



## Full wwPDB EM Validation Report ⓘ

Jul 3, 2023 – 12:37 PM JST

PDB ID : 8IUH  
EMDB ID : EMD-35722  
Title : RNA polymerase III pre-initiation complex open complex 1  
Authors : Hou, H.; Jin, Q.; Ren, Y.; Wang, Q.; Xu, Y.  
Deposited on : 2023-03-24  
Resolution : 3.40 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>.

---

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

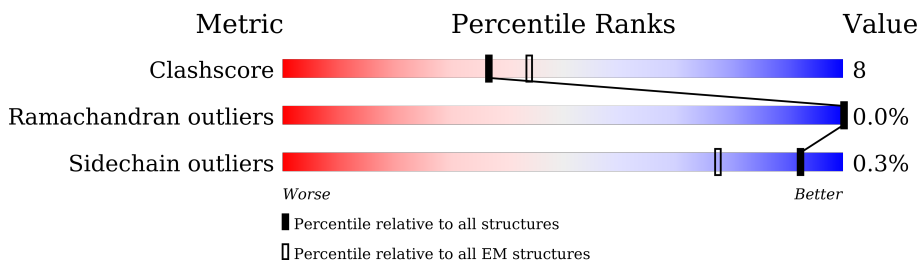
EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.34

# 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 3.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1	368	
2	3	411	
3	4	1469	
4	A	1390	
5	B	1133	
6	C	346	
7	D	148	
8	E	210	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	F	127	54% 6% 40%
10	G	204	60% 21% 19%
11	H	150	79% 19%
12	I	108	22% 74% 25%
13	J	67	76% 21%
14	K	133	68% 9% 23%
15	L	58	55% 24% 21%
16	M	708	5% 50% 9% 40%
17	N	317	36% 10% 54%
18	O	534	7% 84% 12%
19	P	316	18% 79% 16%
20	Q	223	34% 5% 61%
21	U	339	46% 6% 48%
22	V	419	7% 72% 14% 14%
23	W	2624	96%
24	X	464	6% 12% 83%
25	Y	464	8% 10% 83%

## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 58239 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 snRNA-activating protein complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	146	1233	804	212	209	8	0	0

- Molecule 2 is a protein called snRNA-activating protein complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	374	3037	1925	521	570	21	0	0

- Molecule 3 is a protein called snRNA-activating protein complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	365	3058	1921	573	555	9	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	1378	10814	6850	1886	2005	73	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase III subunit RPC2.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC9.

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

- Molecule 8 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		
8	E	209	1715	1083	300	324	8	0	0

- Molecule 9 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		
9	F	76	610	392	103	110	5	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerase III subunit RPC8.

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

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

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

- Molecule 12 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	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 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 14 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

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

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	422	Total	C	N	O	S	0	0
			3382	2138	588	636	20		

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

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

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	LYS	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	PHE	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	GLY	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	ARG	deletion	UNP P05423
N	?	-	ASN	deletion	UNP P05423

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	ASP	deletion	UNP P05423
N	?	-	THR	deletion	UNP P05423
N	?	-	ARG	deletion	UNP P05423
N	?	-	ASN	deletion	UNP P05423
N	?	-	MET	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	GLN	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	HIS	deletion	UNP P05423
N	?	-	SER	deletion	UNP P05423
N	?	-	GLY	deletion	UNP P05423
N	?	-	TRP	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	PHE	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	ASN	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	TRP	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	GLY	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	MET	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	ILE	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	ARG	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	MET	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	ARG	deletion	UNP P05423

- Molecule 18 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	O	512	4075	2565	712	774	24	0	0

- Molecule 19 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	P	303	2403	1516	411	460	16	0	0

- Molecule 20 is a protein called DNA-directed RNA polymerase III subunit RPC7.



Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	87	Total	C	N	O	S	0	0
			754	488	126	134	6		

- Molecule 21 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	176	Total	C	N	O	S	1	0
			1396	907	244	238	7		

- Molecule 22 is a protein called Transcription factor IIIB 50 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	361	Total	C	N	O	S	1	0
			2853	1792	507	531	23		

- Molecule 23 is a protein called Transcription factor TFIIB component B' homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	111	Total	C	N	O	S	0	0
			943	606	163	170	4		

- Molecule 24 is a DNA chain called DNA (81-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	81	Total	C	N	O	P	0	0
			1661	795	288	497	81		

- Molecule 25 is a DNA chain called DNA (81-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	81	Total	C	N	O	P	0	0
			1666	793	317	475	81		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
26	A	2	Total	Zn	0
			2	2	
26	B	1	Total	Zn	0
			1	1	
26	I	2	Total	Zn	0
			2	2	

*Continued on next page...*

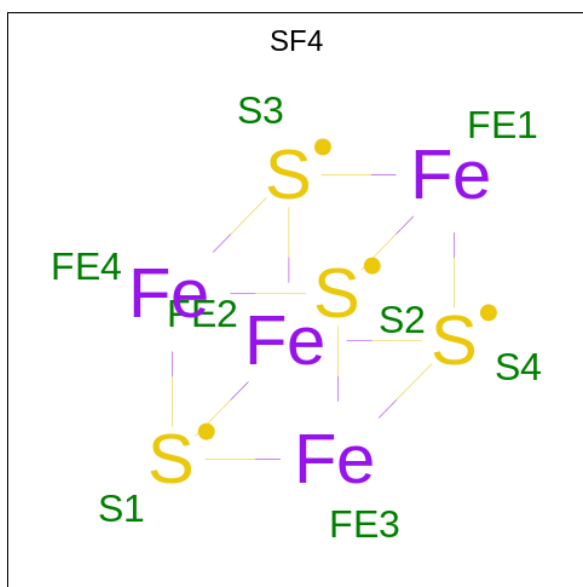
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
26	J	1	Total	Zn	0
			1	1	
26	L	1	Total	Zn	0
			1	1	
26	V	1	Total	Zn	0
			1	1	

- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 28 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

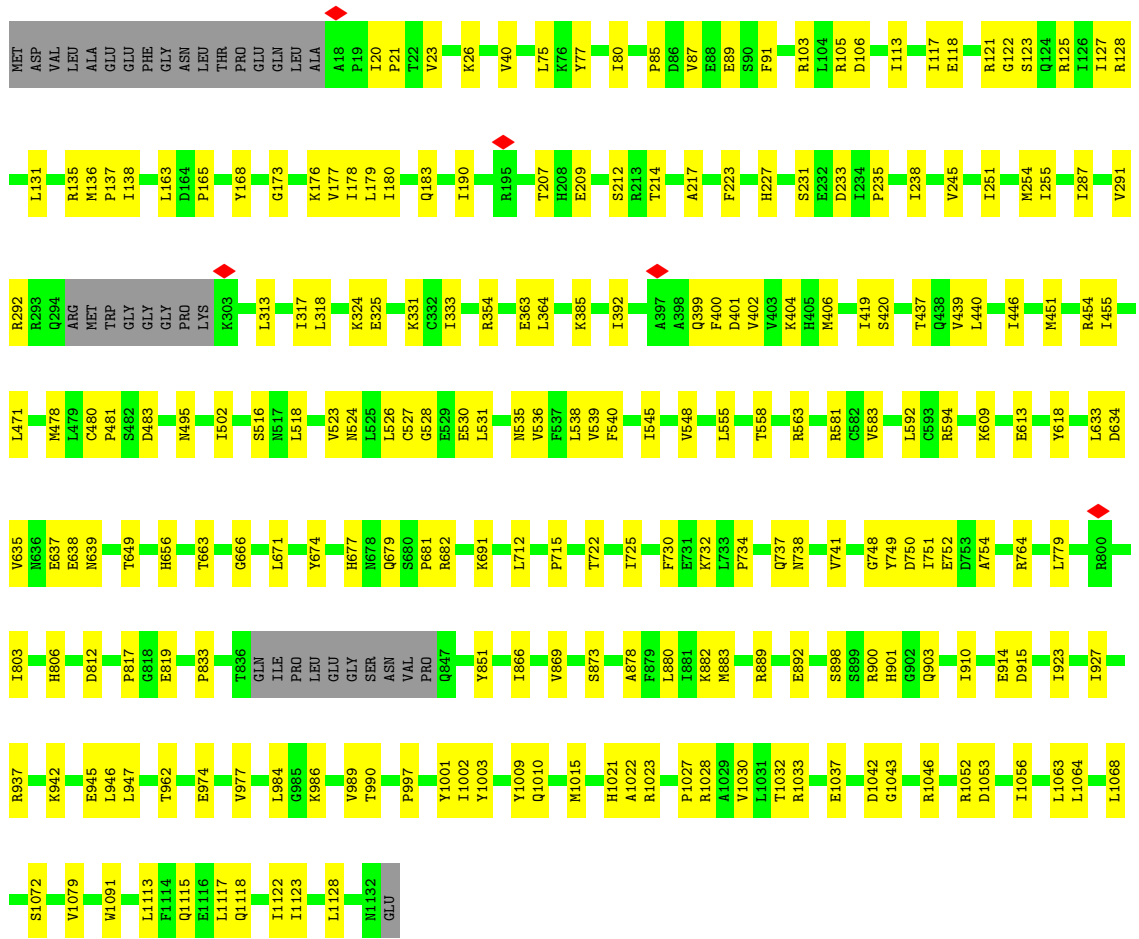
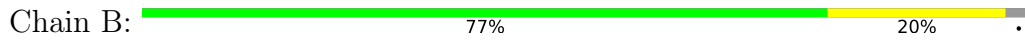




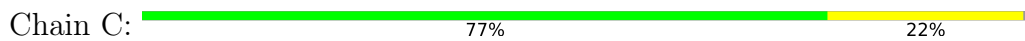


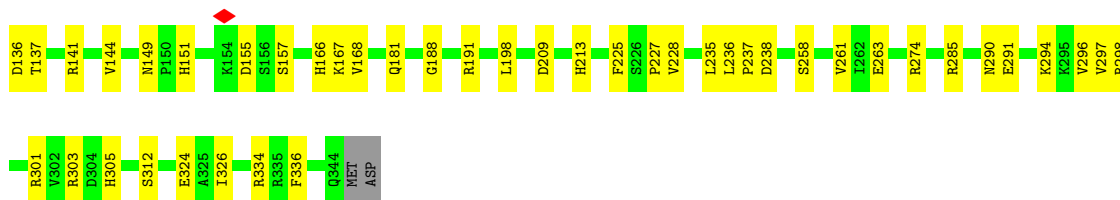


• Molecule 5: DNA-directed RNA polymerase III subunit RPC2

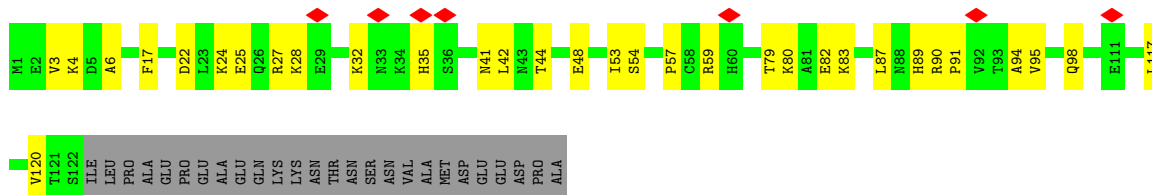


• Molecule 6: DNA-directed RNA polymerases I and III subunit RPAC1

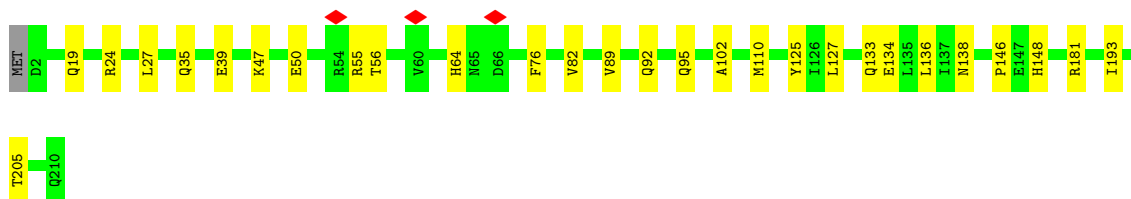
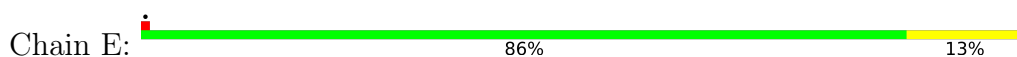




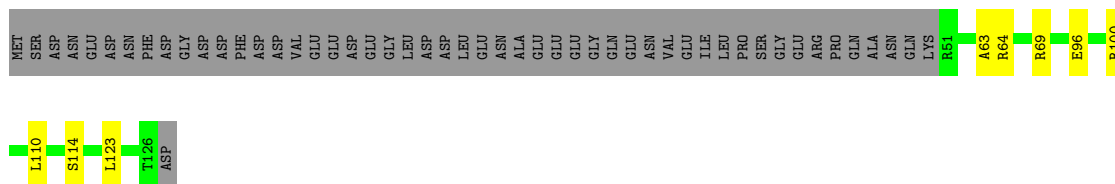
• Molecule 7: DNA-directed RNA polymerase III subunit RPC9



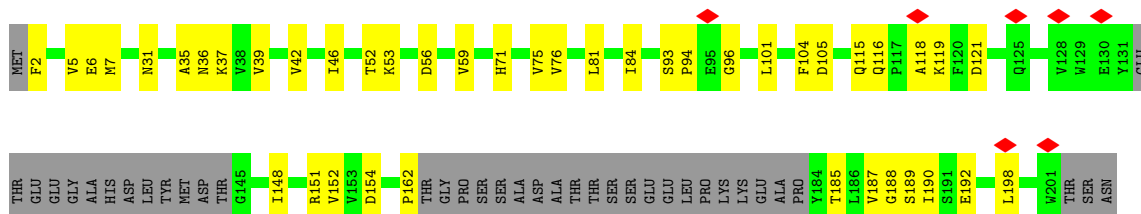
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC1




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

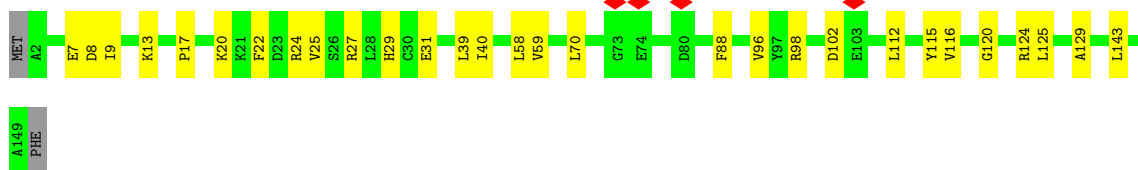


• Molecule 10: DNA-directed RNA polymerase III subunit RPC8



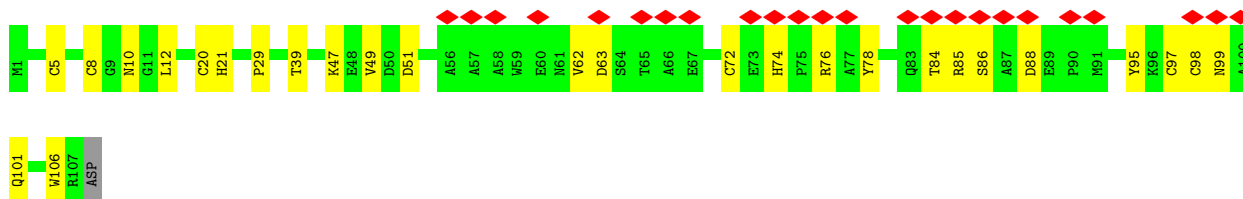
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  79% 19%



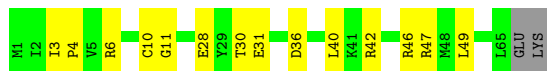
- Molecule 12: DNA-directed RNA polymerase III subunit RPC10

Chain I:  22% 74% 25%



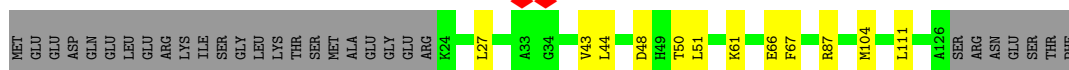
- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  76% 21%



- Molecule 14: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:  68% 9% 23%



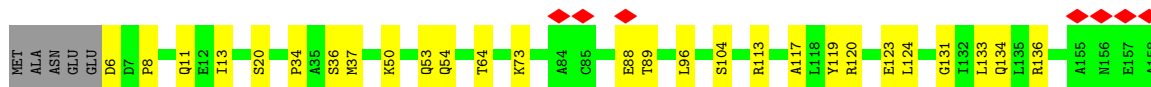
- Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:  55% 24% 21%

