



## Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 07:20 AM JST

PDB ID : 7FJI  
EMDB ID : EMD-31621  
Title : human Pol III elongation 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](mailto: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>.

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

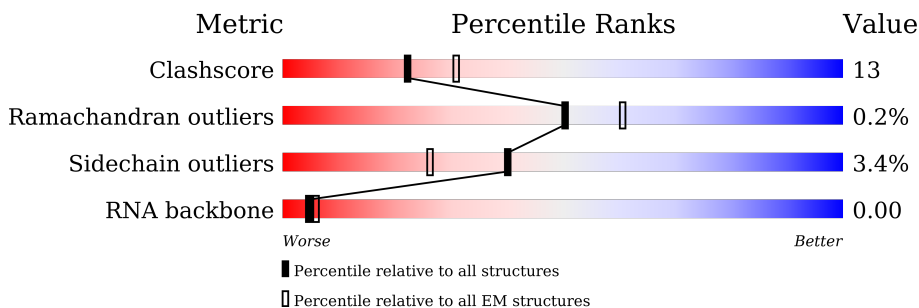
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.60 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.






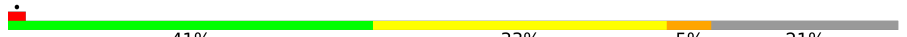

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 83% 14% ..
2	B	1133	 87% 9% .
3	C	346	 74% 23% ..
4	D	148	 35% 33% 14% 18%
5	E	210	 81% 17% .
6	F	127	 47% 11% . 40%
7	G	204	 54% 26% . 19%

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Mol	Chain	Length	Quality of chain
8	H	150	 88% 10% ..
9	I	108	 16% 70% 27% ..
10	J	67	 69% 21% 6% ..
11	K	133	 54% 22% 23%
12	L	58	 41% 33% 5% 21%
13	M	708	 26% 70%
14	N	398	 32% 5% 63%
15	O	534	 61% 20% 17%
16	P	316	 5% 27% 13% 59%
17	Q	223	 10% 21% 15% 61%
18	R	10	 20% 10% 30% 60%
19	X	54	 15% 17% 69%
20	Y	54	 13% 28% 59%

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	SF4	P	401	-	-	X	-

## 2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 39536 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1367	10732	6798	1874	1987	73	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1097	8680	5499	1516	1597	68	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S		
10	J	65	512	331	87	88	6	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	209	1682	1059	286	327	10	0	0

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	P		
18	R	4	86	38	15	29	4	0	0

- Molecule 19 is a DNA chain called non\_template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
19	X	17	349	165	66	101	17	0	0

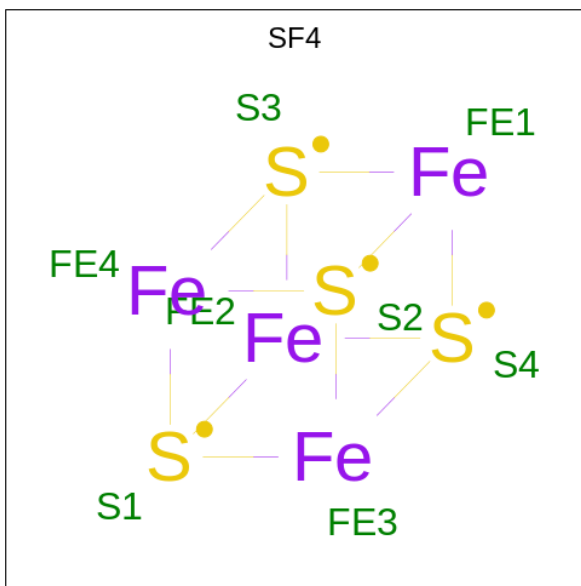
- Molecule 20 is a DNA chain called template.

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

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 22 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).

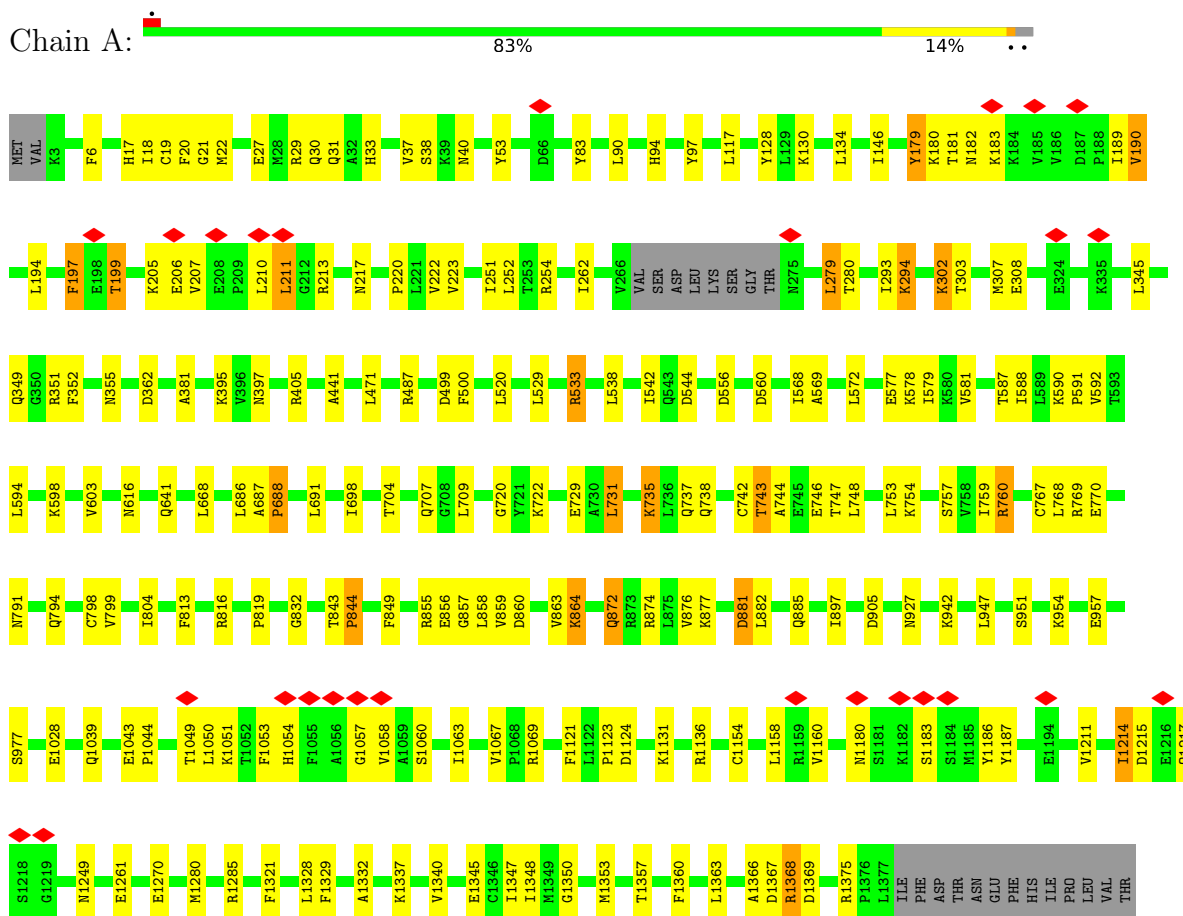


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
22	P	1	8	4	4	0

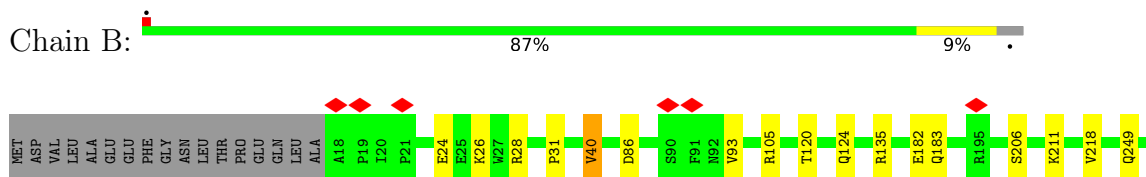
### 3 Residue-property plots [i](#)

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

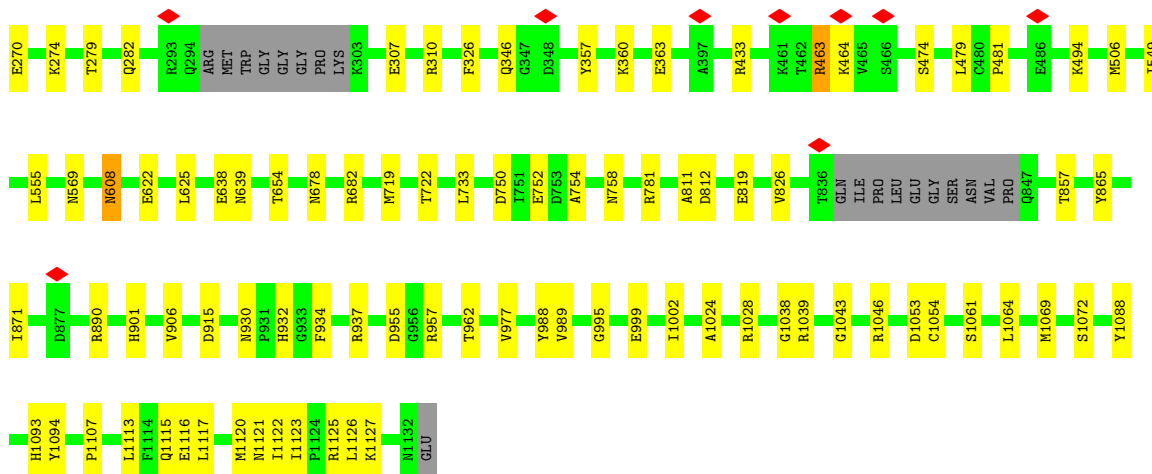
- Molecule 1: DNA-directed RNA polymerase III subunit RPC1



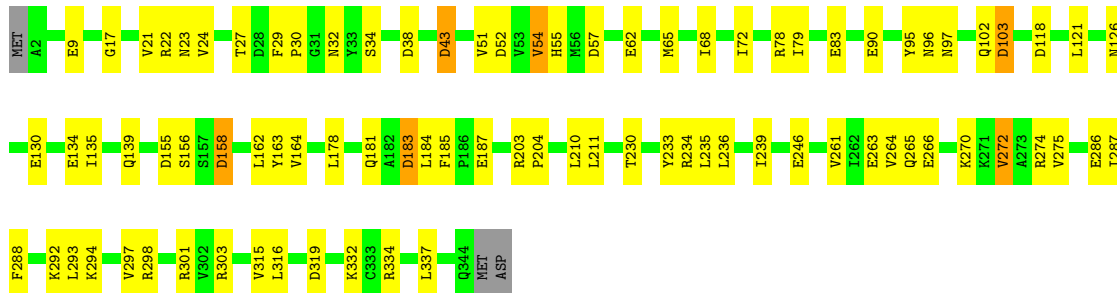
- Molecule 2: DNA-directed RNA polymerase III subunit RPC2



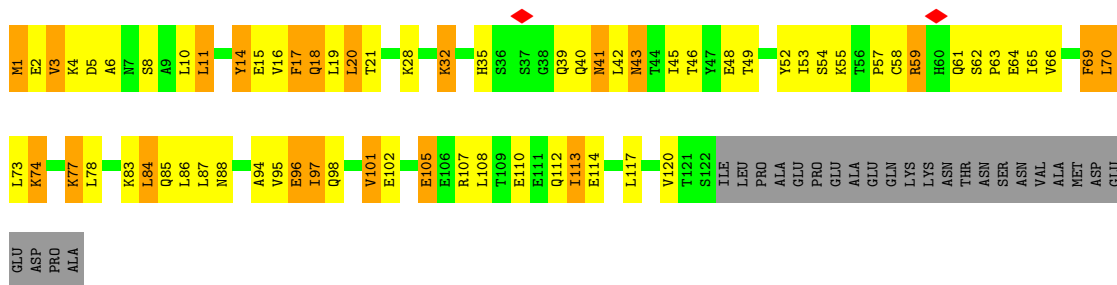




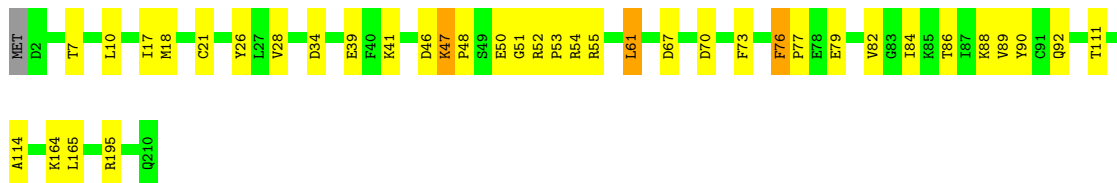
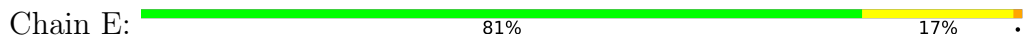
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



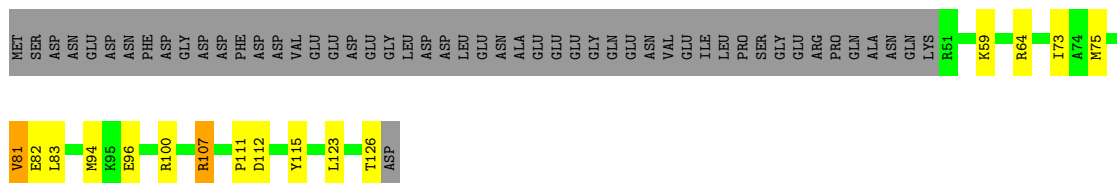
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9



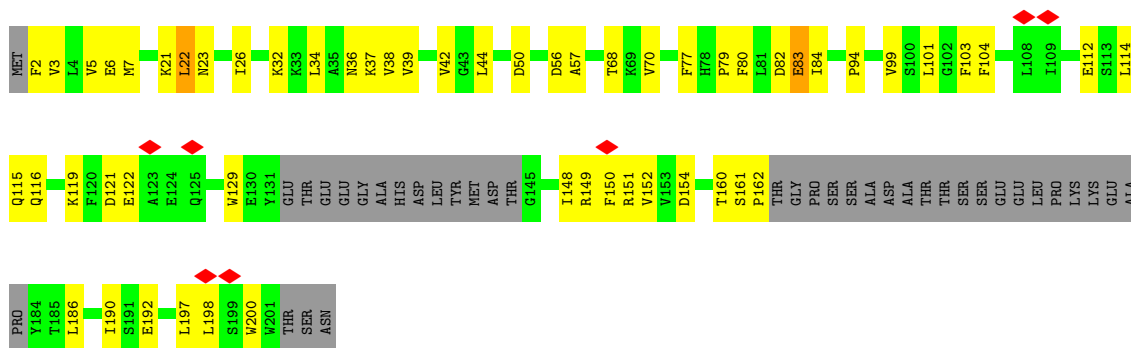
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



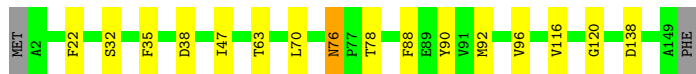
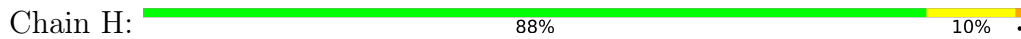
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



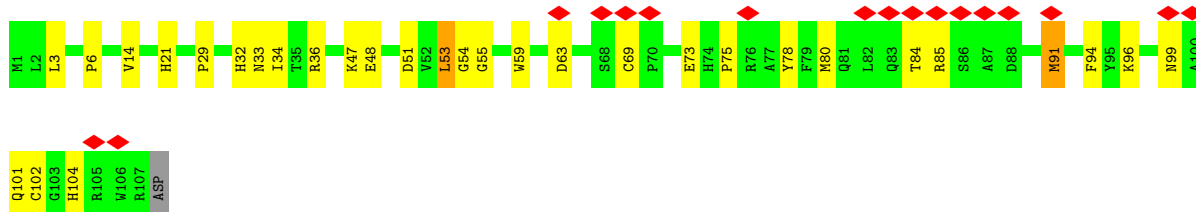
• Molecule 7: DNA-directed RNA polymerase III subunit RPC8



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



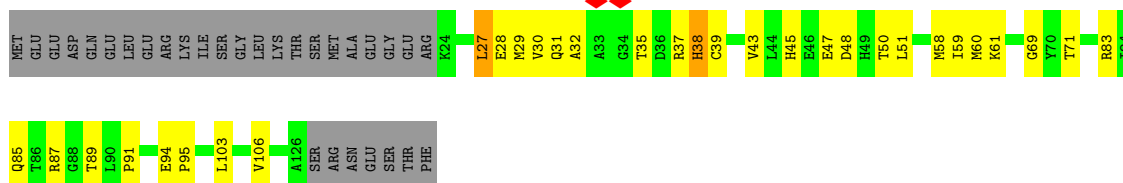
• Molecule 9: DNA-directed RNA polymerase III subunit RPC10



