:CE2	2.39	0.57
3:C:158:ASP:OD1	3:C:158:ASP:N	2.38	0.57
10:J:21:TYR:HB2	10:J:38:LEU:HD11	1.86	0.57
1:A:93:PHE:H	1:A:314:GLN:HE22	1.51	0.57
1:A:328:ILE:H	1:A:328:ILE:CD1	2.16	0.57
12:L:19:CYS:HB3	12:L:36:CYS:SG	2.45	0.57
1:A:484:ARG:O	1:A:484:ARG:HG2	2.05	0.56
1:A:38:SER:HB2	1:A:54:GLY:CA	2.35	0.56
1:A:57:ASP:C	1:A:59:ARG:N	2.63	0.56
4:D:78:LEU:HD13	4:D:86:LEU:HD11	1.86	0.56
15:O:445:ASN:ND2	16:P:304:PRO:CG	2.59	0.56
1:A:39:LYS:HB2	1:A:41:LEU:H	1.71	0.56
1:A:1113:ILE:HB	1:A:1137:ILE:HD11	1.87	0.56
5:E:84:ILE:HG13	5:E:114:ALA:HA	1.88	0.56
10:J:53:VAL:O	10:J:53:VAL:HG13	2.05	0.56
11:K:35:THR:O	11:K:35:THR:HG22	2.06	0.56
1:A:91:PRO:HB3	1:A:251:ILE:HD11	1.87	0.56
15:O:113:ASN:HB2	15:O:116:LEU:HD21	1.86	0.56
1:A:328:ILE:HD12	1:A:328:ILE:N	2.21	0.56
1:A:1124:ASP:HA	9:I:21:HIS:CE1	2.41	0.56
3:C:162:LEU:HD23	3:C:162:LEU:O	2.05	0.56
15:O:409:ILE:CG1	15:O:423:LEU:CD1	2.47	0.56
1:A:1217:GLN:OE1	1:A:1217:GLN:N	2.38	0.56
4:D:100:MET:SD	7:G:147:GLU:OE1	2.64	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:83:LEU:N	6:F:83:LEU:HD23	2.21	0.56
16:P:309:TYR:OH	17:Q:32:LEU:O	2.24	0.56
9:I:3:LEU:HB3	14:N:143:GLU:HG3	1.88	0.56
11:K:60:MET:O	11:K:60:MET:HG3	2.06	0.56
19:X:43:DC:H2'	19:X:44:DT:C7	2.36	0.56
1:A:1119:GLU:CD	1:A:1119:GLU:N	2.63	0.56
2:B:597:ILE:HG13	2:B:659:ILE:HG12	1.88	0.56
17:Q:27:LEU:O	17:Q:28:PRO:C	2.48	0.56
1:A:41:LEU:HG	17:Q:21:PHE:HB3	1.89	0.55
2:B:259:GLU:CD	2:B:259:GLU:N	2.64	0.55
3:C:121:LEU:HD13	3:C:185:PHE:HE1	1.70	0.55
1:A:180:LYS:NZ	1:A:182:ASN:CG	2.64	0.55
2:B:508:ASP:HA	2:B:511:ILE:HD12	1.88	0.55
15:O:374:HIS:HB3	15:O:423:LEU:HD13	1.79	0.55
1:A:1048:MET:HA	1:A:1280:MET:HE1	1.88	0.55
2:B:30:LEU:HD22	2:B:663:THR:HG22	1.89	0.55
2:B:294:GLN:NE2	19:X:24:DT:H4'	2.22	0.55
9:I:105:ARG:NH2	9:I:106:TRP:O	2.39	0.55
20:Y:9:DA:H2''	20:Y:10:DG:H5'	1.89	0.55
20:Y:12:DC:C2'	20:Y:13:DT:H71	2.36	0.55
1:A:1235:VAL:HG12	1:A:1235:VAL:O	2.06	0.55
1:A:335:LYS:HD3	1:A:335:LYS:N	2.21	0.55
1:A:1009:THR:O	1:A:1012:GLU:HG3	2.06	0.55
1:A:1224:LYS:O	1:A:1224:LYS:HG3	2.06	0.55
5:E:46:ASP:HB3	5:E:48:PRO:HD2	1.87	0.55
15:O:265:GLU:OE1	15:O:268:ARG:NH1	2.39	0.55
1:A:7:ARG:HG3	7:G:34:LEU:CD1	2.37	0.55
1:A:370:SER:O	1:A:487:ARG:HA	2.06	0.55
1:A:529:LEU:HD23	1:A:539:ILE:HD12	1.88	0.55
1:A:1061:MET:CG	1:A:1061:MET:O	2.55	0.55
2:B:303:LYS:HA	2:B:303:LYS:HE2	1.89	0.55
18:R:11:G:H1	20:Y:17:DC:N4	1.96	0.55
2:B:249:GLN:NE2	14:N:144:LYS:HE3	2.15	0.55
15:O:99:TYR:OH	15:O:150:ARG:NH1	2.40	0.55
1:A:622:LYS:HD3	1:A:651:ASP:OD1	2.06	0.55
1:A:1357:THR:OG1	2:B:1061:SER:OG	2.22	0.55
4:D:42:LEU:HG	7:G:31:ASN:HB3	1.87	0.55
4:D:57:PRO:C	4:D:59:ARG:N	2.64	0.55
1:A:1124:ASP:HA	9:I:21:HIS:ND1	2.22	0.55
1:A:1232:LEU:HD13	1:A:1248:SER:HB2	1.89	0.55
2:B:725:ILE:HG23	2:B:730:PHE:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:107:ARG:NH2	17:Q:82:GLN:OE1	2.39	0.55
5:E:111:THR:HG21	19:X:44:DT:P	2.47	0.55
15:O:37:ARG:O	15:O:41:HIS:ND1	2.39	0.55
1:A:588:ILE:HB	1:A:594:LEU:HB2	1.88	0.54
1:A:1061:MET:O	1:A:1061:MET:SD	2.65	0.54
2:B:1062:MET:HE3	2:B:1062:MET:HA	1.89	0.54
9:I:3:LEU:HD13	14:N:143:GLU:HG3	1.89	0.54
15:O:410:PRO:HB3	15:O:422:TYR:CE2	2.42	0.54
16:P:283:VAL:O	16:P:283:VAL:HG13	2.07	0.54
16:P:290:CYS:SG	23:P:401:SF4:S4	3.04	0.54
1:A:164:GLY:HA3	1:A:177:GLU:CG	2.37	0.54
1:A:720:GLY:HA3	1:A:759:ILE:HD11	1.88	0.54
1:A:1053:PHE:CG	1:A:1053:PHE:O	2.60	0.54
15:O:86:LEU:HD21	15:O:443:ILE:HD13	1.89	0.54
15:O:357:ARG:HA	16:P:289:LEU:HD13	1.89	0.54
2:B:182:GLU:HG2	2:B:457:SER:HA	1.89	0.54
2:B:896:LYS:HD2	2:B:1012:LEU:HD12	1.89	0.54
11:K:30:VAL:HG11	11:K:35:THR:HG23	1.89	0.54
15:O:412:THR:OG1	15:O:420:THR:HG23	2.08	0.54
1:A:39:LYS:HB2	1:A:41:LEU:HB2	1.90	0.54
2:B:392:ILE:HD12	2:B:392:ILE:O	2.08	0.54
3:C:265:GLN:HG3	3:C:272:VAL:HG12	1.88	0.54
15:O:409:ILE:N	15:O:410:PRO:CD	2.35	0.54
16:P:202:PRO:O	16:P:205:GLN:NE2	2.37	0.54
19:X:26:DT:H4'	19:X:26:DT:OP1	2.07	0.54
1:A:501:ASP:HB2	2:B:904:LYS:HG3	1.90	0.54
2:B:784:ASN:N	2:B:784:ASN:OD1	2.38	0.54
4:D:39:GLN:HG2	7:G:32:LYS:CE	2.38	0.54
4:D:112:GLN:O	4:D:112:GLN:NE2	2.40	0.54
1:A:544:ASP:HA	1:A:547:THR:CG2	2.38	0.54
2:B:213:ARG:HH21	2:B:213:ARG:CB	2.18	0.54
2:B:759:LYS:HG3	2:B:910:ILE:HG22	1.90	0.54
7:G:154:ASP:OD1	7:G:154:ASP:N	2.39	0.54
11:K:27:LEU:HG	11:K:43:VAL:HB	1.90	0.54
13:M:245:TYR:CD2	14:N:344:VAL:HG21	2.43	0.54
1:A:1088:GLN:HB3	1:A:1242:LYS:HG2	1.88	0.54
4:D:39:GLN:HG2	7:G:32:LYS:HE2	1.90	0.54
4:D:96:GLU:O	4:D:101:VAL:N	2.36	0.54
1:A:1066:GLY:HA2	1:A:1278:HIS:CE1	2.43	0.54
2:B:233:ASP:N	2:B:233:ASP:OD1	2.41	0.54
3:C:246:GLU:HG2	3:C:272:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:227:LYS:O	16:P:240:ASN:ND2	2.41	0.54
19:X:43:DC:N4	20:Y:0:DA:N1	2.56	0.54
2:B:1080:CYS:HB3	2:B:1083:CYS:SG	2.48	0.53
15:O:407:GLN:O	15:O:410:PRO:CG	2.56	0.53
1:A:154:ASN:HB3	1:A:162:PHE:CE1	2.43	0.53
1:A:183:LYS:HD3	1:A:183:LYS:N	2.22	0.53
1:A:1045:GLY:HA2	1:A:1048:MET:HE3	1.90	0.53
1:A:1137:ILE:HD13	1:A:1137:ILE:N	2.24	0.53
2:B:526:LEU:HD12	2:B:526:LEU:O	2.09	0.53
15:O:239:LEU:HA	15:O:242:PHE:HD2	1.73	0.53
7:G:44:LEU:HB3	7:G:77:PHE:HB3	1.89	0.53
15:O:419:ARG:HD2	15:O:422:TYR:CZ	2.44	0.53
13:M:64:THR:HG21	13:M:96:LEU:HD13	1.89	0.53
1:A:987:TYR:OH	8:H:102:ASP:N	2.41	0.53
2:B:812:ASP:HB3	12:L:15:MET:HG3	1.89	0.53
4:D:35:HIS:HD2	7:G:32:LYS:HE3	1.73	0.53
1:A:42:TYR:O	1:A:43:SER:HB3	2.08	0.53
1:A:1125:ASP:N	9:I:21:HIS:CE1	2.66	0.53
11:K:48:ASP:N	11:K:48:ASP:OD1	2.40	0.53
15:O:115:LYS:HE2	15:O:160:CYS:HB2	1.89	0.53
19:X:43:DC:H2'	19:X:44:DT:H72	1.91	0.53
1:A:7:ARG:HE	4:D:1:MET:HG2	1.74	0.53
1:A:15:ILE:HD13	2:B:1126:LEU:HD22	1.90	0.53
1:A:1137:ILE:HD12	1:A:1142:LEU:HD11	1.89	0.53
2:B:705:ILE:HG22	2:B:705:ILE:O	2.08	0.53
4:D:62:SER:HB2	4:D:65:ILE:HG23	1.90	0.53
15:O:171:PRO:O	15:O:174:PRO:HD2	2.07	0.53
16:P:290:CYS:HB2	16:P:293:PHE:HB2	1.90	0.53
1:A:1186:TYR:CG	1:A:1186:TYR:O	2.62	0.53
2:B:375:ASP:OD1	2:B:375:ASP:C	2.52	0.53
3:C:266:GLU:OE1	3:C:266:GLU:N	2.35	0.53
16:P:286:PRO:HG2	16:P:313:TRP:CG	2.44	0.53
8:H:96:VAL:HG22	8:H:116:VAL:HG22	1.91	0.53
13:M:249:LEU:HD13	14:N:389:PHE:HE1	1.74	0.53
15:O:24:ILE:HD11	15:O:45:THR:HG21	1.90	0.53
1:A:37:VAL:O	1:A:37:VAL:HG22	2.08	0.52
1:A:547:THR:HG21	2:B:932:HIS:NE2	2.24	0.52
1:A:882:LEU:HB2	1:A:1034:GLY:HA3	1.91	0.52
1:A:952:ILE:HA	1:A:955:LYS:HD3	1.90	0.52
4:D:14:TYR:CE2	4:D:18:GLN:HG2	2.44	0.52
4:D:42:LEU:HD13	4:D:42:LEU:C	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:MET:HE2	1:A:1031:SER:HB2	1.90	0.52
1:A:1212:ILE:HD11	1:A:1223:TYR:HD2	1.74	0.52
7:G:32:LYS:CB	7:G:32:LYS:NZ	2.72	0.52
15:O:409:ILE:CG1	15:O:423:LEU:CG	2.84	0.52
1:A:51:LEU:HG	1:A:58:HIS:CD2	2.45	0.52
2:B:384:MET:HG2	2:B:402:VAL:HG12	1.91	0.52
4:D:39:GLN:CG	7:G:32:LYS:CE	2.87	0.52
13:M:33:ARG:HD2	13:M:37:MET:HB2	1.91	0.52
16:P:286:PRO:HG3	17:Q:38:PHE:CD2	2.44	0.52
1:A:51:LEU:HB3	1:A:56:LEU:O	2.09	0.52
1:A:886:TYR:HB3	6:F:53:THR:HG22	1.91	0.52
1:A:1073:ILE:O	1:A:1294:MET:HE1	2.10	0.52
1:A:1161:LYS:N	1:A:1162:PRO:HD2	2.25	0.52
3:C:130:GLU:CD	3:C:130:GLU:H	2.15	0.52
11:K:47:GLU:OE1	11:K:47:GLU:HA	2.08	0.52
1:A:463:ASN:HB2	1:A:473:ILE:HG12	1.90	0.52
4:D:4:LYS:HE2	4:D:4:LYS:CA	2.31	0.52
4:D:59:ARG:NE	4:D:59:ARG:H	2.07	0.52
5:E:77:PRO:HG3	5:E:90:TYR:HE2	1.74	0.52
6:F:107:ARG:O	6:F:107:ARG:HG3	2.09	0.52
8:H:63:THR:HB	8:H:70:LEU:HD13	1.91	0.52
12:L:57:ALA:O	12:L:58:ARG:C	2.53	0.52
13:M:11:GLN:HB2	14:N:331:ILE:HD12	1.92	0.52
15:O:127:ASP:HB3	15:O:128:ARG:HH11	1.75	0.52
1:A:151:ARG:HG3	1:A:151:ARG:HH11	1.74	0.52
4:D:48:GLU:OE1	7:G:103:PHE:CB	2.57	0.52
4:D:48:GLU:CD	7:G:103:PHE:CG	2.87	0.52
15:O:376:GLU:HG3	15:O:424:TYR:HB2	1.91	0.52
1:A:1214:ILE:HG13	1:A:1214:ILE:O	2.09	0.52
4:D:11:LEU:HD21	7:G:3:VAL:CA	2.37	0.52
17:Q:80:GLU:HA	17:Q:86:ARG:HD3	1.92	0.52
3:C:263:GLU:HG3	3:C:274:ARG:HG2	1.92	0.51
13:M:37:MET:HE3	14:N:151:THR:HG21	1.92	0.51
15:O:440:TYR:OH	15:O:524:GLU:OE2	2.27	0.51
1:A:1375:ARG:NH1	1:A:1376:PRO:O	2.43	0.51
13:M:234:GLU:HA	13:M:234:GLU:OE2	2.09	0.51
1:A:834:VAL:O	1:A:834:VAL:HG23	2.10	0.51
1:A:1185:MET:HB3	9:I:14:VAL:O	2.10	0.51
3:C:287:ILE:HG12	3:C:297:VAL:HG21	1.91	0.51
15:O:460:LEU:HB3	15:O:499:LEU:HD11	1.92	0.51
2:B:412:THR:OG1	2:B:413:ASN:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:48:GLU:OE1	7:G:103:PHE:CD2	2.63	0.51
15:O:22:GLU:O	15:O:26:VAL:N	2.40	0.51
1:A:221:LEU:HD21	15:O:400:SER:HA	1.92	0.51
1:A:898:ILE:HG22	1:A:899:GLN:HG3	1.91	0.51
1:A:1119:GLU:HA	1:A:1128:ILE:HA	1.93	0.51
1:A:1179:GLU:OE2	1:A:1179:GLU:HA	2.10	0.51
3:C:103:ASP:OD1	3:C:103:ASP:N	2.44	0.51
15:O:5:GLU:HG3	15:O:83:LEU:HD11	1.93	0.51
16:P:286:PRO:HA	17:Q:38:PHE:HD2	1.75	0.51
1:A:1363:LEU:HD21	7:G:56:ASP:HB2	1.92	0.51
2:B:196:LYS:CD	20:Y:9:DA:OP1	2.59	0.51
1:A:6:PHE:CE2	7:G:157:PHE:HA	2.44	0.51
1:A:398:LYS:O	1:A:398:LYS:HG2	2.11	0.51
3:C:135:ILE:HD12	3:C:135:ILE:N	2.23	0.51
4:D:105:GLU:CD	4:D:105:GLU:H	2.19	0.51
5:E:67:ASP:HB3	5:E:70:ASP:HB2	1.93	0.51
6:F:75:MET:CB	7:G:15:PRO:HG2	2.40	0.51
12:L:34:ILE:H	12:L:34:ILE:CD1	2.14	0.51
14:N:269:LEU:HD12	14:N:269:LEU:O	2.11	0.51
15:O:407:GLN:N	15:O:407:GLN:CD	2.69	0.51
15:O:409:ILE:CB	15:O:423:LEU:CD2	2.67	0.51
1:A:17:HIS:O	1:A:17:HIS:CG	2.63	0.51
1:A:1129:LEU:HB2	1:A:1175:VAL:HG22	1.92	0.51
5:E:7:THR:HG21	5:E:41:LYS:HE3	1.93	0.51
5:E:26:TYR:HB3	5:E:61:LEU:HB3	1.93	0.51
15:O:60:HIS:NE2	15:O:112:LEU:O	2.44	0.51
1:A:601:PHE:CE2	1:A:650:MET:HE3	2.46	0.51
2:B:455:ILE:HD11	2:B:496:LEU:HG	1.92	0.51
3:C:51:VAL:HG22	3:C:65:MET:HG2	1.92	0.51
4:D:39:GLN:HB2	7:G:32:LYS:HG2	1.93	0.51
5:E:79:GLU:OE1	5:E:79:GLU:N	2.44	0.51
1:A:151:ARG:HB2	1:A:151:ARG:CZ	2.41	0.50
1:A:1363:LEU:HA	7:G:57:ALA:O	2.11	0.50
12:L:52:LEU:C	12:L:52:LEU:HD23	2.37	0.50
1:A:7:ARG:HG2	1:A:7:ARG:HH11	1.75	0.50
1:A:36:VAL:HG21	1:A:257:VAL:HG21	1.93	0.50
1:A:469:HIS:CD2	1:A:471:LEU:HB2	2.46	0.50
1:A:1260:ILE:HD13	5:E:207:ARG:NH1	2.25	0.50
1:A:1357:THR:HG1	2:B:1061:SER:HG	1.57	0.50
3:C:286:GLU:OE1	3:C:286:GLU:HA	2.11	0.50
3:C:292:LYS:HD2	3:C:293:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:99:VAL:HG11	7:G:148:ILE:HG12	1.92	0.50
8:H:32:SER:OG	8:H:35:PHE:O	2.27	0.50
1:A:1112:GLU:OE1	9:I:47:LYS:CE	2.58	0.50
1:A:1225:LEU:HD12	1:A:1225:LEU:O	2.11	0.50
2:B:135:ARG:H	2:B:412:THR:HG22	1.75	0.50
7:G:148:ILE:CG2	7:G:190:ILE:HG23	2.29	0.50
20:Y:2:DC:H2''	20:Y:3:DG:C8	2.46	0.50
1:A:7:ARG:HG2	1:A:7:ARG:NH1	2.27	0.50
1:A:583:LEU:HD23	1:A:583:LEU:H	1.76	0.50
1:A:1360:PHE:O	1:A:1360:PHE:CD1	2.64	0.50
2:B:306:ILE:HD13	2:B:306:ILE:N	2.17	0.50
3:C:263:GLU:HG3	3:C:263:GLU:O	2.10	0.50
7:G:39:VAL:HB	7:G:42:VAL:HB	1.93	0.50
16:P:296:CYS:SG	16:P:297:HIS:N	2.79	0.50
1:A:424:ARG:HE	1:A:447:GLY:HA3	1.75	0.50
1:A:1368:ARG:HB3	7:G:22:LEU:HB2	1.93	0.50
2:B:307:GLU:O	2:B:311:GLU:HG2	2.11	0.50
2:B:724:THR:HA	2:B:727:LEU:HD12	1.93	0.50
4:D:1:MET:SD	7:G:7:MET:HE3	2.51	0.50
4:D:102:GLU:N	4:D:102:GLU:OE2	2.40	0.50
18:R:11:G:H8	18:R:11:G:O5'	1.94	0.50
5:E:47:LYS:C	5:E:47:LYS:HD2	2.37	0.50
16:P:286:PRO:HG2	16:P:313:TRP:CD2	2.47	0.50
18:R:11:G:O5'	18:R:11:G:C8	2.65	0.50
1:A:1239:HIS:HE1	5:E:8:TYR:CZ	2.29	0.50
3:C:163:TYR:HE1	3:C:204:PRO:HG3	1.76	0.50
4:D:2:GLU:OE1	4:D:2:GLU:N	2.27	0.50
4:D:85:GLN:HG2	7:G:80:PHE:HZ	1.77	0.50
1:A:16:SER:HB3	2:B:1127:LYS:HD2	1.94	0.50
1:A:596:THR:CG2	8:H:119:GLY:O	2.44	0.50
1:A:645:LEU:HD22	1:A:650:MET:HE2	1.93	0.50
1:A:897:ILE:O	1:A:897:ILE:HG22	2.12	0.50
2:B:133:ILE:CG2	2:B:133:ILE:O	2.60	0.50
5:E:84:ILE:HG22	5:E:88:LYS:HG2	1.94	0.50
7:G:115:GLN:NE2	7:G:192:GLU:O	2.45	0.50
1:A:180:LYS:HZ3	1:A:182:ASN:CG	2.11	0.50
1:A:211:LEU:HD12	1:A:211:LEU:C	2.36	0.50
2:B:555:LEU:C	2:B:555:LEU:HD23	2.36	0.50
13:M:7:ASP:OD1	13:M:7:ASP:N	2.32	0.50
15:O:436:LEU:HB2	15:O:523:LEU:HD22	1.92	0.50
1:A:49:ALA:N	1:A:50:PRO:HD3	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:TYR:HE1	1:A:140:ARG:HE	1.59	0.49
1:A:1194:GLU:OE1	1:A:1194:GLU:HA	2.10	0.49
12:L:52:LEU:HD23	12:L:52:LEU:O	2.12	0.49
13:M:63:ASP:OD1	13:M:63:ASP:N	2.45	0.49
15:O:405:SER:HB3	15:O:425:THR:O	2.12	0.49
15:O:450:ARG:O	15:O:454:THR:OG1	2.29	0.49
15:O:378:LYS:HD2	15:O:379:GLN:HE21	1.77	0.49
1:A:136:TYR:O	1:A:136:TYR:CD1	2.63	0.49
1:A:345:LEU:HD11	2:B:1120:MET:HE1	1.93	0.49
1:A:727:TYR:CG	1:A:751:LEU:HD21	2.48	0.49
1:A:801:GLN:HA	1:A:833:PHE:HA	1.95	0.49
1:A:1185:MET:SD	1:A:1185:MET:N	2.86	0.49
2:B:721:LYS:HZ3	2:B:731:GLU:CD	2.19	0.49
15:O:118:MET:SD	17:Q:108:ARG:NH2	2.74	0.49
1:A:958:PHE:HB3	1:A:966:LEU:HD11	1.95	0.49
2:B:409:ASP:N	2:B:409:ASP:OD1	2.43	0.49
2:B:594:ARG:NH2	2:B:663:THR:OG1	2.45	0.49
5:E:47:LYS:N	5:E:48:PRO:CD	2.76	0.49
5:E:76:PHE:CD1	5:E:76:PHE:N	2.80	0.49
16:P:222:GLU:O	16:P:226:SER:OG	2.27	0.49
1:A:164:GLY:HA3	1:A:177:GLU:HG3	1.95	0.49
1:A:232:ALA:HB2	15:O:6:ILE:CD1	2.42	0.49
1:A:1089:LEU:HD21	1:A:1225:LEU:HD21	1.95	0.49
2:B:567:TYR:HB3	13:M:250:MET:HG2	1.94	0.49
10:J:40:LEU:HD22	10:J:45:CYS:HB3	1.94	0.49
15:O:410:PRO:HB3	15:O:422:TYR:CD2	2.47	0.49
15:O:460:LEU:HA	15:O:463:LYS:HG2	1.94	0.49
16:P:252:ILE:HG23	16:P:257:GLU:HB3	1.93	0.49
17:Q:27:LEU:CD2	17:Q:27:LEU:N	2.63	0.49
1:A:183:LYS:H	1:A:183:LYS:HE2	1.77	0.49
1:A:1048:MET:HE2	1:A:1280:MET:SD	2.53	0.49
17:Q:72:PRO:HA	17:Q:75:ILE:HG22	1.95	0.49
2:B:715:PRO:HB2	2:B:734:PRO:HG2	1.95	0.49
15:O:409:ILE:CD1	15:O:423:LEU:CD1	2.63	0.49
1:A:91:PRO:HG2	1:A:221:LEU:HD13	1.95	0.49
1:A:143:LYS:HB2	1:A:239:LEU:HD13	1.95	0.49
1:A:442:GLN:HA	1:A:442:GLN:NE2	2.26	0.49
1:A:776:SER:N	1:A:777:PRO:HD2	2.28	0.49
1:A:1236:MET:HE3	1:A:1246:THR:HG22	1.94	0.49
2:B:65:VAL:HG23	2:B:75:LEU:O	2.13	0.49
16:P:308:ILE:HD13	17:Q:31:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1369:ASP:OD1	1:A:1369:ASP:N	2.45	0.49
3:C:57:ASP:C	3:C:57:ASP:OD1	2.56	0.49
5:E:52:ARG:N	5:E:53:PRO:HD2	2.27	0.49
11:K:58:MET:HE3	11:K:58:MET:CA	2.42	0.49
15:O:416:ALA:HA	15:O:422:TYR:OH	2.13	0.49
1:A:1346:CYS:HB3	1:A:1351:ILE:O	2.13	0.48
7:G:161:SER:HB2	7:G:162:PRO:CD	2.43	0.48
1:A:534:ASN:HB2	1:A:536:GLU:HG3	1.94	0.48
1:A:1204:ILE:HD12	1:A:1204:ILE:N	2.28	0.48
2:B:139:MET:SD	2:B:167:GLY:HA2	2.53	0.48
2:B:1080:CYS:CB	2:B:1083:CYS:SG	3.01	0.48
15:O:400:SER:OG	15:O:401:GLU:OE1	2.31	0.48