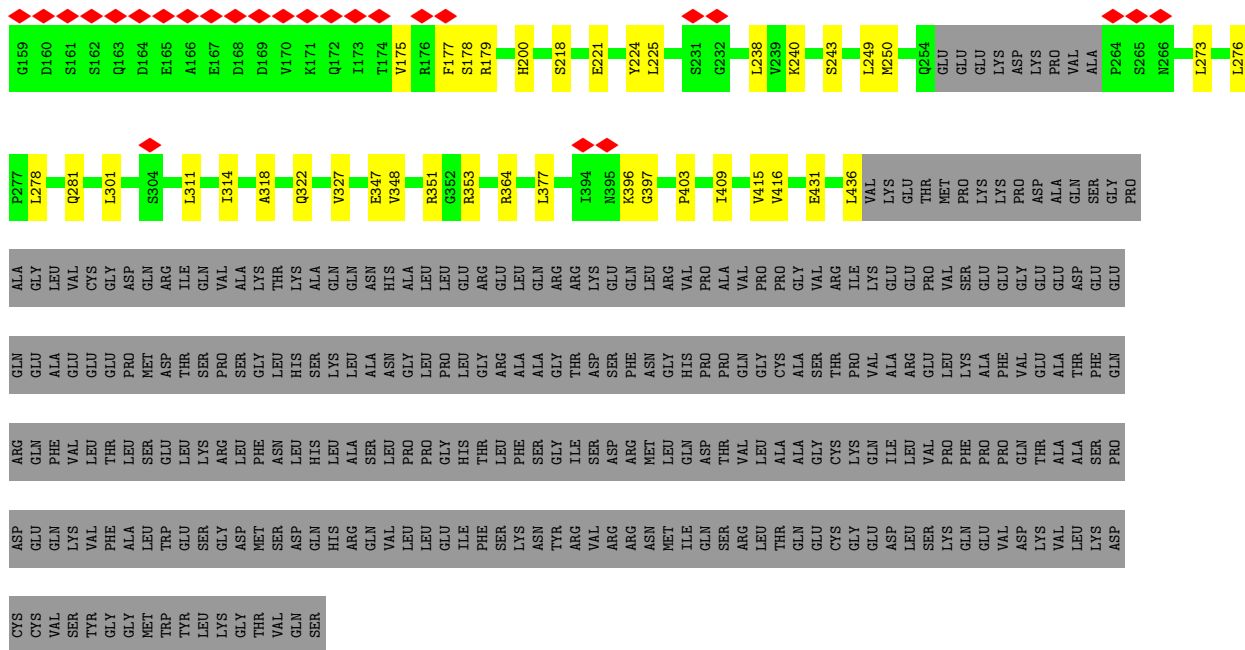


- Molecule 16: DNA-directed RNA polymerase III subunit RPC5

Chain M:  5% 50% 9% 40%

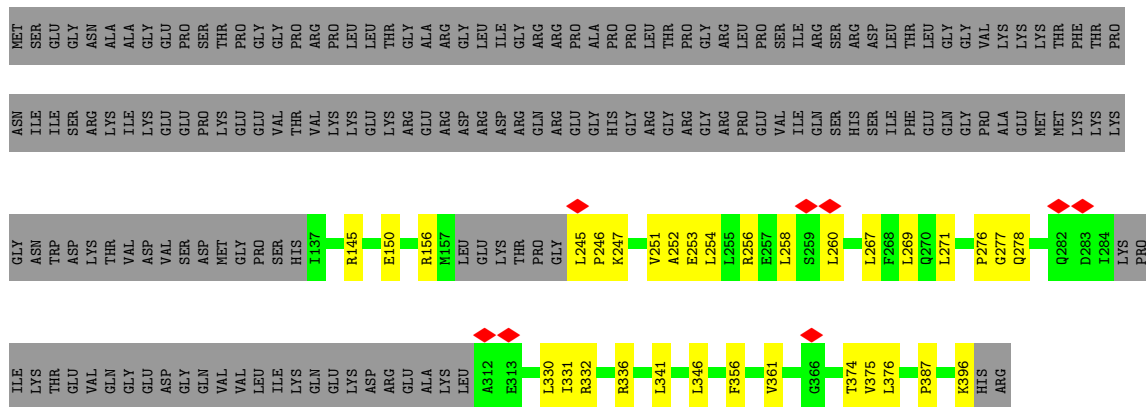






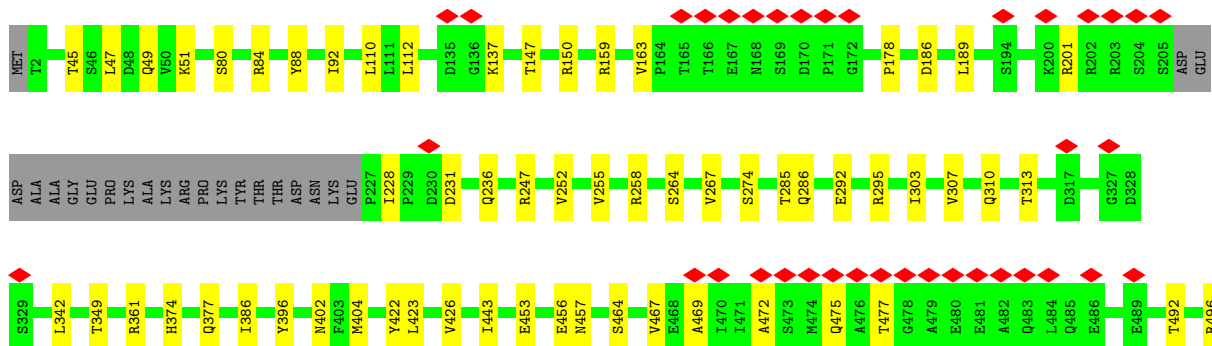
● Molecule 17: DNA-directed RNA polymerase III subunit RPC4

Chain N: 36% 10% 54%



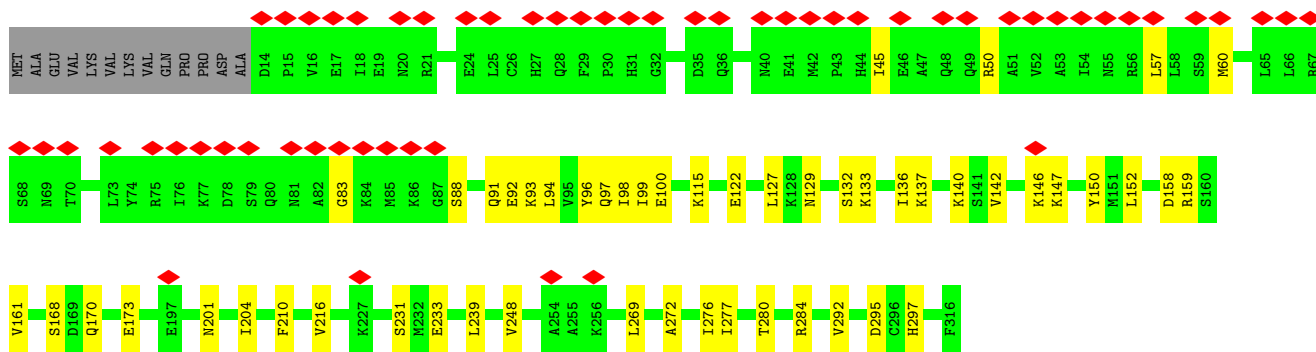
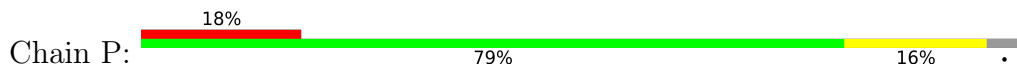
● Molecule 18: DNA-directed RNA polymerase III subunit RPC3

Chain O: 7% 84% 12%

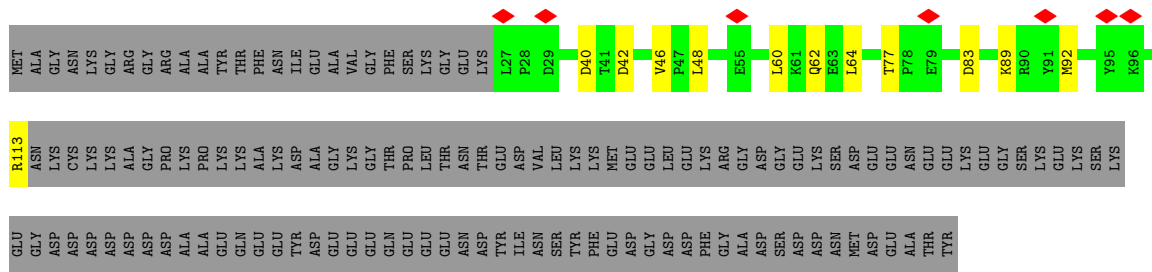




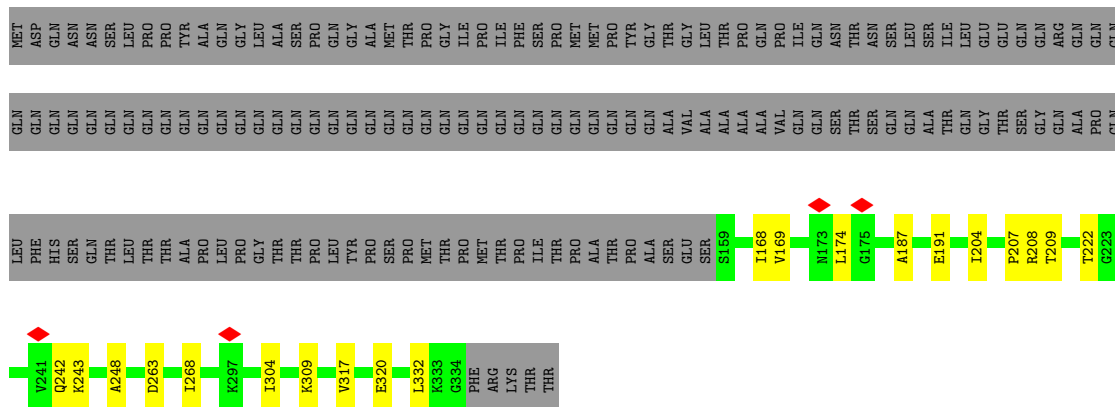
• Molecule 19: DNA-directed RNA polymerase III subunit RPC6



• Molecule 20: DNA-directed RNA polymerase III subunit RPC7



• Molecule 21: TATA-box-binding protein



• Molecule 22: Transcription factor IIIB 50 kDa subunit









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107630	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.271	Depositor
Minimum map value	-0.107	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size ( $\text{\AA}$ )	426.88, 426.88, 426.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.334, 1.334, 1.334	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.24	0/1266	0.38	0/1708
2	3	0.24	0/3112	0.41	0/4206
3	4	0.23	0/3121	0.38	0/4181
4	A	0.24	0/11008	0.40	0/14842
5	B	0.24	0/8845	0.40	0/11930
6	C	0.23	0/2790	0.40	0/3782
7	D	0.23	0/997	0.39	0/1343
8	E	0.23	0/1745	0.39	0/2358
9	F	0.22	0/620	0.38	0/839
10	G	0.24	0/1374	0.42	0/1868
11	H	0.24	0/1207	0.42	0/1628
12	I	0.23	0/869	0.42	0/1174
13	J	0.23	0/521	0.36	0/703
14	K	0.23	0/837	0.41	0/1129
15	L	0.23	0/394	0.42	0/524
16	M	0.23	0/3455	0.38	0/4673
17	N	0.23	0/1137	0.44	0/1530
18	O	0.23	0/4141	0.39	0/5592
19	P	0.23	0/2446	0.36	0/3301
20	Q	0.23	0/777	0.38	0/1050
21	U	0.24	0/1424	0.43	0/1918
22	V	0.23	0/2904	0.39	0/3941
23	W	0.24	0/967	0.38	0/1293
24	X	0.52	0/1858	0.96	0/2865
25	Y	0.48	0/1872	0.86	0/2884
All	All	0.26	0/59687	0.45	0/81262

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.



There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1233	0	1231	46	0
2	3	3037	0	2911	75	0
3	4	3058	0	3064	56	0
4	A	10814	0	11057	215	0
5	B	8680	0	8805	179	0
6	C	2736	0	2712	55	0
7	D	985	0	1006	24	0
8	E	1715	0	1733	20	0
9	F	610	0	642	5	0
10	G	1337	0	1306	34	0
11	H	1186	0	1147	18	0
12	I	848	0	809	20	0
13	J	512	0	525	14	0
14	K	822	0	810	11	0
15	L	388	0	394	10	0
16	M	3382	0	3376	52	0
17	N	1128	0	1181	26	0
18	O	4075	0	4149	43	0
19	P	2403	0	2409	42	0
20	Q	754	0	759	13	0
21	U	1396	0	1490	18	0
22	V	2853	0	2892	71	0
23	W	943	0	924	16	0
24	X	1661	0	922	61	0
25	Y	1666	0	911	32	0
26	A	2	0	0	0	0
26	B	1	0	0	0	0
26	I	2	0	0	0	0
26	J	1	0	0	0	0
26	L	1	0	0	0	0
26	V	1	0	0	0	0
27	A	1	0	0	0	0
28	P	8	0	0	0	0
All	All	58239	0	57165	949	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 8.

All (949) 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)
2:3:191:ILE:HB	3:4:176:PHE:CZ	1.59	1.36
22:V:111:LEU:HD13	24:X:-17:DT:OP2	1.24	1.30
1:1:63:TRP:HE3	1:1:82:LEU:CD1	1.51	1.24
5:B:113:ILE:HD11	5:B:136:MET:CB	1.73	1.17
2:3:101:ARG:HA	2:3:104:CYS:SG	1.83	1.16
4:A:41:LEU:HD12	4:A:42:TYR:CD1	1.81	1.16
4:A:41:LEU:CD1	4:A:42:TYR:CD1	2.29	1.15
4:A:41:LEU:HD12	4:A:42:TYR:CG	1.81	1.15
1:1:26:PHE:CD2	1:1:121:ASP:CB	2.30	1.14
4:A:41:LEU:HD13	4:A:42:TYR:CE1	1.86	1.11
1:1:90:LEU:HD11	2:3:109:LEU:HD21	1.32	1.10
2:3:101:ARG:O	2:3:104:CYS:SG	2.09	1.10
22:V:282:TRP:O	22:V:286:LEU:HD13	1.49	1.09
13:J:30:THR:HG22	13:J:31:GLU:H	1.18	1.08
4:A:41:LEU:CD1	4:A:42:TYR:CG	2.39	1.06
5:B:401:ASP:OD2	5:B:404:LYS:NZ	1.89	1.05
1:1:43:CYS:HG	2:3:119:GLU:N	1.55	1.03
2:3:191:ILE:CB	3:4:176:PHE:HZ	1.70	1.03
22:V:111:LEU:HD13	24:X:-17:DT:P	1.98	1.03
1:1:26:PHE:CE2	1:1:121:ASP:HB3	1.94	1.02
1:1:63:TRP:CE3	1:1:82:LEU:CD1	2.42	1.02
4:A:76:LEU:CD2	22:V:40:LEU:HD23	1.90	1.02
4:A:41:LEU:HD11	4:A:42:TYR:CD2	1.95	1.01
5:B:113:ILE:HD11	5:B:136:MET:HB2	1.02	1.00
1:1:63:TRP:HE3	1:1:82:LEU:HD13	1.27	0.99
4:A:41:LEU:CD1	4:A:42:TYR:CE1	2.43	0.98
4:A:41:LEU:HD11	4:A:42:TYR:CE2	1.98	0.97
4:A:41:LEU:HG	22:V:58:SER:OG	1.64	0.96
4:A:48:HIS:HA	22:V:55:TYR:CE1	1.99	0.96
22:V:111:LEU:CD1	24:X:-17:DT:OP2	2.13	0.95
1:1:26:PHE:CD2	1:1:121:ASP:HB3	2.02	0.95
6:C:236:LEU:HD13	6:C:305:HIS:CE1	2.03	0.94
5:B:23:VAL:HG23	5:B:26:LYS:HB2	1.50	0.94
1:1:26:PHE:HD2	1:1:121:ASP:OD2	1.50	0.94
1:1:26:PHE:HD2	1:1:121:ASP:CG	1.70	0.93
5:B:113:ILE:CD1	5:B:136:MET:HB2	1.96	0.93
2:3:101:ARG:CA	2:3:104:CYS:SG	2.56	0.92