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



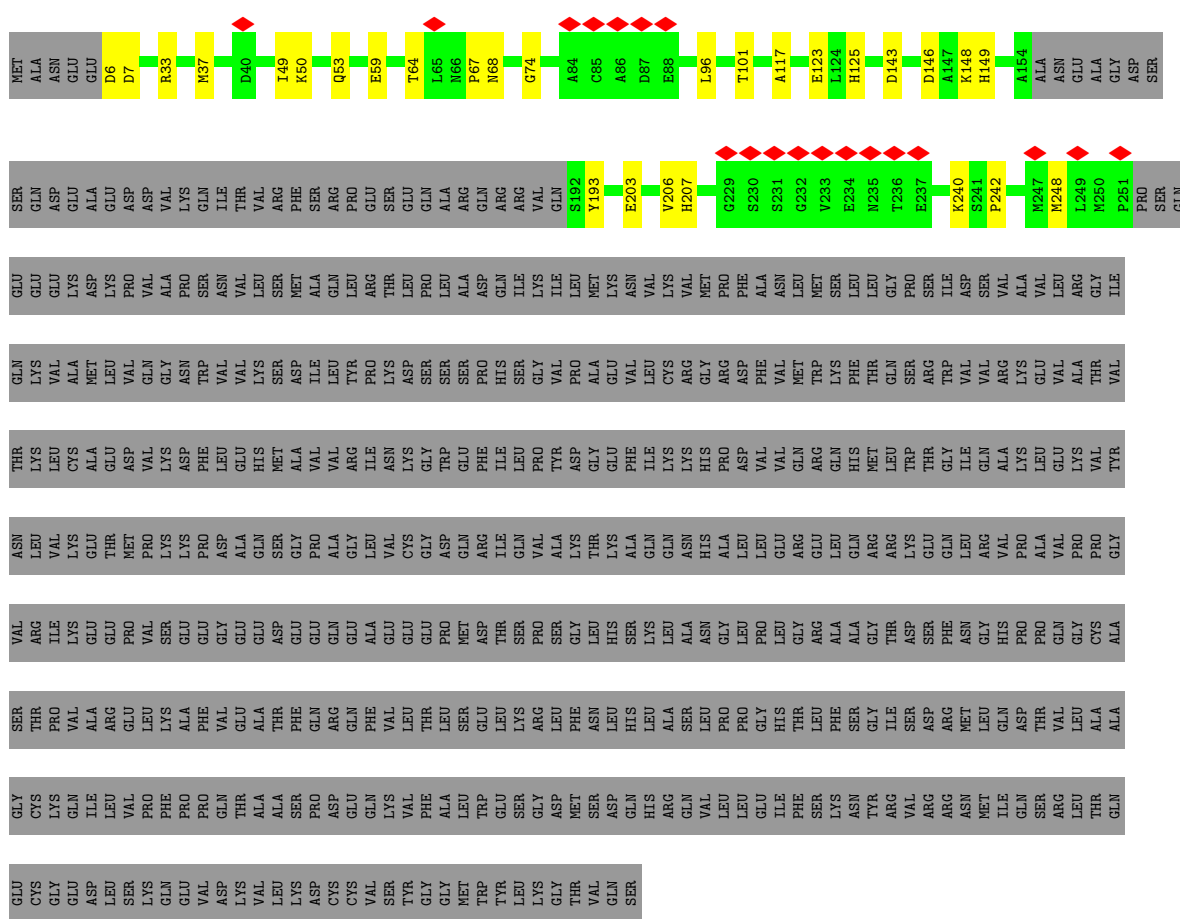
• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2



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

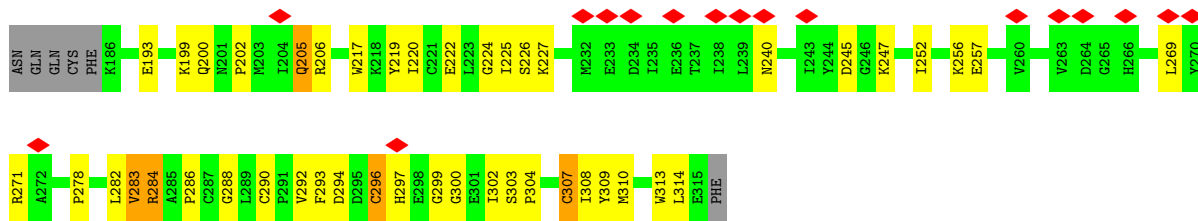


• Molecule 13: DNA-directed RNA polymerase III subunit RPC5

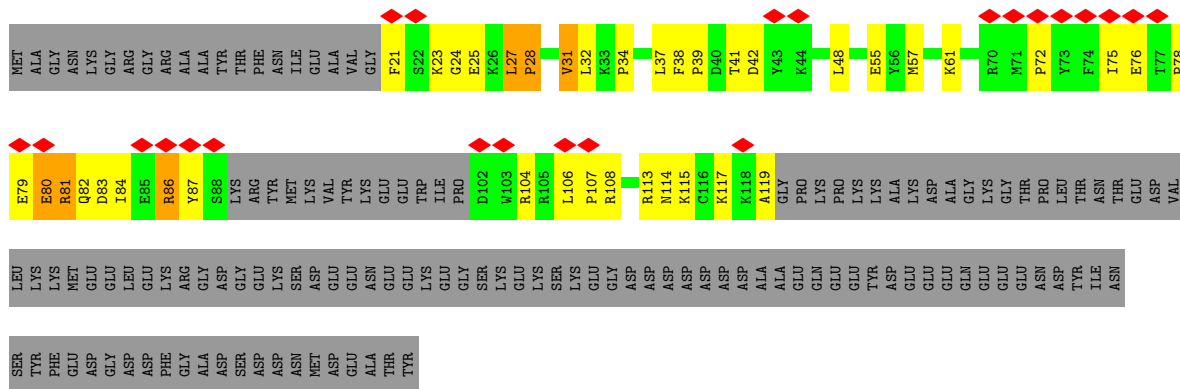


• Molecule 14: DNA-directed RNA polymerase III subunit RPC4





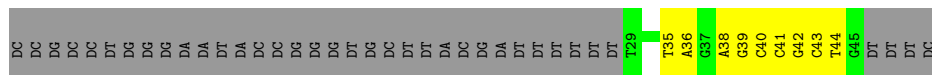
• Molecule 17: DNA-directed RNA polymerase III subunit RPC7



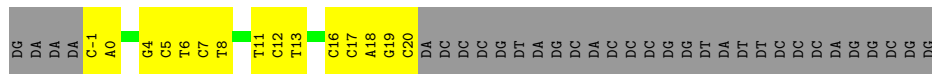
• Molecule 18: RNA (5'-R(\*CP\*CP\*GP\*GP\*GP\*UP\*GP\*CP\*UP\*G)-3')



• Molecule 19: non\_template DNA



• Molecule 20: template



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40590	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	0.071	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	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: SF4, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.48	0/10924	0.67	0/14727
2	B	0.44	0/8845	0.61	0/11930
3	C	0.58	0/2790	0.69	0/3782
4	D	0.58	0/997	0.79	0/1343
5	E	0.46	0/1745	0.64	0/2358
6	F	0.59	0/620	0.66	0/839
7	G	0.51	0/1374	0.69	0/1868
8	H	0.43	0/1207	0.67	0/1628
9	I	0.41	0/869	0.66	0/1174
10	J	0.56	0/521	0.81	2/703 (0.3%)
11	K	0.56	0/837	0.69	0/1129
12	L	0.58	0/394	0.67	0/524
13	M	0.36	0/1720	0.58	0/2326
14	N	0.57	0/1137	0.70	0/1530
15	O	0.40	0/3604	0.60	0/4872
16	P	0.45	0/1028	0.73	0/1391
17	Q	0.46	0/742	0.69	0/996
18	R	0.92	0/95	1.27	0/146
19	X	0.64	0/391	0.90	0/601
20	Y	0.68	0/499	0.95	0/767
All	All	0.48	0/40339	0.67	2/54634 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	10	CYS	CA-CB-SG	-6.11	103.00	114.00
10	J	10	CYS	CB-CA-C	5.73	121.87	110.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10732	0	10976	296	0
2	B	8680	0	8805	154	0
3	C	2736	0	2712	85	0
4	D	985	0	1006	108	0
5	E	1715	0	1733	34	0
6	F	610	0	642	22	0
7	G	1337	0	1306	92	0
8	H	1186	0	1147	28	0
9	I	848	0	812	64	0
10	J	512	0	525	17	0
11	K	822	0	810	64	0
12	L	388	0	395	36	0
13	M	1682	0	1641	24	0
14	N	1128	0	1181	24	0
15	O	3546	0	3585	161	0
16	P	1008	0	998	62	0
17	Q	724	0	734	64	0
18	R	86	0	44	6	0
19	X	349	0	191	13	0
20	Y	447	0	248	27	0
21	A	2	0	0	0	0
21	B	1	0	0	0	0
21	I	2	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0
22	P	8	0	0	4	0
All	All	39536	0	39491	1006	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 13.