20:Y:-1:DC:H2''	20:Y:0:DA:C8	2.47	0.48
1:A:571:ILE:HD11	1:A:686:LEU:HB2	1.94	0.48
1:A:882:LEU:HD11	1:A:1293:LEU:HD12	1.96	0.48
1:A:1140:LEU:HD22	9:I:52:VAL:CG1	2.41	0.48
1:A:1233:ARG:CD	5:E:134:GLU:HG2	2.40	0.48
12:L:37:ARG:O	12:L:38:GLU:HB2	2.13	0.48
14:N:269:LEU:HB3	14:N:383:LEU:HB2	1.95	0.48
19:X:37:DG:H2'	19:X:38:DA:H8	1.76	0.48
1:A:55:VAL:O	1:A:60:MET:HE1	2.14	0.48
1:A:1139:LEU:HD11	9:I:53:LEU:HD21	1.94	0.48
11:K:58:MET:HE2	11:K:102:GLU:HB3	1.94	0.48
16:P:219:TYR:HD2	16:P:271:ARG:HB3	1.78	0.48
16:P:286:PRO:HA	17:Q:38:PHE:CD2	2.48	0.48
19:X:38:DA:H61	20:Y:6:DT:H3	1.60	0.48
1:A:1048:MET:CG	1:A:1280:MET:HE1	2.43	0.48
1:A:1269:ASN:O	1:A:1273:TYR:N	2.43	0.48
3:C:43:ASP:OD1	3:C:43:ASP:N	2.46	0.48
1:A:1297:LYS:HB3	1:A:1301:LEU:HD11	1.96	0.48
1:A:1347:ILE:HD13	2:B:1052:ARG:HD2	1.96	0.48
2:B:253:GLN:HG3	14:N:146:GLU:OE2	2.14	0.48
2:B:672:ILE:HG12	2:B:686:GLN:HG3	1.94	0.48
3:C:210:LEU:C	3:C:210:LEU:HD12	2.39	0.48
4:D:61:GLN:HA	4:D:61:GLN:NE2	2.28	0.48
7:G:84:ILE:HD11	7:G:149:ARG:HH21	1.77	0.48
15:O:445:ASN:CG	23:P:401:SF4:S2	2.97	0.48
1:A:213:ARG:H	1:A:213:ARG:CD	2.27	0.48
1:A:331:ASN:ND2	1:A:331:ASN:C	2.68	0.48
1:A:385:HIS:HB2	2:B:1020:MET:HE1	1.95	0.48
2:B:75:LEU:HD13	2:B:119:TYR:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:781:ARG:NH2	2:B:781:ARG:HB3	2.29	0.48
3:C:332:LYS:HB3	11:K:51:LEU:HD22	1.95	0.48
4:D:11:LEU:HD22	7:G:4:LEU:HD22	1.96	0.48
4:D:43:ASN:HD22	4:D:43:ASN:N	2.01	0.48
6:F:126:THR:O	6:F:126:THR:OG1	2.23	0.48
16:P:220:ILE:CD1	16:P:271:ARG:HD2	2.43	0.48
17:Q:57:MET:O	17:Q:61:LYS:N	2.38	0.48
1:A:587:THR:HG23	1:A:599:GLN:OE1	2.12	0.48
1:A:1033:VAL:HG13	1:A:1289:LEU:HD22	1.95	0.48
1:A:1239:HIS:CE1	5:E:8:TYR:CZ	3.02	0.48
2:B:184:LEU:HD23	2:B:190:ILE:HD13	1.96	0.48
2:B:303:LYS:HE2	2:B:303:LYS:CA	2.44	0.48
2:B:530:GLU:OE1	2:B:530:GLU:N	2.46	0.48
3:C:23:ASN:O	3:C:303:ARG:NH2	2.47	0.48
3:C:97:ASN:C	3:C:97:ASN:OD1	2.55	0.48
3:C:264:VAL:HG23	3:C:264:VAL:O	2.13	0.48
3:C:319:ASP:OD1	3:C:319:ASP:N	2.44	0.48
20:Y:2:DC:C5	20:Y:2:DC:OP2	2.66	0.48
2:B:196:LYS:HD2	20:Y:9:DA:OP1	2.14	0.48
7:G:151:ARG:NH1	7:G:152:VAL:HG12	2.29	0.48
8:H:76:ASN:ND2	11:K:87:ARG:NE	2.53	0.48
20:Y:4:DG:H2'	20:Y:5:DC:C6	2.48	0.48
1:A:1239:HIS:HE1	5:E:8:TYR:CE1	2.32	0.47
4:D:52:TYR:O	4:D:55:LYS:HB2	2.14	0.47
5:E:82:VAL:HG13	5:E:86:THR:HB	1.96	0.47
7:G:161:SER:HB2	7:G:162:PRO:HD3	1.96	0.47
11:K:37:ARG:HB3	11:K:91:PRO:HA	1.95	0.47
11:K:89:THR:HG22	11:K:89:THR:O	2.14	0.47
1:A:386:VAL:HG22	2:B:1022:ALA:HB2	1.96	0.47
1:A:474:MET:HE2	1:A:525:THR:HG22	1.95	0.47
1:A:574:GLY:O	1:A:575:LYS:HB3	2.13	0.47
2:B:40:VAL:HG12	2:B:40:VAL:O	2.14	0.47
2:B:505:ASP:OD1	2:B:505:ASP:N	2.44	0.47
2:B:551:ASP:O	2:B:551:ASP:CG	2.56	0.47
15:O:84:ARG:NH2	15:O:524:GLU:OE1	2.46	0.47
15:O:414:ASP:OD1	15:O:414:ASP:N	2.44	0.47
1:A:35:GLN:HG2	1:A:37:VAL:HB	1.97	0.47
1:A:1065:LEU:O	1:A:1274:THR:OG1	2.33	0.47
1:A:1261:GLU:CG	5:E:193:ILE:HD13	2.40	0.47
9:I:8:CYS:HB2	13:M:139:PHE:HE1	1.79	0.47
1:A:183:LYS:H	1:A:183:LYS:CE	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1295:THR:O	1:A:1295:THR:OG1	2.27	0.47
2:B:242:ALA:HB1	2:B:284:LEU:CD2	2.44	0.47
2:B:514:LEU:HD22	2:B:568:ILE:HD11	1.95	0.47
2:B:686:GLN:HA	2:B:686:GLN:NE2	2.29	0.47
9:I:44:PRO:O	9:I:86:SER:OG	2.32	0.47
1:A:563:LYS:O	1:A:567:ILE:HG12	2.15	0.47
2:B:106:ASP:HA	2:B:173:GLY:HA3	1.97	0.47
9:I:1:MET:HE1	14:N:153:GLN:OE1	2.15	0.47
12:L:25:GLU:CD	12:L:25:GLU:N	2.69	0.47
19:X:43:DC:H42	20:Y:1:DG:H1	1.61	0.47
1:A:34:ILE:HD12	1:A:34:ILE:HA	1.71	0.47
1:A:197:PHE:O	1:A:197:PHE:CD1	2.64	0.47
1:A:205:LYS:NZ	1:A:205:LYS:HB3	2.29	0.47
1:A:630:ASP:OD1	1:A:630:ASP:N	2.47	0.47
1:A:868:THR:HG21	1:A:1046:THR:HG22	1.96	0.47
2:B:562:MET:CE	13:M:250:MET:HE3	2.44	0.47
2:B:1053:ASP:HA	2:B:1056:ILE:HD12	1.96	0.47
6:F:107:ARG:HD3	6:F:115:TYR:HB2	1.97	0.47
15:O:20:ILE:HD11	17:Q:68:MET:HG3	1.95	0.47
15:O:156:PHE:HA	15:O:241:ARG:HG2	1.96	0.47
15:O:412:THR:CG2	15:O:413:PRO:HD2	2.45	0.47
1:A:196:SER:HB2	15:O:373:LYS:CE	2.40	0.47
1:A:941:SER:CB	1:A:980:ILE:HG21	2.42	0.47
1:A:1048:MET:CA	1:A:1280:MET:HE1	2.44	0.47
1:A:1112:GLU:HB3	9:I:47:LYS:HG2	1.95	0.47
1:A:1192:LEU:O	1:A:1196:LEU:N	2.47	0.47
2:B:424:TRP:HB2	2:B:436:VAL:HG21	1.96	0.47
4:D:43:ASN:ND2	4:D:43:ASN:N	2.57	0.47
6:F:78:PRO:HD2	7:G:18:PHE:HB2	1.96	0.47
7:G:160:THR:O	7:G:160:THR:CG2	2.63	0.47
13:M:59:GLU:HG2	13:M:101:THR:HG22	1.96	0.47
15:O:357:ARG:HA	16:P:289:LEU:CD1	2.44	0.47
16:P:283:VAL:O	16:P:283:VAL:CG1	2.62	0.47
1:A:104:ILE:HG23	1:A:238:LEU:HD22	1.96	0.47
1:A:210:LEU:HB3	15:O:411:LYS:HD2	1.96	0.47
1:A:427:GLN:N	1:A:427:GLN:CD	2.73	0.47
1:A:1235:VAL:O	1:A:1241:VAL:HG11	2.14	0.47
2:B:828:VAL:HG22	2:B:856:ILE:HB	1.97	0.47
4:D:1:MET:HE1	7:G:7:MET:HE3	1.96	0.47
15:O:406:LEU:N	15:O:406:LEU:HD23	2.30	0.47
1:A:149:LYS:O	1:A:152:LYS:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ASN:HD22	1:A:323:SER:N	2.13	0.47
1:A:954:LYS:NZ	1:A:954:LYS:HB2	2.30	0.47
5:E:55:ARG:N	5:E:55:ARG:CD	2.77	0.47
10:J:16:ASN:OD1	10:J:16:ASN:N	2.47	0.47
13:M:245:TYR:HD2	14:N:344:VAL:HG21	1.80	0.47
17:Q:86:ARG:HB2	17:Q:86:ARG:HH11	1.80	0.47
1:A:703:VAL:HG13	1:A:795:MET:HB3	1.97	0.47
4:D:48:GLU:OE1	7:G:103:PHE:HB3	2.15	0.47
5:E:61:LEU:N	5:E:61:LEU:HD13	2.30	0.46
6:F:115:TYR:CD1	6:F:115:TYR:C	2.92	0.46
16:P:308:ILE:HD13	17:Q:31:VAL:CG1	2.45	0.46
1:A:291:ASP:HB2	17:Q:23:LYS:HE2	1.97	0.46
2:B:757:LEU:HD23	2:B:762:LEU:HD21	1.97	0.46
2:B:920:ASP:OD2	3:C:301:ARG:NH2	2.47	0.46
3:C:65:MET:HE2	3:C:68:ILE:CG2	2.43	0.46
3:C:203:ARG:HB3	3:C:204:PRO:HD2	1.97	0.46
4:D:1:MET:O	4:D:1:MET:HG3	2.15	0.46
1:A:1034:GLY:HA2	1:A:1289:LEU:HD21	1.97	0.46
1:A:1215:ASP:C	1:A:1215:ASP:OD1	2.58	0.46
2:B:384:MET:HE2	2:B:384:MET:HB2	1.39	0.46
2:B:733:LEU:N	2:B:733:LEU:CD2	2.78	0.46
2:B:973:CYS:HB2	2:B:983:TYR:HB2	1.97	0.46
7:G:94:PRO:HA	7:G:121:ASP:HB2	1.96	0.46
15:O:26:VAL:HA	15:O:29:ILE:HD12	1.97	0.46
16:P:269:LEU:HD23	16:P:269:LEU:HA	1.78	0.46
1:A:36:VAL:O	1:A:36:VAL:CG1	2.62	0.46
1:A:481:LYS:HB2	1:A:487:ARG:HH21	1.80	0.46
2:B:133:ILE:O	2:B:133:ILE:HG22	2.15	0.46
2:B:1112:LEU:O	2:B:1116:GLU:HG2	2.14	0.46
7:G:79:PRO:HG2	7:G:150:PHE:CD2	2.51	0.46
14:N:139:ASN:O	14:N:142:LYS:NZ	2.42	0.46
16:P:294:ASP:OD1	16:P:294:ASP:C	2.58	0.46
17:Q:81:ARG:HE	17:Q:84:ILE:HD11	1.81	0.46
20:Y:3:DG:H2''	20:Y:4:DG:O4'	2.16	0.46
1:A:91:PRO:CB	1:A:251:ILE:HD11	2.45	0.46
2:B:854:VAL:HG12	2:B:854:VAL:O	2.16	0.46
7:G:80:PHE:CE2	7:G:82:ASP:HB2	2.51	0.46
10:J:31:GLU:OE1	10:J:31:GLU:HA	2.15	0.46
1:A:39:LYS:CA	17:Q:24:GLY:HA3	2.45	0.46
1:A:881:ASP:OD1	1:A:881:ASP:N	2.27	0.46
1:A:1080:ILE:HD13	1:A:1249:ASN:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:HIS:N	7:G:57:ALA:O	2.49	0.46
2:B:338:MET:O	2:B:342:VAL:HG23	2.16	0.46
2:B:957:ARG:NH1	2:B:957:ARG:HB2	2.31	0.46
3:C:29:PHE:HB2	3:C:32:ASN:ND2	2.30	0.46
3:C:275:VAL:O	3:C:275:VAL:HG23	2.16	0.46
4:D:32:LYS:HD3	4:D:32:LYS:H	1.80	0.46
15:O:147:THR:HA	15:O:150:ARG:HB2	1.98	0.46
20:Y:9:DA:H2''	20:Y:10:DG:C5'	2.46	0.46
1:A:1145:ASN:HB3	1:A:1148:THR:HG23	1.98	0.46
15:O:170:ASP:O	15:O:173:PRO:HD2	2.15	0.46
15:O:409:ILE:HG22	15:O:409:ILE:O	2.15	0.46
20:Y:3:DG:H2'	20:Y:4:DG:C8	2.50	0.46
2:B:613:GLU:HA	2:B:613:GLU:OE1	2.15	0.46
4:D:84:LEU:O	4:D:84:LEU:HD12	2.16	0.46
15:O:19:GLU:OE2	17:Q:70:ARG:NE	2.47	0.46
2:B:131:LEU:HD11	2:B:403:VAL:HG13	1.96	0.46
2:B:335:THR:O	2:B:339:VAL:HG23	2.15	0.46
3:C:155:ASP:N	3:C:155:ASP:OD1	2.49	0.46
6:F:75:MET:HB3	7:G:15:PRO:HG2	1.98	0.46
11:K:58:MET:HA	11:K:58:MET:CE	2.46	0.46
19:X:42:DG:H2''	19:X:43:DC:O4'	2.15	0.46
20:Y:11:DT:H2''	20:Y:12:DC:C6	2.50	0.46
1:A:105:LEU:HD13	1:A:218:LEU:HD13	1.98	0.46
1:A:183:LYS:H	1:A:183:LYS:CD	2.28	0.46
2:B:294:GLN:HE21	19:X:24:DT:H4'	1.80	0.46
2:B:486:GLU:HG2	2:B:486:GLU:O	2.15	0.46
15:O:412:THR:HG22	15:O:413:PRO:HD2	1.98	0.46
1:A:115:ILE:CD1	1:A:237:LEU:HB3	2.46	0.45
1:A:378:ASP:OD1	1:A:379:GLU:HG3	2.15	0.45
2:B:536:VAL:HG13	2:B:548:VAL:HG13	1.98	0.45
2:B:542:ASN:ND2	2:B:587:SER:H	2.13	0.45
2:B:578:LEU:HD23	2:B:578:LEU:N	2.25	0.45
3:C:337:LEU:HD23	3:C:337:LEU:HA	1.82	0.45
20:Y:9:DA:H2'	20:Y:10:DG:C8	2.51	0.45
1:A:446:TYR:N	1:A:446:TYR:CD1	2.84	0.45
1:A:1135:GLU:O	1:A:1139:LEU:N	2.36	0.45
1:A:1228:GLU:N	1:A:1228:GLU:OE1	2.49	0.45
2:B:520:VAL:HA	2:B:549:ILE:HG23	1.97	0.45
15:O:59:GLN:NE2	15:O:113:ASN:O	2.42	0.45
1:A:45:ASP:N	1:A:50:PRO:O	2.43	0.45
1:A:412:PRO:O	1:A:453:HIS:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:TYR:CD1	2:B:119:TYR:N	2.84	0.45
2:B:196:LYS:HD3	20:Y:9:DA:P	2.56	0.45
2:B:464:LYS:HE3	19:X:30:DC:H5"	1.98	0.45
2:B:743:VAL:HG22	2:B:743:VAL:O	2.16	0.45
2:B:984:LEU:HD12	2:B:984:LEU:HA	1.77	0.45
4:D:85:GLN:NE2	7:G:83:GLU:CA	2.69	0.45
11:K:31:GLN:C	11:K:31:GLN:CD	2.82	0.45
11:K:38:HIS:CE1	11:K:89:THR:HA	2.52	0.45
13:M:67:PRO:HD2	14:N:138:ILE:HG12	1.97	0.45
13:M:238:LEU:CD1	14:N:341:LEU:HG	2.44	0.45
14:N:261:THR:HG22	14:N:263:GLU:H	1.82	0.45
15:O:406:LEU:N	15:O:406:LEU:CD2	2.79	0.45
15:O:445:ASN:HD22	16:P:304:PRO:CG	2.26	0.45
2:B:65:VAL:HG23	2:B:75:LEU:HB3	1.98	0.45
2:B:478:MET:HB3	2:B:592:LEU:HD13	1.98	0.45
4:D:7:ASN:ND2	17:Q:78:PRO:HG3	2.29	0.45
5:E:21:CYS:SG	5:E:61:LEU:HG	2.57	0.45
5:E:61:LEU:H	5:E:61:LEU:CD2	2.12	0.45
19:X:40:DC:H6	19:X:40:DC:OP2	1.99	0.45
1:A:794:GLN:HG2	1:A:799:VAL:HA	1.98	0.45
1:A:1135:GLU:OE1	1:A:1135:GLU:HA	2.16	0.45
1:A:1315:VAL:O	1:A:1319:ALA:N	2.47	0.45
2:B:189:ILE:H	2:B:189:ILE:HG13	1.56	0.45
11:K:27:LEU:HD21	11:K:45:HIS:CE1	2.52	0.45
2:B:574:ILE:HD13	2:B:574:ILE:N	2.31	0.45
2:B:623:ASP:OD1	2:B:623:ASP:N	2.50	0.45
4:D:59:ARG:HB3	4:D:59:ARG:NH2	2.32	0.45
10:J:19:GLU:OE1	10:J:19:GLU:N	2.50	0.45
10:J:28:GLU:C	10:J:28:GLU:CD	2.84	0.45
11:K:94:GLU:HB3	11:K:95:PRO:HD3	1.98	0.45
1:A:94:HIS:CD2	1:A:96:GLY:H	2.34	0.45
1:A:700:ILE:HD11	2:B:944:ILE:HG12	1.99	0.45
1:A:1017:THR:HG22	1:A:1021:LYS:HD2	1.99	0.45
1:A:1150:ARG:HD2	1:A:1167:VAL:HG13	1.98	0.45
1:A:1328:LEU:HD23	1:A:1328:LEU:HA	1.83	0.45
2:B:883:MET:HE2	2:B:883:MET:HB2	1.66	0.45
3:C:266:GLU:N	3:C:266:GLU:CD	2.75	0.45
3:C:292:LYS:O	3:C:292:LYS:HD3	2.16	0.45
7:G:160:THR:O	7:G:160:THR:HG22	2.15	0.45
15:O:416:ALA:HB3	15:O:417:PRO:HD3	1.98	0.45
15:O:423:LEU:HD23	15:O:423:LEU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LEU:HB3	1:A:122:LYS:HG3	1.99	0.45
1:A:575:LYS:O	1:A:575:LYS:HG2	2.15	0.45
2:B:384:MET:SD	2:B:406:MET:HG2	2.57	0.45
15:O:63:VAL:HG22	15:O:77:ALA:HB2	1.99	0.45
1:A:176:HIS:CE1	1:A:178:LYS:HB2	2.52	0.45
1:A:1074:ILE:CD1	1:A:1290:LEU:HD21	2.47	0.45
1:A:1305:ARG:HD2	1:A:1323:LYS:HE3	1.99	0.45
2:B:989:VAL:CG2	2:B:998:LEU:HD12	2.47	0.45
5:E:46:ASP:C	5:E:48:PRO:HD2	2.41	0.45
5:E:82:VAL:O	5:E:111:THR:HG22	2.17	0.45
7:G:151:ARG:CZ	7:G:152:VAL:HG12	2.47	0.45
20:Y:10:DG:H2''	20:Y:11:DT:C5'	2.43	0.45
1:A:7:ARG:HG3	7:G:34:LEU:HD13	1.97	0.45
1:A:990:ASN:CG	1:A:990:ASN:O	2.60	0.45
1:A:1196:LEU:N	1:A:1197:PRO:HD2	2.32	0.45
2:B:570:GLU:H	2:B:570:GLU:HG3	1.50	0.45
6:F:69:ARG:HD2	6:F:69:ARG:HA	1.74	0.45
9:I:32:HIS:NE2	14:N:137:ILE:HG12	2.31	0.45
15:O:447:ILE:O	15:O:451:GLN:N	2.47	0.45
15:O:459:ARG:HG2	15:O:460:LEU:HD23	1.99	0.45
16:P:293:PHE:CD2	23:P:401:SF4:S1	3.10	0.45
1:A:1206:GLU:CD	1:A:1231:ASN:HB2	2.42	0.44
2:B:128:ARG:CZ	2:B:403:VAL:HG11	2.47	0.44
7:G:161:SER:CB	7:G:162:PRO:CD	2.95	0.44
4:D:117:LEU:HA	4:D:120:VAL:HG12	1.98	0.44
8:H:38:ASP:OD1	8:H:38:ASP:N	2.42	0.44
1:A:99:ARG:HA	1:A:102:ILE:HD12	2.00	0.44
1:A:1132:LEU:HD11	1:A:1149:VAL:HG21	1.99	0.44
2:B:1062:MET:HE3	2:B:1062:MET:CA	2.48	0.44
10:J:33:ASP:OD1	10:J:33:ASP:C	2.60	0.44
13:M:50:LYS:HD3	13:M:203:GLU:HB3	1.98	0.44
1:A:29:ARG:HD2	16:P:301:GLU:OE2	2.18	0.44
2:B:245:VAL:HG22	2:B:245:VAL:O	2.16	0.44
3:C:118:ASP:C	3:C:118:ASP:OD1	2.59	0.44
3:C:181:GLN:HG2	3:C:185:PHE:HE2	1.82	0.44
4:D:58:CYS:CA	4:D:61:GLN:HB2	2.39	0.44
1:A:142:LEU:HD23	1:A:142:LEU:HA	1.76	0.44
1:A:651:ASP:CG	1:A:783:CYS:HA	2.41	0.44
1:A:1239:HIS:CE1	5:E:8:TYR:CE2	3.06	0.44
2:B:598:ILE:HD12	2:B:628:SER:O	2.17	0.44
3:C:17:GLY:HA3	3:C:22:ARG:HH12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:107:ARG:NH2	7:G:56:ASP:OD2	2.41	0.44
7:G:56:ASP:OD1	7:G:56:ASP:N	2.41	0.44
13:M:240:LYS:NZ	13:M:248:MET:SD	2.87	0.44
1:A:44:GLN:OE1	1:A:44:GLN:HA	2.18	0.44
1:A:760:ARG:HH22	1:A:794:GLN:HG3	1.83	0.44
2:B:446:ILE:H	2:B:446:ILE:HG12	1.66	0.44
7:G:26:ILE:HG21	7:G:70:VAL:HG21	1.98	0.44
15:O:357:ARG:HD2	16:P:288:GLY:O	2.16	0.44
18:R:9:C:H2'	18:R:10:U:C6	2.52	0.44
1:A:118:SER:O	1:A:122:LYS:N	2.42	0.44
1:A:237:LEU:HD12	1:A:237:LEU:HA	1.70	0.44
1:A:410:ASN:HB3	1:A:414:VAL:HB	1.99	0.44
1:A:1140:LEU:O	1:A:1142:LEU:HD23	2.17	0.44
2:B:59:MET:HE1	2:B:79:ASN:N	2.33	0.44
15:O:406:LEU:HD23	15:O:406:LEU:H	1.83	0.44
15:O:415:HIS:HB2	15:O:418:SER:O	2.18	0.44
16:P:256:LYS:HE2	16:P:278:PRO:HA	1.99	0.44
1:A:1161:LYS:N	1:A:1161:LYS:HD3	2.33	0.44
1:A:1297:LYS:HE2	1:A:1297:LYS:HB2	1.87	0.44
2:B:303:LYS:HA	2:B:303:LYS:CE	2.48	0.44
2:B:707:THR:HA	2:B:774:ASN:HB3	1.99	0.44
3:C:38:ASP:O	11:K:61:LYS:NZ	2.51	0.44
3:C:96:ASN:CG	3:C:96:ASN:O	2.60	0.44
11:K:67:PHE:CD1	11:K:67:PHE:C	2.95	0.44
15:O:434:MET:HE2	15:O:434:MET:HB3	1.86	0.44
17:Q:78:PRO:HD2	17:Q:79:GLU:CD	2.43	0.44
2:B:1108:TYR:CD1	2:B:1108:TYR:C	2.96	0.44
13:M:66:ASN:HB2	14:N:138:ILE:HG13	2.00	0.44
15:O:345:LEU:HD23	15:O:345:LEU:HA	1.89	0.44
1:A:229:ARG:HD2	15:O:433:ARG:HB3	2.00	0.43
1:A:782:LEU:HD23	1:A:789:PHE:HZ	1.83	0.43
1:A:1082:THR:N	1:A:1083:PRO:HD3	2.33	0.43
2:B:262:MET:HB3	9:I:2:LEU:HD12	2.00	0.43
2:B:1115:GLN:OE1	2:B:1115:GLN:CA	2.65	0.43
4:D:100:MET:SD	7:G:147:GLU:OE2	2.76	0.43
13:M:6:ASP:OD1	13:M:6:ASP:N	2.50	0.43
1:A:516:LYS:HB3	1:A:516:LYS:HE2	1.64	0.43
2:B:303:LYS:HE2	2:B:303:LYS:H	1.83	0.43
2:B:312:LEU:HG	2:B:316:THR:HG21	2.01	0.43
3:C:29:PHE:HB2	3:C:32:ASN:HD21	1.82	0.43
3:C:49:PHE:CZ	3:C:65:MET:HE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:239:ILE:HD12	3:C:239:ILE:N	2.26	0.43
7:G:115:GLN:HG3	7:G:116:GLN:HG3	2.00	0.43
1:A:206:GLU:OE1	1:A:206:GLU:N	2.46	0.43
1:A:991:ASP:OD1	1:A:991:ASP:N	2.51	0.43
3:C:337:LEU:HD12	11:K:104:MET:HE1	1.99	0.43
4:D:39:GLN:CG	7:G:32:LYS:HE2	2.48	0.43