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:257:VAL:HG23	4:A:283:LEU:CD1	2.00	0.91
4:A:76:LEU:HD21	22:V:40:LEU:HD23	1.48	0.91
5:B:401:ASP:OD1	5:B:404:LYS:HG2	1.69	0.91
1:1:26:PHE:HD2	1:1:121:ASP:CB	1.73	0.90
4:A:41:LEU:HG	22:V:58:SER:HG	1.32	0.90
4:A:257:VAL:HG23	4:A:283:LEU:HD13	1.53	0.89
22:V:282:TRP:O	22:V:286:LEU:CD1	2.20	0.88
13:J:30:THR:HG22	13:J:31:GLU:N	1.86	0.88
22:V:111:LEU:CD1	24:X:-17:DT:H5'	2.04	0.85
2:3:191:ILE:CB	3:4:176:PHE:CZ	2.50	0.84
1:1:63:TRP:CE3	1:1:82:LEU:HD13	2.12	0.84
4:A:489:ASN:O	4:A:492:VAL:HG12	1.78	0.84
4:A:41:LEU:CD1	4:A:42:TYR:CD2	2.59	0.83
5:B:113:ILE:CD1	5:B:136:MET:N	2.41	0.83
1:1:26:PHE:CD2	1:1:121:ASP:HB2	2.11	0.83
2:3:221:CYS:O	2:3:224:ASP:OD1	1.96	0.83
6:C:133:THR:O	6:C:137:THR:HG22	1.77	0.83
23:W:331:HIS:NE2	23:W:375:LEU:HD21	1.95	0.82
2:3:279:GLU:OE1	2:3:287:LYS:HE2	1.79	0.81
4:A:76:LEU:HD23	22:V:40:LEU:HD23	1.63	0.81
1:1:26:PHE:CD2	1:1:121:ASP:OD2	2.35	0.80
2:3:101:ARG:C	2:3:104:CYS:HG	1.85	0.80
4:A:41:LEU:CD1	4:A:42:TYR:CZ	2.64	0.80
13:J:30:THR:CG2	13:J:31:GLU:H	1.94	0.80
1:1:88:THR:HG22	2:3:109:LEU:HD13	1.65	0.79
17:N:251:VAL:HG23	17:N:331:ILE:HG21	1.65	0.79
14:K:66:GLU:HG2	14:K:87:ARG:HG2	1.65	0.79
22:V:189:VAL:HG23	22:V:253:LEU:HD11	1.65	0.78
8:E:56:THR:HG22	8:E:76:PHE:CD1	2.18	0.77
2:3:191:ILE:N	3:4:176:PHE:HE2	1.81	0.77
2:3:101:ARG:C	2:3:104:CYS:SG	2.62	0.77
18:O:92:ILE:HG21	20:Q:60:LEU:HD21	1.66	0.76
4:A:776:SER:OG	4:A:777:PRO:HD3	1.84	0.76
4:A:720:GLY:HA3	4:A:759:ILE:HD11	1.69	0.75
4:A:41:LEU:HD13	4:A:42:TYR:CZ	2.23	0.74
4:A:266:VAL:HB	4:A:275:ASN:HB2	1.70	0.74
11:H:98:ARG:HB3	11:H:115:TYR:HB2	1.68	0.74
8:E:56:THR:HG22	8:E:76:PHE:CE1	2.24	0.73
3:4:198:SER:HB3	22:V:286:LEU:HD11	1.70	0.73
4:A:41:LEU:CD1	4:A:42:TYR:CE2	2.72	0.73
6:C:98:THR:O	6:C:98:THR:HG22	1.87	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:49:LEU:HD13	2:3:153:GLU:HB3	1.71	0.72
2:3:234:THR:HG23	2:3:234:THR:O	1.88	0.72
5:B:715:PRO:HB2	5:B:734:PRO:HG2	1.72	0.72
2:3:191:ILE:N	3:4:176:PHE:CE2	2.58	0.71
6:C:49:PHE:HA	6:C:66:VAL:O	1.90	0.71
4:A:494:THR:OG1	4:A:495:PRO:HD3	1.90	0.71
4:A:1049:THR:HG22	12:I:85:ARG:HD2	1.72	0.71
16:M:221:GLU:HB3	17:N:374:THR:HG21	1.73	0.70
7:D:41:ASN:HB2	10:G:36:ASN:HD22	1.56	0.70
16:M:249:LEU:HD12	16:M:250:MET:HG2	1.73	0.70
2:3:313:HIS:O	2:3:317:CYS:HB3	1.91	0.70
6:C:91:LYS:HB2	6:C:213:HIS:HB2	1.74	0.70
4:A:1215:ASP:O	4:A:1221:GLU:HA	1.92	0.70
3:4:408:GLU:OE2	3:4:442:ARG:NH1	2.25	0.70
4:A:414:VAL:HG12	4:A:416:PRO:HD2	1.73	0.70
5:B:404:LYS:HD2	22:V:141:LEU:HA	1.74	0.69
19:P:146:LYS:HG3	19:P:147:LYS:HD3	1.74	0.69
4:A:76:LEU:CD2	22:V:40:LEU:CD2	2.71	0.69
24:X:8:DC:H2'	24:X:9:DT:C6	2.27	0.69
17:N:251:VAL:HG23	17:N:331:ILE:CG2	2.23	0.68
4:A:48:HIS:HA	22:V:55:TYR:HE1	1.57	0.68
16:M:178:SER:H	19:P:94:LEU:HD11	1.59	0.68
4:A:485:THR:OG1	4:A:487:ARG:NH1	2.27	0.68
3:4:163:GLU:HA	3:4:166:ARG:HH21	1.59	0.67
1:1:26:PHE:CD2	1:1:121:ASP:CG	2.57	0.67
2:3:297:THR:HG22	2:3:298:PHE:N	2.10	0.67
22:V:267:GLN:NE2	24:X:-38:DT:OP1	2.27	0.67
4:A:76:LEU:HD21	22:V:40:LEU:CD2	2.24	0.67
4:A:471:LEU:HD22	4:A:538:LEU:HD12	1.76	0.67
2:3:191:ILE:HB	3:4:176:PHE:HZ	0.91	0.67
5:B:113:ILE:HD11	5:B:136:MET:N	2.08	0.67
18:O:349:THR:HG23	19:P:280:THR:HG21	1.75	0.66
4:A:257:VAL:CG2	4:A:283:LEU:HD13	2.26	0.66
5:B:535:ASN:HD21	17:N:247:LYS:HE2	1.60	0.66
4:A:464:ARG:HG2	4:A:466:PRO:HD2	1.77	0.66
21:U:243:LYS:HG3	22:V:389:ILE:HG21	1.78	0.66
24:X:13:DG:N7	24:X:14:DC:N4	2.43	0.65
2:3:310:LEU:HD11	2:3:318:GLU:HB2	1.78	0.65
2:3:279:GLU:OE2	2:3:287:LYS:HD3	1.96	0.65
4:A:995:THR:HG22	4:A:997:PRO:HD2	1.77	0.65
19:P:216:VAL:HG21	19:P:239:LEU:HD11	1.78	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:180:ILE:HB	5:B:455:ILE:HG12	1.78	0.64
4:A:1273:TYR:O	4:A:1277:ASN:ND2	2.30	0.64
4:A:461:LEU:HD23	4:A:473:ILE:HD11	1.78	0.64
5:B:190:ILE:HG21	5:B:354:ARG:HE	1.62	0.64
5:B:725:ILE:HG23	5:B:730:PHE:HB3	1.78	0.64
18:O:374:HIS:HB3	18:O:423:LEU:HD23	1.78	0.64
21:U:169:VAL:HG22	21:U:222:THR:HG22	1.79	0.64
5:B:915:ASP:OD1	6:C:78:ARG:NH2	2.31	0.64
5:B:178:ILE:HG12	5:B:437:THR:HG22	1.78	0.64
2:3:310:LEU:HD13	3:4:152:ASP:HA	1.78	0.64
5:B:231:SER:HA	5:B:292:ARG:HE	1.63	0.64
21:U:169:VAL:HG11	24:X:-27:DA:H1'	1.79	0.63
4:A:1044:PRO:HG2	4:A:1282:ILE:HD11	1.80	0.63
11:H:112:LEU:HD13	11:H:129:ALA:HB2	1.79	0.63
21:U:168:ILE:HB	21:U:224:ALA:HB3	1.79	0.63
4:A:23:LYS:HG3	5:B:1123:ILE:HG13	1.80	0.63
5:B:23:VAL:CG2	5:B:26:LYS:HB2	2.26	0.63
5:B:113:ILE:HD11	5:B:136:MET:CA	2.28	0.63
4:A:861:THR:HG21	12:I:86:SER:H	1.62	0.63
1:1:83:TYR:OH	2:3:101:ARG:NH1	2.32	0.63
4:A:41:LEU:CG	22:V:58:SER:OG	2.44	0.63
24:X:-14:DA:N1	24:X:-13:DA:N6	2.47	0.63
4:A:461:LEU:HD21	5:B:1063:LEU:HD21	1.79	0.63
22:V:189:VAL:CG2	22:V:253:LEU:HD11	2.27	0.63
16:M:50:LYS:NZ	16:M:200:HIS:O	2.32	0.62
3:4:373:ARG:HH11	3:4:384:SER:HB2	1.64	0.62
4:A:41:LEU:HD11	4:A:42:TYR:CZ	2.31	0.62
1:1:36:MET:HG3	1:1:36:MET:O	2.00	0.62
2:3:190:VAL:HG22	3:4:176:PHE:HD2	1.63	0.62
5:B:113:ILE:HD12	5:B:136:MET:N	2.14	0.62
7:D:17:PHE:HB2	7:D:53:ILE:HG21	1.80	0.62
4:A:381:ALA:HB3	4:A:487:ARG:HB2	1.82	0.62
16:M:175:VAL:HG23	19:P:97:GLN:CD	2.19	0.62
1:1:147:ARG:HD3	2:3:199:LYS:HG2	1.80	0.62
5:B:679:GLN:HG2	5:B:681:PRO:HD2	1.82	0.61
4:A:1132:LEU:HB2	4:A:1171:ALA:HB1	1.82	0.61
18:O:472:ALA:HA	18:O:475:GLN:HE21	1.64	0.61
4:A:1069:ARG:HH12	4:A:1080:ILE:HD12	1.66	0.61
24:X:-17:DT:H2''	24:X:-16:DG:C8	2.36	0.61
4:A:44:GLN:HB2	22:V:59:THR:HG21	1.81	0.61
4:A:49:ALA:N	22:V:55:TYR:OH	2.33	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:874:ARG:HH22	4:A:1071:LYS:HG3	1.65	0.61
18:O:507:ASN:OD1	20:Q:62:GLN:NE2	2.34	0.61
4:A:492:VAL:HG22	4:A:492:VAL:O	1.99	0.61
12:I:62:VAL:HG11	12:I:78:TYR:CD1	2.35	0.61
6:C:326:ILE:HG21	14:K:111:LEU:HB2	1.83	0.61
7:D:3:VAL:HG12	10:G:7:MET:HG2	1.83	0.61
4:A:29:ARG:HH21	4:A:254:ARG:HH21	1.49	0.60
4:A:1119:GLU:HG3	4:A:1128:ILE:HG12	1.82	0.60
19:P:83:GLY:N	19:P:92:GLU:OE2	2.30	0.60
11:H:20:LYS:NZ	11:H:22:PHE:O	2.34	0.60
4:A:1194:GLU:O	4:A:1198:LYS:NZ	2.34	0.60
22:V:111:LEU:HD11	24:X:-17:DT:H5'	1.82	0.60
4:A:354:GLY:HA2	5:B:1046:ARG:HH22	1.67	0.60
5:B:77:TYR:HA	5:B:117:ILE:HG22	1.83	0.60
5:B:682:ARG:HD2	5:B:937:ARG:HB3	1.83	0.60
4:A:534:ASN:O	4:A:660:LYS:NZ	2.34	0.59
4:A:855:ARG:NH2	5:B:481:PRO:O	2.34	0.59
4:A:942:LYS:HG3	4:A:977:SER:HB2	1.84	0.59
18:O:258:ARG:HD3	19:P:276:ILE:HG12	1.82	0.59
19:P:142:VAL:HG23	19:P:170:GLN:HA	1.84	0.59
19:P:159:ARG:NH1	19:P:233:GLU:OE2	2.30	0.59
1:1:67:LEU:HB3	1:1:69:PRO:HD2	1.84	0.59
4:A:41:LEU:HD21	22:V:53:VAL:HG11	1.82	0.59
5:B:750:ASP:HA	5:B:754:ALA:HB3	1.83	0.59
18:O:159:ARG:NH2	18:O:189:LEU:O	2.35	0.59
6:C:236:LEU:CD1	6:C:305:HIS:CE1	2.83	0.59
1:1:63:TRP:CE3	1:1:82:LEU:HD12	2.36	0.59
24:X:16:DG:H22	25:Y:-15:DT:H3	1.50	0.59
4:A:6:PHE:HB2	10:G:37:LYS:HB3	1.84	0.59
10:G:187:VAL:HG13	10:G:188:GLY:N	2.18	0.59
24:X:-29:DT:H5'	24:X:-29:DT:C6	2.37	0.59
18:O:92:ILE:HG21	20:Q:60:LEU:CD2	2.33	0.59
2:3:190:VAL:HG22	3:4:176:PHE:CD2	2.38	0.59
13:J:36:ASP:OD1	13:J:46:ARG:NH1	2.35	0.59
5:B:113:ILE:CD1	5:B:136:MET:H	2.14	0.58
5:B:986:LYS:O	6:C:285:ARG:NH2	2.36	0.58
5:B:313:LEU:HD23	5:B:317:ILE:HD12	1.84	0.58
5:B:392:ILE:HD13	5:B:400:PHE:HB3	1.85	0.58
5:B:741:VAL:HG22	5:B:927:ILE:HB	1.85	0.58
6:C:93:LEU:HD23	15:L:52:LEU:HD11	1.85	0.58
22:V:173:VAL:HG21	22:V:208:VAL:HG21	1.85	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:284:GLU:OE2	23:W:285:ARG:HB2	2.02	0.58
4:A:631:LEU:HD11	11:H:124:ARG:HD3	1.84	0.58
4:A:1360:PHE:O	9:F:64:ARG:NH1	2.36	0.58
4:A:303:THR:OG1	18:O:377:GLN:NE2	2.36	0.58
5:B:128:ARG:NH2	23:W:287:SER:OG	2.36	0.58
24:X:6:DC:H2'	24:X:7:DG:C8	2.38	0.58
4:A:470:LYS:HB3	4:A:1039:GLN:HE22	1.67	0.58
4:A:937:GLU:OE1	4:A:1007:THR:OG1	2.21	0.58
5:B:594:ARG:NH2	5:B:663:THR:OG1	2.31	0.58
5:B:903:GLN:OE1	5:B:937:ARG:NH1	2.36	0.58
2:3:234:THR:HG23	2:3:237:GLN:HB2	1.84	0.58
4:A:125:PHE:HZ	4:A:149:LYS:HD2	1.68	0.58
17:N:332:ARG:HB2	17:N:336:ARG:HB2	1.86	0.58
1:1:63:TRP:HE3	1:1:82:LEU:HD11	1.58	0.58
4:A:43:SER:O	22:V:55:TYR:CD2	2.56	0.58
6:C:157:SER:HB3	16:M:377:LEU:HA	1.86	0.58
3:4:354:ASP:OD1	3:4:390:ARG:NH1	2.36	0.58
5:B:674:TYR:HB3	5:B:677:HIS:HD2	1.68	0.58
6:C:86:THR:HG21	6:C:227:PRO:HB3	1.84	0.58
1:1:88:THR:HG22	2:3:109:LEU:CD1	2.34	0.57
5:B:531:LEU:HD22	5:B:538:LEU:HD21	1.86	0.57
6:C:89:VAL:HB	6:C:111:GLY:HA2	1.84	0.57
13:J:28:GLU:OE2	16:M:397:GLY:N	2.37	0.57
5:B:89:GLU:HG3	5:B:105:ARG:HH22	1.69	0.57
10:G:115:GLN:NE2	10:G:192:GLU:O	2.37	0.57
23:W:335:ILE:O	23:W:339:ASN:ND2	2.36	0.57
4:A:1102:LYS:HB2	4:A:1212:ILE:HD11	1.86	0.57
8:E:95:GLN:OE1	8:E:125:TYR:OH	2.21	0.57
2:3:310:LEU:HB3	3:4:153:LYS:HD2	1.86	0.57
4:A:5:GLN:HB2	10:G:185:THR:HG21	1.85	0.57
5:B:113:ILE:HD12	5:B:136:MET:H	1.68	0.57
6:C:78:ARG:HE	14:K:50:THR:HG22	1.69	0.57
24:X:-70:DA:H2''	24:X:-69:DT:C4	2.40	0.57
24:X:1:DG:H2'	24:X:2:DT:H71	1.86	0.57
19:P:140:LYS:NZ	25:Y:16:DC:OP1	2.36	0.57
18:O:292:GLU:HA	18:O:295:ARG:HG2	1.87	0.57
4:A:43:SER:O	22:V:59:THR:OG1	2.18	0.57
4:A:499:ASP:OD1	4:A:499:ASP:N	2.38	0.57
4:A:760:ARG:NH2	4:A:794:GLN:OE1	2.38	0.57
4:A:899:GLN:NE2	4:A:1292:ASP:OD2	2.28	0.56
5:B:207:THR:HG23	5:B:209:GLU:H	1.70	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:401:ASP:OD1	5:B:404:LYS:CG	2.50	0.56
16:M:177:PHE:HE1	19:P:97:GLN:HB3	1.70	0.56
4:A:891:ARG:HG2	4:A:897:ILE:HG12	1.87	0.56
16:M:218:SER:HA	17:N:374:THR:HG23	1.85	0.56
4:A:108:ILE:HA	4:A:115:ILE:HA	1.87	0.56
4:A:360:ARG:HG2	5:B:1046:ARG:HB2	1.88	0.56
4:A:431:PHE:N	22:V:32:GLY:O	2.37	0.56
16:M:409:ILE:HG23	16:M:416:VAL:HG21	1.88	0.56
25:Y:25:DT:H2''	25:Y:26:DA:H5'	1.88	0.56
5:B:722:THR:HG23	5:B:962:THR:HA	1.85	0.56
9:F:69:ARG:NE	9:F:96:GLU:OE1	2.37	0.56
3:4:353:GLU:HG3	3:4:390:ARG:HH12	1.70	0.56
4:A:598:LYS:HD2	11:H:120:GLY:HA3	1.88	0.56
6:C:28:ASP:O	14:K:61:LYS:NZ	2.38	0.56
16:M:311:LEU:HD21	16:M:415:VAL:HG21	1.86	0.56
18:O:457:ASN:HD22	18:O:502:LEU:HD13	1.71	0.56
2:3:191:ILE:CG2	3:4:176:PHE:HZ	2.19	0.56
6:C:9:GLU:OE2	6:C:298:ARG:NH1	2.39	0.56
7:D:80:LYS:HD2	7:D:83:LYS:HD2	1.88	0.56
4:A:481:LYS:HB2	4:A:487:ARG:HH21	1.70	0.56
22:V:111:LEU:HD13	24:X:-17:DT:H5'	1.87	0.56
2:3:103:VAL:HG12	2:3:107:ASP:OD2	2.06	0.56
5:B:85:PRO:HG3	5:B:138:ILE:HG13	1.88	0.56
6:C:236:LEU:HD13	6:C:305:HIS:ND1	2.20	0.56
16:M:117:ALA:HB1	16:M:124:LEU:HD11	1.88	0.56
5:B:87:VAL:HG22	5:B:89:GLU:H	1.71	0.56
21:U:204:ILE:HG13	21:U:207:PRO:HD2	1.88	0.55
24:X:-58:DT:H2''	24:X:-57:DA:C8	2.41	0.55
1:1:67:LEU:O	1:1:75:ARG:NH1	2.37	0.55
13:J:3:ILE:HD12	13:J:4:PRO:HD2	1.87	0.55
16:M:327:VAL:O	16:M:353:ARG:NH1	2.37	0.55
19:P:137:LYS:NZ	19:P:152:LEU:O	2.39	0.55
4:A:459:VAL:HB	4:A:516:LYS:HG3	1.87	0.55
5:B:40:VAL:HG12	5:B:40:VAL:O	2.06	0.55
5:B:914:GLU:HB2	6:C:78:ARG:HG2	1.89	0.55
10:G:115:GLN:O	10:G:119:LYS:NZ	2.35	0.55
22:V:68:SER:OG	24:X:-16:DG:OP2	2.23	0.55
3:4:295:GLN:O	3:4:328:ARG:NH1	2.40	0.55
18:O:147:THR:HG22	18:O:150:ARG:HH22	1.72	0.55
24:X:-59:DG:C8	25:Y:61:DG:H5''	2.41	0.55
2:3:216:ARG:NH2	2:3:248:LYS:O	2.39	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:254:MET:HA	5:B:528:GLY:HA3	1.89	0.54
6:C:141:ARG:NH1	6:C:209:ASP:OD1	2.40	0.54
14:K:50:THR:OG1	14:K:51:LEU:N	2.39	0.54
1:1:130:ARG:O	1:1:133:ARG:NH2	2.38	0.54
22:V:294:VAL:HA	22:V:297:ILE:HG13	1.89	0.54
5:B:634:ASP:OD1	5:B:635:VAL:N	2.37	0.54
5:B:1023:ARG:NH1	5:B:1042:ASP:O	2.41	0.54
10:G:93:SER:OG	10:G:96:GLY:O	2.23	0.54
3:4:388:ILE:HD13	25:Y:55:DG:H2'	1.90	0.54
4:A:1107:LYS:HG3	4:A:1200:VAL:HG23	1.89	0.54
4:A:1136:ARG:NH2	12:I:47:LYS:O	2.40	0.54
10:G:81:LEU:HD22	10:G:152:VAL:HA	1.89	0.54
16:M:273:LEU:HD11	16:M:281:GLN:HA	1.90	0.54
3:4:435:SER:H	3:4:438:GLN:HE21	1.56	0.54
4:A:1069:ARG:HH21	4:A:1270:GLU:HG2	1.72	0.54
4:A:903:GLY:HA3	4:A:1285:ARG:HG2	1.90	0.54
5:B:1028:ARG:NH1	5:B:1072:SER:O	2.41	0.54
4:A:553:THR:HG21	4:A:650:MET:HG2	1.90	0.54
5:B:313:LEU:O	5:B:331:LYS:NZ	2.34	0.54
4:A:361:VAL:HG12	5:B:1072:SER:HB3	1.88	0.53
6:C:188:GLY:O	6:C:191:ARG:NH1	2.36	0.53
9:F:100:ARG:NH2	9:F:123:LEU:O	2.38	0.53
10:G:2:PHE:HA	10:G:76:VAL:O	2.08	0.53
21:U:187:ALA:O	22:V:394:ARG:NH1	2.41	0.53
22:V:224:PRO:HD3	23:W:291:TYR:HE1	1.72	0.53
25:Y:13:DT:H2''	25:Y:14:DT:C5	2.44	0.53
12:I:20:CYS:SG	12:I:21:HIS:N	2.81	0.53
4:A:542:ILE:HG13	4:A:543:GLN:H	1.72	0.53
4:A:1332:ALA:HB2	5:B:1122:ILE:HG23	1.89	0.53
5:B:889:ARG:NH1	5:B:1015:MET:SD	2.79	0.53
12:I:84:THR:O	12:I:84:THR:HG23	2.08	0.53
4:A:471:LEU:HB3	4:A:495:PRO:HB3	1.90	0.53
5:B:318:LEU:HD12	5:B:331:LYS:HG3	1.90	0.53
5:B:483:ASP:OD2	5:B:495:ASN:ND2	2.42	0.53
5:B:539:VAL:HG12	5:B:583:VAL:HB	1.89	0.53
18:O:361:ARG:HH21	18:O:386:ILE:HG23	1.72	0.53
24:X:-20:DT:H2''	24:X:-19:DT:H71	1.89	0.53
2:3:369:ASP:OD1	2:3:370:SER:N	2.42	0.53
5:B:524:ASN:O	16:M:134:GLN:NE2	2.42	0.53
18:O:255:VAL:HG21	18:O:267:VAL:HG11	1.89	0.53
3:4:203:ARG:NH1	3:4:260:SER:O	2.42	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:405:ALA:HB1	3:4:408:GLU:HB3	1.89	0.53
4:A:799:VAL:HG23	4:A:837:SER:HA	1.91	0.53
6:C:98:THR:O	6:C:98:THR:CG2	2.56	0.53
19:P:284:ARG:HG2	20:Q:46:VAL:HB	1.91	0.53
4:A:583:LEU:HD12	4:A:584:PRO:HD2	1.91	0.53
12:I:49:VAL:HG12	12:I:51:ASP:H	1.74	0.53
3:4:399:LEU:HA	3:4:433:GLY:HA2	1.89	0.53
17:N:254:LEU:HD12	17:N:331:ILE:HD11	1.90	0.53
24:X:10:DT:H2'	24:X:11:DC:C6	2.44	0.53
25:Y:60:DG:H2''	25:Y:61:DG:C8	2.44	0.53
9:F:110:LEU:HD12	9:F:114:SER:HB3	1.90	0.52
14:K:66:GLU:OE2	14:K:87:ARG:NH1	2.42	0.52
1:1:114:LEU:HD13	1:1:122:ALA:HB1	1.91	0.52
12:I:8:CYS:SG	12:I:10:ASN:ND2	2.74	0.52
21:U:317:VAL:HG12	21:U:320:GLU:HG3	1.90	0.52
2:3:324:THR:HG23	2:3:325:ASP:N	2.24	0.52
5:B:712:LEU:HD21	5:B:737:GLN:HG3	1.92	0.52
17:N:253:GLU:OE2	17:N:256:ARG:NH2	2.41	0.52
4:A:590:LYS:NZ	11:H:88:PHE:O	2.43	0.52
5:B:649:THR:HG22	5:B:649:THR:O	2.09	0.52
5:B:1021:HIS:NE2	5:B:1043:GLY:O	2.34	0.52
18:O:137:LYS:O	18:O:201:ARG:NH2	2.43	0.52
19:P:210:PHE:HB3	19:P:269:LEU:HB3	1.92	0.52
2:3:297:THR:CG2	2:3:298:PHE:N	2.73	0.52
5:B:526:LEU:HD13	5:B:530:GLU:HB2	1.91	0.52
5:B:869:VAL:HG22	5:B:883:MET:HG3	1.91	0.52
6:C:133:THR:OG1	6:C:136:ASP:OD1	2.27	0.52
18:O:47:LEU:HG	18:O:51:LYS:HE3	1.92	0.52
19:P:98:ILE:HD13	19:P:115:LYS:HD3	1.91	0.52
19:P:248:VAL:HG12	19:P:272:ALA:HA	1.92	0.52
2:3:347:HIS:O	2:3:411:ASN:ND2	2.42	0.52
5:B:803:ILE:HG13	5:B:806:HIS:H	1.75	0.52
22:V:55:TYR:O	22:V:59:THR:OG1	2.27	0.52
4:A:656:GLY:O	4:A:662:ASN:ND2	2.43	0.52
5:B:137:PRO:HG2	5:B:419:ILE:HD12	1.91	0.52