All (1006) 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:581:VAL:HG23	11:K:85:GLN:NE2	1.29	1.43
1:A:577:GLU:OE2	11:K:29:MET:CE	1.65	1.42
8:H:76:ASN:HD21	11:K:87:ARG:CZ	1.34	1.38
4:D:48:GLU:OE1	7:G:103:PHE:CG	1.77	1.37
4:D:48:GLU:CB	7:G:103:PHE:HB3	1.55	1.35
3:C:263:GLU:OE2	3:C:274:ARG:HD3	1.26	1.26
15:O:409:ILE:CD1	15:O:423:LEU:HD11	1.67	1.24
2:B:781:ARG:HH21	12:L:31:ARG:NH2	1.32	1.23
15:O:374:HIS:HB3	15:O:423:LEU:CD1	1.70	1.22
15:O:409:ILE:CG1	15:O:423:LEU:HD11	1.67	1.21
2:B:865:TYR:CE2	12:L:55:PHE:HE2	1.58	1.21
8:H:78:THR:CB	11:K:87:ARG:HH22	1.54	1.21
2:B:865:TYR:CE2	12:L:55:PHE:CE2	2.30	1.20
1:A:30:GLN:NE2	2:B:1094:TYR:O	1.74	1.19
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	1.17
4:D:48:GLU:HB3	7:G:103:PHE:CB	1.73	1.17
15:O:409:ILE:HG13	15:O:423:LEU:CD1	1.76	1.16
3:C:287:ILE:HD11	3:C:293:LEU:HB3	1.26	1.16
10:J:26:GLN:HA	10:J:26:GLN:HE21	1.00	1.15
4:D:48:GLU:CB	7:G:103:PHE:O	1.94	1.14
1:A:97:TYR:OH	2:B:1121:ASN:O	1.65	1.14
1:A:577:GLU:CD	11:K:29:MET:CE	2.15	1.13
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
17:Q:106:LEU:HD12	17:Q:107:PRO:HD2	1.25	1.12
1:A:1053:PHE:CZ	9:I:78:TYR:CZ	2.37	1.11
15:O:409:ILE:N	15:O:410:PRO:HD2	1.58	1.11
8:H:78:THR:HB	11:K:87:ARG:HH12	1.14	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
8:H:78:THR:OG1	11:K:87:ARG:NH2	1.84	1.09
15:O:352:SER:O	15:O:356:GLU:HG2	1.51	1.09
15:O:409:ILE:CB	15:O:423:LEU:HD21	1.83	1.08
7:G:148:ILE:HG23	7:G:190:ILE:CG2	1.84	1.08
2:B:93:VAL:HG11	12:L:35:ARG:HH22	1.06	1.08
4:D:48:GLU:CD	7:G:103:PHE:CG	2.26	1.07
1:A:572:LEU:HD13	11:K:83:ARG:HD2	1.29	1.07
15:O:410:PRO:HB2	15:O:419:ARG:HH21	0.93	1.07
1:A:581:VAL:CG2	11:K:85:GLN:NE2	2.18	1.06
8:H:76:ASN:ND2	11:K:87:ARG:CZ	2.19	1.06
2:B:865:TYR:HE2	12:L:55:PHE:CE2	1.68	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:48:GLU:OE1	7:G:103:PHE:CD2	2.08	1.05
1:A:577:GLU:CD	11:K:29:MET:HE3	1.77	1.05
8:H:78:THR:HB	11:K:87:ARG:NH1	1.72	1.04
4:D:39:GLN:HG3	7:G:32:LYS:HB3	1.07	1.04
4:D:48:GLU:HB3	7:G:103:PHE:O	1.53	1.04
4:D:11:LEU:HD23	4:D:11:LEU:H	1.18	1.04
13:M:67:PRO:HD2	14:N:138:ILE:HD11	1.39	1.04
10:J:26:GLN:HA	10:J:26:GLN:NE2	1.71	1.03
4:D:48:GLU:OE1	7:G:103:PHE:CB	2.07	1.03
2:B:93:VAL:CG1	12:L:35:ARG:HH22	1.73	1.02
2:B:781:ARG:NH2	12:L:31:ARG:NH2	2.07	1.02
16:P:299:GLY:HA2	16:P:303:SER:CB	1.89	1.02
8:H:76:ASN:HD21	11:K:87:ARG:NH2	1.58	1.01
15:O:407:GLN:HB3	15:O:422:TYR:HB3	1.41	1.01
1:A:1217:GLN:HG3	9:I:101:GLN:HG2	1.39	1.01
15:O:409:ILE:HG21	15:O:423:LEU:HD21	1.39	1.00
1:A:577:GLU:OE2	11:K:29:MET:HE1	0.81	0.99
7:G:148:ILE:HG23	7:G:190:ILE:HG23	1.42	0.99
1:A:180:LYS:NZ	1:A:182:ASN:OD1	1.96	0.97
15:O:377:GLN:HB3	15:O:421:PHE:HZ	1.27	0.97
17:Q:27:LEU:HD22	17:Q:27:LEU:H	1.26	0.97
1:A:1328:LEU:HD13	2:B:1117:LEU:HD21	1.45	0.97
15:O:356:GLU:OE1	17:Q:39:PRO:HD3	1.65	0.97
2:B:819:GLU:OE2	12:L:51:ARG:HD3	1.63	0.97
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
4:D:48:GLU:HB3	7:G:103:PHE:HB3	0.97	0.96
1:A:37:VAL:O	17:Q:23:LYS:HE3	1.66	0.95
4:D:48:GLU:HB2	7:G:103:PHE:O	1.64	0.95
19:X:43:DC:C6	19:X:44:DT:H72	2.01	0.95
1:A:577:GLU:CD	11:K:29:MET:HE1	1.78	0.95
1:A:1053:PHE:CE2	9:I:78:TYR:CE2	2.55	0.95
1:A:1357:THR:O	6:F:64:ARG:NH1	2.00	0.95
8:H:78:THR:CB	11:K:87:ARG:NH2	2.29	0.95
1:A:211:LEU:HD12	1:A:211:LEU:H	1.33	0.93
15:O:409:ILE:H	15:O:410:PRO:HD2	0.79	0.93
4:D:48:GLU:CG	7:G:103:PHE:HB3	1.98	0.93
16:P:284:ARG:HA	16:P:284:ARG:NE	1.80	0.93
1:A:857:GLY:HA2	9:I:84:THR:C	1.90	0.92
16:P:299:GLY:HA2	16:P:303:SER:HB3	1.51	0.92
4:D:39:GLN:HG3	7:G:32:LYS:CB	1.97	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:412:THR:HB	15:O:419:ARG:HA	1.50	0.92
13:M:68:ASN:OD1	14:N:138:ILE:HB	1.69	0.92
2:B:781:ARG:HH21	12:L:31:ARG:HH21	1.12	0.91
3:C:288:PHE:HA	3:C:294:LYS:HG2	1.52	0.91
5:E:61:LEU:H	5:E:61:LEU:HD22	1.35	0.91
1:A:816:ARG:NH2	2:B:639:ASN:O	2.03	0.91
4:D:17:PHE:HB2	4:D:53:ILE:HG21	1.53	0.91
15:O:409:ILE:HB	15:O:423:LEU:HD21	1.49	0.91
4:D:48:GLU:CD	7:G:103:PHE:CD1	2.43	0.90
1:A:17:HIS:CE1	2:B:1127:LYS:CB	2.54	0.90
16:P:284:ARG:HA	16:P:284:ARG:HE	1.33	0.90
4:D:11:LEU:H	4:D:11:LEU:CD2	1.84	0.90
3:C:9:GLU:OE2	3:C:298:ARG:NH1	2.05	0.90
4:D:4:LYS:HE2	4:D:4:LYS:HA	1.52	0.90
1:A:581:VAL:HG23	11:K:85:GLN:HE21	1.38	0.89
1:A:1329:PHE:CD1	2:B:1122:ILE:HD11	2.07	0.89
1:A:38:SER:HB2	17:Q:24:GLY:HA3	1.53	0.89
15:O:407:GLN:O	15:O:410:PRO:HD2	1.73	0.89
17:Q:106:LEU:HD12	17:Q:107:PRO:CD	2.00	0.89
4:D:45:ILE:HB	7:G:36:ASN:OD1	1.73	0.89
1:A:1121:PHE:CE1	9:I:14:VAL:HG21	2.08	0.88
4:D:97:ILE:HA	4:D:101:VAL:HB	1.54	0.88
1:A:1332:ALA:HB2	2:B:1122:ILE:HG23	1.55	0.88
17:Q:27:LEU:H	17:Q:27:LEU:CD2	1.86	0.87
8:H:78:THR:CB	11:K:87:ARG:HH12	1.87	0.87
8:H:76:ASN:ND2	11:K:87:ARG:NH2	2.23	0.86
1:A:17:HIS:CE1	2:B:1127:LYS:HB3	2.10	0.86
1:A:180:LYS:NZ	1:A:182:ASN:HD21	1.73	0.85
15:O:377:GLN:HB3	15:O:421:PHE:CZ	2.10	0.85
1:A:19:CYS:N	2:B:1125:ARG:O	2.08	0.85
4:D:43:ASN:H	4:D:43:ASN:HD22	1.25	0.85
15:O:407:GLN:O	15:O:410:PRO:CD	2.24	0.85
15:O:374:HIS:CB	15:O:423:LEU:HD12	2.06	0.85
15:O:507:ASN:ND2	17:Q:55:GLU:OE2	2.09	0.85
1:A:1053:PHE:CZ	9:I:78:TYR:OH	2.30	0.84
15:O:356:GLU:HG3	16:P:284:ARG:HB2	1.57	0.84
13:M:68:ASN:OD1	14:N:138:ILE:CB	2.25	0.84
1:A:22:MET:HA	2:B:1123:ILE:HG12	1.58	0.84
1:A:581:VAL:CG2	11:K:85:GLN:HE22	1.83	0.84
4:D:85:GLN:HE22	7:G:84:ILE:H	1.25	0.84
15:O:409:ILE:HG13	15:O:423:LEU:CG	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:445:ASN:ND2	16:P:304:PRO:HG3	1.92	0.83
4:D:58:CYS:HA	4:D:61:GLN:HB2	1.60	0.83
9:I:53:LEU:HD12	9:I:54:GLY:H	1.44	0.83
1:A:6:PHE:CE2	4:D:1:MET:HG2	2.13	0.82
15:O:415:HIS:O	15:O:419:ARG:HG3	1.78	0.82
1:A:858:LEU:HD12	1:A:858:LEU:H	1.44	0.82
4:D:11:LEU:HD23	4:D:11:LEU:N	1.91	0.81
15:O:409:ILE:HB	15:O:423:LEU:CD2	2.09	0.81
8:H:78:THR:HB	11:K:87:ARG:CZ	2.11	0.81
7:G:148:ILE:HG23	7:G:190:ILE:HG21	1.60	0.81
1:A:180:LYS:NZ	1:A:182:ASN:ND2	2.27	0.81
1:A:579:ILE:O	11:K:83:ARG:NH2	2.14	0.81
16:P:299:GLY:HA2	16:P:303:SER:HB2	1.61	0.81
1:A:17:HIS:NE2	2:B:1127:LYS:HD3	1.95	0.80
15:O:407:GLN:CB	15:O:422:TYR:HB3	2.11	0.80
2:B:93:VAL:HG11	12:L:35:ARG:NH2	1.92	0.80
3:C:287:ILE:HD11	3:C:293:LEU:CB	2.10	0.80
1:A:18:ILE:HG12	2:B:1126:LEU:CD2	2.12	0.80
3:C:263:GLU:OE2	3:C:274:ARG:CD	2.21	0.80
1:A:17:HIS:CE1	2:B:1127:LYS:HB2	2.17	0.79
1:A:1049:THR:HG22	9:I:85:ARG:CD	2.12	0.79
13:M:68:ASN:OD1	14:N:138:ILE:CG1	2.30	0.79
4:D:48:GLU:HB3	7:G:103:PHE:C	2.02	0.79
1:A:1049:THR:HG22	9:I:85:ARG:HD2	1.64	0.78
15:O:138:THR:HG21	17:Q:104:ARG:HB2	1.63	0.78
1:A:1028:GLU:OE1	6:F:59:LYS:HG2	1.83	0.78
1:A:199:THR:HG22	15:O:378:LYS:HZ1	1.49	0.78
1:A:581:VAL:HG23	11:K:85:GLN:HE22	0.96	0.78
4:D:10:LEU:HD23	4:D:10:LEU:O	1.83	0.77
15:O:508:LYS:HE3	17:Q:41:THR:HB	1.66	0.77
3:C:287:ILE:CD1	3:C:293:LEU:HB3	2.09	0.77
8:H:78:THR:HB	11:K:87:ARG:NH2	1.98	0.77
16:P:300:GLY:N	16:P:303:SER:HB3	1.97	0.77
1:A:720:GLY:HA3	1:A:759:ILE:HD11	1.67	0.77
4:D:54:SER:HA	4:D:59:ARG:NH1	2.00	0.77
2:B:999:GLU:HG2	3:C:24:VAL:HG21	1.68	0.76
3:C:239:ILE:HD12	3:C:239:ILE:H	1.50	0.76
7:G:151:ARG:HD2	7:G:151:ARG:O	1.85	0.76
1:A:581:VAL:H	11:K:85:GLN:HE22	1.33	0.76
1:A:1121:PHE:CD1	9:I:14:VAL:HG11	2.21	0.76
5:E:84:ILE:HD12	5:E:84:ILE:H	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:67:PRO:HD2	14:N:138:ILE:CD1	2.15	0.76
1:A:1123:PRO:HA	9:I:21:HIS:H	1.51	0.76
6:F:82:GLU:O	6:F:82:GLU:HG2	1.84	0.76
1:A:33:HIS:CE1	2:B:1088:TYR:OH	2.39	0.75
17:Q:106:LEU:CD1	17:Q:107:PRO:HD2	2.13	0.75
17:Q:27:LEU:HD22	17:Q:27:LEU:N	2.00	0.75
1:A:180:LYS:NZ	1:A:182:ASN:CG	2.40	0.75
1:A:1123:PRO:O	9:I:21:HIS:ND1	2.18	0.74
3:C:288:PHE:O	3:C:294:LYS:HD3	1.87	0.74
15:O:445:ASN:OD1	22:P:401:SF4:S2	2.45	0.74
7:G:32:LYS:HB3	7:G:32:LYS:HZ3	1.52	0.74
7:G:99:VAL:HG21	7:G:148:ILE:HD11	1.70	0.74
16:P:293:PHE:HE2	16:P:307:CYS:HB2	1.51	0.74
2:B:865:TYR:CD2	12:L:55:PHE:HE2	2.04	0.74
1:A:1057:GLY:HA2	9:I:59:TRP:CZ3	2.22	0.74
1:A:1053:PHE:CE2	9:I:78:TYR:CZ	2.75	0.74
13:M:68:ASN:OD1	14:N:138:ILE:HG12	1.88	0.74
1:A:38:SER:HB2	17:Q:24:GLY:CA	2.17	0.73
1:A:1369:ASP:H	7:G:23:ASN:HD21	1.35	0.73
1:A:1183:SER:O	2:B:274:LYS:NZ	2.16	0.73
7:G:79:PRO:HG2	7:G:150:PHE:CE2	2.24	0.73
9:I:32:HIS:HA	14:N:137:ILE:HD11	1.70	0.73
3:C:163:TYR:CE1	3:C:204:PRO:HD3	2.23	0.73
5:E:55:ARG:H	5:E:55:ARG:HD3	1.52	0.73
3:C:163:TYR:CD1	3:C:204:PRO:HD3	2.24	0.73
15:O:356:GLU:OE2	16:P:282:LEU:HD22	1.87	0.73
1:A:1123:PRO:C	9:I:21:HIS:HD1	1.92	0.72
5:E:79:GLU:H	5:E:79:GLU:CD	1.92	0.72
1:A:1348:ILE:O	2:B:1107:PRO:HG2	1.89	0.72
1:A:94:HIS:NE2	2:B:1120:MET:O	2.22	0.72
15:O:141:TYR:CZ	17:Q:106:LEU:O	2.41	0.72
3:C:135:ILE:H	3:C:135:ILE:HD12	1.54	0.72
1:A:1053:PHE:HZ	9:I:78:TYR:CZ	2.03	0.72
1:A:1217:GLN:CG	9:I:101:GLN:HG2	2.19	0.72
4:D:77:LYS:O	4:D:77:LYS:HG3	1.90	0.72
1:A:872:GLN:HE21	1:A:872:GLN:HA	1.54	0.71
1:A:578:LYS:HB3	11:K:31:GLN:O	1.90	0.71
4:D:48:GLU:CD	7:G:103:PHE:HB3	2.11	0.71
1:A:19:CYS:O	2:B:1125:ARG:N	2.24	0.71
2:B:1046:ARG:HD3	20:Y:18:DA:H5'	1.71	0.71
9:I:3:LEU:HB3	14:N:143:GLU:HG3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:78:ARG:HE	11:K:50:THR:HG22	1.57	0.70
1:A:1214:ILE:HG12	9:I:55:GLY:HA2	1.72	0.70
1:A:791:ASN:HD21	9:I:91:MET:HG2	1.56	0.69
2:B:93:VAL:CG1	12:L:35:ARG:NH2	2.53	0.69
1:A:1329:PHE:CG	2:B:1122:ILE:HD11	2.27	0.69
12:L:25:GLU:H	12:L:25:GLU:CD	1.95	0.69
20:Y:11:DT:H2 <sup>?</sup>	20:Y:12:DC:C5	2.28	0.69
4:D:1:MET:O	4:D:1:MET:SD	2.51	0.68
15:O:409:ILE:HG21	15:O:423:LEU:CD2	2.18	0.68
1:A:858:LEU:HD12	1:A:858:LEU:N	2.07	0.68
15:O:409:ILE:HG13	15:O:423:LEU:HG	1.75	0.68
4:D:85:GLN:NE2	7:G:83:GLU:HA	2.08	0.68
1:A:864:LYS:HD2	1:A:1067:VAL:HG21	1.76	0.68
2:B:608:ASN:H	2:B:608:ASN:HD22	1.40	0.68
8:H:78:THR:HB	11:K:87:ARG:HH22	1.51	0.68
10:J:26:GLN:HE21	10:J:26:GLN:CA	1.82	0.68
2:B:865:TYR:HE2	12:L:55:PHE:CD2	2.12	0.68
2:B:871:ILE:HD12	12:L:17:TYR:CE2	2.28	0.67
4:D:48:GLU:OE1	7:G:103:PHE:HB3	1.86	0.67
16:P:299:GLY:CA	16:P:303:SER:HB3	2.24	0.67
5:E:47:LYS:N	5:E:48:PRO:HD2	2.09	0.67
1:A:18:ILE:HG12	2:B:1126:LEU:HD22	1.76	0.67
1:A:27:GLU:HB3	2:B:1094:TYR:HE1	1.60	0.67
15:O:412:THR:CB	15:O:419:ARG:HA	2.24	0.67
5:E:55:ARG:HD3	5:E:55:ARG:N	2.09	0.67
4:D:48:GLU:HB3	7:G:103:PHE:CA	2.24	0.67
19:X:39:DG:H2 <sup>?</sup>	19:X:40:DC:H5 <sup>?</sup>	1.75	0.67
2:B:1039:ARG:N	20:Y:20:DC:OP1	2.27	0.67
2:B:40:VAL:HG12	2:B:40:VAL:O	1.94	0.66
15:O:157:VAL:O	17:Q:115:LYS:HG2	1.95	0.66
1:A:1123:PRO:HG3	9:I:34:ILE:O	1.95	0.66
15:O:505:ASN:HA	16:P:314:LEU:HD22	1.77	0.66
7:G:151:ARG:HD2	7:G:151:ARG:C	2.16	0.66
1:A:180:LYS:HZ2	1:A:182:ASN:HD21	1.40	0.66
4:D:85:GLN:HE22	7:G:84:ILE:N	1.93	0.66
9:I:36:ARG:NH1	14:N:155:LEU:O	2.28	0.66
1:A:742:CYS:SG	1:A:747:THR:OG1	2.53	0.65
4:D:48:GLU:CD	7:G:103:PHE:CB	2.61	0.65
1:A:19:CYS:O	2:B:1125:ARG:HB2	1.95	0.65
1:A:251:ILE:HD12	1:A:251:ILE:H	1.62	0.65
1:A:858:LEU:H	1:A:858:LEU:CD1	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:VAL:HG21	15:O:406:LEU:HD13	1.79	0.65
1:A:1051:LYS:NZ	9:I:94:PHE:CG	2.61	0.65
4:D:39:GLN:HG3	7:G:32:LYS:HZ3	1.61	0.65
17:Q:86:ARG:NH1	17:Q:86:ARG:HB2	2.12	0.65
20:Y:11:DT:H2'	20:Y:11:DT:O2	1.95	0.65
1:A:1058:VAL:HG22	9:I:53:LEU:HG	1.78	0.65
13:M:49:ILE:HD13	14:N:363:VAL:HG11	1.79	0.65
1:A:1158:LEU:O	1:A:1158:LEU:HD23	1.97	0.64
1:A:1328:LEU:HD13	2:B:1117:LEU:CD2	2.26	0.64
4:D:11:LEU:HD21	7:G:3:VAL:HA	1.78	0.64
1:A:1328:LEU:CD1	2:B:1117:LEU:HD21	2.25	0.64
1:A:1053:PHE:HE2	9:I:78:TYR:CE2	2.11	0.64
13:M:242:PRO:HB3	14:N:392:LEU:HD23	1.80	0.64
9:I:78:TYR:HB3	9:I:96:LYS:HB3	1.78	0.64
1:A:581:VAL:N	11:K:85:GLN:HE22	1.96	0.64
3:C:270:LYS:NZ	3:C:270:LYS:HB3	2.13	0.64
16:P:220:ILE:HD11	16:P:271:ARG:HD2	1.80	0.63
19:X:36:DA:H61	20:Y:8:DT:H3	1.44	0.63
1:A:180:LYS:HZ1	1:A:182:ASN:HD21	1.44	0.63
1:A:882:LEU:H	1:A:882:LEU:HD12	1.62	0.63
3:C:139:GLN:HG2	3:C:211:LEU:HD11	1.80	0.63
1:A:252:LEU:O	1:A:252:LEU:HD12	1.98	0.63
4:D:16:VAL:HG11	7:G:2:PHE:CE2	2.34	0.63
1:A:6:PHE:CD1	7:G:34:LEU:HD13	2.34	0.63
2:B:865:TYR:HE2	12:L:55:PHE:HE2	1.07	0.63
1:A:1329:PHE:CE1	2:B:1122:ILE:HD11	2.33	0.63
3:C:288:PHE:HA	3:C:294:LYS:CG	2.27	0.63
13:M:117:ALA:HB3	14:N:267:LEU:HB2	1.80	0.63
15:O:407:GLN:CG	15:O:422:TYR:HB3	2.29	0.63
16:P:293:PHE:CE1	17:Q:31:VAL:HG12	2.34	0.63
1:A:885:GLN:HE21	6:F:111:PRO:HG3	1.64	0.62
3:C:54:VAL:CG1	3:C:62:GLU:HG2	2.29	0.62
3:C:102:GLN:OE1	3:C:102:GLN:N	2.31	0.62
7:G:79:PRO:CG	7:G:150:PHE:CE2	2.82	0.62
1:A:743:THR:HG23	1:A:746:GLU:HB2	1.80	0.62
1:A:855:ARG:HA	1:A:858:LEU:HD13	1.81	0.62
4:D:41:ASN:OD1	4:D:41:ASN:N	2.30	0.62
4:D:73:LEU:HD13	4:D:83:LYS:HB2	1.78	0.62
10:J:26:GLN:NE2	10:J:26:GLN:CA	2.49	0.62
3:C:134:GLU:HG2	3:C:181:GLN:HG3	1.81	0.62
8:H:78:THR:CB	11:K:87:ARG:NH1	2.52	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:308:ILE:HD13	17:Q:31:VAL:HG11	1.80	0.62
19:X:41:DC:H2''	19:X:42:DG:H5'	1.81	0.62
4:D:49:THR:HG23	7:G:104:PHE:CE2	2.34	0.62
15:O:159:ARG:HA	15:O:235:TRP:HB3	1.80	0.62
15:O:445:ASN:HD22	16:P:304:PRO:HG3	1.65	0.62
1:A:180:LYS:HZ1	1:A:182:ASN:ND2	1.96	0.62
1:A:1367:ASP:O	7:G:21:LYS:HG3	1.99	0.62
4:D:17:PHE:HB2	4:D:53:ILE:CG2	2.28	0.62
1:A:572:LEU:HD13	11:K:83:ARG:CD	2.18	0.62
16:P:199:LYS:NZ	16:P:245:ASP:O	2.32	0.62
10:J:9:THR:OG1	10:J:10:CYS:SG	2.57	0.61
1:A:1154:CYS:HA	1:A:1160:VAL:HG23	1.82	0.61
4:D:16:VAL:HG21	7:G:2:PHE:HD2	1.65	0.61
1:A:21:GLY:N	2:B:1123:ILE:O	2.33	0.61
4:D:14:TYR:HD2	4:D:18:GLN:HE21	1.47	0.61
1:A:27:GLU:CD	2:B:1094:TYR:OH	2.39	0.61
2:B:26:LYS:NZ	2:B:26:LYS:HB3	2.15	0.61
5:E:61:LEU:H	5:E:61:LEU:CD2	2.12	0.61
7:G:151:ARG:HG3	7:G:152:VAL:HG13	1.82	0.61
16:P:293:PHE:CE2	16:P:307:CYS:HB2	2.34	0.61
4:D:20:LEU:HD11	4:D:46:THR:HB	1.82	0.61
4:D:48:GLU:OE2	7:G:103:PHE:CD1	2.53	0.61
18:R:10:U:H3'	18:R:11:G:H8	1.65	0.61
15:O:91:TYR:OH	15:O:243:HIS:NE2	2.33	0.61
1:A:881:ASP:N	1:A:881:ASP:OD1	2.34	0.61
1:A:22:MET:HA	2:B:1123:ILE:CG1	2.30	0.60
1:A:180:LYS:HZ2	1:A:182:ASN:ND2	1.98	0.60
1:A:520:LEU:HD23	6:F:94:MET:CE	2.32	0.60
1:A:572:LEU:CD1	11:K:83:ARG:HD2	2.19	0.60
2:B:812:ASP:HB3	12:L:15:MET:HG3	1.82	0.60
2:B:995:GLY:O	3:C:233:TYR:OH	2.18	0.60
9:I:6:PRO:HG3	14:N:142:LYS:O	2.02	0.60
2:B:722:THR:HG23	2:B:962:THR:HA	1.83	0.60
16:P:302:ILE:HG22	16:P:302:ILE:O	2.00	0.60
12:L:34:ILE:HG22	12:L:44:MET:HG3	1.82	0.60
1:A:577:GLU:CG	11:K:29:MET:HE3	2.31	0.60
1:A:804:ILE:HG23	1:A:856:GLU:HG3	1.83	0.59
1:A:1053:PHE:O	9:I:80:MET:CE	2.49	0.59
4:D:5:ASP:HB2	7:G:6:GLU:CG	2.32	0.59
4:D:43:ASN:H	4:D:43:ASN:ND2	1.96	0.59
4:D:110:GLU:OE2	4:D:110:GLU:HA	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1187:TYR:HD2	2:B:270:GLU:OE2	1.86	0.59
4:D:108:LEU:O	4:D:113:ILE:HG22	2.02	0.59
15:O:508:LYS:CE	17:Q:41:THR:HB	2.32	0.59
2:B:819:GLU:OE2	12:L:51:ARG:CD	2.46	0.59
2:B:871:ILE:CD1	12:L:17:TYR:CE2	2.85	0.59
7:G:79:PRO:CG	7:G:150:PHE:CD2	2.86	0.59
17:Q:80:GLU:HA	17:Q:86:ARG:CD	2.32	0.59
3:C:54:VAL:HG11	3:C:62:GLU:HG2	1.85	0.59
4:D:18:GLN:OE1	4:D:18:GLN:HA	2.01	0.59
4:D:35:HIS:HD2	7:G:32:LYS:HE3	1.68	0.59
1:A:1053:PHE:O	9:I:80:MET:HE3	2.02	0.59
2:B:206:SER:CB	2:B:211:LYS:HG2	2.32	0.59
15:O:364:ARG:NH2	15:O:384:ALA:O	2.35	0.59
1:A:1353:MET:HG2	2:B:1061:SER:HB2	1.83	0.59
3:C:139:GLN:HB2	3:C:178:LEU:HD11	1.85	0.59
4:D:1:MET:O	4:D:1:MET:CG	2.51	0.59
1:A:1049:THR:HG22	9:I:85:ARG:HD3	1.84	0.58
3:C:183:ASP:OD1	3:C:183:ASP:N	2.35	0.58
2:B:988:TYR:CE2	3:C:301:ARG:NH1	2.71	0.58
3:C:163:TYR:CE1	3:C:204:PRO:CD	2.86	0.58
15:O:284:PHE:HA	15:O:338:LEU:HB2	1.83	0.58
1:A:31:GLN:O	2:B:1093:HIS:ND1	2.36	0.58
1:A:251:ILE:HD12	1:A:251:ILE:N	2.19	0.58
2:B:463:ARG:NH2	2:B:464:LYS:O	2.36	0.58
1:A:1347:ILE:HD11	2:B:1064:LEU:HD21	1.84	0.58
2:B:1039:ARG:H	20:Y:20:DC:P	2.26	0.58
4:D:54:SER:HA	4:D:59:ARG:CZ	2.34	0.58
1:A:641:GLN:NE2	8:H:138:ASP:OD1	2.36	0.58
3:C:316:LEU:N	3:C:316:LEU:HD23	2.18	0.58
7:G:114:LEU:HD21	7:G:192:GLU:H	1.68	0.58
1:A:94:HIS:CE1	2:B:1120:MET:O	2.57	0.58
1:A:205:LYS:NZ	1:A:205:LYS:HB3	2.19	0.58
1:A:37:VAL:O	17:Q:23:LYS:HG3	2.03	0.58
4:D:39:GLN:CG	7:G:32:LYS:HZ3	2.16	0.58
15:O:410:PRO:CB	15:O:419:ARG:NH2	2.40	0.58
1:A:857:GLY:HA2	9:I:84:THR:CA	2.34	0.57
17:Q:113:ARG:HH21	17:Q:117:LYS:HA	1.67	0.57
7:G:99:VAL:CG2	7:G:148:ILE:HD11	2.34	0.57
10:J:21:TYR:HB2	10:J:38:LEU:HD11	1.86	0.57
19:X:38:DA:H2'	19:X:39:DG:O4'	2.04	0.57
1:A:1121:PHE:HD1	9:I:14:VAL:HG11	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:16:VAL:HG21	7:G:2:PHE:CD2	2.39	0.57
1:A:616:ASN:OD1	1:A:927:ASN:ND2	2.37	0.57
7:G:32:LYS:CB	7:G:32:LYS:HZ3	2.17	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
1:A:303:THR:OG1	15:O:424:TYR:OH	2.21	0.57
12:L:19:CYS:HB3	12:L:36:CYS:SG	2.45	0.57
3:C:158:ASP:OD1	3:C:158:ASP:N	2.38	0.57
1:A:20:PHE:HA	2:B:1123:ILE:O	2.04	0.57
1:A:577:GLU:CG	11:K:29:MET:CE	2.83	0.57
1:A:1360:PHE:HB2	6:F:107:ARG:O	2.05	0.57
9:I:33:ASN:H	14:N:137:ILE:HD13	1.69	0.57
3:C:187:GLU:H	3:C:187:GLU:CD	2.09	0.56
11:K:35:THR:O	11:K:35:THR:HG22	2.05	0.56
10:J:53:VAL:O	10:J:53:VAL:HG13	2.05	0.56
15:O:356:GLU:CG	16:P:284:ARG:HB2	2.32	0.56
1:A:37:VAL:O	17:Q:23:LYS:CE	2.48	0.56
1:A:217:ASN:ND2	15:O:410:PRO:HG2	2.20	0.56
3:C:162:LEU:HD23	3:C:162:LEU:O	2.05	0.56
3:C:319:ASP:OD1	3:C:319:ASP:N	2.37	0.56
4:D:78:LEU:HD13	4:D:86:LEU:HD11	1.86	0.56
15:O:113:ASN:HB2	15:O:116:LEU:HD21	1.86	0.56
15:O:158:GLN:HA	17:Q:115:LYS:HG2	1.87	0.56
1:A:40:ASN:OD1	17:Q:21:PHE:HB3	2.06	0.56
2:B:206:SER:OG	2:B:211:LYS:HG2	2.06	0.56
15:O:409:ILE:CG1	15:O:423:LEU:CD1	2.47	0.56
1:A:882:LEU:HD12	1:A:882:LEU:N	2.19	0.56
9:I:47:LYS:HE3	9:I:47:LYS:O	2.06	0.56
9:I:53:LEU:HD12	9:I:54:GLY:N	2.18	0.56
15:O:138:THR:OG1	17:Q:104:ARG:HD2	2.05	0.56
1:A:592:VAL:HG21	8:H:47:ILE:HG21	1.88	0.56
15:O:374:HIS:HB3	15:O:423:LEU:HD13	1.79	0.56
16:P:286:PRO:HA	17:Q:38:PHE:CD2	2.40	0.56
1:A:294:LYS:HB3	1:A:294:LYS:NZ	2.21	0.56
5:E:46:ASP:HB3	5:E:48:PRO:HD2	1.87	0.56
6:F:83:LEU:N	6:F:83:LEU:HD23	2.21	0.56
1:A:1375:ARG:HG3	7:G:50:ASP:OD1	2.05	0.55
2:B:781:ARG:NH2	12:L:31:ARG:CZ	2.68	0.55
5:E:84:ILE:HG13	5:E:114:ALA:HA	1.88	0.55
1:A:520:LEU:HD23	6:F:94:MET:HE3	1.87	0.55
7:G:112:GLU:OE1	7:G:119:LYS:NZ	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:X:43:DC:H2'	19:X:44:DT:C7	2.36	0.55
4:D:2:GLU:H	4:D:2:GLU:CD	2.07	0.55
11:K:60:MET:O	11:K:60:MET:HG3	2.05	0.55
15:O:357:ARG:NH1	16:P:288:GLY:O	2.39	0.55
1:A:1329:PHE:CD1	2:B:1122:ILE:CD1	2.86	0.55
2:B:183:GLN:NE2	2:B:363:GLU:OE1	2.39	0.55
1:A:37:VAL:HG23	17:Q:24:GLY:HA2	1.89	0.55
3:C:121:LEU:HD13	3:C:185:PHE:HE1	1.70	0.55
4:D:96:GLU:O	4:D:101:VAL:N	2.36	0.55
15:O:265:GLU:OE1	15:O:268:ARG:NH1	2.39	0.55
1:A:405:ARG:NH2	1:A:441:ALA:O	2.39	0.55
1:A:813:PHE:CZ	2:B:474:SER:HA	2.42	0.55
13:M:64:THR:HG21	13:M:96:LEU:HD13	1.88	0.55
15:O:152:ALA:HB1	17:Q:114:ASN:HB2	1.89	0.55
10:J:19:GLU:CD	10:J:19:GLU:H	2.09	0.55
1:A:687:ALA:HB3	1:A:688:PRO:HD3	1.89	0.55
11:K:48:ASP:N	11:K:48:ASP:OD1	2.40	0.55
15:O:99:TYR:OH	15:O:150:ARG:NH1	2.40	0.55
20:Y:4:DG:H2''	20:Y:5:DC:C6	2.42	0.55
1:A:1328:LEU:O	2:B:1122:ILE:HG21	2.07	0.55
15:O:37:ARG:O	15:O:41:HIS:ND1	2.39	0.55
1:A:872:GLN:HA	1:A:872:GLN:NE2	2.20	0.55
16:P:283:VAL:O	16:P:283:VAL:HG13	2.07	0.55
1:A:21:GLY:O	2:B:1123:ILE:N	2.32	0.54
15:O:118:MET:SD	17:Q:108:ARG:NH2	2.74	0.54
15:O:410:PRO:HB3	15:O:422:TYR:CE2	2.42	0.54
3:C:265:GLN:HG3	3:C:272:VAL:HG12	1.88	0.54
16:P:202:PRO:O	16:P:205:GLN:NE2	2.37	0.54
16:P:290:CYS:SG	22:P:401:SF4:S4	3.04	0.54
7:G:154:ASP:OD1	7:G:154:ASP:N	2.39	0.54
15:O:86:LEU:HD21	15:O:443:ILE:HD13	1.89	0.54
15:O:412:THR:OG1	15:O:420:THR:HG23	2.08	0.54
2:B:26:LYS:HB3	2:B:26:LYS:HZ2	1.72	0.54
11:K:27:LEU:HG	11:K:43:VAL:HB	1.90	0.54
15:O:409:ILE:N	15:O:410:PRO:CD	2.35	0.54
1:A:1136:ARG:NH1	9:I:48:GLU:HA	2.22	0.54
4:D:112:GLN:O	4:D:112:GLN:NE2	2.40	0.54
15:O:141:TYR:OH	17:Q:106:LEU:O	2.24	0.54
1:A:882:LEU:H	1:A:882:LEU:CD1	2.20	0.54
2:B:249:GLN:OE1	14:N:144:LYS:HE3	2.08	0.54
9:I:32:HIS:CD2	14:N:137:ILE:HG12	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:18:DA:H8	20:Y:18:DA:H5''	1.72	0.54
1:A:217:ASN:HD22	15:O:410:PRO:HG2	1.72	0.54
11:K:30:VAL:HG11	11:K:35:THR:HG23	1.89	0.54
15:O:407:GLN:O	15:O:410:PRO:CG	2.56	0.54
16:P:227:LYS:O	16:P:240:ASN:ND2	2.41	0.54
20:Y:19:DG:H4'	20:Y:19:DG:OP1	2.07	0.54
1:A:19:CYS:HA	1:A:1337:LYS:HA	1.90	0.53
1:A:707:GLN:HA	1:A:707:GLN:NE2	2.24	0.53
3:C:246:GLU:HG2	3:C:272:VAL:HG23	1.89	0.53
8:H:78:THR:CB	11:K:87:ARG:CZ	2.78	0.53
1:A:351:ARG:HA	1:A:355:ASN:HD22	1.74	0.53
5:E:111:THR:HG21	19:X:44:DT:OP2	2.08	0.53
15:O:138:THR:HG21	17:Q:104:ARG:CB	2.35	0.53
15:O:419:ARG:HD2	15:O:422:TYR:CZ	2.44	0.53
2:B:506:MET:SD	2:B:569:ASN:ND2	2.82	0.53
7:G:44:LEU:HB3	7:G:77:PHE:HB3	1.89	0.53
1:A:1217:GLN:HG3	9:I:101:GLN:CG	2.24	0.53
15:O:171:PRO:O	15:O:174:PRO:HD2	2.07	0.53
15:O:239:LEU:HA	15:O:242:PHE:HD2	1.73	0.53
1:A:183:LYS:H	1:A:183:LYS:HE2	1.73	0.53
2:B:86:ASP:O	2:B:135:ARG:NH2	2.42	0.53
15:O:115:LYS:HE2	15:O:160:CYS:HB2	1.89	0.53
16:P:290:CYS:HB2	16:P:293:PHE:HB2	1.89	0.53
1:A:1044:PRO:HB3	1:A:1280:MET:HG3	1.90	0.53
8:H:96:VAL:HG22	8:H:116:VAL:HG22	1.91	0.53
11:K:47:GLU:OE1	11:K:47:GLU:HA	2.08	0.53
4:D:62:SER:HB2	4:D:65:ILE:HG23	1.89	0.53
15:O:24:ILE:HD11	15:O:45:THR:HG21	1.90	0.53
1:A:556:ASP:OD1	8:H:22:PHE:HB3	2.09	0.53
4:D:3:VAL:HG11	7:G:42:VAL:HG21	1.91	0.53
5:E:77:PRO:HG3	5:E:90:TYR:HE2	1.74	0.53
14:N:269:LEU:HB3	14:N:383:LEU:HB2	1.91	0.53
16:P:286:PRO:HG2	16:P:313:TRP:CG	2.44	0.53
4:D:4:LYS:HE2	4:D:4:LYS:CA	2.31	0.53
4:D:102:GLU:N	4:D:102:GLU:CD	2.62	0.53
13:M:33:ARG:HD2	13:M:37:MET:HB2	1.91	0.53
19:X:43:DC:H2'	19:X:44:DT:H72	1.91	0.53
1:A:33:HIS:NE2	2:B:1088:TYR:OH	2.42	0.52
3:C:266:GLU:OE1	3:C:266:GLU:N	2.35	0.52
7:G:32:LYS:CB	7:G:32:LYS:NZ	2.72	0.52
13:M:7:ASP:OD1	13:M:7:ASP:N	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:ARG:NH2	2:B:481:PRO:O	2.42	0.52
8:H:63:THR:HB	8:H:70:LEU:HD13	1.91	0.52
15:O:445:ASN:CG	22:P:401:SF4:S2	2.87	0.52
1:A:1366:ALA:HB1	7:G:22:LEU:HD23	1.90	0.52
4:D:14:TYR:CE2	4:D:18:GLN:HG2	2.44	0.52
4:D:59:ARG:NE	4:D:59:ARG:H	2.07	0.52
15:O:409:ILE:CG1	15:O:423:LEU:CG	2.84	0.52
1:A:183:LYS:HD3	1:A:183:LYS:N	2.24	0.52
4:D:6:ALA:O	7:G:5:VAL:HG22	2.10	0.52
20:Y:12:DC:H2'	20:Y:13:DT:H72	1.91	0.52
6:F:107:ARG:O	6:F:107:ARG:HG3	2.09	0.52
15:O:127:ASP:HB3	15:O:128:ARG:HH11	1.75	0.52
1:A:1053:PHE:HZ	9:I:78:TYR:CE1	2.27	0.52
2:B:206:SER:OG	2:B:211:LYS:HE2	2.10	0.52
15:O:376:GLU:HG3	15:O:424:TYR:HB2	1.91	0.52
1:A:816:ARG:HH21	2:B:639:ASN:C	2.11	0.52
1:A:864:LYS:HD2	1:A:1067:VAL:CG2	2.39	0.52
3:C:135:ILE:HD12	3:C:135:ILE:N	2.23	0.52
1:A:211:LEU:H	1:A:211:LEU:CD1	2.10	0.51
1:A:1053:PHE:CZ	9:I:78:TYR:CE2	2.87	0.51
2:B:1028:ARG:NH1	2:B:1072:SER:O	2.43	0.51
15:O:440:TYR:OH	15:O:524:GLU:OE2	2.28	0.51
15:O:460:LEU:HB3	15:O:499:LEU:HD11	1.92	0.51
17:Q:80:GLU:HA	17:Q:86:ARG:HD3	1.92	0.51
1:A:587:THR:O	8:H:92:MET:HA	2.09	0.51
3:C:263:GLU:HG3	3:C:274:ARG:HG2	1.92	0.51
1:A:767:CYS:SG	1:A:768:LEU:N	2.83	0.51
15:O:22:GLU:O	15:O:26:VAL:N	2.40	0.51
2:B:871:ILE:HD12	12:L:17:TYR:CD2	2.46	0.51
2:B:955:ASP:OD2	2:B:957:ARG:NH2	2.43	0.51