4:D:57:PRO:C	4:D:59:ARG:H	2.25	0.43
4:D:59:ARG:HB3	4:D:59:ARG:HH21	1.83	0.43
15:O:170:ASP:OD1	15:O:170:ASP:N	2.48	0.43
15:O:399:LEU:HD12	15:O:404:MET:HB3	2.00	0.43
1:A:397:ASN:O	1:A:398:LYS:HB3	2.18	0.43
1:A:618:ARG:HE	1:A:618:ARG:HB2	1.57	0.43
1:A:691:LEU:HD12	1:A:691:LEU:HA	1.86	0.43
2:B:562:MET:HE2	13:M:250:MET:HE3	2.00	0.43
2:B:1049:GLU:H	2:B:1049:GLU:HG2	1.61	0.43
2:B:1062:MET:HA	2:B:1062:MET:CE	2.43	0.43
4:D:114:GLU:N	4:D:114:GLU:OE2	2.51	0.43
15:O:89:PRO:HG2	17:Q:54:GLU:HG2	2.00	0.43
1:A:90:LEU:HD23	1:A:90:LEU:HA	1.78	0.43
1:A:530:VAL:HG13	1:A:535:GLY:HA2	2.00	0.43
1:A:753:LEU:HD12	1:A:753:LEU:HA	1.81	0.43
2:B:62:ASN:C	2:B:62:ASN:HD22	2.27	0.43
2:B:78:LEU:N	2:B:78:LEU:HD12	2.34	0.43
4:D:11:LEU:HD13	7:G:4:LEU:HD22	2.01	0.43
4:D:48:GLU:HB2	7:G:103:PHE:O	2.16	0.43
4:D:87:LEU:N	4:D:87:LEU:HD23	2.32	0.43
4:D:96:GLU:H	4:D:96:GLU:HG2	1.43	0.43
11:K:38:HIS:ND1	11:K:38:HIS:N	2.67	0.43
12:L:15:MET:HE3	12:L:15:MET:HA	2.00	0.43
13:M:238:LEU:HB3	14:N:341:LEU:O	2.19	0.43
15:O:159:ARG:NH1	17:Q:112:PRO:O	2.50	0.43
1:A:211:LEU:HA	15:O:411:LYS:HZ1	1.83	0.43
1:A:727:TYR:CE1	1:A:751:LEU:HD11	2.53	0.43
2:B:37:LYS:HA	2:B:41:LYS:HG2	2.00	0.43
2:B:39:LEU:HD23	2:B:39:LEU:HA	1.91	0.43
2:B:60:LYS:HD3	2:B:60:LYS:HA	1.81	0.43
2:B:251:ILE:O	2:B:255:ILE:HG12	2.19	0.43
2:B:674:TYR:HB3	2:B:677:HIS:HD2	1.83	0.43
3:C:234:ARG:O	3:C:234:ARG:HG3	2.19	0.43
15:O:409:ILE:HD12	15:O:423:LEU:CD1	2.31	0.43
1:A:51:LEU:HD21	1:A:67:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:VAL:HG22	1:A:480:VAL:HG12	2.01	0.43
1:A:797:ALA:O	1:A:837:SER:HB3	2.18	0.43
1:A:899:GLN:HG2	1:A:1292:ASP:OD2	2.18	0.43
1:A:1048:MET:HE3	1:A:1067:VAL:HG22	2.00	0.43
1:A:1104:ARG:O	1:A:1203:GLY:HA2	2.18	0.43
2:B:234:ILE:HB	2:B:239:ILE:HD11	1.99	0.43
2:B:404:LYS:HD3	2:B:404:LYS:HA	1.57	0.43
2:B:509:GLY:N	2:B:510:PRO:HD2	2.33	0.43
2:B:606:VAL:HG12	2:B:608:ASN:H	1.84	0.43
2:B:1105:ARG:HB2	2:B:1105:ARG:CZ	2.48	0.43
3:C:72:ILE:HD13	11:K:106:VAL:HG11	2.01	0.43
4:D:81:ALA:HB1	7:G:80:PHE:CE2	2.54	0.43
15:O:416:ALA:N	15:O:417:PRO:CD	2.81	0.43
1:A:171:LEU:HD21	1:A:329:PRO:HG3	1.99	0.43
1:A:1083:PRO:HA	1:A:1249:ASN:OD1	2.19	0.43
1:A:1198:LYS:H	1:A:1198:LYS:HG2	1.59	0.43
1:A:1235:VAL:O	1:A:1235:VAL:CG1	2.66	0.43
2:B:118:GLU:O	2:B:118:GLU:HG2	2.16	0.43
2:B:175:GLU:H	2:B:175:GLU:HG2	1.55	0.43
2:B:307:GLU:OE1	2:B:307:GLU:HA	2.18	0.43
3:C:49:PHE:CE1	3:C:65:MET:HE3	2.54	0.43
3:C:141:ARG:C	3:C:141:ARG:HD2	2.43	0.43
4:D:5:ASP:HB2	7:G:6:GLU:CG	2.49	0.43
17:Q:34:PRO:HG2	17:Q:37:LEU:HD23	2.01	0.43
1:A:112:CYS:HB3	1:A:159:CYS:SG	2.59	0.43
3:C:235:LEU:N	3:C:235:LEU:HD12	2.34	0.43
4:D:95:VAL:HA	4:D:98:GLN:HB2	2.01	0.43
5:E:10:LEU:HD21	5:E:52:ARG:HG2	2.00	0.43
7:G:57:ALA:HA	7:G:68:THR:HG22	2.01	0.43
15:O:413:PRO:O	15:O:415:HIS:HD2	2.01	0.43
1:A:155:ILE:HG22	1:A:156:CYS:H	1.84	0.43
1:A:1317:MET:HG3	1:A:1344:SER:HB2	1.99	0.43
2:B:30:LEU:HD22	2:B:663:THR:CG2	2.49	0.43
3:C:79:ILE:HG23	3:C:83:GLU:HB2	2.01	0.43
7:G:151:ARG:C	7:G:151:ARG:CD	2.85	0.43
18:R:11:G:H2'	18:R:11:G:N3	2.33	0.43
1:A:55:VAL:HG21	1:A:280:THR:HG23	2.00	0.42
1:A:174:ILE:HG22	1:A:218:LEU:HB2	2.00	0.42
1:A:183:LYS:N	1:A:183:LYS:CD	2.80	0.42
1:A:864:LYS:NZ	1:A:1048:MET:HB2	2.29	0.42
2:B:192:GLU:O	2:B:192:GLU:CG	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:GLU:O	2:B:247:SER:HB3	2.18	0.42
3:C:315:VAL:HG12	3:C:316:LEU:HD22	1.99	0.42
1:A:52:LEU:HD13	1:A:52:LEU:HA	1.76	0.42
1:A:116:MET:HG3	1:A:150:CYS:HB3	2.02	0.42
2:B:274:LYS:HE2	2:B:274:LYS:HB3	1.90	0.42
2:B:518:LEU:HD11	2:B:558:THR:HG21	2.00	0.42
3:C:184:LEU:HD12	3:C:184:LEU:O	2.19	0.42
11:K:92:ALA:C	11:K:95:PRO:HD2	2.44	0.42
16:P:222:GLU:HA	16:P:225:ILE:HG22	2.01	0.42
1:A:151:ARG:HH11	1:A:151:ARG:CG	2.33	0.42
1:A:257:VAL:HA	1:A:258:PRO:HD3	1.79	0.42
1:A:591:PRO:HD3	8:H:90:TYR:HA	2.01	0.42
2:B:88:GLU:CD	2:B:88:GLU:N	2.76	0.42
2:B:128:ARG:HD3	2:B:403:VAL:HG21	2.01	0.42
2:B:372:LEU:HD21	2:B:415:MET:HA	1.99	0.42
2:B:1108:TYR:CD1	2:B:1108:TYR:O	2.72	0.42
18:R:10:U:H3'	18:R:11:G:C8	2.50	0.42
19:X:39:DG:H2'	19:X:40:DC:C6	2.55	0.42
1:A:94:HIS:HD2	1:A:96:GLY:H	1.66	0.42
1:A:194:LEU:HD11	1:A:214:ALA:CB	2.49	0.42
1:A:224:LEU:HG	1:A:251:ILE:HG12	2.01	0.42
1:A:590:LYS:O	1:A:591:PRO:C	2.60	0.42
1:A:1074:ILE:HD12	1:A:1290:LEU:HD21	2.01	0.42
1:A:1080:ILE:HD11	1:A:1249:ASN:OD1	2.20	0.42
2:B:395:GLN:HE21	2:B:395:GLN:HB3	1.63	0.42
2:B:1092:CYS:C	2:B:1094:TYR:H	2.27	0.42
4:D:17:PHE:CE1	4:D:21:THR:CG2	3.03	0.42
2:B:712:LEU:HD23	2:B:712:LEU:HA	1.76	0.42
15:O:370:LEU:HD23	15:O:370:LEU:HA	1.93	0.42
15:O:459:ARG:H	15:O:459:ARG:HD3	1.85	0.42
17:Q:34:PRO:HG2	17:Q:37:LEU:CD2	2.49	0.42
1:A:1065:LEU:HD12	1:A:1065:LEU:HA	1.77	0.42
2:B:1115:GLN:OE1	2:B:1115:GLN:N	2.53	0.42
3:C:156:SER:HB2	3:C:162:LEU:HG	2.02	0.42
3:C:235:LEU:HD23	3:C:303:ARG:HA	2.01	0.42
4:D:69:PHE:HD1	4:D:69:PHE:O	2.02	0.42
4:D:102:GLU:CD	4:D:102:GLU:H	2.25	0.42
14:N:350:MET:HE3	14:N:350:MET:HB3	1.93	0.42
15:O:124:LYS:HA	15:O:124:LYS:HD3	1.75	0.42
16:P:220:ILE:O	16:P:224:GLY:N	2.50	0.42
1:A:222:VAL:CG2	15:O:406:LEU:HD13	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:THR:O	1:A:598:LYS:HE2	2.19	0.42
1:A:735:LYS:HB2	1:A:735:LYS:HE2	1.90	0.42
1:A:1185:MET:HB2	1:A:1186:TYR:H	1.63	0.42
1:A:1372:PRO:HA	1:A:1373:PRO:HD3	1.89	0.42
2:B:262:MET:HE3	2:B:262:MET:HB2	1.81	0.42
4:D:2:GLU:HG2	4:D:2:GLU:O	2.19	0.42
4:D:17:PHE:CD2	4:D:18:GLN:NE2	2.86	0.42
6:F:81:VAL:HG11	6:F:96:GLU:HA	2.01	0.42
7:G:197:LEU:HD13	7:G:200:TRP:CH2	2.54	0.42
11:K:59:ILE:HG12	11:K:59:ILE:O	2.20	0.42
15:O:459:ARG:NH1	15:O:460:LEU:HB2	2.34	0.42
1:A:6:PHE:CD2	7:G:157:PHE:HA	2.54	0.42
1:A:38:SER:HA	17:Q:24:GLY:HA2	2.02	0.42
1:A:375:LEU:HD11	1:A:381:ALA:HB2	2.02	0.42
1:A:533:ARG:O	1:A:1283:ASP:HB2	2.20	0.42
2:B:28:ARG:HD3	2:B:28:ARG:HA	1.86	0.42
4:D:3:VAL:O	4:D:3:VAL:CG2	2.68	0.42
6:F:83:LEU:N	6:F:83:LEU:CD2	2.83	0.42
12:L:26:ASN:ND2	12:L:36:CYS:HB3	2.35	0.42
15:O:174:PRO:N	15:O:175:PRO:HD2	2.34	0.42
1:A:942:LYS:HD2	1:A:942:LYS:HA	1.75	0.42
1:A:1212:ILE:HD11	1:A:1223:TYR:CD2	2.53	0.42
1:A:1343:VAL:HG21	2:B:1056:ILE:HD13	2.02	0.42
2:B:253:GLN:CG	14:N:146:GLU:OE2	2.68	0.42
4:D:48:GLU:CG	7:G:103:PHE:HB3	2.50	0.42
4:D:65:ILE:C	4:D:65:ILE:HD12	2.44	0.42
4:D:90:ARG:O	4:D:91:PRO:C	2.63	0.42
7:G:38:VAL:HG11	7:G:186:LEU:HB2	2.02	0.42
10:J:53:VAL:O	10:J:53:VAL:CG1	2.67	0.42
15:O:170:ASP:CG	15:O:173:PRO:HG2	2.45	0.42
19:X:39:DG:C2'	19:X:40:DC:H5'	2.42	0.42
1:A:233:GLU:O	1:A:236:PRO:HD2	2.20	0.42
1:A:324:GLU:OE2	1:A:343:GLN:NE2	2.53	0.42
1:A:523:MET:HB3	1:A:523:MET:HE3	1.57	0.42
1:A:700:ILE:O	1:A:704:THR:HG23	2.20	0.42
2:B:131:LEU:HD22	2:B:131:LEU:HA	1.69	0.42
15:O:409:ILE:HB	15:O:423:LEU:CG	2.49	0.42
1:A:38:SER:CA	17:Q:24:GLY:HA2	2.50	0.41
1:A:112:CYS:SG	1:A:159:CYS:SG	3.18	0.41
1:A:1223:TYR:CD1	1:A:1223:TYR:N	2.88	0.41
2:B:260:HIS:H	2:B:260:HIS:CD2	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:494:LYS:HB2	2:B:494:LYS:HE2	1.67	0.41
2:B:1062:MET:SD	7:G:61:PRO:HB3	2.60	0.41
5:E:89:VAL:O	5:E:92:GLN:HG3	2.19	0.41
7:G:79:PRO:HG3	7:G:150:PHE:CE2	2.55	0.41
13:M:207:HIS:O	14:N:370:THR:HA	2.20	0.41
16:P:200:GLN:NE2	16:P:257:GLU:OE2	2.53	0.41
16:P:206:ARG:CZ	16:P:217:TRP:HE1	2.33	0.41
1:A:412:PRO:HG3	1:A:433:LYS:HB2	2.02	0.41
1:A:1000:LEU:HD13	1:A:1000:LEU:HA	1.77	0.41
2:B:640:ASP:OD1	2:B:640:ASP:N	2.53	0.41
2:B:721:LYS:NZ	2:B:731:GLU:OE1	2.49	0.41
2:B:1093:HIS:O	2:B:1093:HIS:CG	2.74	0.41
4:D:28:LYS:HE2	4:D:28:LYS:HB3	1.83	0.41
4:D:45:ILE:HG13	7:G:46:ILE:HG23	2.02	0.41
4:D:66:VAL:O	4:D:70:LEU:HB2	2.20	0.41
10:J:44:CYS:O	10:J:47:ARG:HG2	2.20	0.41
15:O:102:THR:HA	15:O:129:LEU:HD11	2.02	0.41
15:O:353:VAL:HG21	15:O:435:LEU:HD21	2.03	0.41
15:O:399:LEU:CD1	15:O:404:MET:HB3	2.50	0.41
1:A:662:ASN:O	1:A:666:ILE:HG12	2.20	0.41
1:A:704:THR:HG22	1:A:839:TYR:CE1	2.56	0.41
2:B:344:LEU:HD13	2:B:344:LEU:HA	1.80	0.41
4:D:74:LYS:HB3	4:D:74:LYS:HE3	1.63	0.41
13:M:123:GLU:HG3	13:M:125:HIS:CE1	2.55	0.41
19:X:35:DT:H2'	19:X:36:DA:C8	2.55	0.41
1:A:1050:LEU:HD23	1:A:1050:LEU:O	2.21	0.41
1:A:1193:LYS:NZ	9:I:42:LYS:HD3	2.35	0.41
2:B:241:LYS:HD3	2:B:246:GLU:HG2	2.01	0.41
2:B:916:MET:HG3	2:B:917:PRO:HD2	2.02	0.41
5:E:51:GLY:O	5:E:55:ARG:HB2	2.20	0.41
1:A:232:ALA:HB2	15:O:6:ILE:HD11	2.03	0.41
1:A:563:LYS:HE3	1:A:567:ILE:HD11	2.03	0.41
1:A:625:CYS:SG	1:A:627:LYS:O	2.78	0.41
2:B:236:ILE:HD12	2:B:240:PHE:HE2	1.86	0.41
2:B:522:ASP:OD1	2:B:523:VAL:N	2.53	0.41
2:B:551:ASP:OD1	2:B:551:ASP:N	2.50	0.41
2:B:988:TYR:CD1	2:B:988:TYR:C	2.99	0.41
11:K:27:LEU:HD23	11:K:27:LEU:N	2.36	0.41
15:O:269:THR:HG21	15:O:298:PRO:HD3	2.01	0.41
15:O:432:ALA:HB1	15:O:523:LEU:HD21	2.01	0.41
16:P:227:LYS:HD2	16:P:240:ASN:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:286:PRO:CB	17:Q:38:PHE:CD2	3.04	0.41
1:A:94:HIS:HE1	2:B:1120:MET:O	2.03	0.41
1:A:554:LEU:HD12	1:A:554:LEU:HA	1.77	0.41
1:A:687:ALA:HB3	1:A:688:PRO:HD3	2.02	0.41
1:A:864:LYS:NZ	1:A:1048:MET:CB	2.83	0.41
2:B:513:LYS:HE3	2:B:513:LYS:HB2	1.72	0.41
2:B:876:GLU:H	2:B:876:GLU:CD	2.24	0.41
3:C:264:VAL:O	3:C:264:VAL:CG2	2.69	0.41
6:F:100:ARG:NH2	6:F:123:LEU:O	2.54	0.41
1:A:255:LEU:HD21	1:A:320:TYR:CE2	2.55	0.41
1:A:717:LEU:HA	1:A:717:LEU:HD13	1.81	0.41
2:B:133:ILE:HD13	2:B:380:PHE:CE2	2.56	0.41
2:B:249:GLN:HE22	14:N:144:LYS:NZ	2.19	0.41
4:D:48:GLU:CD	7:G:103:PHE:CD1	2.99	0.41
4:D:94:ALA:HA	4:D:117:LEU:HD22	2.03	0.41
13:M:239:VAL:HG13	14:N:343:LYS:NZ	2.35	0.41
15:O:449:ARG:HB2	16:P:310:MET:HE1	2.01	0.41
1:A:95:VAL:HG21	1:A:325:LEU:HD13	2.02	0.41
1:A:1236:MET:HG3	5:E:137:ILE:HG21	2.02	0.41
2:B:265:PHE:O	2:B:269:LEU:HG	2.21	0.41
2:B:499:MET:HE2	2:B:663:THR:HG21	2.01	0.41
3:C:287:ILE:CD1	3:C:293:LEU:CB	2.86	0.41
15:O:376:GLU:HB3	15:O:424:TYR:HD1	1.86	0.41
15:O:377:GLN:HA	15:O:380:VAL:HG12	2.03	0.41
1:A:6:PHE:HZ	7:G:155:GLU:HB3	1.86	0.41
1:A:259:PRO:O	1:A:262:ILE:HG12	2.20	0.41
1:A:378:ASP:OD2	1:A:526:LYS:HE3	2.19	0.41
1:A:1155:THR:O	1:A:1155:THR:CG2	2.68	0.41
2:B:239:ILE:HG22	2:B:243:MET:HE2	2.02	0.41
2:B:555:LEU:HD23	2:B:555:LEU:O	2.21	0.41
2:B:686:GLN:HA	2:B:686:GLN:HE21	1.85	0.41
2:B:957:ARG:HB2	2:B:957:ARG:HH11	1.86	0.41
6:F:75:MET:HB2	7:G:15:PRO:HG2	2.01	0.41
12:L:31:ARG:NE	12:L:31:ARG:HA	2.35	0.41
1:A:6:PHE:CZ	7:G:155:GLU:HB3	2.56	0.41
1:A:580:LYS:HB2	11:K:31:GLN:HG2	2.03	0.41
1:A:1375:ARG:HA	1:A:1376:PRO:HD3	1.95	0.41
2:B:618:TYR:HD1	2:B:618:TYR:HA	1.83	0.41
4:D:54:SER:O	4:D:55:LYS:C	2.63	0.41
4:D:100:MET:SD	7:G:147:GLU:CD	3.04	0.41
11:K:28:GLU:OE1	11:K:28:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:MET:O	1:A:153:LYS:HD3	2.21	0.40
1:A:1121:PHE:HB2	9:I:38:VAL:HG13	2.02	0.40
2:B:548:VAL:O	2:B:548:VAL:HG12	2.20	0.40
2:B:990:THR:HA	2:B:997:PRO:HA	2.03	0.40
5:E:17:ILE:HD13	5:E:17:ILE:HA	1.89	0.40
10:J:47:ARG:HH11	10:J:47:ARG:HG3	1.85	0.40
11:K:50:THR:OG1	11:K:51:LEU:N	2.54	0.40
11:K:106:VAL:O	11:K:110:VAL:HG12	2.21	0.40
13:M:67:PRO:HD2	14:N:138:ILE:CG1	2.51	0.40
1:A:39:LYS:HE3	1:A:41:LEU:HB2	2.03	0.40
1:A:183:LYS:HD3	1:A:183:LYS:H	1.85	0.40
1:A:963:ASP:N	1:A:963:ASP:OD1	2.54	0.40
1:A:1304:THR:OG1	1:A:1306:PHE:N	2.51	0.40
2:B:88:GLU:N	2:B:88:GLU:OE2	2.54	0.40
2:B:196:LYS:HD3	20:Y:9:DA:OP1	2.20	0.40
2:B:973:CYS:SG	2:B:974:GLU:N	2.94	0.40
2:B:1078:ASP:HB3	2:B:1101:VAL:CG1	2.51	0.40
4:D:16:VAL:HG21	7:G:2:PHE:CD2	2.57	0.40
7:G:80:PHE:CD2	7:G:82:ASP:HB2	2.56	0.40
9:I:8:CYS:HB2	13:M:139:PHE:CE1	2.56	0.40
1:A:222:VAL:HG21	15:O:406:LEU:HD13	2.02	0.40
1:A:263:ARG:HD3	1:A:279:LEU:HD23	2.02	0.40
1:A:1364:HIS:ND1	1:A:1366:ALA:HB2	2.37	0.40
2:B:1063:LEU:HD12	2:B:1063:LEU:O	2.21	0.40
3:C:334:ARG:O	3:C:334:ARG:HD3	2.21	0.40
9:I:1:MET:SD	14:N:153:GLN:OE1	2.79	0.40
14:N:269:LEU:HA	14:N:383:LEU:O	2.20	0.40
15:O:345:LEU:HB3	15:O:522:LEU:HD21	2.03	0.40
15:O:356:GLU:O	16:P:289:LEU:HD11	2.21	0.40
1:A:39:LYS:N	17:Q:24:GLY:CA	2.84	0.40
1:A:406:LYS:HE2	1:A:406:LYS:HB3	1.96	0.40
1:A:556:ASP:OD1	8:H:22:PHE:HB3	2.21	0.40
1:A:973:ILE:HD13	1:A:973:ILE:HA	1.90	0.40
1:A:1051:LYS:HE3	1:A:1051:LYS:C	2.44	0.40
1:A:1134:LEU:HD12	1:A:1134:LEU:HA	1.94	0.40
3:C:163:TYR:CE1	3:C:204:PRO:HG3	2.56	0.40
4:D:3:VAL:HG11	7:G:42:VAL:HG21	2.02	0.40
7:G:192:GLU:OE2	7:G:197:LEU:HD11	2.21	0.40
13:M:67:PRO:HD2	14:N:138:ILE:HD11	2.02	0.40
15:O:392:LYS:HD2	15:O:395:LEU:HD12	2.03	0.40
15:O:514:ILE:HD11	17:Q:54:GLU:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:76:GLU:O	17:Q:78:PRO:HD3	2.22	0.40
19:X:37:DG:H2''	19:X:38:DA:O5'	2.22	0.40
1:A:39:LYS:NZ	1:A:39:LYS:HB3	2.36	0.40
1:A:133:GLY:O	1:A:138:GLN:NE2	2.52	0.40
1:A:331:ASN:C	1:A:331:ASN:HD22	2.24	0.40
1:A:860:ASP:OD1	2:B:465:VAL:HG21	2.22	0.40
1:A:1216:GLU:OE1	1:A:1216:GLU:HA	2.20	0.40
1:A:1363:LEU:HB3	6:F:105:ILE:HB	2.04	0.40
2:B:404:LYS:NZ	2:B:404:LYS:N	2.69	0.40
2:B:812:ASP:OD1	2:B:813:GLY:N	2.54	0.40
7:G:5:VAL:HG12	7:G:7:MET:HG3	2.03	0.40
9:I:4:PHE:HE2	14:N:146:GLU:OE1	2.05	0.40
13:M:242:PRO:O	14:N:392:LEU:HD22	2.22	0.40
14:N:389:PHE:O	14:N:393:LEU:HB3	2.22	0.40
15:O:68:HIS:CE1	15:O:70:ARG:HH21	2.39	0.40
15:O:106:ILE:HD13	15:O:125:VAL:HG11	2.03	0.40
15:O:376:GLU:O	15:O:421:PHE:HE1	2.04	0.40
17:Q:80:GLU:HA	17:Q:86:ARG:HD2	2.03	0.40
17:Q:86:ARG:HB2	17:Q:86:ARG:CZ	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1356/1390 (98%)	1274 (94%)	69 (5%)	13 (1%)	12	45
2	B	1091/1133 (96%)	1026 (94%)	57 (5%)	8 (1%)	18	51
3	C	341/346 (99%)	338 (99%)	3 (1%)	0	100	100
4	D	120/148 (81%)	109 (91%)	10 (8%)	1 (1%)	16	49
5	E	207/210 (99%)	200 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	74/127 (58%)	72 (97%)	2 (3%)	0	100	100
7	G	160/204 (78%)	137 (86%)	23 (14%)	0	100	100
8	H	146/150 (97%)	141 (97%)	5 (3%)	0	100	100
9	I	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
10	J	63/67 (94%)	63 (100%)	0	0	100	100
11	K	101/133 (76%)	100 (99%)	1 (1%)	0	100	100
12	L	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
13	M	198/708 (28%)	189 (96%)	8 (4%)	1 (0%)	24	57
14	N	140/398 (35%)	140 (100%)	0	0	100	100
15	O	435/534 (82%)	416 (96%)	18 (4%)	1 (0%)	43	72
16	P	128/316 (40%)	102 (80%)	25 (20%)	1 (1%)	16	49
17	Q	82/223 (37%)	72 (88%)	9 (11%)	1 (1%)	10	41
All	All	4791/6253 (77%)	4519 (94%)	246 (5%)	26 (0%)	26	57