6:C:50:ARG:NH1	6:C:52:ASP:OD2	2.43	0.52
7:D:25:GLU:HA	7:D:28:LYS:HG2	1.92	0.52
4:A:1105:ILE:HG22	4:A:1238:THR:HG21	1.92	0.52
4:A:1185:MET:SD	4:A:1185:MET:N	2.82	0.52
6:C:109:ARG:NH2	6:C:198:LEU:O	2.43	0.52
6:C:228:VAL:HA	6:C:312:SER:HA	1.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:9:DT:H2'	24:X:10:DT:C6	2.44	0.52
7:D:87:LEU:O	7:D:90:ARG:NH1	2.43	0.52
15:L:26:ASN:ND2	15:L:36:CYS:SG	2.80	0.52
4:A:374:ASN:ND2	5:B:749:TYR:OH	2.43	0.52
4:A:1340:VAL:HA	4:A:1345:GLU:HG3	1.92	0.52
5:B:40:VAL:HG21	5:B:165:PRO:HB2	1.91	0.52
5:B:1030:VAL:HG22	22:V:40:LEU:HG	1.92	0.52
4:A:590:LYS:HB3	4:A:591:PRO:HD3	1.91	0.51
5:B:779:LEU:O	5:B:878:ALA:HA	2.10	0.51
7:D:89:HIS:HE1	10:G:84:ILE:HB	1.74	0.51
11:H:96:VAL:HA	11:H:116:VAL:HG22	1.92	0.51
1:1:26:PHE:HE2	1:1:121:ASP:HB3	1.68	0.51
2:3:186:ILE:HG22	2:3:321:ILE:HG12	1.92	0.51
4:A:383:PRO:HB3	4:A:484:ARG:HA	1.92	0.51
5:B:518:LEU:HD21	5:B:558:THR:HG21	1.93	0.51
15:L:19:CYS:SG	15:L:23:HIS:N	2.83	0.51
16:M:175:VAL:HG23	19:P:97:GLN:HG2	1.93	0.51
25:Y:46:DT:H2''	25:Y:47:DA:H5''	1.93	0.51
16:M:53:GLN:OE1	16:M:200:HIS:ND1	2.43	0.51
16:M:240:LYS:HE3	17:N:278:GLN:HB2	1.92	0.51
5:B:89:GLU:OE2	15:L:42:ARG:NE	2.43	0.51
7:D:42:LEU:HD11	10:G:31:ASN:HB3	1.92	0.51
19:P:284:ARG:HD3	20:Q:48:LEU:HA	1.91	0.51
22:V:212:ASN:HD22	22:V:217:VAL:HG21	1.75	0.51
25:Y:-5:DA:H2''	25:Y:-4:DG:N7	2.25	0.51
3:4:508:ARG:HH11	3:4:511:ARG:HH21	1.58	0.51
5:B:526:LEU:HD12	5:B:527:CYS:O	2.09	0.51
11:H:70:LEU:HD23	11:H:70:LEU:H	1.75	0.51
5:B:20:ILE:HD12	5:B:21:PRO:HD2	1.93	0.51
3:4:372:TYR:CE1	3:4:388:ILE:HG23	2.45	0.51
4:A:1107:LYS:HD3	4:A:1205:PRO:HA	1.93	0.51
8:E:56:THR:CG2	8:E:76:PHE:CD1	2.91	0.51
19:P:100:GLU:HG3	19:P:152:LEU:HD11	1.93	0.51
5:B:880:LEU:HD21	5:B:882:LYS:HE3	1.93	0.51
5:B:1023:ARG:NH2	5:B:1027:PRO:O	2.42	0.51
22:V:263:SER:O	22:V:266:LEU:HB3	2.11	0.51
5:B:471:LEU:HD21	5:B:481:PRO:HB3	1.92	0.51
5:B:764:ARG:HD3	13:J:6:ARG:HB3	1.93	0.51
6:C:235:LEU:HB2	6:C:301:ARG:HH11	1.76	0.51
18:O:477:THR:HG23	18:O:477:THR:O	2.09	0.51
4:A:56:LEU:HA	4:A:260:LEU:HD21	1.91	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:212:SER:HB2	5:B:227:HIS:HE2	1.75	0.50
6:C:236:LEU:HD23	6:C:237:PRO:O	2.11	0.50
18:O:92:ILE:CG2	20:Q:60:LEU:HD21	2.39	0.50
23:W:276:VAL:O	23:W:276:VAL:HG13	2.11	0.50
16:M:175:VAL:CG2	19:P:97:GLN:CD	2.79	0.50
22:V:111:LEU:CD1	24:X:-17:DT:C5'	2.83	0.50
24:X:-61:DC:H2''	24:X:-60:DC:C5	2.45	0.50
4:A:257:VAL:HG23	4:A:283:LEU:HD11	1.92	0.50
5:B:923:ILE:HD11	13:J:42:ARG:HB2	1.92	0.50
6:C:149:ASN:ND2	6:C:151:HIS:O	2.44	0.50
24:X:-63:DT:O2	24:X:-62:DA:N6	2.45	0.50
6:C:296:VAL:HG23	6:C:297:VAL:HG13	1.93	0.50
11:H:58:LEU:HD11	11:H:143:LEU:HD11	1.93	0.50
17:N:251:VAL:HG13	17:N:252:ALA:N	2.27	0.50
24:X:4:DC:H2''	24:X:5:DT:C5	2.47	0.50
4:A:26:GLU:HG2	19:P:297:HIS:HB2	1.93	0.50
4:A:36:VAL:HB	4:A:86:ILE:HG12	1.93	0.50
15:L:17:TYR:HB3	15:L:44:MET:HG3	1.93	0.50
16:M:347:GLU:OE2	16:M:351:ARG:NH2	2.45	0.50
22:V:15:LEU:H	22:V:15:LEU:HD23	1.76	0.50
23:W:325:ILE:HG22	23:W:337:ILE:HD13	1.94	0.50
24:X:11:DC:H2''	24:X:12:DG:H5'	1.93	0.50
1:1:90:LEU:CD1	2:3:109:LEU:HD21	2.23	0.50
6:C:115:ILE:HG22	6:C:117:ALA:H	1.76	0.50
18:O:464:SER:HA	18:O:467:VAL:HG22	1.93	0.50
21:U:268[A]:ILE:HD13	21:U:332:LEU:HD22	1.92	0.50
21:U:268[B]:ILE:HD13	21:U:332:LEU:HD22	1.92	0.50
22:V:15:LEU:HD12	22:V:26:LEU:HD22	1.94	0.50
22:V:214:THR:HA	22:V:312:PHE:HZ	1.75	0.50
24:X:-18:DG:H4'	24:X:-17:DT:OP1	2.12	0.50
2:3:343:LEU:HD22	2:3:346:LYS:HE2	1.93	0.50
4:A:1152:SER:OG	4:A:1200:VAL:O	2.28	0.50
13:J:28:GLU:OE2	16:M:396:LYS:N	2.44	0.50
22:V:222:PRO:O	22:V:226:ILE:HG12	2.12	0.50
23:W:284:GLU:CD	23:W:285:ARG:HB2	2.31	0.50
10:G:154:ASP:OD1	10:G:154:ASP:N	2.45	0.50
12:I:29:PRO:HA	16:M:73:LYS:HD3	1.93	0.50
12:I:85:ARG:NH1	12:I:88:ASP:OD1	2.45	0.50
3:4:416:VAL:HG22	3:4:443:TYR:HE1	1.76	0.50
5:B:738:ASN:HB2	13:J:47:ARG:HD3	1.94	0.50
2:3:175:ILE:HG12	2:3:337:ARG:HB2	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:265:LYS:HG2	3:4:269:ILE:HD12	1.94	0.49
4:A:811:ASP:OD1	4:A:811:ASP:N	2.44	0.49
5:B:103:ARG:NH2	5:B:168:TYR:OH	2.44	0.49
5:B:214:THR:HB	5:B:227:HIS:HD2	1.77	0.49
18:O:469:ALA:HA	18:O:472:ALA:HB3	1.92	0.49
4:A:192:ASN:HA	4:A:195:GLN:HG2	1.93	0.49
5:B:812:ASP:OD2	15:L:46:LYS:NZ	2.43	0.49
7:D:57:PRO:HB2	7:D:90:ARG:HE	1.76	0.49
6:C:334:ARG:NH2	14:K:104:MET:SD	2.86	0.49
7:D:54:SER:HA	7:D:59:ARG:HD2	1.94	0.49
1:1:63:TRP:CE3	1:1:82:LEU:HD11	2.40	0.49
3:4:264:GLU:O	3:4:268:ASN:ND2	2.35	0.49
4:A:168:LYS:NZ	4:A:170:GLY:O	2.45	0.49
4:A:555:LYS:HG2	11:H:25:VAL:HG21	1.93	0.49
4:A:558:PHE:HB3	4:A:594:LEU:HD13	1.94	0.49
4:A:1044:PRO:HA	4:A:1047:GLN:HB2	1.93	0.49
16:M:104:SER:HB2	16:M:133:LEU:HB3	1.95	0.49
18:O:404:MET:HB3	18:O:426:VAL:HG22	1.95	0.49
24:X:-62:DA:H1'	24:X:-61:DC:H5'	1.93	0.49
3:4:366:VAL:HG13	3:4:366:VAL:O	2.13	0.49
4:A:855:ARG:HD2	5:B:471:LEU:HB2	1.93	0.49
8:E:56:THR:HG22	8:E:56:THR:O	2.12	0.49
24:X:-24:DT:H1'	24:X:-23:DA:C8	2.46	0.49
4:A:40:ASN:HB3	22:V:58:SER:O	2.12	0.49
4:A:593:THR:HB	6:C:32:ASN:HA	1.94	0.49
4:A:604:ILE:HG23	4:A:682:ARG:HB2	1.93	0.49
5:B:1079:VAL:HB	5:B:1128:LEU:HD11	1.93	0.49
16:M:322:GLN:HE22	16:M:364:ARG:HA	1.77	0.49
4:A:731:LEU:HB2	4:A:736:LEU:HD22	1.94	0.49
5:B:526:LEU:CD1	5:B:527:CYS:O	2.60	0.49
5:B:901:HIS:CD2	5:B:942:LYS:HZ3	2.30	0.49
10:G:187:VAL:HG13	10:G:188:GLY:H	1.77	0.49
16:M:175:VAL:HG23	19:P:97:GLN:CG	2.42	0.49
17:N:145:ARG:HH21	17:N:150:GLU:HB3	1.77	0.49
4:A:739:GLN:HG3	4:A:747:THR:HG23	1.94	0.49
4:A:918:PRO:HB2	4:A:919:LEU:HD12	1.95	0.49
6:C:8:GLU:HA	6:C:11:ARG:HG2	1.95	0.49
6:C:263:GLU:OE2	6:C:274:ARG:NH1	2.46	0.49
16:M:13:ILE:HD13	16:M:119:TYR:HE1	1.78	0.49
16:M:243:SER:HB2	17:N:396:LYS:HD2	1.94	0.49
1:1:21:THR:OG1	1:1:73:GLN:NE2	2.44	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:470:LYS:HE3	4:A:532:PRO:HG3	1.95	0.49
4:A:556:ASP:HB3	11:H:24:ARG:HH11	1.78	0.49
5:B:235:PRO:HD2	5:B:238:ILE:HD12	1.94	0.49
6:C:134:GLU:O	6:C:181:GLN:NE2	2.45	0.49
16:M:431:GLU:HG2	16:M:436:LEU:HB2	1.95	0.49
4:A:940:LEU:HB2	4:A:1006:ILE:HG23	1.94	0.49
5:B:125:ARG:HG2	23:W:279:ASN:HD22	1.78	0.49
16:M:225:LEU:HD11	17:N:376:LEU:HD13	1.94	0.49
25:Y:23:DT:H2''	25:Y:24:DA:H5''	1.95	0.49
25:Y:54:DA:H2''	25:Y:55:DG:C8	2.47	0.49
2:3:184:VAL:HG23	2:3:321:ILE:HG23	1.95	0.48
5:B:1042:ASP:HB3	22:V:22:SER:HB2	1.95	0.48
2:3:63:LEU:O	2:3:63:LEU:HD12	2.13	0.48
14:K:27:LEU:HG	14:K:43:VAL:HB	1.93	0.48
25:Y:42:DG:H2''	25:Y:43:DA:C8	2.47	0.48
2:3:158:GLU:CB	3:4:366:VAL:HG23	2.42	0.48
5:B:563:ARG:NH2	5:B:637:GLU:OE2	2.41	0.48
24:X:-30:DT:H2'	24:X:-29:DT:H72	1.95	0.48
1:1:124:TYR:HE2	2:3:101:ARG:HH21	1.60	0.48
4:A:529:LEU:HA	4:A:539:ILE:HD13	1.93	0.48
10:G:148:ILE:HG23	10:G:190:ILE:HG23	1.95	0.48
16:M:364:ARG:HH22	16:M:403:PRO:HA	1.78	0.48
21:U:191:GLU:OE2	23:W:323:SER:N	2.46	0.48
2:3:216:ARG:HE	2:3:250:ALA:HB3	1.78	0.48
6:C:155:ASP:HB3	16:M:348:VAL:HG21	1.94	0.48
5:B:217:ALA:O	5:B:223:PHE:HA	2.14	0.48
16:M:177:PHE:CZ	19:P:98:ILE:HB	2.48	0.48
5:B:121:ARG:HG2	5:B:399:GLN:HB2	1.96	0.48
16:M:34:PRO:HA	17:N:356:PHE:HA	1.96	0.48
22:V:115:GLU:HG2	22:V:142:LEU:HG	1.96	0.48
1:1:52:ASN:OD1	1:1:95:GLN:NE2	2.46	0.48
3:4:443:TYR:CE1	3:4:447:LEU:HD22	2.49	0.48
4:A:1105:ILE:HD13	4:A:1225:LEU:HD13	1.95	0.47
4:A:1217:GLN:OE1	12:I:101:GLN:NE2	2.46	0.47
7:D:89:HIS:CE1	10:G:84:ILE:HB	2.48	0.47
21:U:204:ILE:CG2	21:U:209:THR:OG1	2.62	0.47
25:Y:28:DA:H1'	25:Y:29:DA:C5	2.49	0.47
3:4:483:LEU:HB3	3:4:486:ARG:HB2	1.96	0.47
4:A:616:ASN:HA	4:A:640:ILE:O	2.14	0.47
5:B:176:LYS:HE2	5:B:439:VAL:HG22	1.95	0.47
8:E:35:GLN:NE2	8:E:39:GLU:OE1	2.47	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:27:ARG:HD2	11:H:40:ILE:HG22	1.96	0.47
16:M:134:GLN:OE1	16:M:136:ARG:NH2	2.46	0.47
18:O:112:LEU:HD11	20:Q:64:LEU:HD22	1.96	0.47
23:W:331:HIS:NE2	23:W:375:LEU:CD2	2.74	0.47
24:X:-41:DG:H2''	24:X:-40:DA:C8	2.49	0.47
1:1:43:CYS:SG	2:3:119:GLU:N	2.72	0.47
1:1:71:THR:O	1:1:75:ARG:HG3	2.15	0.47
4:A:389:ILE:HD12	5:B:1022:ALA:HB3	1.97	0.47
4:A:523:MET:HA	4:A:528:ASN:HD21	1.79	0.47
5:B:245:VAL:HG13	5:B:245:VAL:O	2.14	0.47
22:V:76:VAL:HG22	22:V:118:VAL:HG13	1.95	0.47
1:1:15:LEU:HD22	1:1:74:ILE:HD12	1.95	0.47
4:A:356:LEU:HD11	5:B:1113:LEU:HD22	1.96	0.47
4:A:669:ARG:NH2	4:A:910:ALA:O	2.48	0.47
5:B:40:VAL:HG11	5:B:165:PRO:O	2.14	0.47
5:B:318:LEU:HB2	5:B:331:LYS:HE2	1.97	0.47
5:B:898:SER:HB3	5:B:1010:GLN:HG3	1.97	0.47
2:3:140:ARG:HG3	2:3:144:ILE:HB	1.96	0.47
4:A:1087:ALA:HA	4:A:1246:THR:HG22	1.95	0.47
4:A:1117:ILE:HG12	4:A:1130:VAL:HG13	1.94	0.47
5:B:176:LYS:NZ	5:B:420:SER:O	2.47	0.47
5:B:1032:THR:HG23	5:B:1032:THR:O	2.14	0.47
12:I:5:CYS:HB2	12:I:12:LEU:HD21	1.96	0.47
18:O:274:SER:OG	18:O:285:THR:OG1	2.26	0.47
25:Y:61:DG:H2''	25:Y:62:DT:H5''	1.96	0.47
4:A:76:LEU:HD23	22:V:40:LEU:CD2	2.39	0.47
4:A:907:LEU:HD13	4:A:918:PRO:HB3	1.97	0.47
16:M:64:THR:HG21	16:M:96:LEU:HD13	1.96	0.47
19:P:231:SER:OG	19:P:233:GLU:OE2	2.33	0.47
25:Y:-15:DT:H2''	25:Y:-14:DG:C8	2.49	0.47
7:D:91:PRO:HD2	7:D:120:VAL:HG21	1.96	0.47
8:E:193:ILE:HB	8:E:205:THR:HG23	1.97	0.47
11:H:8:ASP:OD1	11:H:9:ILE:N	2.48	0.47
25:Y:37:DA:H2''	25:Y:38:DA:C8	2.50	0.47
1:1:67:LEU:C	1:1:75:ARG:HH12	2.18	0.47
2:3:308:PRO:HB2	3:4:149:TYR:HE2	1.80	0.47
3:4:303:GLU:N	3:4:303:GLU:OE1	2.47	0.47
4:A:1347:ILE:HD13	5:B:1052:ARG:HD2	1.96	0.47
5:B:23:VAL:HG23	5:B:23:VAL:O	2.15	0.47
18:O:110:LEU:HD12	18:O:236:GLN:HA	1.97	0.47
4:A:1374:LYS:HE3	10:G:52:THR:HG22	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:974:GLU:HA	5:B:977:VAL:HG12	1.97	0.47
16:M:175:VAL:HG23	16:M:175:VAL:O	2.14	0.47
22:V:276:MET:HB3	22:V:307:LEU:HD13	1.96	0.47
24:X:-61:DC:H2''	24:X:-60:DC:C4	2.50	0.47
4:A:701:GLY:HA3	5:B:984:LEU:HD13	1.98	0.46
8:E:89:VAL:O	8:E:92:GLN:HG3	2.15	0.46
4:A:459:VAL:HG21	4:A:520:LEU:HB2	1.97	0.46
4:A:772:ASP:OD1	4:A:773:LYS:N	2.45	0.46
3:4:371:PRO:HB2	3:4:374:ARG:HG2	1.96	0.46
4:A:60:MET:HA	4:A:82:HIS:HB2	1.98	0.46
5:B:900:ARG:NH2	5:B:945:GLU:OE2	2.39	0.46
5:B:1118:GLN:HA	5:B:1123:ILE:HD13	1.97	0.46
4:A:43:SER:O	22:V:55:TYR:CE2	2.68	0.46
4:A:262:ILE:HD11	5:B:1115:GLN:HB3	1.98	0.46
4:A:518:GLU:HA	9:F:63:ALA:HB1	1.96	0.46
4:A:996:GLU:HB3	4:A:997:PRO:HD3	1.96	0.46
12:I:62:VAL:HG22	12:I:63:ASP:N	2.30	0.46
18:O:443:ILE:HG23	18:O:513:GLU:HG3	1.98	0.46
19:P:276:ILE:HG22	19:P:277:ILE:HG23	1.97	0.46
21:U:208:ARG:HE	23:W:345:GLU:HB3	1.80	0.46
5:B:901:HIS:NE2	5:B:945:GLU:OE1	2.43	0.46
6:C:86:THR:HA	6:C:119:PRO:HB3	1.98	0.46
7:D:24:LYS:HG3	7:D:27:ARG:HH21	1.80	0.46
7:D:94:ALA:HB2	7:D:117:LEU:HD11	1.97	0.46
16:M:238:LEU:HD13	17:N:341:LEU:HG	1.96	0.46
17:N:256:ARG:HA	17:N:260:LEU:HD23	1.96	0.46
2:3:229:GLY:H	3:4:171:GLN:HG2	1.80	0.46
4:A:384:VAL:HG13	4:A:415:HIS:CD2	2.51	0.46
5:B:118:GLU:HB3	5:B:127:ILE:HG22	1.97	0.46
17:N:245:LEU:HD12	17:N:246:PRO:HD2	1.97	0.46
18:O:303:ILE:HG13	18:O:307:VAL:HB	1.97	0.46
21:U:242:GLN:NE2	21:U:248:ALA:O	2.41	0.46
2:3:297:THR:HG22	2:3:298:PHE:H	1.79	0.46
8:E:134:GLU:OE1	8:E:181:ARG:NH2	2.46	0.46
19:P:168:SER:OG	19:P:173:GLU:OE2	2.32	0.46
4:A:1313:GLU:OE2	4:A:1336:GLN:NE2	2.49	0.46
22:V:111:LEU:HD13	24:X:-17:DT:C5'	2.46	0.46
3:4:383:ASP:OD1	3:4:386:GLN:NE2	2.41	0.46
5:B:135:ARG:HD2	22:V:84:GLN:NE2	2.31	0.46
12:I:76:ARG:NH2	12:I:98:CYS:O	2.49	0.46
19:P:158:ASP:HB3	19:P:161:VAL:HG22	1.97	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:324:LYS:HD2	5:B:325:GLU:HG3	1.98	0.46
5:B:518:LEU:HD13	5:B:555:LEU:HD12	1.98	0.46
5:B:613:GLU:HB3	5:B:618:TYR:HB2	1.97	0.46
24:X:8:DC:H2'	24:X:9:DT:H6	1.79	0.46
1:1:128:LYS:HG3	2:3:101:ARG:CZ	2.46	0.45
3:4:219:GLN:HA	3:4:222:VAL:HG12	1.98	0.45
3:4:256:ASN:H	3:4:259:ASP:HB2	1.81	0.45
4:A:1049:THR:HB	12:I:84:THR:HG23	1.97	0.45
6:C:144:VAL:HG11	6:C:168:VAL:HG22	1.97	0.45
8:E:102:ALA:HB3	8:E:127:LEU:HG	1.97	0.45
24:X:2:DT:H2''	24:X:3:DG:C8	2.51	0.45
2:3:268:ARG:NH1	3:4:163:GLU:OE2	2.49	0.45
4:A:838:PHE:O	5:B:677:HIS:ND1	2.40	0.45
4:A:868:THR:HG21	4:A:1046:THR:N	2.31	0.45
4:A:987:TYR:OH	11:H:102:ASP:N	2.48	0.45
16:M:238:LEU:HD23	17:N:277:GLY:HA3	1.98	0.45
25:Y:64:DA:H2''	25:Y:65:DG:C8	2.50	0.45
2:3:279:GLU:OE1	2:3:287:LYS:CE	2.60	0.45
4:A:700:ILE:HG21	5:B:947:LEU:HD22	1.97	0.45
5:B:128:ARG:HH12	5:B:131:LEU:HD13	1.80	0.45
18:O:247:ARG:HG3	18:O:342:LEU:HD21	1.97	0.45
22:V:257:ASP:OD1	22:V:257:ASP:N	2.49	0.45
22:V:280:LEU:HD12	22:V:283:LEU:HD12	1.98	0.45
23:W:328:LEU:HD13	23:W:367:PHE:HZ	1.81	0.45
24:X:-70:DA:H2''	24:X:-69:DT:C5	2.51	0.45
5:B:251:ILE:O	5:B:255:ILE:HG12	2.16	0.45
11:H:13:LYS:NZ	11:H:31:GLU:OE1	2.50	0.45
25:Y:-8:DG:H1'	25:Y:-7:DC:H5'	1.98	0.45
5:B:402:VAL:O	5:B:406:MET:HG2	2.16	0.45
5:B:451:MET:HA	5:B:454:ARG:HG3	1.99	0.45
5:B:990:THR:HA	5:B:997:PRO:HA	1.97	0.45
6:C:238:ASP:OD1	6:C:238:ASP:N	2.49	0.45
4:A:1054:HIS:CD2	4:A:1065:LEU:HD12	2.52	0.45
7:D:32:LYS:HB2	7:D:35:HIS:HB2	1.98	0.45
19:P:83:GLY:HA2	19:P:133:LYS:HD2	1.99	0.45
25:Y:34:DA:H2''	25:Y:35:DA:C8	2.51	0.45
2:3:204:MET:HG2	2:3:343:LEU:HG	1.99	0.45
6:C:86:THR:OG1	6:C:225:PHE:O	2.34	0.45
7:D:6:ALA:HA	10:G:5:VAL:HG22	1.99	0.45
18:O:80:SER:O	18:O:84:ARG:HG2	2.17	0.45
4:A:74:LYS:HB3	4:A:78:ASP:HB2	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:40:VAL:O	5:B:40:VAL:CG1	2.65	0.45
5:B:480:CYS:SG	5:B:666:GLY:N	2.89	0.45
5:B:946:LEU:HD22	5:B:1003:TYR:CZ	2.52	0.45
17:N:361:VAL:HG12	17:N:375:VAL:HA	1.98	0.45
22:V:294:VAL:HG23	22:V:297:ILE:HD12	1.99	0.45
2:3:306:GLY:N	2:3:323:ILE:O	2.49	0.45
3:4:490:GLN:O	3:4:494:LYS:NZ	2.45	0.45
4:A:282:LYS:NZ	4:A:316:GLN:OE1	2.33	0.45
10:G:101:LEU:HB3	10:G:104:PHE:HB3	1.99	0.45
1:1:4:PRO:HB2	1:1:7:LEU:HD13	1.98	0.45
1:1:121:ASP:OD1	1:1:121:ASP:N	2.50	0.45
19:P:57:LEU:HD23	19:P:60:MET:HE1	1.99	0.45
2:3:188:TYR:HB2	2:3:319:HIS:ND1	2.32	0.44
5:B:75:LEU:HD11	5:B:117:ILE:HD12	1.98	0.44
5:B:613:GLU:HG2	5:B:618:TYR:HD2	1.82	0.44
6:C:336:PHE:HE1	14:K:44:LEU:HD22	1.81	0.44
24:X:3:DG:H2''	24:X:4:DC:H5'	1.98	0.44
4:A:579:ILE:HB	4:A:608:SER:HB3	1.98	0.44
5:B:817:PRO:HG3	5:B:869:VAL:HG23	1.99	0.44
10:G:59:VAL:O	10:G:59:VAL:HG13	2.18	0.44
4:A:48:HIS:HA	22:V:55:TYR:CZ	2.49	0.44
4:A:875:LEU:HD23	4:A:1303:ILE:HG21	1.99	0.44
16:M:276:LEU:O	16:M:281:GLN:NE2	2.50	0.44
5:B:986:LYS:HB3	5:B:1001:TYR:HB2	2.00	0.44
6:C:120:ARG:NH1	6:C:324:GLU:OE2	2.43	0.44
19:P:96:TYR:HA	19:P:99:ILE:HB	1.99	0.44
19:P:99:ILE:HD13	19:P:136:ILE:HG21	1.99	0.44
20:Q:89:LYS:HA	20:Q:92:MET:HG2	1.99	0.44
24:X:-57:DA:H2	25:Y:58:DA:H2	1.65	0.44