3:C:51:VAL:HG22	3:C:65:MET:HG2	1.92	0.51
15:O:356:GLU:OE1	17:Q:39:PRO:CD	2.48	0.51
1:A:210:LEU:HD23	1:A:213:ARG:HG2	1.93	0.51
4:D:2:GLU:OE1	4:D:2:GLU:N	2.27	0.51
13:M:207:HIS:O	14:N:370:THR:HA	2.10	0.51
17:Q:27:LEU:O	17:Q:28:PRO:C	2.48	0.51
5:E:67:ASP:HB3	5:E:70:ASP:HB2	1.93	0.51
15:O:5:GLU:HG3	15:O:83:LEU:HD11	1.93	0.51
1:A:206:GLU:OE1	1:A:206:GLU:N	2.38	0.51
1:A:207:VAL:HA	15:O:411:LYS:HE3	1.93	0.51
3:C:103:ASP:OD1	3:C:103:ASP:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:57:PRO:C	4:D:59:ARG:N	2.64	0.51
1:A:794:GLN:HG3	1:A:799:VAL:HA	1.93	0.51
1:A:1363:LEU:HD11	6:F:107:ARG:NH2	2.26	0.51
8:H:78:THR:CG2	11:K:87:ARG:HH12	2.22	0.51
15:O:60:HIS:NE2	15:O:112:LEU:O	2.44	0.51
15:O:505:ASN:ND2	16:P:314:LEU:HD13	2.26	0.51
1:A:262:ILE:HD11	2:B:1115:GLN:OE1	2.11	0.50
3:C:286:GLU:OE1	3:C:286:GLU:HA	2.11	0.50
3:C:287:ILE:HG12	3:C:297:VAL:HG21	1.91	0.50
5:E:164:LYS:HE3	6:F:112:ASP:OD2	2.10	0.50
7:G:99:VAL:HG11	7:G:148:ILE:HG12	1.92	0.50
15:O:409:ILE:CB	15:O:423:LEU:CD2	2.67	0.50
16:P:296:CYS:SG	16:P:297:HIS:N	2.79	0.50
5:E:7:THR:HG21	5:E:41:LYS:HE3	1.93	0.50
7:G:39:VAL:HB	7:G:42:VAL:HB	1.93	0.50
1:A:951:SER:HA	1:A:954:LYS:HE3	1.93	0.50
8:H:32:SER:OG	8:H:35:PHE:O	2.27	0.50
1:A:302:LYS:HE2	1:A:302:LYS:H	1.77	0.50
1:A:569:ALA:CB	11:K:69:GLY:HA3	2.41	0.50
18:R:11:G:H8	18:R:11:G:O5'	1.94	0.50
1:A:874:ARG:HG2	1:A:1321:PHE:HZ	1.77	0.50
16:P:282:LEU:HB2	17:Q:42:ASP:OD2	2.11	0.50
18:R:11:G:O5'	18:R:11:G:C8	2.65	0.50
1:A:362:ASP:HB2	2:B:1024:ALA:O	2.12	0.50
3:C:163:TYR:HE1	3:C:204:PRO:HG3	1.77	0.50
3:C:263:GLU:HG3	3:C:263:GLU:O	2.10	0.50
3:C:292:LYS:HD2	3:C:293:LEU:HD12	1.93	0.50
16:P:286:PRO:HG2	16:P:313:TRP:CD2	2.47	0.50
1:A:791:ASN:ND2	9:I:91:MET:HG2	2.27	0.50
2:B:182:GLU:OE2	2:B:360:LYS:NZ	2.36	0.50
3:C:334:ARG:O	3:C:334:ARG:HD3	2.12	0.50
7:G:115:GLN:NE2	7:G:192:GLU:O	2.45	0.50
10:J:40:LEU:HD22	10:J:45:CYS:HB3	1.93	0.50
15:O:436:LEU:HB2	15:O:523:LEU:HD22	1.92	0.50
16:P:286:PRO:HB3	17:Q:38:PHE:CD2	2.47	0.50
1:A:30:GLN:O	2:B:1093:HIS:ND1	2.45	0.50
1:A:303:THR:H	15:O:377:GLN:HE22	1.59	0.49
5:E:26:TYR:HB3	5:E:61:LEU:HB3	1.93	0.49
2:B:750:ASP:O	2:B:930:ASN:ND2	2.45	0.49
5:E:76:PHE:CD1	5:E:76:PHE:N	2.80	0.49
7:G:148:ILE:CG2	7:G:190:ILE:HG23	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:378:LYS:HD2	15:O:379:GLN:HE21	1.77	0.49
15:O:450:ARG:O	15:O:454:THR:OG1	2.28	0.49
16:P:222:GLU:O	16:P:226:SER:OG	2.27	0.49
1:A:6:PHE:HE2	4:D:1:MET:HG2	1.72	0.49
1:A:533:ARG:NH2	1:A:1043:GLU:OE1	2.44	0.49
1:A:591:PRO:HD3	8:H:90:TYR:HA	1.94	0.49
2:B:307:GLU:OE2	2:B:310:ARG:NH2	2.46	0.49
4:D:43:ASN:ND2	4:D:43:ASN:N	2.57	0.49
5:E:84:ILE:HG22	5:E:88:LYS:HG2	1.94	0.49
15:O:405:SER:HB3	15:O:425:THR:O	2.13	0.49
1:A:381:ALA:HB3	1:A:487:ARG:HB2	1.94	0.49
1:A:729:GLU:HA	1:A:729:GLU:OE1	2.12	0.49
5:E:52:ARG:N	5:E:53:PRO:HD2	2.27	0.49
15:O:460:LEU:HA	15:O:463:LYS:HG2	1.94	0.49
15:O:505:ASN:OD1	16:P:314:LEU:HB3	2.12	0.49
1:A:598:LYS:HD2	8:H:120:GLY:HA3	1.93	0.49
4:D:102:GLU:N	4:D:102:GLU:OE2	2.40	0.49
12:L:52:LEU:HD23	12:L:52:LEU:O	2.12	0.49
15:O:410:PRO:HB3	15:O:422:TYR:CD2	2.47	0.49
20:Y:0:DA:C8	20:Y:0:DA:OP2	2.65	0.49
4:D:48:GLU:CA	7:G:103:PHE:HB3	2.38	0.49
15:O:141:TYR:CE2	17:Q:108:ARG:HG2	2.48	0.49
15:O:409:ILE:CD1	15:O:423:LEU:CD1	2.63	0.49
1:A:1054:HIS:HD2	1:A:1063:ILE:HG13	1.78	0.49
1:A:1121:PHE:CZ	9:I:14:VAL:HG21	2.46	0.49
16:P:252:ILE:HG23	16:P:257:GLU:HB3	1.93	0.49
17:Q:57:MET:O	17:Q:61:LYS:N	2.38	0.49
17:Q:72:PRO:HA	17:Q:75:ILE:HG22	1.95	0.49
4:D:61:GLN:HA	4:D:61:GLN:NE2	2.28	0.49
2:B:608:ASN:H	2:B:608:ASN:ND2	2.10	0.48
2:B:999:GLU:O	3:C:21:VAL:HG23	2.13	0.48
15:O:416:ALA:HA	15:O:422:TYR:OH	2.13	0.48
1:A:1039:GLN:HE22	2:B:1054:CYS:HA	1.79	0.48
1:A:1329:PHE:CZ	2:B:1120:MET:HE2	2.48	0.48
3:C:38:ASP:O	11:K:61:LYS:NZ	2.46	0.48
6:F:126:THR:O	6:F:126:THR:OG1	2.23	0.48
7:G:161:SER:HB2	7:G:162:PRO:CD	2.43	0.48
16:P:286:PRO:CB	17:Q:38:PHE:CD2	2.96	0.48
1:A:117:LEU:HD11	1:A:146:ILE:HG23	1.96	0.48
3:C:23:ASN:O	3:C:303:ARG:NH2	2.47	0.48
3:C:264:VAL:HG23	3:C:264:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:219:TYR:HD2	16:P:271:ARG:HB3	1.78	0.48
16:P:220:ILE:CD1	16:P:271:ARG:HD2	2.43	0.48
1:A:183:LYS:H	1:A:183:LYS:CE	2.27	0.48
15:O:159:ARG:HD2	17:Q:113:ARG:CZ	2.44	0.48
17:Q:27:LEU:CD2	17:Q:27:LEU:N	2.63	0.48
1:A:1187:TYR:HD2	2:B:270:GLU:CD	2.17	0.48
2:B:120:THR:HG23	2:B:124:GLN:HA	1.96	0.48
5:E:47:LYS:N	5:E:48:PRO:CD	2.76	0.48
1:A:1057:GLY:HA2	9:I:59:TRP:HZ3	1.78	0.48
3:C:43:ASP:OD1	3:C:43:ASP:N	2.46	0.48
7:G:84:ILE:HD11	7:G:149:ARG:HH21	1.77	0.48
11:K:89:THR:HG22	11:K:89:THR:O	2.14	0.48
4:D:5:ASP:HB2	7:G:6:GLU:HG3	1.96	0.48
1:A:1329:PHE:HA	2:B:1122:ILE:HG12	1.96	0.47
4:D:52:TYR:O	4:D:55:LYS:HB2	2.14	0.47
12:L:37:ARG:O	12:L:38:GLU:HB2	2.14	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
2:B:915:ASP:OD1	3:C:78:ARG:NH2	2.46	0.47
4:D:43:ASN:HD22	4:D:43:ASN:N	2.01	0.47
7:G:151:ARG:NH1	7:G:152:VAL:HG12	2.29	0.47
7:G:161:SER:HB2	7:G:162:PRO:HD3	1.96	0.47
1:A:17:HIS:HE1	2:B:1127:LYS:HB2	1.77	0.47
12:L:57:ALA:O	12:L:58:ARG:C	2.53	0.47
1:A:27:GLU:OE2	2:B:1094:TYR:OH	2.32	0.47
15:O:156:PHE:HA	15:O:241:ARG:HG2	1.96	0.47
9:I:75:PRO:HD2	9:I:99:ASN:HD22	1.79	0.47
10:J:16:ASN:OD1	10:J:16:ASN:N	2.47	0.47
15:O:412:THR:CG2	15:O:413:PRO:HD2	2.45	0.47
1:A:1215:ASP:N	1:A:1215:ASP:OD1	2.47	0.47
2:B:105:ARG:NH2	12:L:42:ARG:HD2	2.30	0.47
2:B:915:ASP:OD1	3:C:78:ARG:NH1	2.47	0.47
15:O:508:LYS:HG3	16:P:313:TRP:CZ2	2.50	0.47
1:A:499:ASP:OD1	1:A:499:ASP:N	2.48	0.47
1:A:760:ARG:CZ	1:A:760:ARG:O	2.63	0.47
2:B:678:ASN:HD21	2:B:901:HIS:CD2	2.33	0.47
4:D:42:LEU:HD13	4:D:42:LEU:C	2.35	0.47
5:E:79:GLU:N	5:E:79:GLU:OE1	2.44	0.47
6:F:107:ARG:HD3	6:F:115:TYR:HB2	1.97	0.47
7:G:160:THR:O	7:G:160:THR:CG2	2.63	0.47
9:I:102:CYS:HG	9:I:104:HIS:CD2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:37:ARG:HB3	11:K:91:PRO:HA	1.95	0.47
16:P:283:VAL:O	16:P:283:VAL:CG1	2.62	0.47
20:Y:-1:DC:P	20:Y:-1:DC:H2'	2.55	0.47
2:B:218:VAL:HG11	2:B:346:GLN:HE22	1.79	0.47
14:N:139:ASN:O	14:N:142:LYS:NZ	2.42	0.47
1:A:686:LEU:O	1:A:686:LEU:HD23	2.15	0.47
1:A:1328:LEU:O	2:B:1122:ILE:CG2	2.63	0.47
1:A:1350:GLY:HA3	2:B:1069:MET:SD	2.55	0.47
4:D:32:LYS:HD3	4:D:32:LYS:H	1.79	0.47
15:O:406:LEU:N	15:O:406:LEU:HD23	2.30	0.47
1:A:757:SER:HB2	9:I:63:ASP:HB3	1.96	0.47
1:A:857:GLY:HA2	9:I:85:ARG:N	2.30	0.47
2:B:989:VAL:HG21	2:B:1002:ILE:HB	1.97	0.47
5:E:111:THR:CG2	19:X:44:DT:OP2	2.63	0.47
16:P:286:PRO:HA	17:Q:38:PHE:HD2	1.78	0.47
1:A:279:LEU:HD23	1:A:279:LEU:HA	1.71	0.46
1:A:520:LEU:CD2	6:F:94:MET:HE1	2.45	0.46
2:B:279:THR:HG21	13:M:143:ASP:HB2	1.97	0.46
5:E:55:ARG:N	5:E:55:ARG:CD	2.77	0.46
10:J:31:GLU:OE1	10:J:31:GLU:HA	2.15	0.46
17:Q:86:ARG:HB2	17:Q:86:ARG:HH11	1.80	0.46
1:A:1051:LYS:NZ	9:I:94:PHE:CD2	2.73	0.46
3:C:29:PHE:HB2	3:C:32:ASN:ND2	2.30	0.46
3:C:65:MET:HB3	3:C:65:MET:HE2	1.69	0.46
3:C:275:VAL:O	3:C:275:VAL:HG23	2.16	0.46
4:D:1:MET:O	4:D:1:MET:HG3	2.15	0.46
17:Q:81:ARG:HE	17:Q:84:ILE:HD11	1.81	0.46
1:A:294:LYS:HB3	1:A:294:LYS:HZ3	1.80	0.46
2:B:865:TYR:CE2	12:L:55:PHE:CD2	2.94	0.46
4:D:1:MET:HE3	4:D:1:MET:HB2	1.46	0.46
5:E:82:VAL:HG13	5:E:86:THR:HB	1.96	0.46
7:G:79:PRO:HG2	7:G:150:PHE:CD2	2.51	0.46
1:A:876:VAL:HG11	2:B:1053:ASP:CG	2.36	0.46
1:A:942:LYS:HG3	1:A:977:SER:HB2	1.97	0.46
15:O:26:VAL:HA	15:O:29:ILE:HD12	1.97	0.46
3:C:203:ARG:HB3	3:C:204:PRO:HD2	1.97	0.46
15:O:374:HIS:CE1	15:O:425:THR:HG1	2.29	0.46
16:P:269:LEU:HD23	16:P:269:LEU:HA	1.78	0.46
1:A:17:HIS:ND1	2:B:1127:LYS:HB3	2.31	0.46
2:B:357:TYR:HE2	2:B:479:LEU:HD22	1.80	0.46
4:D:35:HIS:HD2	7:G:32:LYS:CE	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:80:PHE:CE2	7:G:82:ASP:HB2	2.51	0.46
7:G:94:PRO:HA	7:G:121:ASP:HB2	1.96	0.46
13:M:59:GLU:HG2	13:M:101:THR:HG22	1.96	0.46
2:B:1038:GLY:O	2:B:1043:GLY:N	2.46	0.46
3:C:130:GLU:CD	3:C:130:GLU:H	2.15	0.46
4:D:84:LEU:O	4:D:84:LEU:HD12	2.16	0.46
15:O:147:THR:HA	15:O:150:ARG:HB2	1.98	0.46
16:P:309:TYR:OH	17:Q:32:LEU:O	2.34	0.46
2:B:1038:GLY:CA	20:Y:20:DC:OP1	2.63	0.46
5:E:47:LYS:C	5:E:47:LYS:HD2	2.36	0.46
15:O:170:ASP:O	15:O:173:PRO:HD2	2.15	0.46
20:Y:0:DA:OP2	20:Y:0:DA:H8	1.99	0.46
20:Y:11:DT:H2"	20:Y:12:DC:C6	2.50	0.46
1:A:529:LEU:HD12	1:A:668:LEU:HD13	1.98	0.46
1:A:709:LEU:O	1:A:709:LEU:HD12	2.15	0.46
1:A:957:GLU:OE1	1:A:957:GLU:N	2.33	0.46
4:D:105:GLU:CD	4:D:105:GLU:H	2.19	0.46
5:E:61:LEU:N	5:E:61:LEU:HD13	2.30	0.46
12:L:52:LEU:HD23	12:L:52:LEU:C	2.37	0.46
15:O:409:ILE:HG22	15:O:409:ILE:O	2.16	0.46
1:A:19:CYS:O	2:B:1125:ARG:CB	2.62	0.46
15:O:412:THR:HG22	15:O:413:PRO:HD2	1.98	0.46
15:O:449:ARG:HH11	16:P:310:MET:HE3	1.81	0.46
3:C:155:ASP:N	3:C:155:ASP:OD1	2.49	0.45
1:A:29:ARG:HH11	1:A:254:ARG:HH11	1.64	0.45
1:A:194:LEU:HD12	1:A:197:PHE:CE1	2.51	0.45
1:A:743:THR:OG1	1:A:744:ALA:N	2.47	0.45
1:A:832:GLY:HA2	1:A:849:PHE:CD2	2.51	0.45
1:A:857:GLY:HA2	9:I:84:THR:HA	1.98	0.45
1:A:857:GLY:CA	9:I:84:THR:HA	2.47	0.45
1:A:1187:TYR:CD2	2:B:270:GLU:OE1	2.68	0.45
9:I:32:HIS:HA	14:N:137:ILE:CD1	2.42	0.45
15:O:505:ASN:CG	16:P:314:LEU:HD13	2.37	0.45
1:A:1329:PHE:CZ	2:B:1120:MET:CE	2.99	0.45
2:B:282:GLN:NE2	13:M:146:ASP:OD2	2.49	0.45
3:C:97:ASN:C	3:C:97:ASN:OD1	2.55	0.45
3:C:292:LYS:O	3:C:292:LYS:HD3	2.16	0.45
4:D:96:GLU:H	4:D:96:GLU:HG2	1.43	0.45
5:E:21:CYS:SG	5:E:61:LEU:HG	2.57	0.45
9:I:29:PRO:HG3	13:M:74:GLY:HA2	1.97	0.45
15:O:406:LEU:N	15:O:406:LEU:CD2	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:GLU:HA	1:A:308:GLU:OE1	2.16	0.45
1:A:395:LYS:HE2	6:F:75:MET:CE	2.46	0.45
1:A:731:LEU:HD22	1:A:748:LEU:HD22	1.97	0.45
1:A:1329:PHE:CD1	2:B:1122:ILE:CG1	2.99	0.45
10:J:19:GLU:OE1	10:J:19:GLU:N	2.50	0.45
11:K:58:MET:HE3	11:K:58:MET:HA	1.98	0.45
15:O:400:SER:OG	15:O:401:GLU:OE1	2.31	0.45
20:Y:18:DA:H5''	20:Y:18:DA:C8	2.50	0.45
1:A:181:THR:O	1:A:182:ASN:OD1	2.35	0.45
1:A:560:ASP:OD2	3:C:27:THR:HG22	2.17	0.45
1:A:590:LYS:NZ	8:H:88:PHE:O	2.47	0.45
1:A:757:SER:CB	9:I:63:ASP:HB3	2.46	0.45
2:B:622:GLU:HA	2:B:625:LEU:HD12	1.98	0.45
2:B:750:ASP:HA	2:B:754:ALA:HB3	1.99	0.45
7:G:160:THR:O	7:G:160:THR:HG22	2.15	0.45
9:I:51:ASP:OD1	9:I:51:ASP:C	2.55	0.45
11:K:27:LEU:HD21	11:K:45:HIS:CE1	2.51	0.45
3:C:65:MET:HE1	3:C:68:ILE:HG12	1.98	0.45
4:D:59:ARG:HB3	4:D:59:ARG:NH2	2.32	0.45
15:O:59:GLN:NE2	15:O:113:ASN:O	2.42	0.45
15:O:407:GLN:N	15:O:407:GLN:CD	2.69	0.45
1:A:471:LEU:HD22	1:A:538:LEU:HD12	1.98	0.45
1:A:1211:VAL:HG21	9:I:53:LEU:HD23	1.99	0.45
11:K:38:HIS:CE1	11:K:89:THR:HA	2.52	0.45
13:M:50:LYS:HD3	13:M:203:GLU:HB3	1.98	0.45
14:N:261:THR:HG22	14:N:263:GLU:H	1.82	0.45
15:O:416:ALA:HB3	15:O:417:PRO:HD3	1.98	0.45
18:R:9:C:H2''	18:R:10:U:C6	2.52	0.45
1:A:864:LYS:HZ1	1:A:1050:LEU:HB2	1.82	0.45
7:G:56:ASP:OD1	7:G:56:ASP:N	2.41	0.45
15:O:423:LEU:HD23	15:O:423:LEU:N	2.32	0.45
20:Y:7:DC:H2''	20:Y:8:DT:H71	1.99	0.45
4:D:5:ASP:OD2	7:G:6:GLU:HG3	2.17	0.45
11:K:94:GLU:HB3	11:K:95:PRO:HD3	1.98	0.45
16:P:293:PHE:CD2	22:P:401:SF4:S1	3.10	0.45
16:P:293:PHE:HE1	17:Q:31:VAL:HG12	1.80	0.45
1:A:31:GLN:C	2:B:1093:HIS:HD1	2.19	0.45
2:B:682:ARG:HD2	2:B:937:ARG:HB3	1.98	0.45
7:G:151:ARG:CZ	7:G:152:VAL:HG12	2.47	0.45
11:K:58:MET:HA	11:K:58:MET:CE	2.46	0.45
12:L:13:GLN:HG2	12:L:13:GLN:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:63:VAL:HG22	15:O:77:ALA:HB2	1.99	0.45
15:O:141:TYR:HE2	17:Q:108:ARG:HG2	1.82	0.45
15:O:459:ARG:HG2	15:O:460:LEU:HD23	1.99	0.45
2:B:40:VAL:O	2:B:40:VAL:CG1	2.63	0.44
15:O:434:MET:HB3	15:O:434:MET:HE2	1.79	0.44
15:O:447:ILE:O	15:O:451:GLN:N	2.47	0.44
2:B:494:LYS:HE2	2:B:494:LYS:HB2	1.85	0.44
3:C:332:LYS:HB3	11:K:51:LEU:HD22	1.99	0.44
4:D:58:CYS:CA	4:D:61:GLN:HB2	2.38	0.44
5:E:82:VAL:O	5:E:111:THR:HG22	2.17	0.44
1:A:17:HIS:NE2	2:B:1127:LYS:CD	2.74	0.44
1:A:760:ARG:HE	1:A:798:CYS:HB3	1.82	0.44
3:C:337:LEU:HD23	3:C:337:LEU:HA	1.83	0.44
7:G:161:SER:CB	7:G:162:PRO:CD	2.95	0.44
1:A:769:ARG:HB3	1:A:769:ARG:NH2	2.32	0.44
2:B:826:VAL:HG12	2:B:857:THR:HG22	1.99	0.44
2:B:999:GLU:CG	3:C:24:VAL:HG21	2.44	0.44
3:C:17:GLY:HA3	3:C:22:ARG:HH12	1.83	0.44
4:D:117:LEU:HA	4:D:120:VAL:HG12	1.98	0.44
13:M:6:ASP:OD1	13:M:6:ASP:N	2.51	0.44
15:O:361:ARG:NH1	16:P:193:GLU:OE2	2.50	0.44
1:A:6:PHE:HA	7:G:37:LYS:HD3	2.00	0.44
1:A:1187:TYR:HD2	2:B:270:GLU:OE1	2.00	0.44
1:A:1368:ARG:HH12	7:G:56:ASP:HA	1.83	0.44
13:M:240:LYS:NZ	13:M:248:MET:SD	2.87	0.44
16:P:286:PRO:CA	17:Q:38:PHE:CD2	3.01	0.44
16:P:308:ILE:HD13	17:Q:31:VAL:CG1	2.47	0.44
3:C:239:ILE:HD12	3:C:239:ILE:N	2.26	0.44
16:P:292:VAL:HG21	17:Q:32:LEU:HD12	1.98	0.44
3:C:29:PHE:HB2	3:C:32:ASN:HD21	1.81	0.44
9:I:3:LEU:HD13	14:N:143:GLU:HG3	1.99	0.44
15:O:415:HIS:HB2	15:O:418:SER:O	2.18	0.44
1:A:819:PRO:HB3	2:B:638:GLU:O	2.18	0.44
2:B:183:GLN:NE2	2:B:433:ARG:HH22	2.16	0.44
3:C:181:GLN:HG2	3:C:185:PHE:HE2	1.82	0.44
7:G:26:ILE:HG21	7:G:70:VAL:HG21	1.98	0.44
20:Y:7:DC:H2''	20:Y:8:DT:C6	2.53	0.44
1:A:877:LYS:HG3	1:A:1321:PHE:CD1	2.52	0.44
4:D:87:LEU:N	4:D:87:LEU:HD23	2.32	0.44
8:H:38:ASP:OD1	8:H:38:ASP:N	2.42	0.44
13:M:148:LYS:HE2	13:M:148:LYS:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:406:LEU:HD23	15:O:406:LEU:H	1.83	0.44
2:B:549:ILE:HD13	2:B:555:LEU:HD22	2.00	0.43
3:C:234:ARG:O	3:C:234:ARG:HG3	2.18	0.43
7:G:115:GLN:HG3	7:G:116:GLN:HG3	2.00	0.43
15:O:170:ASP:OD1	15:O:170:ASP:N	2.48	0.43
15:O:356:GLU:HG3	16:P:284:ARG:CB	2.39	0.43
15:O:409:ILE:HD12	15:O:423:LEU:CD1	2.31	0.43
16:P:256:LYS:HE2	16:P:278:PRO:HA	1.99	0.43
1:A:905:ASP:OD2	1:A:1285:ARG:NH2	2.42	0.43
1:A:691:LEU:HD12	1:A:691:LEU:HA	1.79	0.43
1:A:947:LEU:HD23	1:A:947:LEU:C	2.39	0.43
1:A:1261:GLU:OE2	5:E:195:ARG:NH2	2.51	0.43
4:D:59:ARG:HB3	4:D:59:ARG:HH21	1.83	0.43
5:E:10:LEU:HD21	5:E:52:ARG:HG2	2.00	0.43
15:O:345:LEU:HD23	15:O:345:LEU:HA	1.89	0.43
18:R:10:U:H3'	18:R:11:G:C8	2.50	0.43
1:A:753:LEU:HD23	1:A:753:LEU:HA	1.83	0.43
2:B:24:GLU:OE1	2:B:24:GLU:N	2.43	0.43
3:C:57:ASP:C	3:C:57:ASP:OD1	2.56	0.43
15:O:161:PRO:HB3	17:Q:119:ALA:CB	2.48	0.43
1:A:568:ILE:HG23	1:A:603:VAL:HG11	1.99	0.43
1:A:864:LYS:HA	1:A:864:LYS:HD3	1.53	0.43
1:A:1353:MET:HG2	2:B:1061:SER:CB	2.48	0.43
2:B:26:LYS:HZ2	2:B:26:LYS:CB	2.31	0.43
3:C:210:LEU:C	3:C:210:LEU:HD12	2.39	0.43
15:O:399:LEU:HD12	15:O:404:MET:HB3	2.00	0.43
16:P:286:PRO:HB3	17:Q:38:PHE:CE2	2.53	0.43
1:A:38:SER:CB	17:Q:24:GLY:HA3	2.36	0.43
1:A:1249:ASN:ND2	1:A:1270:GLU:OE2	2.52	0.43
11:K:38:HIS:ND1	11:K:38:HIS:N	2.67	0.43
15:O:157:VAL:HG12	17:Q:115:LYS:HE2	2.00	0.43
1:A:130:LYS:HA	1:A:130:LYS:HD3	1.81	0.43
1:A:686:LEU:HD23	1:A:686:LEU:C	2.39	0.43
1:A:1340:VAL:HA	1:A:1345:GLU:HG3	2.00	0.43
3:C:79:ILE:HG23	3:C:83:GLU:HB2	2.01	0.43
4:D:52:TYR:CE1	7:G:101:LEU:HD11	2.54	0.43
7:G:57:ALA:HA	7:G:68:THR:HG22	2.00	0.43
9:I:69:CYS:SG	9:I:73:GLU:N	2.89	0.43
13:M:206:VAL:HG21	14:N:365:LEU:HD21	2.01	0.43
15:O:416:ALA:N	15:O:417:PRO:CD	2.81	0.43
18:R:11:G:H2'	18:R:11:G:N3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:12:DC:C6	20:Y:13:DT:H72	2.54	0.43
1:A:183:LYS:N	1:A:183:LYS:CD	2.81	0.43
17:Q:34:PRO:HG2	17:Q:37:LEU:HD23	2.01	0.43
1:A:83:TYR:OH	2:B:1115:GLN:HG2	2.19	0.43
1:A:1187:TYR:CD2	2:B:270:GLU:OE2	2.71	0.43
4:D:95:VAL:HA	4:D:98:GLN:HB2	2.01	0.43
15:O:413:PRO:O	15:O:415:HIS:HD2	2.01	0.43
1:A:18:ILE:HG12	2:B:1126:LEU:HD23	1.97	0.43
1:A:722:LYS:HE2	1:A:722:LYS:HB3	1.65	0.43
3:C:72:ILE:HD13	11:K:106:VAL:HG11	2.01	0.43
4:D:114:GLU:N	4:D:114:GLU:OE2	2.51	0.43
5:E:89:VAL:O	5:E:92:GLN:HG3	2.19	0.43
16:P:222:GLU:HA	16:P:225:ILE:HG22	2.01	0.43
1:A:352:PHE:HZ	1:A:1328:LEU:HD11	1.83	0.42
1:A:698:ILE:HG21	2:B:934:PHE:HD2	1.84	0.42
3:C:315:VAL:HG12	3:C:316:LEU:HD22	1.99	0.42
9:I:32:HIS:NE2	14:N:137:ILE:HG12	2.33	0.42
19:X:38:DA:H61	20:Y:6:DT:H3	1.67	0.42
1:A:199:THR:HG22	15:O:378:LYS:NZ	2.27	0.42
1:A:735:LYS:NZ	1:A:737:GLN:HA	2.34	0.42
3:C:156:SER:HB2	3:C:162:LEU:HG	2.01	0.42
3:C:235:LEU:N	3:C:235:LEU:HD12	2.34	0.42
1:A:90:LEU:HD23	1:A:293:ILE:HG21	2.02	0.42
3:C:184:LEU:HD12	3:C:184:LEU:O	2.19	0.42
6:F:81:VAL:HG11	6:F:96:GLU:HA	2.01	0.42
13:M:123:GLU:HG3	13:M:125:HIS:CE1	2.55	0.42
4:D:17:PHE:CE1	4:D:21:THR:CG2	3.03	0.42
4:D:69:PHE:HD1	4:D:69:PHE:O	2.02	0.42
5:E:47:LYS:HB3	5:E:47:LYS:HE3	1.89	0.42
17:Q:34:PRO:HG2	17:Q:37:LEU:CD2	2.49	0.42
1:A:179:TYR:HB3	1:A:190:VAL:HB	2.02	0.42
1:A:183:LYS:H	1:A:183:LYS:CD	2.32	0.42
2:B:865:TYR:CD2	12:L:55:PHE:CE2	2.91	0.42
3:C:235:LEU:HD23	3:C:303:ARG:HA	2.01	0.42
5:E:17:ILE:HD13	5:E:17:ILE:HA	1.89	0.42
15:O:124:LYS:HA	15:O:124:LYS:HD3	1.75	0.42
15:O:459:ARG:H	15:O:459:ARG:HD3	1.85	0.42
19:X:40:DC:H6	19:X:40:DC:OP2	2.03	0.42
19:X:43:DC:N4	20:Y:0:DA:N1	2.67	0.42
1:A:542:ILE:HD12	1:A:542:ILE:HA	1.90	0.42
4:D:3:VAL:O	4:D:3:VAL:CG2	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:53:VAL:O	10:J:53:VAL:CG1	2.67	0.42
16:P:294:ASP:OD1	16:P:294:ASP:C	2.58	0.42
1:A:1136:ARG:HH12	9:I:48:GLU:HA	1.82	0.42
4:D:2:GLU:HG2	4:D:2:GLU:O	2.19	0.42
6:F:83:LEU:N	6:F:83:LEU:CD2	2.83	0.42
6:F:115:TYR:CD1	6:F:115:TYR:C	2.93	0.42
7:G:197:LEU:HD13	7:G:200:TRP:CH2	2.54	0.42
11:K:29:MET:HB2	11:K:29:MET:HE2	1.94	0.42
12:L:26:ASN:ND2	12:L:36:CYS:HB3	2.35	0.42
1:A:197:PHE:CD2	1:A:197:PHE:N	2.78	0.42
1:A:588:ILE:HD12	1:A:594:LEU:HD12	2.02	0.42
4:D:107:ARG:HH21	17:Q:82:GLN:HG2	1.85	0.42
7:G:38:VAL:HG11	7:G:186:LEU:HB2	2.02	0.42
16:P:206:ARG:CZ	16:P:217:TRP:HE1	2.33	0.42
1:A:1124:ASP:C	9:I:21:HIS:HE1	2.23	0.42
7:G:79:PRO:HG3	7:G:150:PHE:CE2	2.55	0.42
15:O:174:PRO:N	15:O:175:PRO:HD2	2.34	0.42
15:O:459:ARG:NH1	15:O:460:LEU:HB2	2.34	0.42
16:P:200:GLN:NE2	16:P:257:GLU:OE2	2.53	0.42
16:P:220:ILE:O	16:P:224:GLY:N	2.50	0.42
1:A:345:LEU:CD2	2:B:1116:GLU:OE1	2.68	0.42
1:A:577:GLU:HG2	11:K:29:MET:HE3	2.02	0.42
2:B:326:PHE:CE2	13:M:193:TYR:HB2	2.55	0.42
3:C:30:PRO:CD	11:K:61:LYS:HA	2.50	0.42
3:C:118:ASP:C	3:C:118:ASP:OD1	2.59	0.42
10:J:44:CYS:O	10:J:47:ARG:HG2	2.20	0.42
15:O:409:ILE:HB	15:O:423:LEU:CG	2.49	0.42
20:Y:19:DG:OP1	20:Y:19:DG:C4'	2.68	0.42
1:A:181:THR:C	1:A:182:ASN:OD1	2.59	0.41
2:B:719:MET:CE	10:J:51:ALA:HB2	2.50	0.41
11:K:59:ILE:HG12	11:K:59:ILE:O	2.20	0.41
12:L:25:GLU:CD	12:L:25:GLU:N	2.69	0.41
1:A:19:CYS:O	2:B:1125:ARG:CA	2.68	0.41
1:A:544:ASP:OD1	2:B:932:HIS:NE2	2.53	0.41
1:A:1121:PHE:CD1	9:I:14:VAL:HG21	2.54	0.41
2:B:999:GLU:HG2	3:C:24:VAL:CG2	2.46	0.41
4:D:66:VAL:O	4:D:70:LEU:HB2	2.20	0.41
12:L:31:ARG:NE	12:L:31:ARG:HA	2.35	0.41
15:O:102:THR:HA	15:O:129:LEU:HD11	2.02	0.41
1:A:1124:ASP:C	9:I:21:HIS:CE1	2.94	0.41
15:O:353:VAL:HG21	15:O:435:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:432:ALA:HB1	15:O:523:LEU:HD21	2.01	0.41
20:Y:-1:DC:H2'	20:Y:-1:DC:OP2	2.20	0.41
20:Y:7:DC:C2'	20:Y:8:DT:H71	2.49	0.41
2:B:719:MET:HE1	10:J:51:ALA:HB2	2.02	0.41
11:K:27:LEU:HD23	11:K:27:LEU:N	2.36	0.41
15:O:399:LEU:CD1	15:O:404:MET:HB3	2.51	0.41
16:P:227:LYS:HD2	16:P:240:ASN:HB3	2.03	0.41
1:A:1069:ARG:HH21	1:A:1270:GLU:HG2	1.85	0.41
19:X:35:DT:H2'	19:X:36:DA:C8	2.55	0.41
1:A:33:HIS:HE1	2:B:1088:TYR:OH	1.96	0.41
1:A:307:MET:HB3	15:O:416:ALA:HB1	2.02	0.41
1:A:897:ILE:HD11	5:E:165:LEU:HD21	2.01	0.41
3:C:264:VAL:O	3:C:264:VAL:CG2	2.69	0.41
5:E:51:GLY:O	5:E:55:ARG:HB2	2.19	0.41
6:F:100:ARG:NH2	6:F:123:LEU:O	2.54	0.41
20:Y:17:DC:O5'	20:Y:17:DC:O2	2.39	0.41
10:J:47:ARG:HG3	10:J:47:ARG:HH11	1.85	0.41
1:A:128:TYR:CE2	1:A:134:LEU:HD11	2.56	0.41
1:A:210:LEU:HD12	1:A:210:LEU:HA	1.84	0.41
1:A:397:ASN:ND2	6:F:73:ILE:O	2.52	0.41
4:D:17:PHE:CD2	4:D:18:GLN:NE2	2.87	0.41
11:K:31:GLN:HG3	11:K:32:ALA:N	2.35	0.41
15:O:152:ALA:HB3	17:Q:114:ASN:HD22	1.85	0.41
15:O:269:THR:HG21	15:O:298:PRO:HD3	2.02	0.41
15:O:376:GLU:HB3	15:O:424:TYR:HD1	1.85	0.41
1:A:220:PRO:HA	1:A:223:VAL:HG22	2.02	0.41
1:A:251:ILE:H	1:A:251:ILE:CD1	2.30	0.41
1:A:395:LYS:HE2	6:F:75:MET:HE2	2.03	0.41
1:A:1357:THR:HB	6:F:64:ARG:HD2	2.01	0.41
2:B:28:ARG:O	2:B:31:PRO:HD2	2.21	0.41
2:B:1038:GLY:HA2	20:Y:20:DC:OP1	2.20	0.41
4:D:28:LYS:HE2	4:D:28:LYS:HB3	1.83	0.41
1:A:1053:PHE:CD2	9:I:80:MET:HB2	2.56	0.41
4:D:11:LEU:HD21	7:G:2:PHE:O	2.21	0.41
11:K:31:GLN:HB3	11:K:39:CYS:SG	2.61	0.41
15:O:377:GLN:HA	15:O:380:VAL:HG12	2.03	0.41
1:A:254:ARG:NH2	1:A:254:ARG:HB2	2.36	0.40
1:A:500:PHE:HB2	2:B:752:GLU:O	2.22	0.40
1:A:1329:PHE:CE1	2:B:1122:ILE:CD1	3.03	0.40
2:B:819:GLU:OE1	12:L:51:ARG:CZ	2.69	0.40
4:D:94:ALA:HA	4:D:117:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:76:ASN:ND2	11:K:87:ARG:NE	2.64	0.40
11:K:28:GLU:N	11:K:28:GLU:OE1	2.54	0.40
11:K:50:THR:OG1	11:K:51:LEU:N	2.54	0.40
17:Q:80:GLU:HA	17:Q:86:ARG:HD2	2.03	0.40
1:A:53:TYR:CD2	17:Q:25:GLU:O	2.75	0.40
1:A:345:LEU:HD22	2:B:1113:LEU:HD12	2.03	0.40
1:A:349:GLN:H	1:A:349:GLN:CD	2.24	0.40
15:O:112:LEU:HD22	17:Q:61:LYS:HD3	2.04	0.40
15:O:345:LEU:HB3	15:O:522:LEU:HD21	2.03	0.40
7:G:80:PHE:CD2	7:G:82:ASP:HB2	2.56	0.40
7:G:192:GLU:OE2	7:G:197:LEU:HD11	2.21	0.40
1:A:843:THR:O	1:A:844:PRO:C	2.58	0.40
2:B:811:ALA:HB1	12:L:13:GLN:HB2	2.02	0.40
4:D:1:MET:SD	7:G:7:MET:CE	3.09	0.40
4:D:14:TYR:OH	4:D:63:PRO:HB3	2.21	0.40
15:O:376:GLU:O	15:O:421:PHE:HE1	2.04	0.40
17:Q:76:GLU:O	17:Q:78:PRO:HD3	2.22	0.40
2:B:977:VAL:HG23	3:C:286:GLU:HG3	2.03	0.40
3:C:96:ASN:CG	3:C:96:ASN:O	2.60	0.40
4:D:74:LYS:HB3	4:D:74:LYS:HE3	1.63	0.40
20:Y:16:DC:H2''	20:Y:17:DC:O4'	2.22	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	1363/1390 (98%)	1310 (96%)	50 (4%)	3 (0%)	47	79
2	B	1091/1133 (96%)	1043 (96%)	47 (4%)	1 (0%)	51	83
3	C	341/346 (99%)	338 (99%)	3 (1%)	0	100	100
4	D	120/148 (81%)	109 (91%)	10 (8%)	1 (1%)	19	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	207/210 (99%)	200 (97%)	7 (3%)	0	100	100
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%)	96 (91%)	9 (9%)	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	205/708 (29%)	198 (97%)	7 (3%)	0	100	100
14	N	140/398 (35%)	140 (100%)	0	0	100	100
15	O	435/534 (82%)	416 (96%)	18 (4%)	1 (0%)	47	79
16	P	128/316 (40%)	102 (80%)	25 (20%)	1 (1%)	19	59
17	Q	82/223 (37%)	72 (88%)	9 (11%)	1 (1%)	13	51
All	All	4805/6253 (77%)	4579 (95%)	218 (4%)	8 (0%)	50	79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	8	SER
15	O	409	ILE
16	P	296	CYS
1	A	533	ARG
2	B	40	VAL
1	A	1060	SER
1	A	1186	TYR
17	Q	28	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1190/1212 (98%)	1160 (98%)	30 (2%)	47	75
2	B	959/988 (97%)	952 (99%)	7 (1%)	84	93
3	C	299/302 (99%)	283 (95%)	16 (5%)	22	57
4	D	114/136 (84%)	88 (77%)	26 (23%)	1	5
5	E	191/192 (100%)	181 (95%)	10 (5%)	23	58
6	F	66/111 (60%)	64 (97%)	2 (3%)	41	71
7	G	149/181 (82%)	146 (98%)	3 (2%)	55	79
8	H	129/131 (98%)	128 (99%)	1 (1%)	81	91
9	I	92/93 (99%)	90 (98%)	2 (2%)	52	77
10	J	53/56 (95%)	43 (81%)	10 (19%)	1	9
11	K	92/119 (77%)	88 (96%)	4 (4%)	29	63
12	L	43/55 (78%)	37 (86%)	6 (14%)	3	21
13	M	187/622 (30%)	185 (99%)	2 (1%)	73	88
14	N	131/347 (38%)	129 (98%)	2 (2%)	65	84
15	O	400/476 (84%)	390 (98%)	10 (2%)	47	75
16	P	114/280 (41%)	109 (96%)	5 (4%)	28	63
17	Q	81/195 (42%)	72 (89%)	9 (11%)	6	31
All	All	4290/5496 (78%)	4145 (97%)	145 (3%)	40	69