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	177	GLU
1	A	1185	MET
1	A	1209	ARG
2	B	1096	LYS
4	D	8	SER
15	O	409	ILE
16	P	296	CYS
1	A	485	THR
1	A	628	GLY
1	A	774	SER
1	A	988	GLY
2	B	247	SER
2	B	301	PRO
1	A	942	LYS
2	B	130	ALA
2	B	1099	CYS
13	M	228	PRO
2	B	64	LYS
2	B	123	SER
2	B	322	PRO

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Mol	Chain	Res	Type
17	Q	28	PRO
1	A	38	SER
1	A	590	LYS
1	A	1125	ASP
1	A	1178	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1182/1212 (98%)	1009 (85%)	173 (15%)	3	18
2	B	950/988 (96%)	818 (86%)	132 (14%)	3	19
3	C	299/302 (99%)	275 (92%)	24 (8%)	11	37
4	D	114/136 (84%)	88 (77%)	26 (23%)	1	6
5	E	191/192 (100%)	184 (96%)	7 (4%)	30	56
6	F	66/111 (60%)	60 (91%)	6 (9%)	9	33
7	G	149/181 (82%)	145 (97%)	4 (3%)	39	61
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	92/93 (99%)	92 (100%)	0	100	100
10	J	53/56 (95%)	44 (83%)	9 (17%)	2	13
11	K	92/119 (77%)	85 (92%)	7 (8%)	12	39
12	L	43/55 (78%)	38 (88%)	5 (12%)	5	25
13	M	180/622 (29%)	177 (98%)	3 (2%)	53	69
14	N	131/347 (38%)	128 (98%)	3 (2%)	44	64
15	O	400/476 (84%)	393 (98%)	7 (2%)	51	68
16	P	114/280 (41%)	111 (97%)	3 (3%)	40	62
17	Q	81/195 (42%)	74 (91%)	7 (9%)	10	34
All	All	4266/5496 (78%)	3850 (90%)	416 (10%)	10	31