24:X:-45:DT:H2''	24:X:-44:DT:C5	2.52	0.44
4:A:1186:TYR:C	4:A:1188:VAL:H	2.21	0.44
6:C:57:ASP:N	6:C:57:ASP:OD1	2.49	0.44
7:D:22:ASP:O	7:D:25:GLU:HG3	2.17	0.44
7:D:44:THR:O	7:D:48:GLU:HG2	2.17	0.44
18:O:45:THR:OG1	18:O:49:GLN:OE1	2.35	0.44
20:Q:83:ASP:OD1	20:Q:83:ASP:N	2.51	0.44
24:X:-35:DT:H2'	24:X:-34:DT:C6	2.53	0.44
25:Y:52:DC:H2''	25:Y:53:DA:C8	2.53	0.44
2:3:234:THR:O	2:3:234:THR:CG2	2.59	0.44
4:A:623:GLN:HG2	4:A:636:SER:HB2	2.00	0.44
6:C:96:ASN:HA	15:L:48:ARG:HD3	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:19:GLN:OE1	8:E:138:ASN:ND2	2.51	0.44
16:M:8:PRO:HG3	17:N:330:LEU:HD23	2.00	0.44
22:V:20:HIS:CG	22:V:21:TYR:H	2.35	0.44
25:Y:63:DA:H2''	25:Y:64:DA:C8	2.53	0.44
4:A:1328:LEU:HD13	5:B:1117:LEU:HD21	1.99	0.44
5:B:364:LEU:HD21	5:B:502:ILE:HD12	1.99	0.44
5:B:674:TYR:HB3	5:B:677:HIS:CD2	2.51	0.44
22:V:132:PRO:HG2	22:V:175:THR:HG21	1.98	0.44
25:Y:32:DC:H2''	25:Y:33:DC:C5	2.53	0.44
5:B:105:ARG:NH2	5:B:873:SER:O	2.50	0.44
25:Y:-10:DA:H2''	25:Y:-9:DA:C8	2.53	0.44
4:A:41:LEU:HD22	4:A:56:LEU:HD12	1.99	0.43
4:A:529:LEU:HD12	4:A:668:LEU:HD13	1.98	0.43
4:A:879:LEU:HD12	4:A:1038:ALA:HB2	2.00	0.43
4:A:1131:LYS:HE2	4:A:1172:VAL:HG22	1.99	0.43
4:A:1185:MET:HG2	4:A:1187:TYR:H	1.83	0.43
5:B:91:PHE:O	22:V:175:THR:HG22	2.19	0.43
6:C:291:GLU:HA	6:C:294:LYS:HE2	1.99	0.43
7:D:95:VAL:HG11	10:G:198:LEU:HD22	2.00	0.43
15:L:37:ARG:O	15:L:38:GLU:HG2	2.18	0.43
2:3:86:VAL:HG12	2:3:91:ASP:HB2	2.00	0.43
3:4:474:GLY:H	3:4:479:ILE:HD11	1.83	0.43
4:A:743:THR:HG23	4:A:746:GLU:H	1.82	0.43
5:B:183:GLN:NE2	5:B:363:GLU:OE2	2.51	0.43
7:D:94:ALA:O	7:D:98:GLN:HG2	2.19	0.43
10:G:39:VAL:HB	10:G:42:VAL:HB	1.98	0.43
16:M:6:ASP:OD1	16:M:6:ASP:N	2.51	0.43
21:U:263:ASP:HA	21:U:309:LYS:HA	2.00	0.43
24:X:-27:DA:H2'	24:X:-26:DT:C4	2.53	0.43
25:Y:-12:DC:H2''	25:Y:-11:DG:H5'	2.00	0.43
1:1:28:ASP:OD1	1:1:29:PHE:N	2.50	0.43
2:3:100:LEU:O	2:3:103:VAL:HG22	2.18	0.43
3:4:346:ARG:HE	3:4:381:GLY:HA3	1.83	0.43
4:A:258:PRO:HB2	4:A:262:ILE:HD12	2.00	0.43
4:A:1092:ASP:HB2	4:A:1222:LYS:HB2	2.00	0.43
8:E:50:GLU:OE2	8:E:56:THR:OG1	2.36	0.43
8:E:50:GLU:HG2	8:E:55:ARG:HH21	1.84	0.43
2:3:49:GLU:OE1	2:3:49:GLU:N	2.51	0.43
4:A:41:LEU:HD12	4:A:42:TYR:N	2.34	0.43
4:A:569:ALA:HB2	14:K:67:PHE:HZ	1.82	0.43
4:A:814:GLU:HB2	5:B:639:ASN:HD21	1.83	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:233:ASP:N	5:B:233:ASP:OD1	2.51	0.43
5:B:538:LEU:HD23	5:B:548:VAL:HG12	1.99	0.43
10:G:105:ASP:OD1	10:G:105:ASP:N	2.51	0.43
22:V:281:ALA:O	22:V:284:ARG:HG2	2.19	0.43
2:3:313:HIS:NE2	2:3:317:CYS:SG	2.84	0.43
4:A:324:GLU:OE2	4:A:337:TRP:NE1	2.46	0.43
4:A:526:LYS:HB3	4:A:673:GLN:HB3	2.00	0.43
4:A:1107:LYS:HG3	4:A:1200:VAL:CG2	2.49	0.43
4:A:1118:GLU:OE1	12:I:39:THR:OG1	2.29	0.43
5:B:478:MET:HB3	5:B:592:LEU:HD13	2.00	0.43
6:C:144:VAL:HG21	6:C:168:VAL:HG13	1.99	0.43
10:G:53:LYS:HB3	10:G:71:HIS:HB2	2.01	0.43
22:V:147:ASP:HA	23:W:294:PHE:HE1	1.83	0.43
24:X:-36:DC:H2'	24:X:-35:DT:C6	2.53	0.43
2:3:155:PHE:CD1	3:4:366:VAL:HG11	2.54	0.43
2:3:281:HIS:CE1	22:V:187:PRO:HG2	2.54	0.43
24:X:-69:DT:H2''	24:X:-68:DA:N7	2.34	0.43
4:A:1117:ILE:HG23	4:A:1130:VAL:HG22	2.01	0.43
15:L:34:ILE:O	15:L:42:ARG:NH1	2.51	0.43
16:M:36:SER:OG	16:M:37:MET:SD	2.63	0.43
18:O:159:ARG:NH1	18:O:186:ASP:OD2	2.51	0.43
3:4:473:VAL:HB	3:4:475:HIS:CD2	2.54	0.43
5:B:516:SER:HB2	16:M:113:ARG:HH12	1.82	0.43
5:B:903:GLN:HG3	5:B:942:LYS:HE3	2.00	0.43
6:C:166:HIS:CD2	6:C:167:LYS:HG3	2.53	0.43
12:I:74:HIS:HB2	12:I:97:CYS:SG	2.58	0.43
2:3:297:THR:CG2	2:3:298:PHE:H	2.32	0.43
3:4:434:ARG:HB3	3:4:439:CYS:SG	2.59	0.43
5:B:106:ASP:OD1	5:B:882:LYS:NZ	2.40	0.43
5:B:385:LYS:HE3	5:B:385:LYS:HB3	1.90	0.43
5:B:819:GLU:HG3	15:L:49:THR:HG21	2.01	0.43
6:C:74:ASN:OD1	6:C:77:ARG:NH2	2.46	0.43
7:D:4:LYS:HB2	10:G:6:GLU:HB2	2.01	0.43
8:E:27:LEU:HB2	8:E:64:HIS:HB3	2.01	0.43
10:G:94:PRO:HA	10:G:121:ASP:HB2	2.00	0.43
16:M:117:ALA:HB3	17:N:267:LEU:HB2	2.01	0.43
19:P:201:ASN:HB3	19:P:204:ILE:HB	2.01	0.43
24:X:-24:DT:H4'	24:X:-23:DA:H5'	2.01	0.43
24:X:4:DC:H2''	24:X:5:DT:C6	2.54	0.43
4:A:76:LEU:O	5:B:1033:ARG:NH2	2.52	0.43
4:A:282:LYS:HZ1	4:A:319:LEU:HB2	1.84	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1153:ILE:HG22	4:A:1154:CYS:H	1.83	0.43
4:A:1316:LEU:HD12	4:A:1345:GLU:HB3	2.01	0.43
5:B:287:ILE:O	5:B:291:VAL:HG23	2.19	0.43
5:B:333:ILE:HG21	5:B:523:VAL:HG21	2.01	0.43
6:C:155:ASP:N	6:C:155:ASP:OD1	2.48	0.43
8:E:24:ARG:NH2	8:E:181:ARG:O	2.52	0.43
10:G:187:VAL:CG1	10:G:188:GLY:N	2.82	0.43
19:P:45:ILE:O	19:P:50:ARG:NH1	2.52	0.43
25:Y:27:DT:H2''	25:Y:28:DA:H5'	1.99	0.43
4:A:344:ARG:HH21	4:A:351:ARG:HH21	1.66	0.42
4:A:876:VAL:HG11	5:B:1053:ASP:CG	2.40	0.42
5:B:540:PHE:CE2	5:B:545:ILE:HG12	2.54	0.42
5:B:1091:TRP:CG	10:G:162:PRO:HG3	2.54	0.42
12:I:74:HIS:HD2	12:I:99:ASN:HD22	1.67	0.42
19:P:146:LYS:NZ	24:X:-12:DA:N3	2.62	0.42
24:X:-11:DG:H2'	24:X:-10:DG:C8	2.54	0.42
4:A:758:VAL:HG13	4:A:762:HIS:CE1	2.54	0.42
5:B:80:ILE:HD11	5:B:113:ILE:CG2	2.48	0.42
20:Q:42:ASP:OD1	20:Q:42:ASP:N	2.50	0.42
4:A:756:LEU:HD21	4:A:828:PRO:HB3	2.01	0.42
5:B:741:VAL:HG21	5:B:1009:TYR:CE1	2.54	0.42
10:G:116:GLN:O	10:G:118:ALA:N	2.45	0.42
17:N:253:GLU:O	17:N:256:ARG:HG3	2.19	0.42
19:P:292:VAL:HG22	19:P:295:ASP:HB2	2.00	0.42
2:3:60:ASP:HA	2:3:331:HIS:HB3	2.02	0.42
2:3:191:ILE:HB	3:4:176:PHE:CE2	2.36	0.42
5:B:122:GLY:O	5:B:123:SER:OG	2.33	0.42
5:B:446:ILE:HG13	5:B:671:LEU:HD11	2.02	0.42
5:B:536:VAL:O	5:B:581:ARG:NH1	2.52	0.42
5:B:609:LYS:HE3	5:B:609:LYS:HB3	1.92	0.42
5:B:817:PRO:HA	5:B:866:ILE:HB	2.01	0.42
1:1:10:ASP:HB2	2:3:128:VAL:HB	2.01	0.42
4:A:1054:HIS:HD2	4:A:1065:LEU:HD12	1.85	0.42
6:C:290:ASN:O	6:C:294:LYS:HG3	2.20	0.42
20:Q:77:THR:O	20:Q:77:THR:HG23	2.19	0.42
24:X:-49:DA:H2''	24:X:-48:DG:C8	2.54	0.42
24:X:-12:DA:H2''	24:X:-11:DG:O4'	2.18	0.42
5:B:892:GLU:HA	5:B:910:ILE:HD11	2.01	0.42
6:C:23:ASN:O	6:C:303:ARG:NH2	2.52	0.42
19:P:127:LEU:HD13	19:P:150:TYR:CZ	2.54	0.42
4:A:307:MET:HG3	18:O:422:TYR:CE1	2.55	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:454:ARG:HH21	5:B:691:LYS:HD3	1.84	0.42
11:H:39:LEU:HD13	11:H:125:LEU:HD13	2.02	0.42
4:A:289:LEU:HD11	4:A:316:GLN:HG3	2.02	0.42
5:B:163:LEU:HD21	5:B:732:LYS:HD2	2.02	0.42
6:C:112:LEU:HB3	13:J:6:ARG:HG2	2.02	0.42
17:N:276:PRO:HD2	17:N:341:LEU:HD23	2.01	0.42
17:N:346:LEU:HD22	17:N:387:PRO:HA	2.01	0.42
18:O:163:VAL:HG23	18:O:178:PRO:HB2	2.00	0.42
7:D:41:ASN:ND2	10:G:35:ALA:O	2.52	0.42
12:I:95:TYR:CZ	12:I:106:TRP:HB2	2.54	0.42
16:M:88:GLU:HG2	16:M:89:THR:N	2.34	0.42
22:V:124:ILE:O	22:V:128:GLN:HG2	2.20	0.42
24:X:12:DG:H1'	24:X:13:DG:C8	2.55	0.42
1:1:48:ASN:ND2	1:1:49:LEU:H	2.17	0.42
2:3:186:ILE:HA	2:3:320:VAL:O	2.20	0.42
4:A:537:PRO:HG3	4:A:665:TYR:HB2	2.00	0.42
13:J:30:THR:CG2	13:J:31:GLU:N	2.57	0.42
18:O:92:ILE:CG2	20:Q:60:LEU:CD2	2.97	0.42
21:U:169:VAL:HG21	24:X:-27:DA:N3	2.35	0.42
22:V:115:GLU:OE2	22:V:143:TYR:N	2.52	0.42
4:A:221:LEU:HB3	18:O:402:ASN:HD21	1.84	0.41
4:A:389:ILE:HG12	22:V:21:TYR:CD1	2.54	0.41
5:B:125:ARG:HG3	23:W:281:PRO:HA	2.02	0.41
16:M:278:LEU:HD11	16:M:301:LEU:HD13	2.01	0.41
18:O:285:THR:OG1	18:O:286:GLN:N	2.53	0.41
19:P:122:GLU:OE1	19:P:122:GLU:N	2.53	0.41
22:V:86:PRO:HD2	22:V:89:PHE:CD2	2.55	0.41
4:A:74:LYS:HD2	4:A:78:ASP:HB3	2.01	0.41
4:A:86:ILE:HD13	4:A:287:ILE:HD11	2.00	0.41
6:C:49:PHE:HE1	6:C:68:ILE:HB	1.85	0.41
17:N:269:LEU:HD13	17:N:271:LEU:CD2	2.50	0.41
24:X:6:DC:H2'	24:X:7:DG:H8	1.80	0.41
4:A:599:GLN:O	4:A:603:VAL:HG23	2.20	0.41
5:B:324:LYS:HE3	5:B:324:LYS:HB3	1.92	0.41
5:B:751:ILE:HG22	5:B:752:GLU:HG3	2.01	0.41
5:B:833:PRO:HG3	5:B:851:TYR:CE1	2.56	0.41
18:O:453:GLU:HA	18:O:456:GLU:HG2	2.02	0.41
24:X:-16:DG:N2	25:Y:17:DA:N3	2.68	0.41
22:V:283:LEU:HD22	22:V:288:LEU:HD11	2.01	0.41
1:1:42:PHE:HE2	1:1:90:LEU:HD22	1.84	0.41
2:3:372:ALA:HB1	2:3:377:CYS:SG	2.60	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:365:ARG:HG3	3:4:370:ILE:HG13	2.01	0.41
3:4:446:ARG:HB3	3:4:447:LEU:HD12	2.02	0.41
4:A:143:LYS:HB2	4:A:239:LEU:HG	2.03	0.41
4:A:1295:THR:HG22	4:A:1300:VAL:HG22	2.00	0.41
5:B:177:VAL:HG21	5:B:440:LEU:HD13	2.03	0.41
25:Y:-15:DT:H2''	25:Y:-14:DG:N7	2.35	0.41
1:1:83:TYR:O	1:1:87:ASN:ND2	2.35	0.41
4:A:208:GLU:HB3	4:A:209:PRO:HD3	2.01	0.41
4:A:329:PRO:HD2	4:A:332:MET:HB2	2.03	0.41
4:A:430:ARG:HA	22:V:33:CYS:HA	2.02	0.41
4:A:872:GLN:OE1	4:A:1042:GLY:HA3	2.20	0.41
5:B:633:LEU:HD11	5:B:656:HIS:CD2	2.55	0.41
5:B:635:VAL:HA	5:B:638:GLU:HG2	2.03	0.41
8:E:146:PRO:HD2	8:E:148:HIS:HE1	1.85	0.41
11:H:17:PRO:HG2	11:H:29:HIS:CE1	2.55	0.41
13:J:40:LEU:HD11	13:J:49:LEU:HD12	2.01	0.41
16:M:179:ARG:NE	19:P:115:LYS:O	2.53	0.41
19:P:146:LYS:HD3	24:X:-12:DA:H1'	2.02	0.41
21:U:304:ILE:HD13	21:U:332:LEU:HD21	2.02	0.41
23:W:332:ARG:HH21	23:W:336:GLU:HB3	1.85	0.41
2:3:221:CYS:O	2:3:224:ASP:CG	2.58	0.41
3:4:360:LEU:O	3:4:364:MET:HG2	2.20	0.41
4:A:602:SER:HB2	4:A:644:GLU:HA	2.03	0.41
7:D:79:THR:HG23	7:D:82:GLU:H	1.84	0.41
8:E:47:LYS:HE3	8:E:47:LYS:HB3	1.90	0.41
10:G:46:ILE:HB	10:G:75:VAL:HG23	2.02	0.41
20:Q:40:ASP:OD1	20:Q:40:ASP:N	2.53	0.41
2:3:350:TRP:NE1	24:X:-50:DA:H5'	2.36	0.41
5:B:989:VAL:HG21	5:B:1002:ILE:HB	2.03	0.41
12:I:72:CYS:O	12:I:74:HIS:ND1	2.53	0.41
18:O:88:TYR:O	18:O:92:ILE:HG12	2.21	0.41
24:X:-29:DT:H6	24:X:-29:DT:H2'	1.71	0.41
25:Y:30:DA:H2'	25:Y:31:DG:C8	2.56	0.41
3:4:216:HIS:O	3:4:219:GLN:HG3	2.21	0.41
4:A:360:ARG:HE	5:B:1037:GLU:HG2	1.85	0.41
4:A:492:VAL:O	4:A:495:PRO:HD2	2.21	0.41
4:A:533:ARG:HH11	4:A:1044:PRO:HG3	1.84	0.41
4:A:688:PRO:HB3	5:B:748:GLY:HA3	2.02	0.41
4:A:1237:ALA:HB1	8:E:136:LEU:HD12	2.03	0.41
4:A:1368:ARG:HH12	10:G:56:ASP:HA	1.86	0.41
6:C:79:ILE:HD13	6:C:83:GLU:HG3	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:48:ASP:N	14:K:48:ASP:OD1	2.54	0.41
18:O:228:ILE:HB	18:O:231:ASP:HB2	2.03	0.41
19:P:88:SER:OG	19:P:91:GLN:OE1	2.31	0.41
25:Y:-9:DA:H2''	25:Y:-8:DG:C8	2.56	0.41
2:3:146:ILE:HG21	3:4:425:PHE:HB3	2.03	0.41
2:3:150:CYS:HB2	2:3:153:GLU:HB2	2.03	0.41
3:4:436:ASP:OD1	3:4:437:ALA:N	2.54	0.41
3:4:457:ASN:HD22	3:4:459:LYS:H	1.68	0.41
5:B:633:LEU:HD11	5:B:656:HIS:CG	2.56	0.41
10:G:151:ARG:HB2	10:G:189:SER:OG	2.20	0.41
16:M:54:GLN:HE22	16:M:131:GLY:HA3	1.86	0.41
24:X:-27:DA:H2'	24:X:-26:DT:C5	2.56	0.41
4:A:336:LYS:NZ	22:V:51:ARG:HD3	2.36	0.40
4:A:1149:VAL:O	4:A:1153:ILE:HG13	2.20	0.40
5:B:1064:LEU:HD12	5:B:1068:LEU:HD13	2.03	0.40
13:J:10:CYS:SG	13:J:11:GLY:N	2.94	0.40
19:P:129:ASN:O	19:P:132:SER:OG	2.32	0.40
24:X:-68:DA:H2''	24:X:-67:DT:C6	2.56	0.40
24:X:-22:DT:H2''	24:X:-21:DC:C5	2.56	0.40
1:1:66:PHE:O	1:1:75:ARG:NH2	2.54	0.40
2:3:356:VAL:HG22	3:4:331:PHE:HE1	1.86	0.40
3:4:171:GLN:HE21	3:4:173:ILE:HD11	1.86	0.40
4:A:306:ILE:HG13	18:O:396:TYR:CZ	2.56	0.40
4:A:902:TYR:CZ	4:A:1285:ARG:HB3	2.56	0.40
4:A:1355:ILE:HD11	5:B:1056:ILE:HG23	2.01	0.40
6:C:258:SER:HB3	6:C:261:VAL:HG12	2.04	0.40
10:G:116:GLN:HE22	10:G:118:ALA:HB3	1.85	0.40
16:M:11:GLN:HE22	17:N:258:LEU:HD23	1.87	0.40
21:U:174:LEU:HD22	21:U:248:ALA:HB1	2.03	0.40
21:U:309:LYS:HD2	25:Y:30:DA:H5''	2.04	0.40
5:B:106:ASP:HA	5:B:173:GLY:HA3	2.04	0.40
5:B:179:LEU:HD22	5:B:454:ARG:HB2	2.04	0.40
16:M:120:ARG:HB2	16:M:123:GLU:HG2	2.02	0.40
18:O:492:THR:O	18:O:496:ARG:HG3	2.20	0.40
18:O:496:ARG:HA	18:O:499:LEU:HD12	2.03	0.40
25:Y:49:DT:H2'	25:Y:50:DT:H71	2.03	0.40
4:A:23:LYS:HE3	5:B:1123:ILE:HG21	2.03	0.40
4:A:864:LYS:NZ	4:A:1048:MET:O	2.49	0.40
5:B:483:ASP:OD1	5:B:691:LYS:NZ	2.41	0.40
8:E:82:VAL:HB	8:E:110:MET:SD	2.62	0.40
16:M:20:SER:OG	16:M:224:TYR:O	2.32	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:310:GLN:HA	18:O:313:THR:HG22	2.04	0.40
4:A:731:LEU:HD23	4:A:748:LEU:HD22	2.02	0.40
4:A:882:LEU:HD11	4:A:898:ILE:HG13	2.02	0.40
4:A:1233:ARG:HG2	8:E:133:GLN:HG2	2.03	0.40
7:D:117:LEU:HA	7:D:120:VAL:HG12	2.04	0.40
11:H:7:GLU:HG3	11:H:59:VAL:HG22	2.04	0.40
16:M:314:ILE:HG12	16:M:318:ALA:HB3	2.04	0.40
18:O:252:VAL:HG13	18:O:264:SER:HB2	2.03	0.40
19:P:147:LYS:HE2	19:P:147:LYS:HB2	1.89	0.40
22:V:232:LEU:HD23	22:V:232:LEU:HA	1.90	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	1	144/368 (39%)	142 (99%)	2 (1%)	0	100	100
2	3	368/411 (90%)	352 (96%)	15 (4%)	1 (0%)	41	72
3	4	363/1469 (25%)	353 (97%)	10 (3%)	0	100	100
4	A	1376/1390 (99%)	1350 (98%)	26 (2%)	0	100	100
5	B	1091/1133 (96%)	1062 (97%)	29 (3%)	0	100	100
6	C	341/346 (99%)	336 (98%)	5 (2%)	0	100	100
7	D	120/148 (81%)	115 (96%)	5 (4%)	0	100	100
8	E	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
9	F	74/127 (58%)	72 (97%)	2 (3%)	0	100	100
10	G	160/204 (78%)	144 (90%)	16 (10%)	0	100	100
11	H	146/150 (97%)	145 (99%)	1 (1%)	0	100	100
12	I	105/108 (97%)	98 (93%)	7 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	J	63/67 (94%)	62 (98%)	1 (2%)	0	100	100
14	K	101/133 (76%)	97 (96%)	4 (4%)	0	100	100
15	L	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
16	M	418/708 (59%)	405 (97%)	13 (3%)	0	100	100
17	N	140/317 (44%)	139 (99%)	1 (1%)	0	100	100
18	O	508/534 (95%)	497 (98%)	11 (2%)	0	100	100
19	P	301/316 (95%)	296 (98%)	5 (2%)	0	100	100
20	Q	85/223 (38%)	84 (99%)	1 (1%)	0	100	100
21	U	175/339 (52%)	171 (98%)	4 (2%)	0	100	100
22	V	358/419 (85%)	352 (98%)	6 (2%)	0	100	100
23	W	109/2624 (4%)	105 (96%)	4 (4%)	0	100	100
All	All	6797/11802 (58%)	6622 (97%)	174 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	3	341	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	1	130/334 (39%)	130 (100%)	0	100	100
2	3	330/356 (93%)	323 (98%)	7 (2%)	53	76
3	4	321/1213 (26%)	318 (99%)	3 (1%)	78	90
4	A	1200/1212 (99%)	1197 (100%)	3 (0%)	92	97
5	B	959/988 (97%)	959 (100%)	0	100	100
6	C	299/302 (99%)	299 (100%)	0	100	100
7	D	114/136 (84%)	114 (100%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	E	191/192 (100%)	191 (100%)	0	100	100
9	F	66/111 (60%)	66 (100%)	0	100	100
10	G	149/181 (82%)	149 (100%)	0	100	100
11	H	129/131 (98%)	129 (100%)	0	100	100
12	I	92/93 (99%)	92 (100%)	0	100	100
13	J	53/56 (95%)	53 (100%)	0	100	100
14	K	92/119 (77%)	92 (100%)	0	100	100
15	L	43/55 (78%)	43 (100%)	0	100	100
16	M	377/622 (61%)	377 (100%)	0	100	100
17	N	131/276 (48%)	130 (99%)	1 (1%)	81	91
18	O	458/476 (96%)	457 (100%)	1 (0%)	93	98
19	P	269/280 (96%)	268 (100%)	1 (0%)	91	95
20	Q	84/195 (43%)	83 (99%)	1 (1%)	71	85
21	U	152/293 (52%)	152 (100%)	0	100	100
22	V	325/365 (89%)	323 (99%)	2 (1%)	86	94
23	W	102/2381 (4%)	101 (99%)	1 (1%)	76	88
All	All	6066/10367 (58%)	6046 (100%)	20 (0%)	92	97