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	TYR
1	A	189	ILE
1	A	190	VAL
1	A	197	PHE
1	A	199	THR
1	A	211	LEU
1	A	279	LEU
1	A	280	THR
1	A	294	LYS
1	A	302	LYS
1	A	688	PRO
1	A	704	THR
1	A	731	LEU
1	A	735	LYS
1	A	738	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	743	THR
1	A	754	LYS
1	A	760	ARG
1	A	770	GLU
1	A	844	PRO
1	A	859	VAL
1	A	860	ASP
1	A	863	VAL
1	A	864	LYS
1	A	872	GLN
1	A	881	ASP
1	A	1131	LYS
1	A	1180	ASN
1	A	1214	ILE
1	A	1368	ARG
2	B	463	ARG
2	B	608	ASN
2	B	654	THR
2	B	733	LEU
2	B	758	ASN
2	B	890	ARG
2	B	906	VAL
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	103	ASP
3	C	126	ASN
3	C	158	ASP
3	C	164	VAL
3	C	183	ASP
3	C	230	THR
3	C	236	LEU
3	C	261	VAL
3	C	272	VAL
4	D	1	MET
4	D	3	VAL
4	D	11	LEU
4	D	14	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	D	15	GLU
4	D	17	PHE
4	D	18	GLN
4	D	19	LEU
4	D	20	LEU
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	69	PHE
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	101	VAL
4	D	105	GLU
4	D	113	ILE
5	E	18	MET
5	E	28	VAL
5	E	34	ASP
5	E	39	GLU
5	E	47	LYS
5	E	50	GLU
5	E	54	ARG
5	E	61	LEU
5	E	73	PHE
5	E	76	PHE
6	F	81	VAL
6	F	107	ARG
7	G	22	LEU
7	G	83	GLU
7	G	198	LEU
8	H	76	ASN
9	I	53	LEU
9	I	91	MET
10	J	3	ILE
10	J	5	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	J	9	THR
10	J	10	CYS
10	J	19	GLU
10	J	21	TYR
10	J	26	GLN
10	J	30	THR
10	J	33	ASP
10	J	41	LYS
11	K	27	LEU
11	K	38	HIS
11	K	71	THR
11	K	103	LEU
12	L	13	GLN
12	L	16	ILE
12	L	19	CYS
12	L	28	ILE
12	L	32	ASP
12	L	52	LEU
13	M	53	GLN
13	M	149	HIS
14	N	393	LEU
14	N	395	HIS
15	O	170	ASP
15	O	361	ARG
15	O	378	LYS
15	O	406	LEU
15	O	408	GLU
15	O	409	ILE
15	O	411	LYS
15	O	414	ASP
15	O	423	LEU
15	O	459	ARG
16	P	205	GLN
16	P	247	LYS
16	P	283	VAL
16	P	284	ARG
16	P	307	CYS
17	Q	27	LEU
17	Q	31	VAL
17	Q	48	LEU
17	Q	79	GLU
17	Q	80	GLU