All (416) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PHE
1	A	10	ASP
1	A	15	ILE
1	A	23	LYS
1	A	34	ILE
1	A	39	LYS
1	A	40	ASN
1	A	51	LEU
1	A	52	LEU
1	A	55	VAL
1	A	62	THR
1	A	71	THR
1	A	72	CYS
1	A	86	ILE
1	A	117	LEU
1	A	119	GLN
1	A	120	GLU
1	A	124	GLN
1	A	126	LEU
1	A	134	LEU
1	A	136	TYR
1	A	151	ARG
1	A	159	CYS
1	A	165	THR
1	A	171	LEU
1	A	179	TYR
1	A	189	ILE
1	A	190	VAL
1	A	193	PHE
1	A	194	LEU
1	A	205	LYS
1	A	211	LEU
1	A	221	LEU
1	A	222	VAL
1	A	224	LEU
1	A	225	ASN
1	A	226	LEU
1	A	237	LEU
1	A	240	MET
1	A	248	SER
1	A	251	ILE
1	A	257	VAL
1	A	263	ARG

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Mol	Chain	Res	Type
1	A	293	ILE
1	A	303	THR
1	A	304	GLN
1	A	306	ILE
1	A	316	GLN
1	A	319	LEU
1	A	322	ASN
1	A	328	ILE
1	A	338	THR
1	A	351	ARG
1	A	367	THR
1	A	370	SER
1	A	377	ILE
1	A	421	ILE
1	A	426	THR
1	A	429	LYS
1	A	432	LEU
1	A	433	LYS
1	A	448	ASP
1	A	454	LEU
1	A	462	PHE
1	A	479	ARG
1	A	484	ARG
1	A	485	THR
1	A	507	LEU
1	A	520	LEU
1	A	523	MET
1	A	530	VAL
1	A	534	ASN
1	A	538	LEU
1	A	542	ILE
1	A	544	ASP
1	A	554	LEU
1	A	555	LYS
1	A	571	ILE
1	A	573	VAL
1	A	577	GLU
1	A	579	ILE
1	A	581	VAL
1	A	583	LEU
1	A	593	THR
1	A	596	THR