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	3	47	PHE
2	3	83	ASP
2	3	148	ARG
2	3	167	LYS
2	3	310	LEU
2	3	340	TYR
2	3	386	MET
3	4	152	ASP
3	4	153	LYS
3	4	166	ARG
4	A	136	TYR
4	A	362	ASP
4	A	767	CYS
17	N	156	ARG
18	O	533	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
19	P	93	LYS
20	Q	113	ARG
22	V	55	TYR
22	V	381	ASP
23	W	309	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	48	ASN
1	1	52	ASN
1	1	95	GLN
1	1	111	GLN
1	1	116	ASN
2	3	202	GLN
2	3	226	GLN
2	3	411	ASN
3	4	171	GLN
3	4	229	GLN
3	4	243	GLN
3	4	295	GLN
3	4	312	HIS
3	4	438	GLN
3	4	457	ASN
4	A	119	GLN
4	A	275	ASN
4	A	374	ASN
4	A	415	HIS
4	A	423	GLN
4	A	528	ASN
4	A	599	GLN
4	A	1039	GLN
4	A	1054	HIS
4	A	1213	HIS
4	A	1364	HIS
5	B	395	GLN
5	B	616	GLN
6	C	160	ASN
8	E	108	GLN
8	E	138	ASN
11	H	29	HIS
12	I	83	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	I	99	ASN
12	I	104	HIS
16	M	11	GLN
16	M	197	GLN
18	O	158	GLN
18	O	377	GLN
18	O	402	ASN
18	O	457	ASN
18	O	475	GLN
18	O	497	GLN
19	P	97	GLN
19	P	182	GLN
19	P	201	ASN
19	P	297	HIS
21	U	164	GLN
21	U	166	GLN
21	U	278	GLN
22	V	49	ASN
22	V	206	GLN
22	V	212	ASN
22	V	397	GLN
23	W	279	ASN
23	W	327	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 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 10 ligands modelled in this entry, 9 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
28	SF4	P	401	-	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
28	SF4	P	401	-	-	-	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.