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Mol	Chain	Res	Type
17	Q	81	ARG
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 (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	HIS
1	A	203	HIS
1	A	217	ASN
1	A	316	GLN
1	A	355	ASN
1	A	374	ASN
1	A	476	HIS
1	A	599	GLN
1	A	616	ASN
1	A	693	ASN
1	A	707	GLN
1	A	791	ASN
1	A	836	ASN
1	A	872	GLN
1	A	885	GLN
1	A	927	ASN
1	A	943	ASN
1	A	962	GLN
1	A	1039	GLN
1	A	1180	ASN
1	A	1354	ASN
2	B	183	GLN
2	B	215	ASN
2	B	320	HIS
2	B	346	GLN
2	B	544	ASN
2	B	608	ASN
2	B	683	ASN
2	B	686	GLN
2	B	758	ASN
2	B	903	GLN
2	B	1010	GLN
2	B	1034	GLN
3	C	48	ASN

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Mol	Chain	Res	Type
3	C	180	ASN
4	D	35	HIS
4	D	43	ASN
4	D	61	GLN
4	D	85	GLN
4	D	98	GLN
4	D	112	GLN
7	G	23	ASN
8	H	76	ASN
9	I	40	ASN
9	I	74	HIS
10	J	26	GLN
11	K	85	GLN
12	L	13	GLN
12	L	26	ASN
13	M	125	HIS
15	O	14	GLN
15	O	49	GLN
15	O	113	ASN
15	O	337	ASN
15	O	377	GLN
15	O	379	GLN
15	O	415	HIS
15	O	445	ASN
15	O	451	GLN
15	O	457	ASN
15	O	465	GLN
15	O	507	ASN
16	P	200	GLN
16	P	274	ASN
16	P	306	ASN
17	Q	82	GLN
17	Q	114	ASN