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Mol	Chain	Res	Type
1	A	623	GLN
1	A	627	LYS
1	A	630	ASP
1	A	646	MET
1	A	649	SER
1	A	663	ILE
1	A	668	LEU
1	A	685	ARG
1	A	686	LEU
1	A	707	GLN
1	A	709	LEU
1	A	717	LEU
1	A	729	GLU
1	A	731	LEU
1	A	748	LEU
1	A	751	LEU
1	A	768	LEU
1	A	771	LEU
1	A	773	LYS
1	A	798	CYS
1	A	799	VAL
1	A	822	GLU
1	A	876	VAL
1	A	881	ASP
1	A	882	LEU
1	A	883	CYS
1	A	897	ILE
1	A	901	ILE
1	A	908	ASP
1	A	912	MET
1	A	913	GLU
1	A	944	GLU
1	A	946	ILE
1	A	954	LYS
1	A	966	LEU
1	A	968	GLU
1	A	970	LYS
1	A	974	LYS
1	A	989	ILE
1	A	991	ASP
1	A	1000	LEU
1	A	1011	VAL

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Mol	Chain	Res	Type
1	A	1027	MET
1	A	1033	VAL
1	A	1048	MET
1	A	1050	LEU
1	A	1051	LYS
1	A	1054	HIS
1	A	1055	PHE
1	A	1058	VAL
1	A	1061	MET
1	A	1065	LEU
1	A	1067	VAL
1	A	1074	ILE
1	A	1088	GLN
1	A	1092	ASP
1	A	1093	ASP
1	A	1094	ASP
1	A	1096	ASP
1	A	1099	ARG
1	A	1113	ILE
1	A	1119	GLU
1	A	1126	CYS
1	A	1128	ILE
1	A	1129	LEU
1	A	1132	LEU
1	A	1137	ILE
1	A	1155	THR
1	A	1157	LYS
1	A	1170	GLU
1	A	1173	VAL
1	A	1180	ASN
1	A	1188	VAL
1	A	1191	PHE
1	A	1198	LYS
1	A	1200	VAL
1	A	1211	VAL
1	A	1212	ILE
1	A	1215	ASP
1	A	1225	LEU
1	A	1227	VAL
1	A	1230	ASP
1	A	1233	ARG
1	A	1241	VAL

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Mol	Chain	Res	Type
1	A	1242	LYS
1	A	1244	THR
1	A	1246	THR
1	A	1363	LEU
2	B	24	GLU
2	B	34	LEU
2	B	41	LYS
2	B	42	GLN
2	B	54	GLU
2	B	55	ILE
2	B	59	MET
2	B	62	ASN
2	B	65	VAL
2	B	74	TYR
2	B	81	TYR
2	B	95	ARG
2	B	115	VAL
2	B	119	TYR
2	B	120	THR
2	B	121	ARG
2	B	125	ARG
2	B	131	LEU
2	B	138	ILE
2	B	139	MET
2	B	140	LEU
2	B	148	THR
2	B	181	GLN
2	B	183	GLN
2	B	189	ILE
2	B	191	VAL
2	B	203	VAL
2	B	204	THR
2	B	207	THR
2	B	213	ARG
2	B	214	THR
2	B	216	MET
2	B	218	VAL
2	B	232	GLU
2	B	233	ASP
2	B	234	ILE
2	B	238	ILE
2	B	254	MET

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Mol	Chain	Res	Type
2	B	271	GLU
2	B	279	THR
2	B	303	LYS
2	B	305	LYS
2	B	306	ILE
2	B	316	THR
2	B	317	ILE
2	B	319	THR
2	B	343	ILE
2	B	344	LEU
2	B	348	ASP
2	B	351	VAL
2	B	375	ASP
2	B	377	PHE
2	B	382	SER
2	B	384	MET
2	B	387	ILE
2	B	392	ILE
2	B	394	LYS
2	B	402	VAL
2	B	404	LYS
2	B	409	ASP
2	B	411	ILE
2	B	412	THR
2	B	419	ILE
2	B	440	LEU
2	B	446	ILE
2	B	462	THR
2	B	463	ARG
2	B	494	LYS
2	B	502	ILE
2	B	505	ASP
2	B	506	MET
2	B	507	GLU
2	B	517	ASN
2	B	518	LEU
2	B	525	LEU
2	B	530	GLU
2	B	536	VAL
2	B	542	ASN
2	B	548	VAL
2	B	549	ILE

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Mol	Chain	Res	Type
2	B	552	HIS
2	B	559	PHE
2	B	561	LEU
2	B	570	GLU
2	B	573	SER
2	B	574	ILE
2	B	578	LEU
2	B	583	VAL
2	B	606	VAL
2	B	616	GLN
2	B	619	ARG
2	B	623	ASP
2	B	640	ASP
2	B	643	ILE
2	B	686	GLN
2	B	697	ILE
2	B	708	LEU
2	B	712	LEU
2	B	724	THR
2	B	733	LEU
2	B	743	VAL
2	B	764	ARG
2	B	771	VAL
2	B	777	CYS
2	B	784	ASN
2	B	790	VAL
2	B	791	MET
2	B	800	ARG
2	B	801	LYS
2	B	814	ILE
2	B	815	CYS
2	B	817	PRO
2	B	822	GLU
2	B	828	VAL
2	B	874	ASN
2	B	883	MET
2	B	885	LEU
2	B	906	VAL
2	B	916	MET
2	B	946	LEU
2	B	976	LEU
2	B	984	LEU

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Mol	Chain	Res	Type
2	B	990	THR
2	B	1007	VAL
2	B	1010	GLN
2	B	1030	VAL
2	B	1049	GLU
2	B	1089	SER
2	B	1112	LEU
2	B	1113	LEU
2	B	1115	GLN
2	B	1128	LEU
3	C	21	VAL
3	C	26	THR
3	C	34	SER
3	C	43	ASP
3	C	52	ASP
3	C	54	VAL
3	C	55	HIS
3	C	90	GLU
3	C	95	TYR
3	C	100	ILE
3	C	103	ASP
3	C	126	ASN
3	C	147	THR
3	C	158	ASP
3	C	164	VAL
3	C	183	ASP
3	C	215	VAL
3	C	230	THR
3	C	261	VAL
3	C	270	LYS
3	C	272	VAL
3	C	316	LEU
3	C	319	ASP
3	C	320	VAL
4	D	1	MET
4	D	3	VAL
4	D	11	LEU
4	D	14	TYR
4	D	15	GLU
4	D	18	GLN
4	D	19	LEU
4	D	20	LEU

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Mol	Chain	Res	Type
4	D	32	LYS
4	D	40	GLN
4	D	41	ASN
4	D	43	ASN
4	D	59	ARG
4	D	64	GLU
4	D	65	ILE
4	D	70	LEU
4	D	74	LYS
4	D	77	LYS
4	D	84	LEU
4	D	88	ASN
4	D	96	GLU
4	D	97	ILE
4	D	99	LEU
4	D	101	VAL
4	D	105	GLU
4	D	113	ILE
5	E	28	VAL
5	E	50	GLU
5	E	55	ARG
5	E	61	LEU
5	E	76	PHE
5	E	79	GLU
5	E	177	ASP
6	F	52	ILE
6	F	80	MET
6	F	81	VAL
6	F	82	GLU
6	F	107	ARG
6	F	116	GLU
7	G	22	LEU
7	G	59	VAL
7	G	152	VAL
7	G	198	LEU
10	J	3	ILE
10	J	5	VAL
10	J	9	THR
10	J	19	GLU
10	J	21	TYR
10	J	26	GLN
10	J	30	THR

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Mol	Chain	Res	Type
10	J	33	ASP
10	J	48	MET
11	K	27	LEU
11	K	38	HIS
11	K	71	THR
11	K	77	GLU
11	K	82	LEU
11	K	103	LEU
11	K	110	VAL
12	L	19	CYS
12	L	28	ILE
12	L	34	ILE
12	L	52	LEU
12	L	53	VAL
13	M	7	ASP
13	M	233	VAL
13	M	239	VAL
14	N	269	LEU
14	N	393	LEU
14	N	395	HIS
15	O	170	ASP
15	O	239	LEU
15	O	408	GLU
15	O	409	ILE
15	O	411	LYS
15	O	414	ASP
15	O	423	LEU
16	P	205	GLN
16	P	283	VAL
16	P	284	ARG
17	Q	27	LEU
17	Q	31	VAL
17	Q	79	GLU
17	Q	80	GLU
17	Q	83	ASP
17	Q	86	ARG
17	Q	87	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS

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Mol	Chain	Res	Type
1	A	30	GLN
1	A	58	HIS
1	A	94	HIS
1	A	138	GLN
1	A	157	HIS
1	A	163	ASN
1	A	203	HIS
1	A	225	ASN
1	A	241	ASN
1	A	296	HIS
1	A	314	GLN
1	A	316	GLN
1	A	322	ASN
1	A	331	ASN
1	A	349	GLN
1	A	423	GLN
1	A	442	GLN
1	A	453	HIS
1	A	463	ASN
1	A	511	GLN
1	A	534	ASN
1	A	543	GLN
1	A	611	ASN
1	A	623	GLN
1	A	673	GLN
1	A	707	GLN
1	A	762	HIS
1	A	791	ASN
1	A	794	GLN
1	A	824	HIS
1	A	836	ASN
1	A	872	GLN
1	A	899	GLN
1	A	1039	GLN
1	A	1047	GLN
1	A	1062	ASN
1	A	1180	ASN
1	A	1239	HIS
1	A	1277	ASN
1	A	1278	HIS
1	A	1327	HIS
1	A	1336	GLN

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Mol	Chain	Res	Type
2	B	62	ASN
2	B	92	ASN
2	B	187	ASN
2	B	249	GLN
2	B	260	HIS
2	B	276	GLN
2	B	320	HIS
2	B	395	GLN
2	B	423	ASN
2	B	434	GLN
2	B	458	GLN
2	B	495	ASN
2	B	542	ASN
2	B	569	ASN
2	B	577	ASN
2	B	602	GLN
2	B	608	ASN
2	B	620	ASN
2	B	626	HIS
2	B	677	HIS
2	B	686	GLN
2	B	692	GLN
2	B	703	ASN
2	B	738	ASN
2	B	887	GLN
2	B	1093	HIS
2	B	1118	GLN
3	C	32	ASN
3	C	48	ASN
3	C	180	ASN
4	D	7	ASN
4	D	35	HIS
4	D	39	GLN
4	D	43	ASN
4	D	60	HIS
4	D	61	GLN
4	D	85	GLN
4	D	89	HIS
4	D	98	GLN
8	H	29	HIS
8	H	76	ASN
8	H	131	ASN

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Mol	Chain	Res	Type
9	I	10	ASN
9	I	21	HIS
9	I	61	ASN
10	J	26	GLN
11	K	45	HIS
12	L	26	ASN
13	M	125	HIS
14	N	270	GLN
15	O	3	GLN
15	O	14	GLN
15	O	49	GLN
15	O	113	ASN
15	O	146	ASN
15	O	337	ASN
15	O	355	GLN
15	O	379	GLN
15	O	415	HIS
15	O	445	ASN
15	O	457	ASN
15	O	465	GLN
15	O	507	ASN
16	P	200	GLN
16	P	207	ASN
16	P	240	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	R	4/10 (40%)	3 (75%)	1 (25%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	R	9	C
18	R	10	U
18	R	11	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	R	8	G

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 9 ligands modelled in this entry, 8 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	16	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	16	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

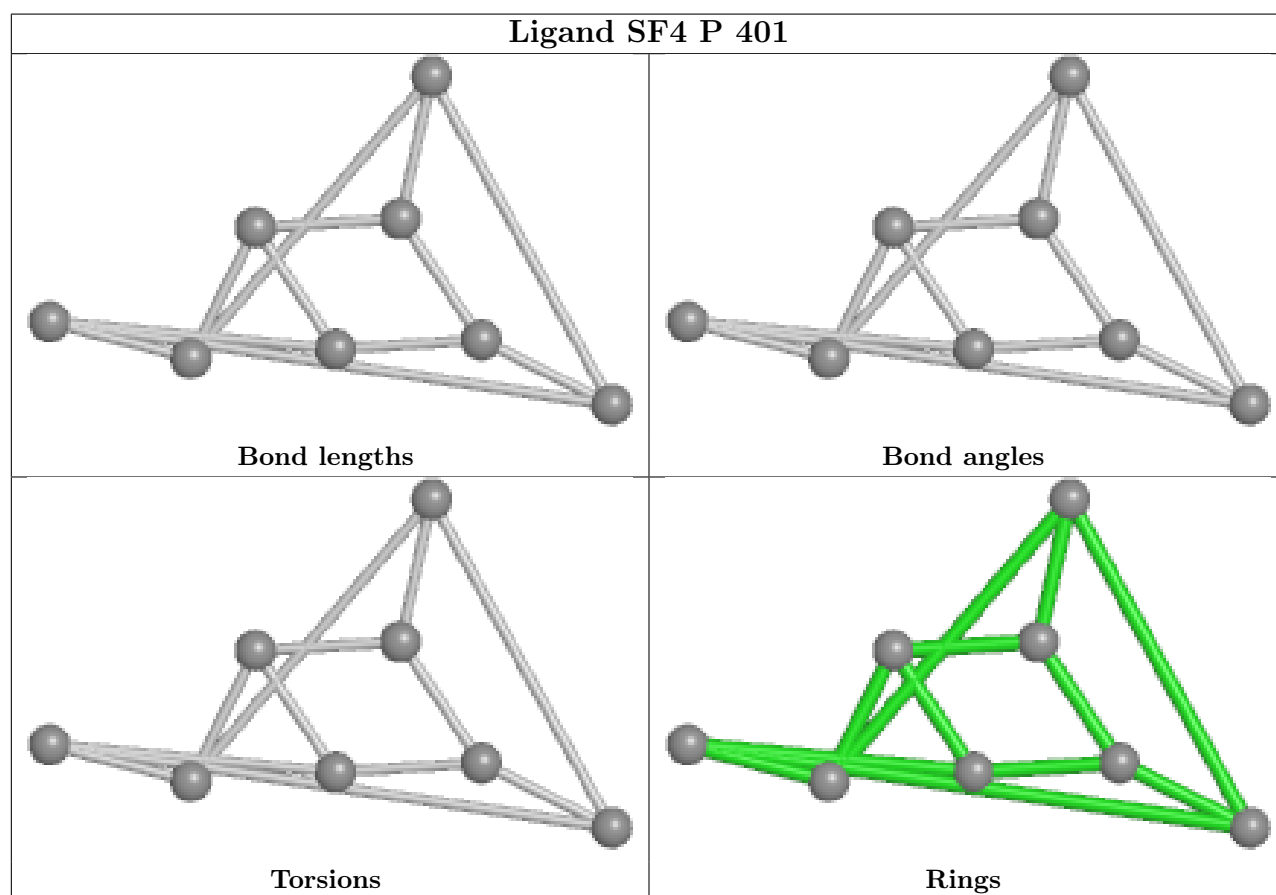
There are no torsion outliers.