No monomer is involved in short contacts.

## 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.

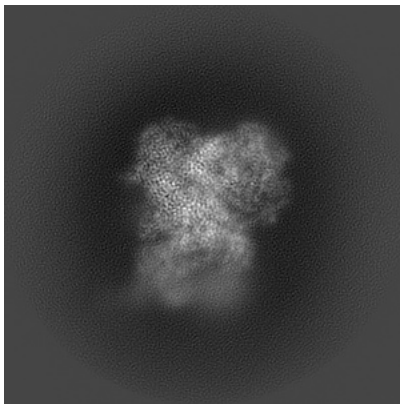
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35722. These allow visual inspection of the internal detail of the map and identification of artifacts.

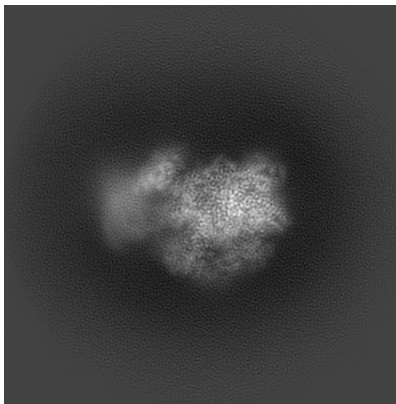
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

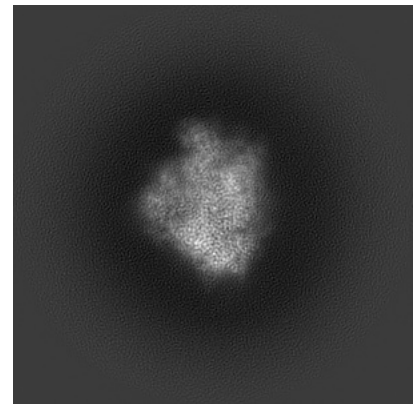
#### 6.1.1 Primary map



X

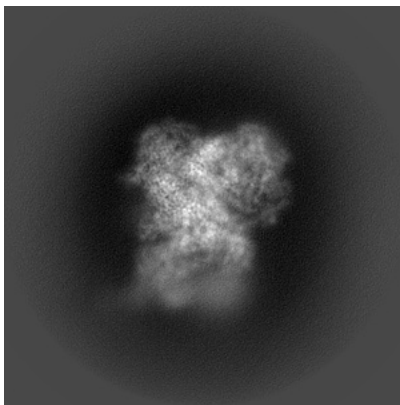


Y

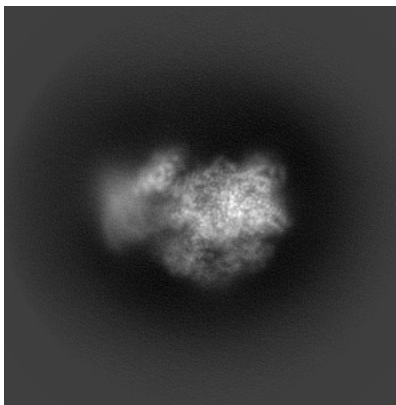


Z

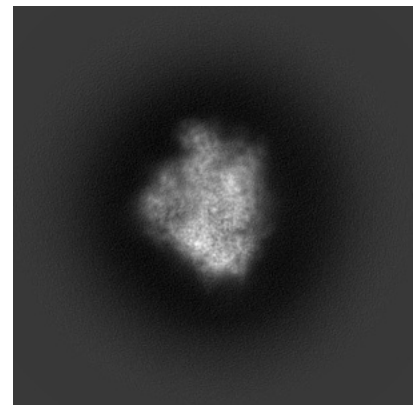
#### 6.1.2 Raw map



X



Y

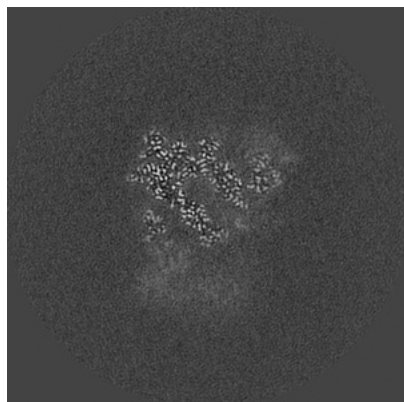


Z

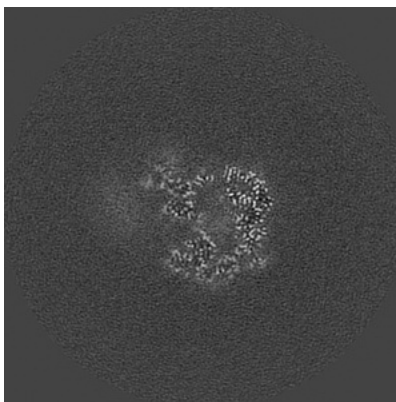
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