### 5.3.3 RNA [i](#)

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
22	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	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.

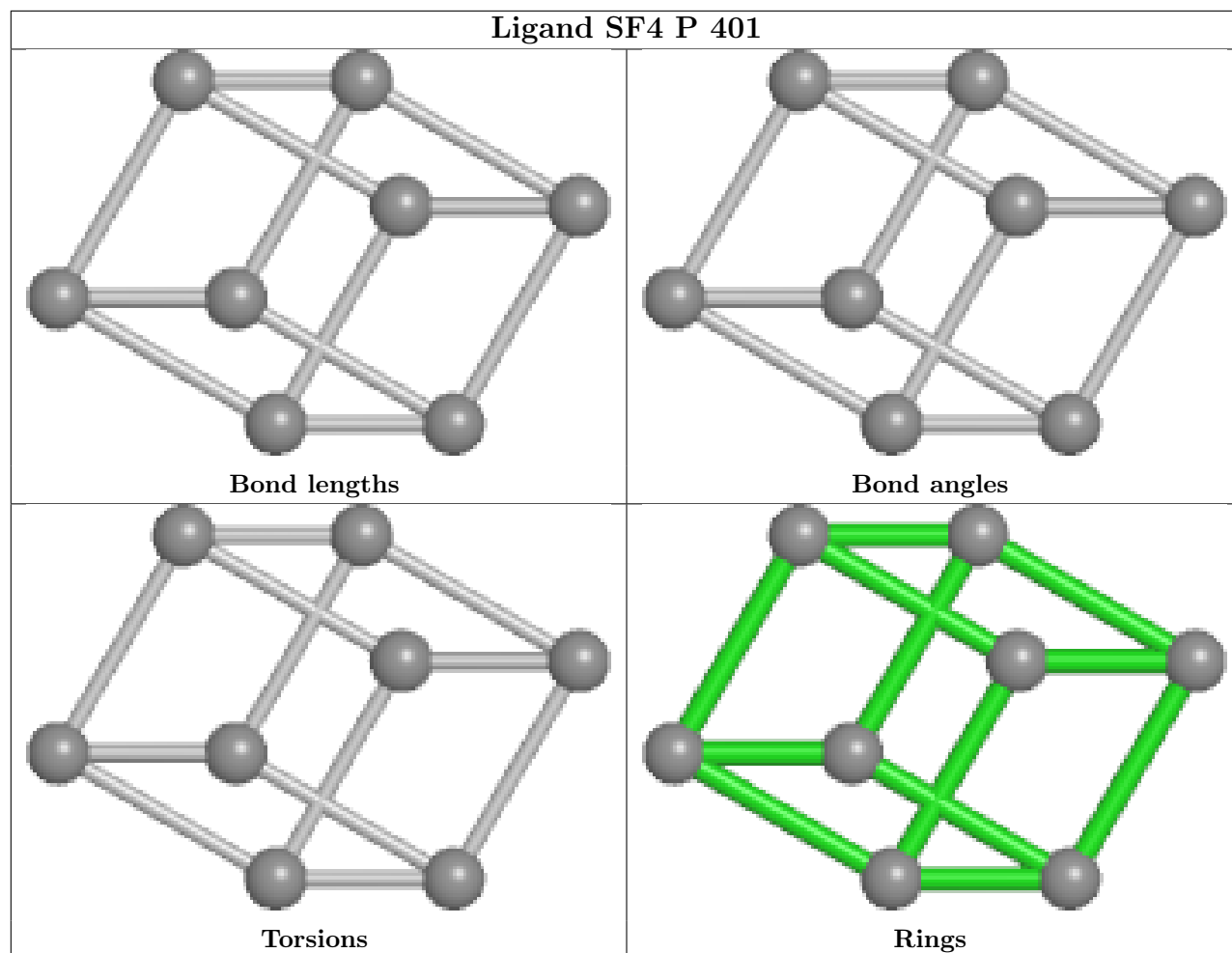
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	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.

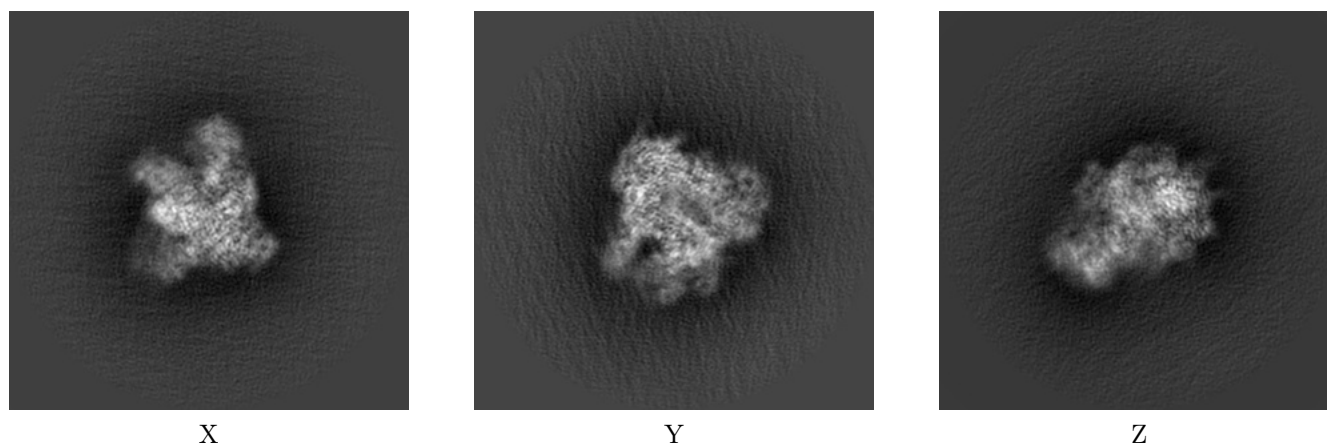
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31621. 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](#)

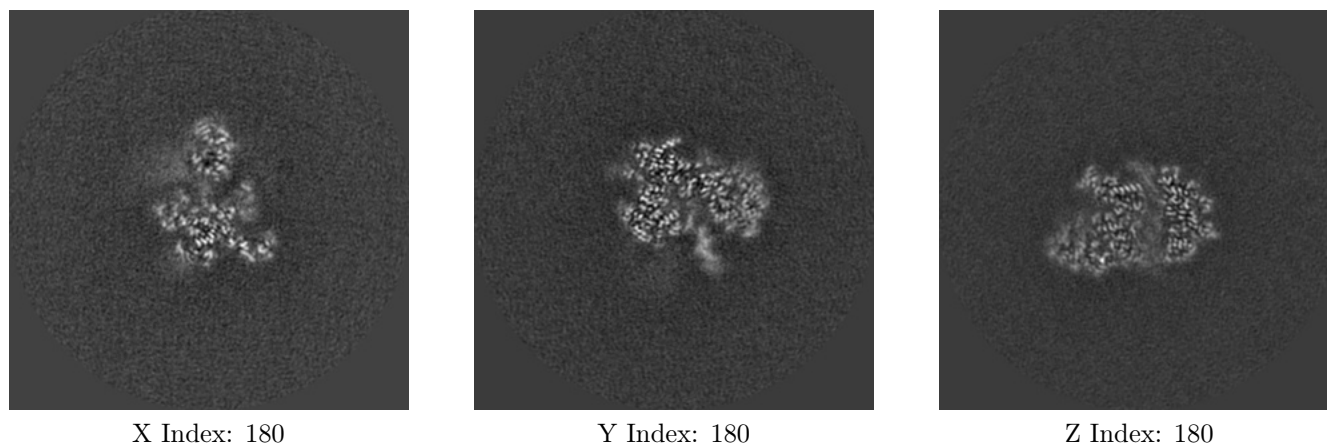
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

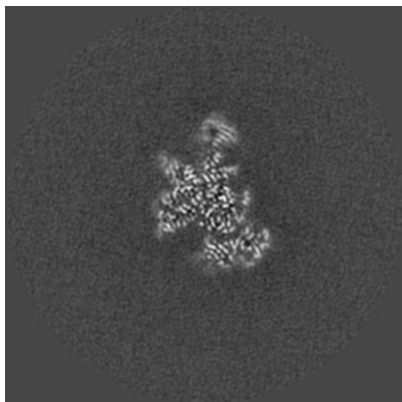
#### 6.2.1 Primary map



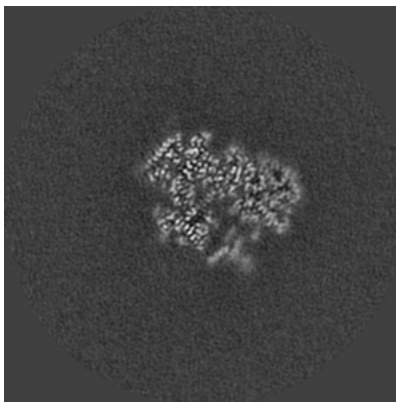
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

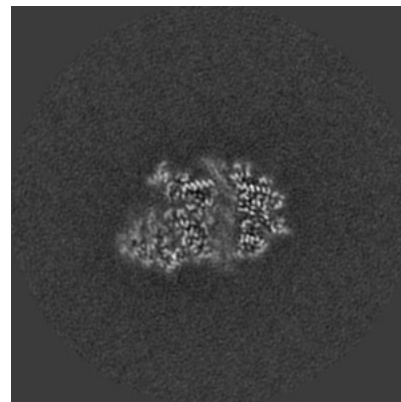
### 6.3.1 Primary map



X Index: 210



Y Index: 187



Z Index: 179

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

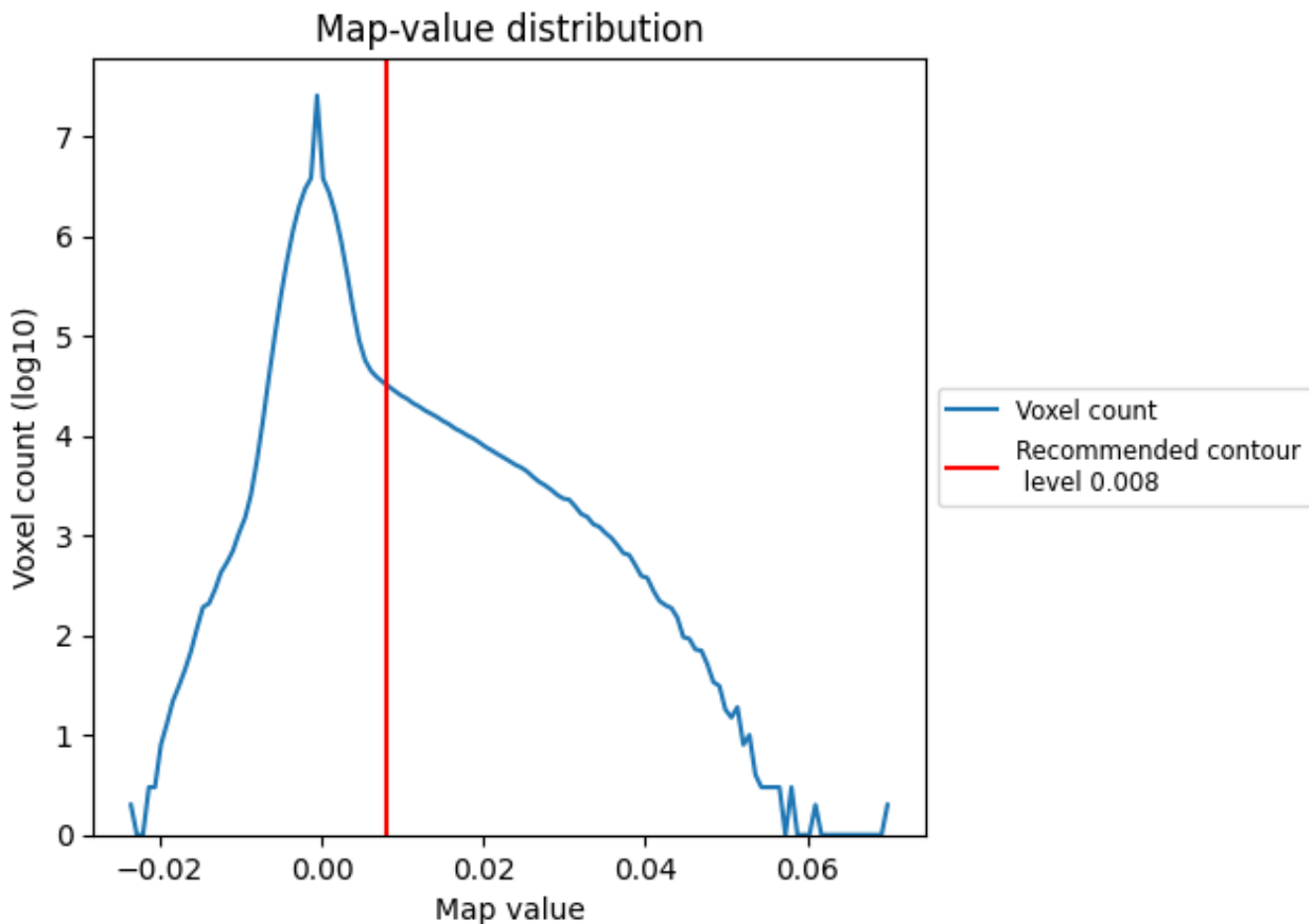
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