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.

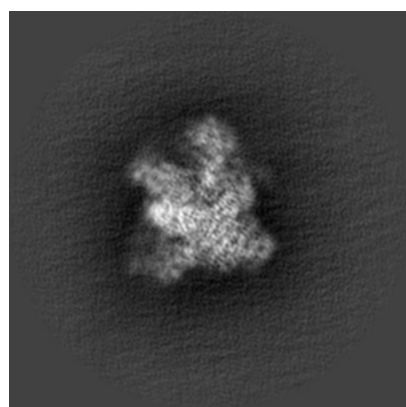
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31622. These allow visual inspection of the internal detail of the map and identification of artifacts.

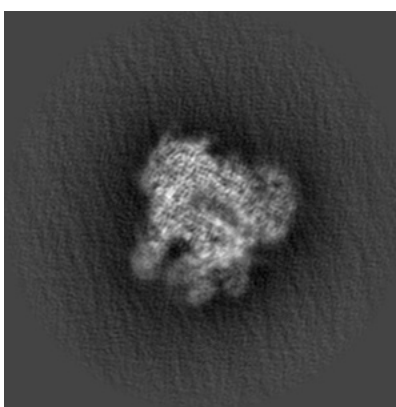
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

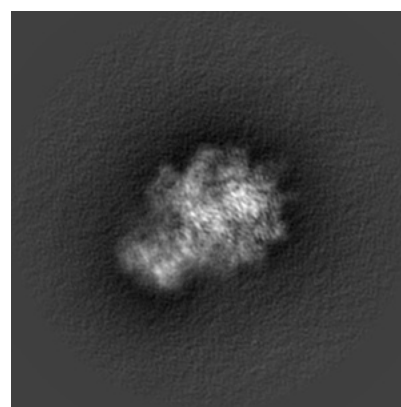
6.1.1 Primary map



X



Y

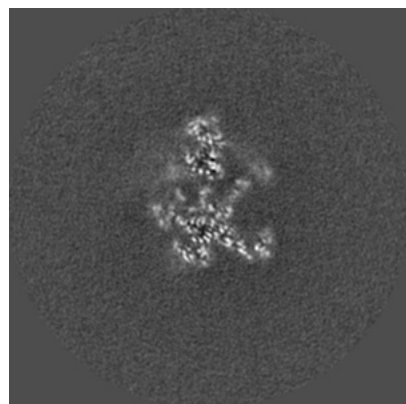


Z

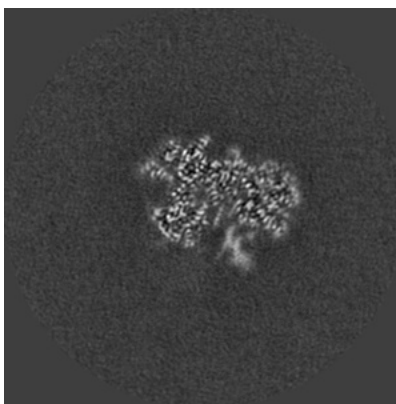
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

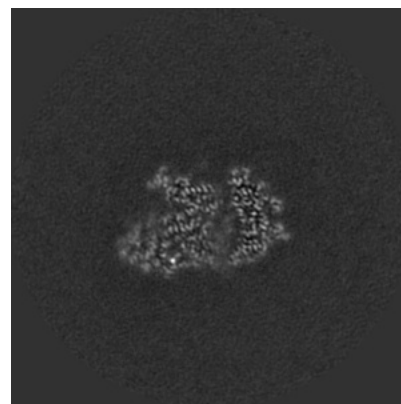
6.2.1 Primary map



X Index: 180



Y Index: 180

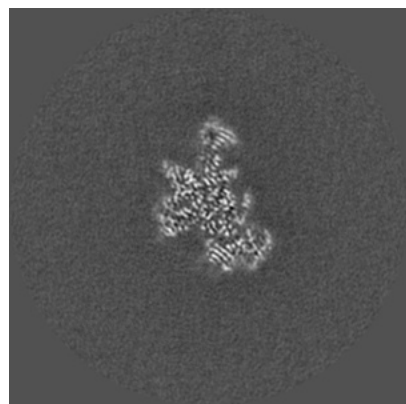


Z Index: 180

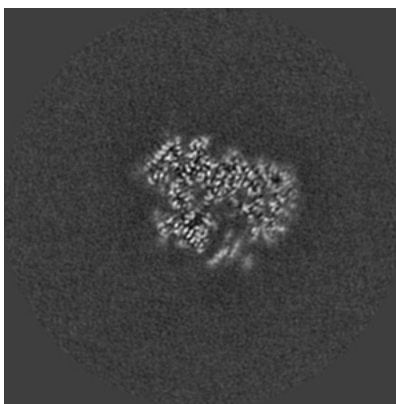
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

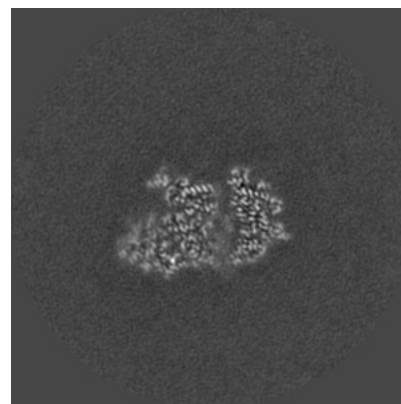
6.3.1 Primary map



X Index: 208



Y Index: 185

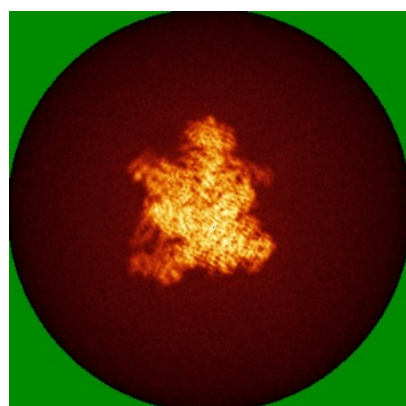


Z Index: 179

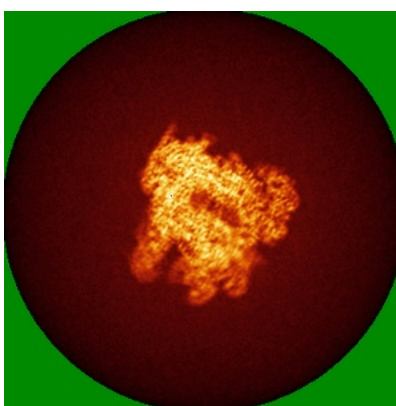
The images above show the largest variance slices of the map in three orthogonal directions.

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

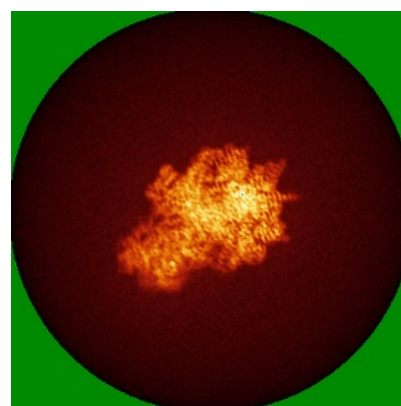
6.4.1 Primary map



X



Y

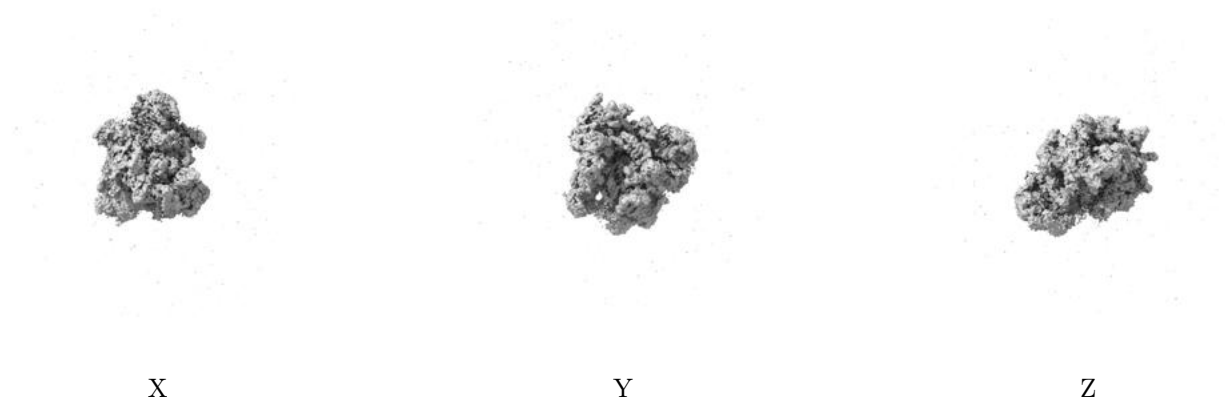


Z

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 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

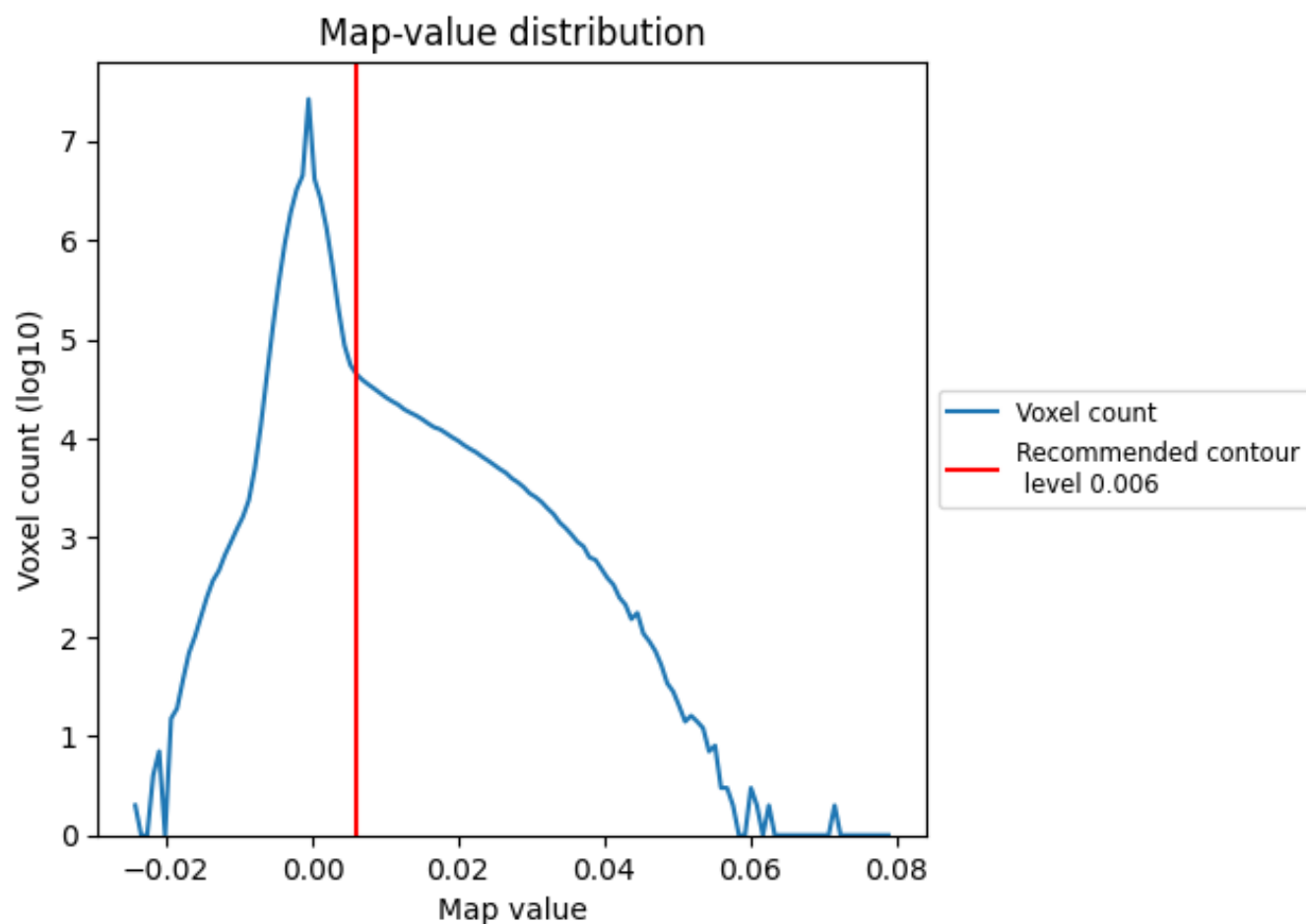
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