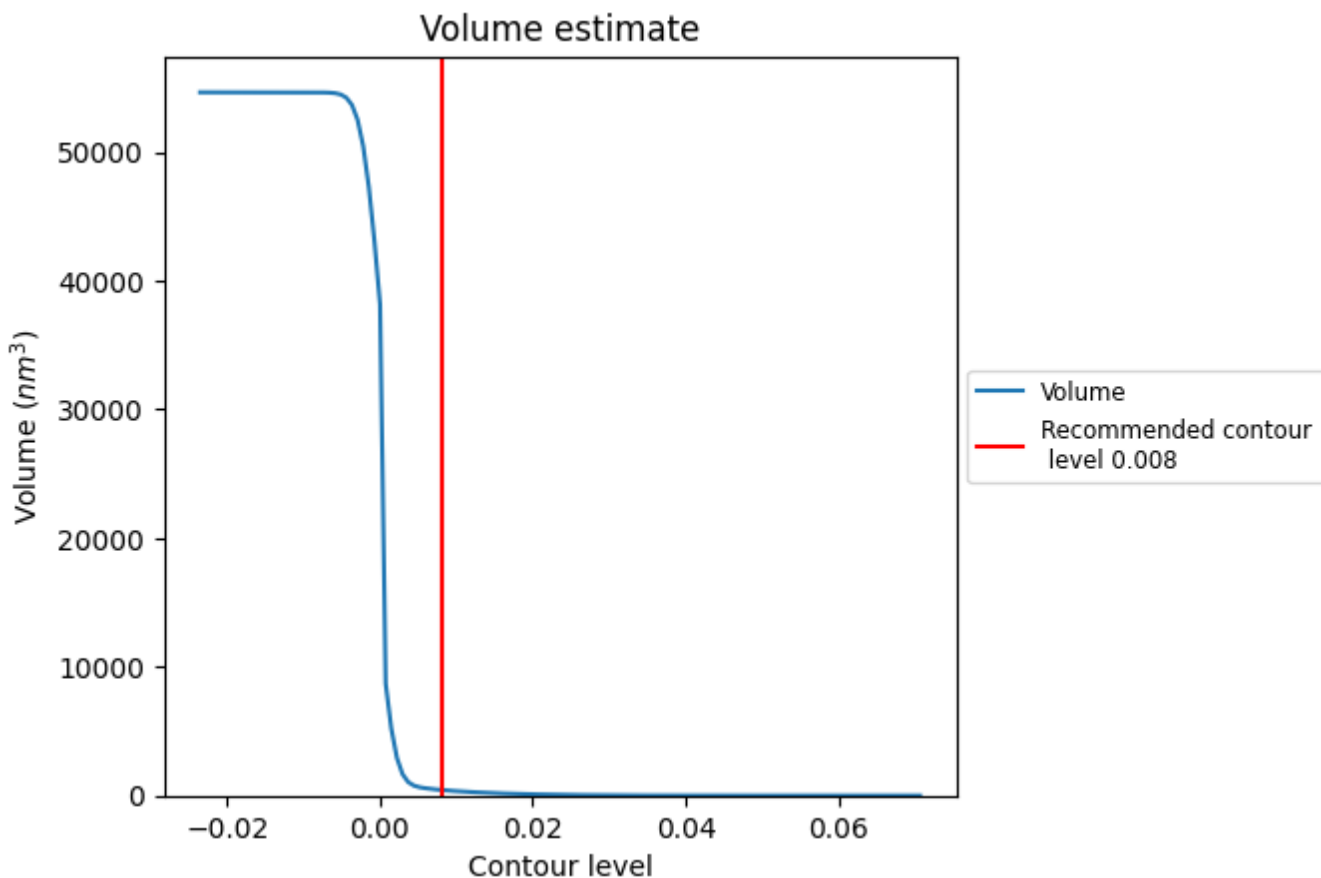
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

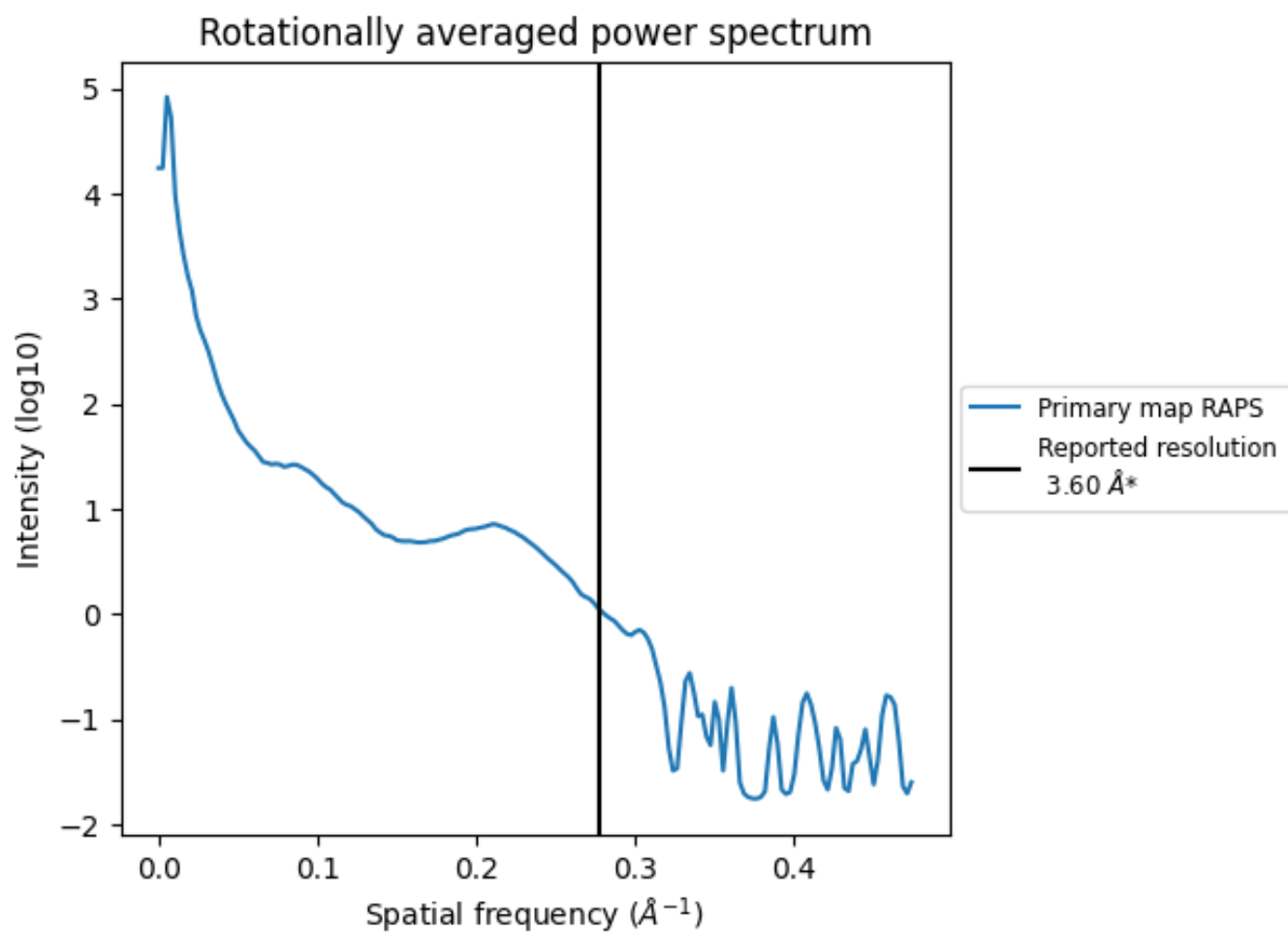


The volume at the recommended contour level is 438 nm<sup>3</sup>; this corresponds to an approximate mass of 396 kDa.

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



### 7.3 Rotationally averaged power spectrum i



\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

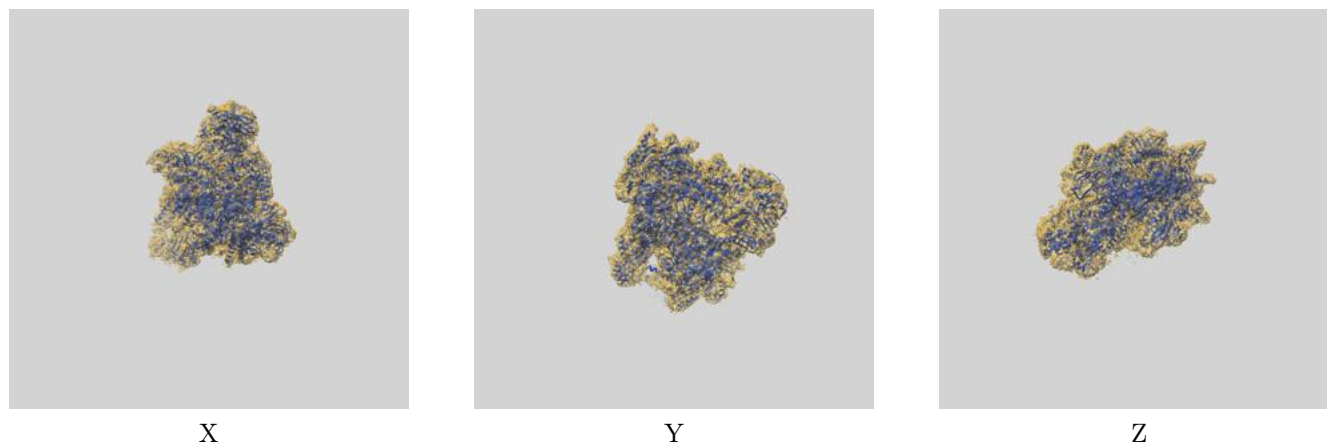
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

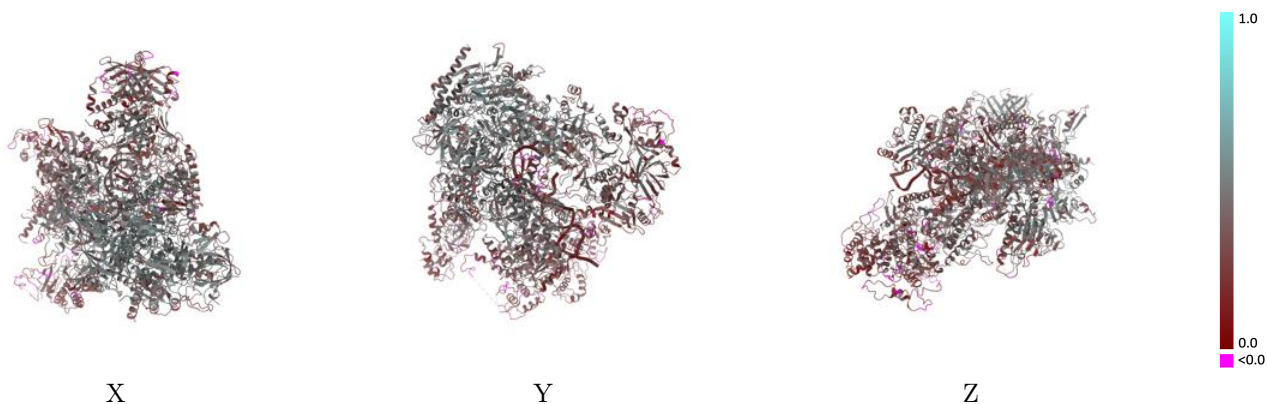
This section contains information regarding the fit between EMDB map EMD-31621 and PDB model 7FJI. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



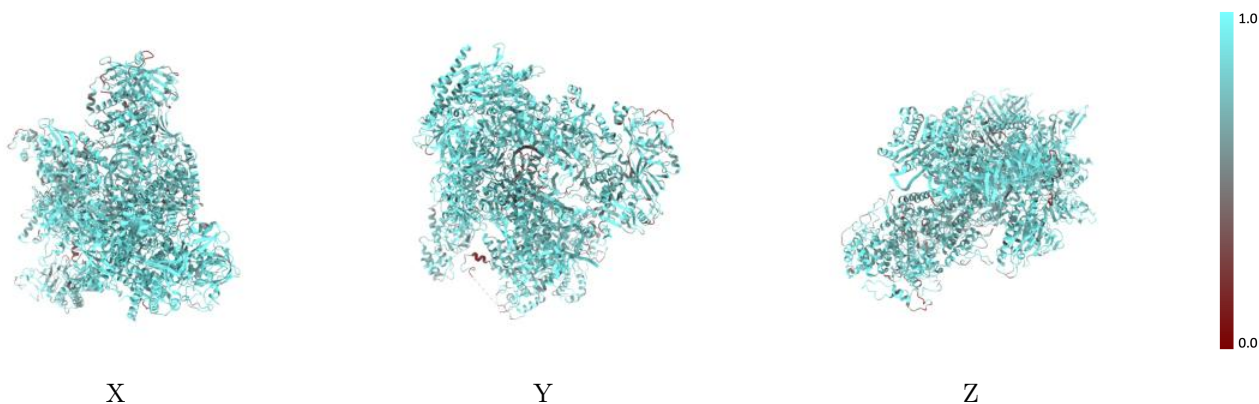
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



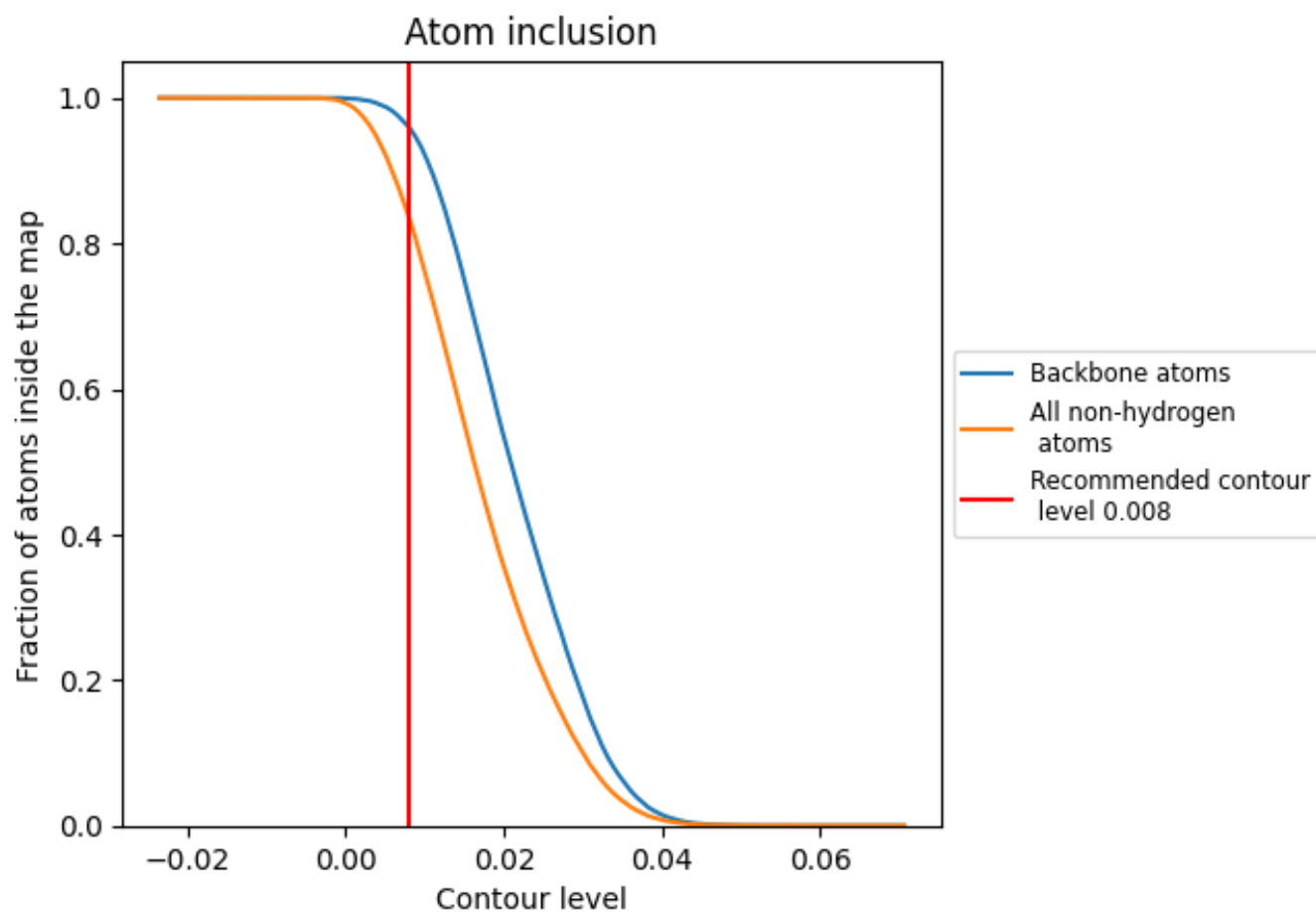
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).











































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 84% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8363	 0.3730
A	 0.8462	 0.4060
B	 0.8585	 0.4200
C	 0.9004	 0.4520
D	 0.7706	 0.2250
E	 0.8680	 0.3830
F	 0.9036	 0.4440
G	 0.8460	 0.3060
H	 0.8723	 0.4350
I	 0.7041	 0.2580
J	 0.9220	 0.4790
K	 0.8850	 0.4260
L	 0.8683	 0.4060
M	 0.7869	 0.3100
N	 0.7186	 0.2980
O	 0.8203	 0.2910
P	 0.7465	 0.2120
Q	 0.5989	 0.1830
R	 0.4884	 0.2330
X	 0.8424	 0.2500
Y	 0.8859	 0.2640