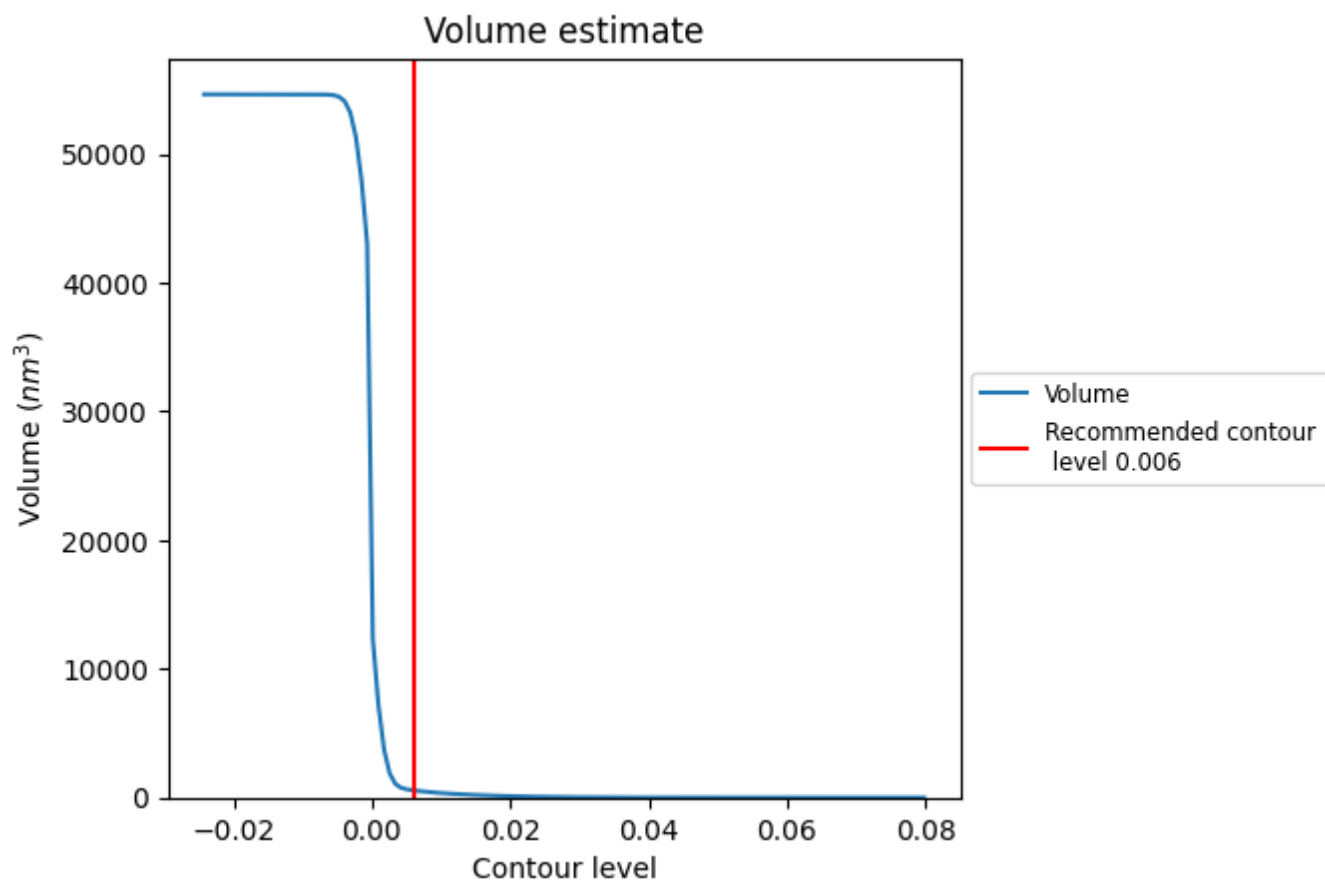
This section contains the results of statistical analysis of the map.

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.

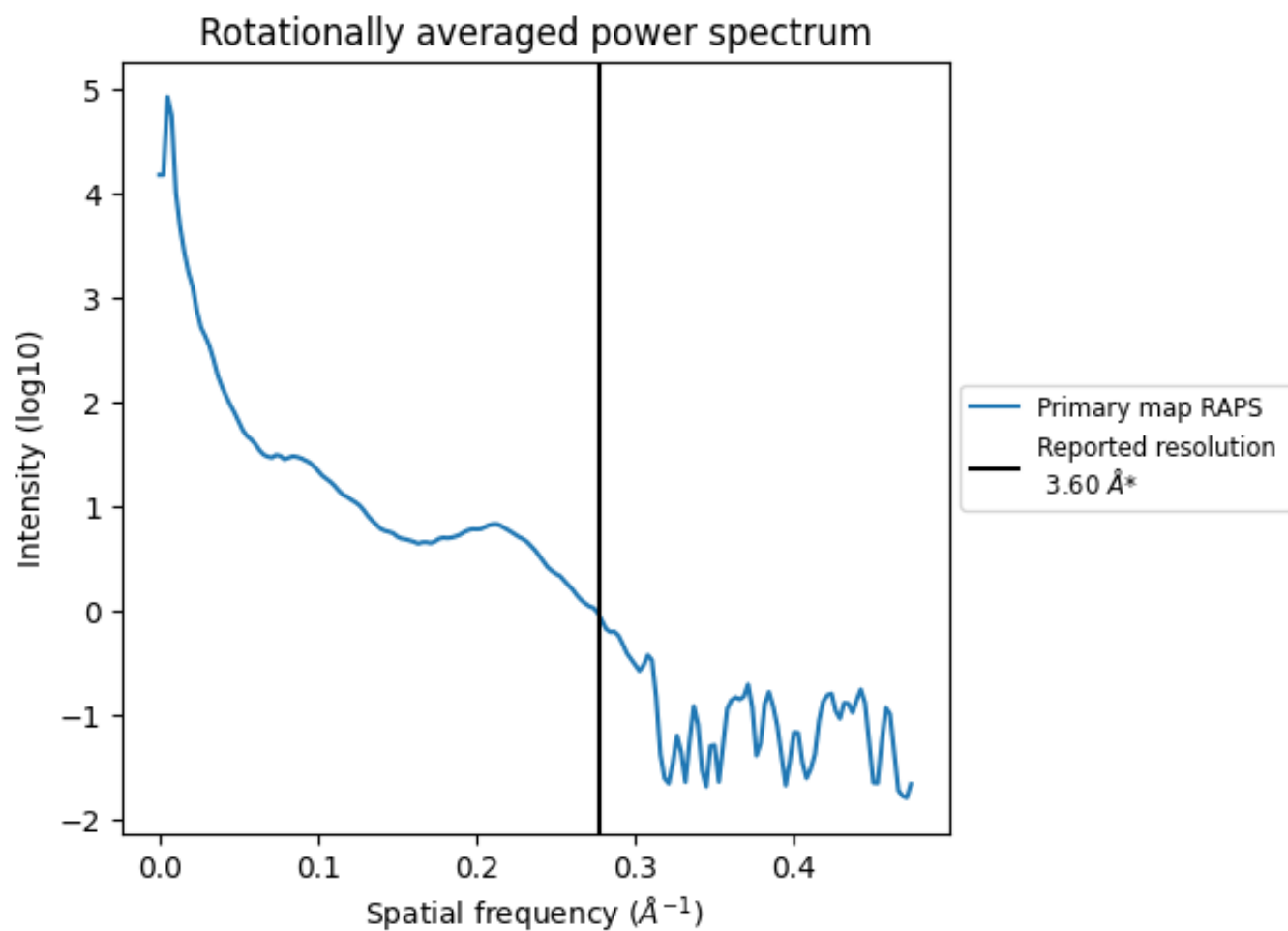
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 558 nm³; this corresponds to an approximate mass of 504 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

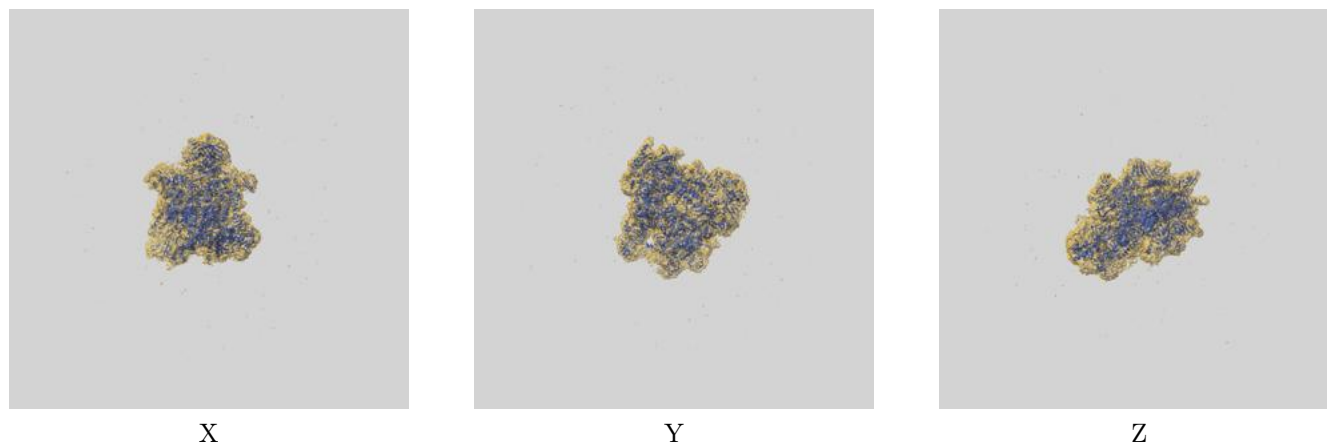
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

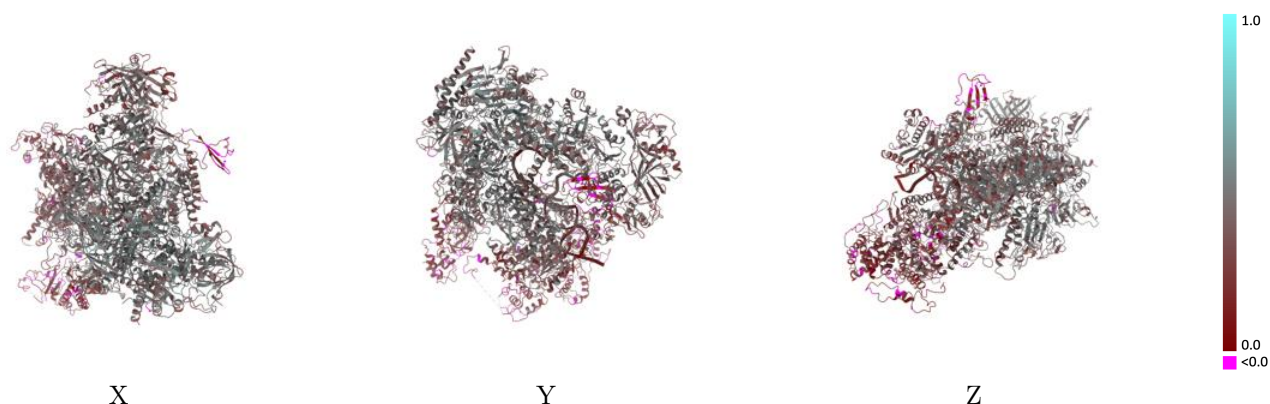
This section contains information regarding the fit between EMDB map EMD-31622 and PDB model 7FJJ. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



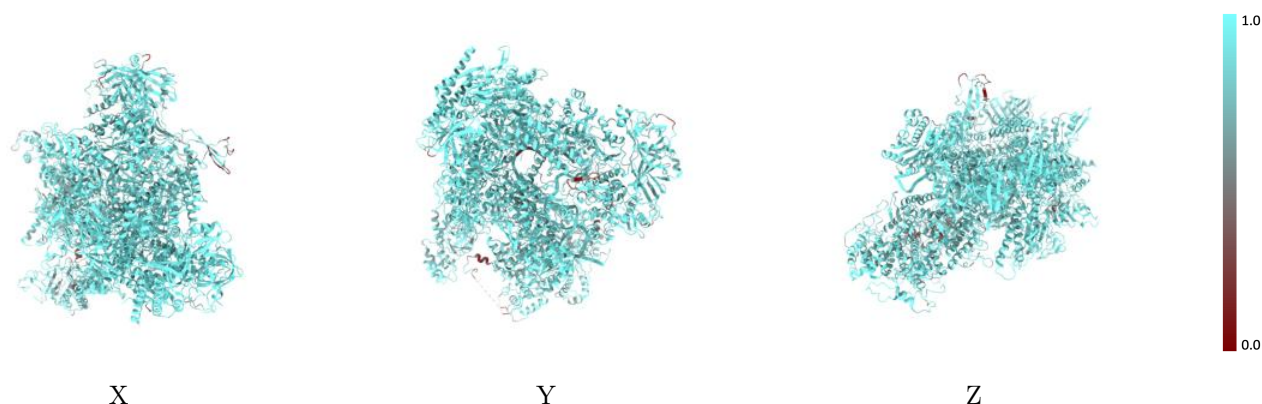
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



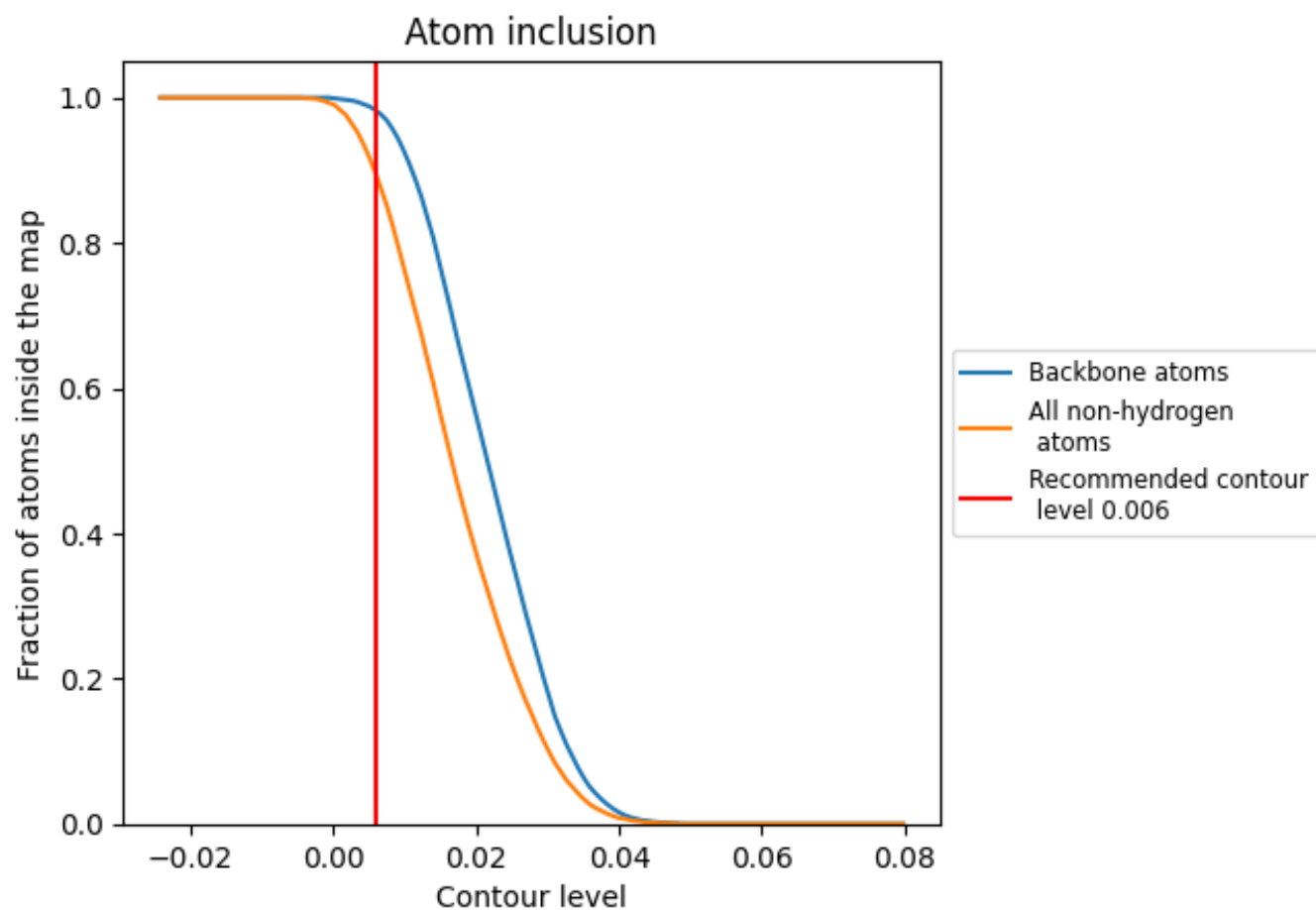
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 89% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8930	 0.3640
A	 0.9020	 0.4020
B	 0.9170	 0.4430
C	 0.9430	 0.4410
D	 0.8260	 0.1330
E	 0.9150	 0.3810
F	 0.9320	 0.4450
G	 0.8720	 0.2100
H	 0.9210	 0.4220
I	 0.7580	 0.2130
J	 0.9440	 0.4590
K	 0.9320	 0.4180
L	 0.9250	 0.3950
M	 0.8760	 0.3480
N	 0.8350	 0.3380
O	 0.8560	 0.2120
P	 0.8440	 0.1840
Q	 0.6810	 0.1280
R	 0.4880	 0.1650
X	 0.9380	 0.3380
Y	 0.9530	 0.2890