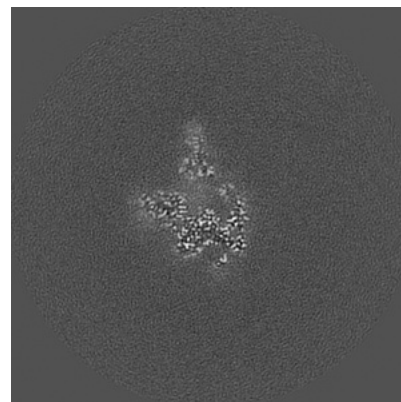
### 6.2.1 Primary map



X Index: 160

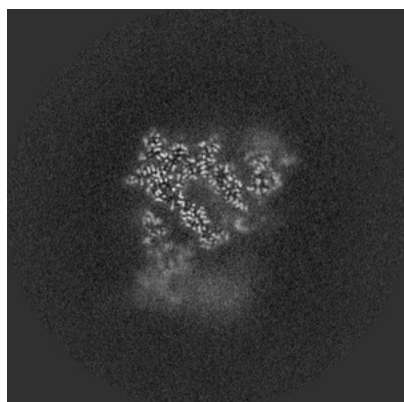


Y Index: 160

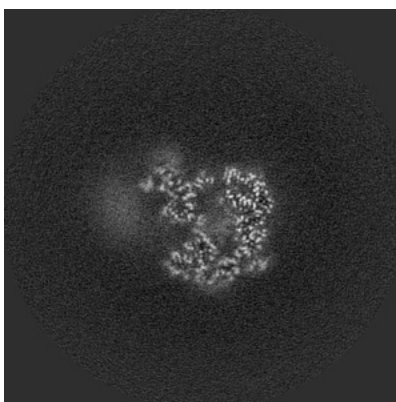


Z Index: 160

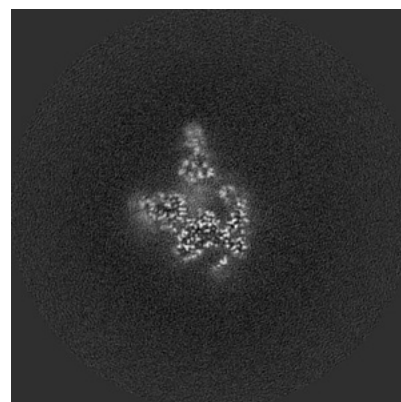
### 6.2.2 Raw map



X Index: 160



Y Index: 160



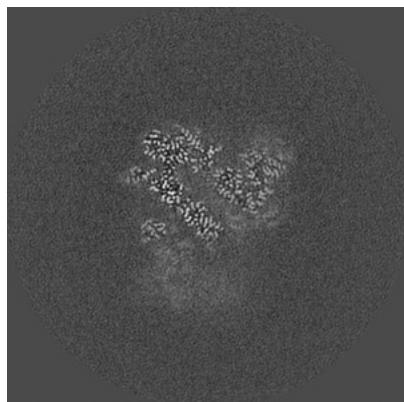
Z Index: 160

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

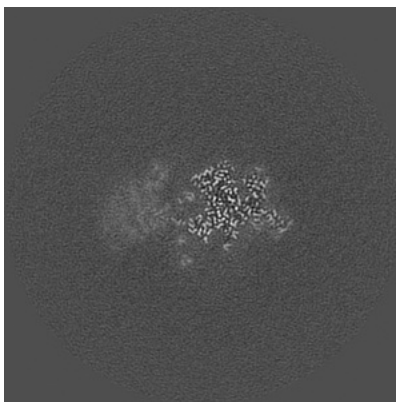


## 6.3 Largest variance slices [i](#)

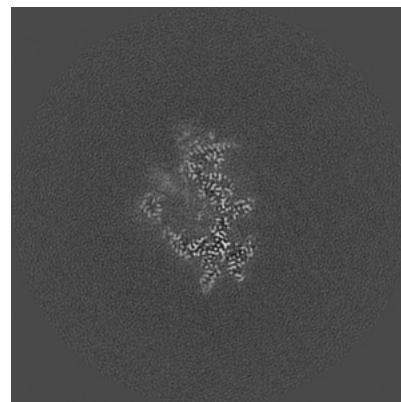
### 6.3.1 Primary map



X Index: 155

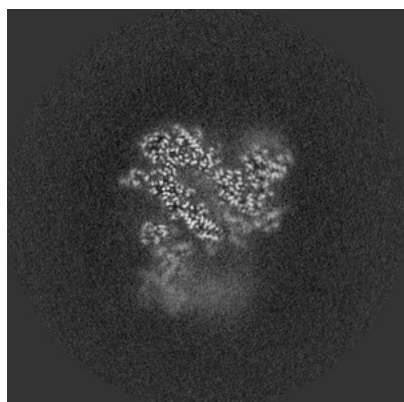


Y Index: 129

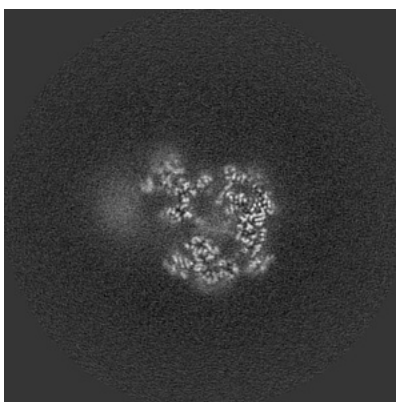


Z Index: 181

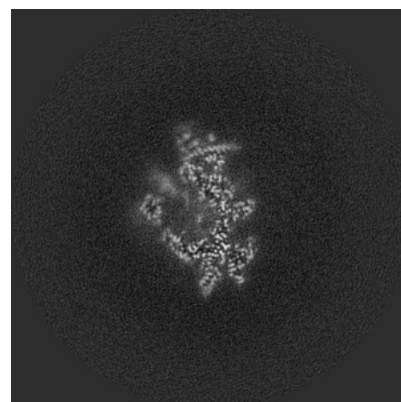
### 6.3.2 Raw map



X Index: 154



Y Index: 162

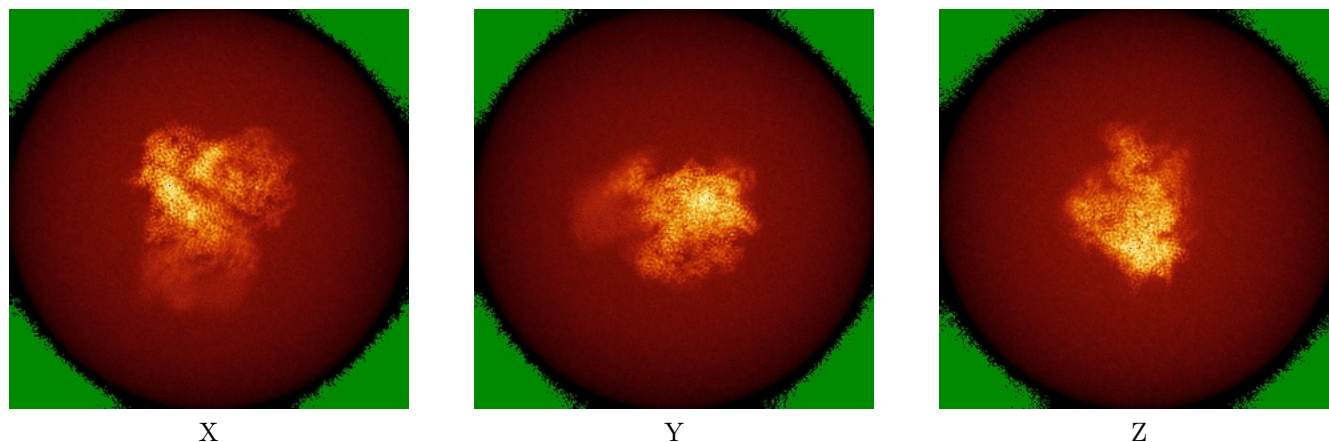


Z Index: 181

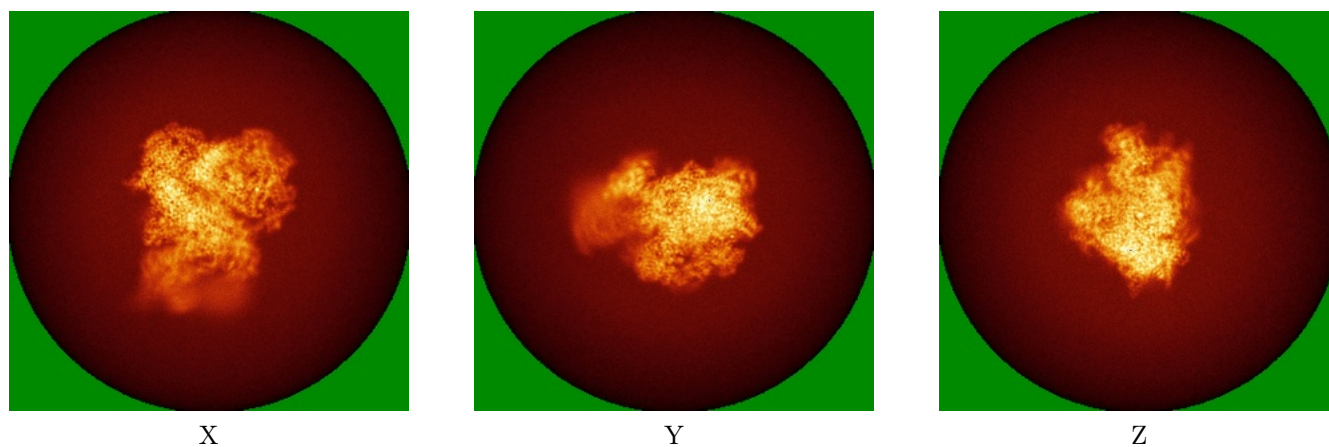
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



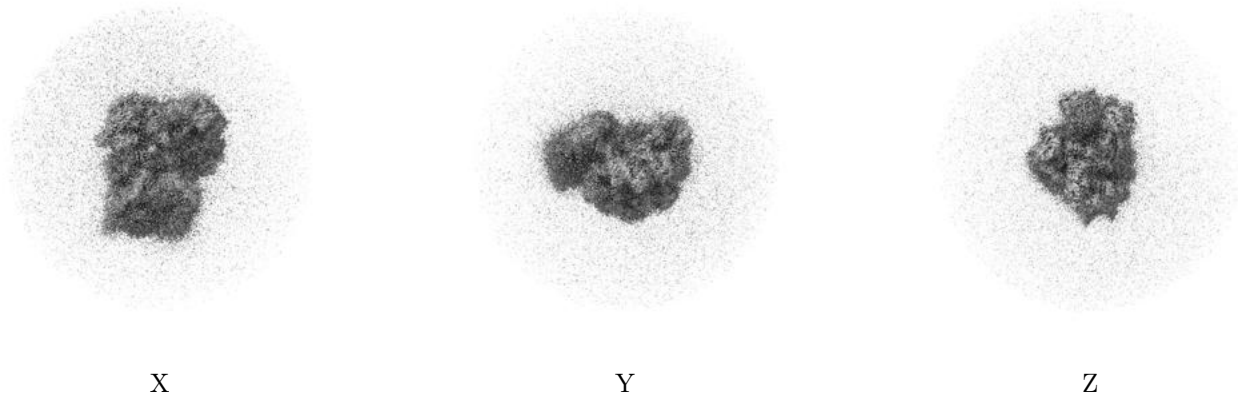
### 6.4.2 Raw map



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.

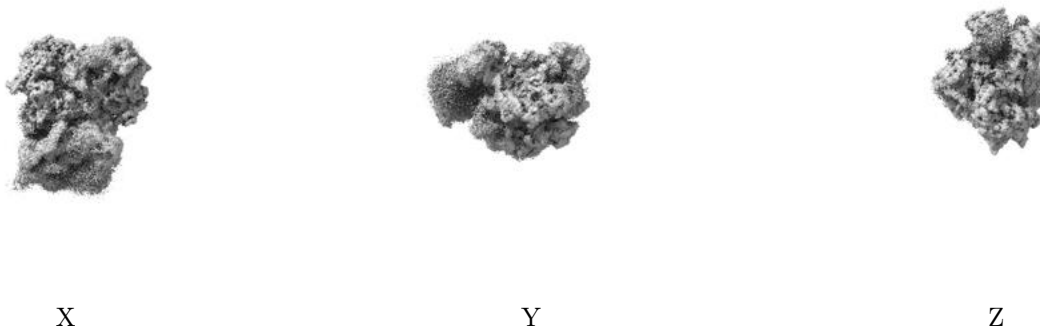
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

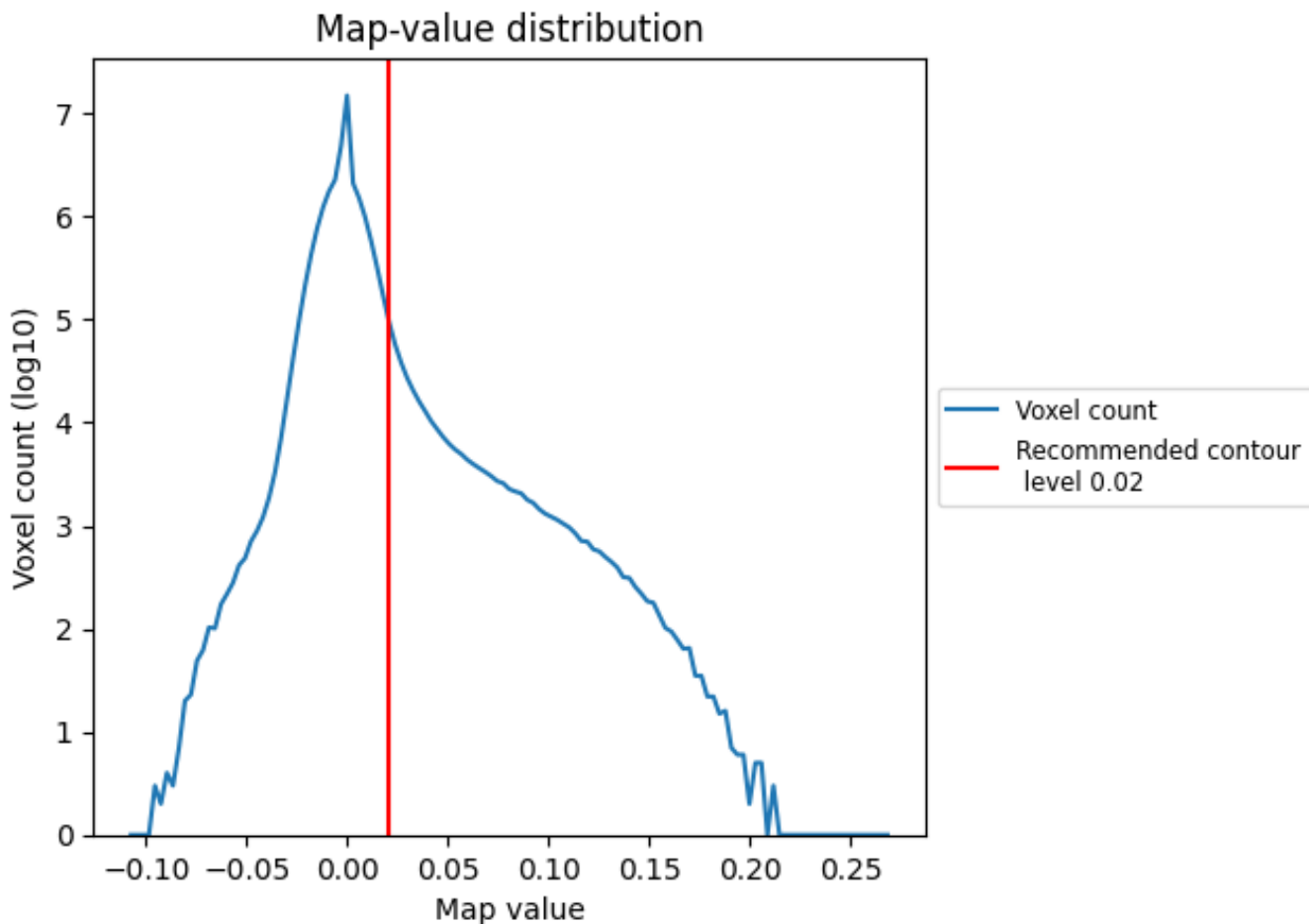
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

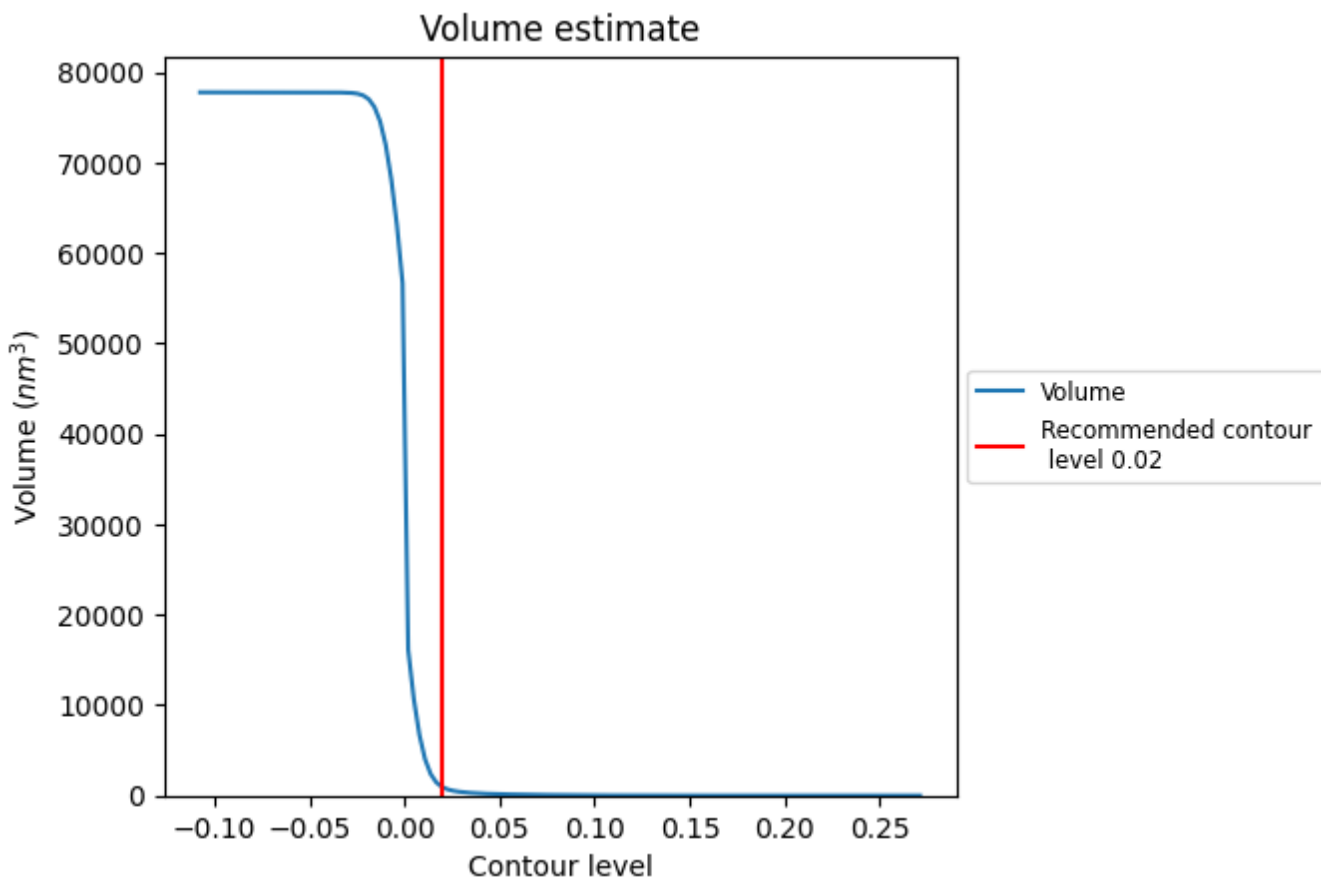
This section contains the results of statistical analysis of the map.

### 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.

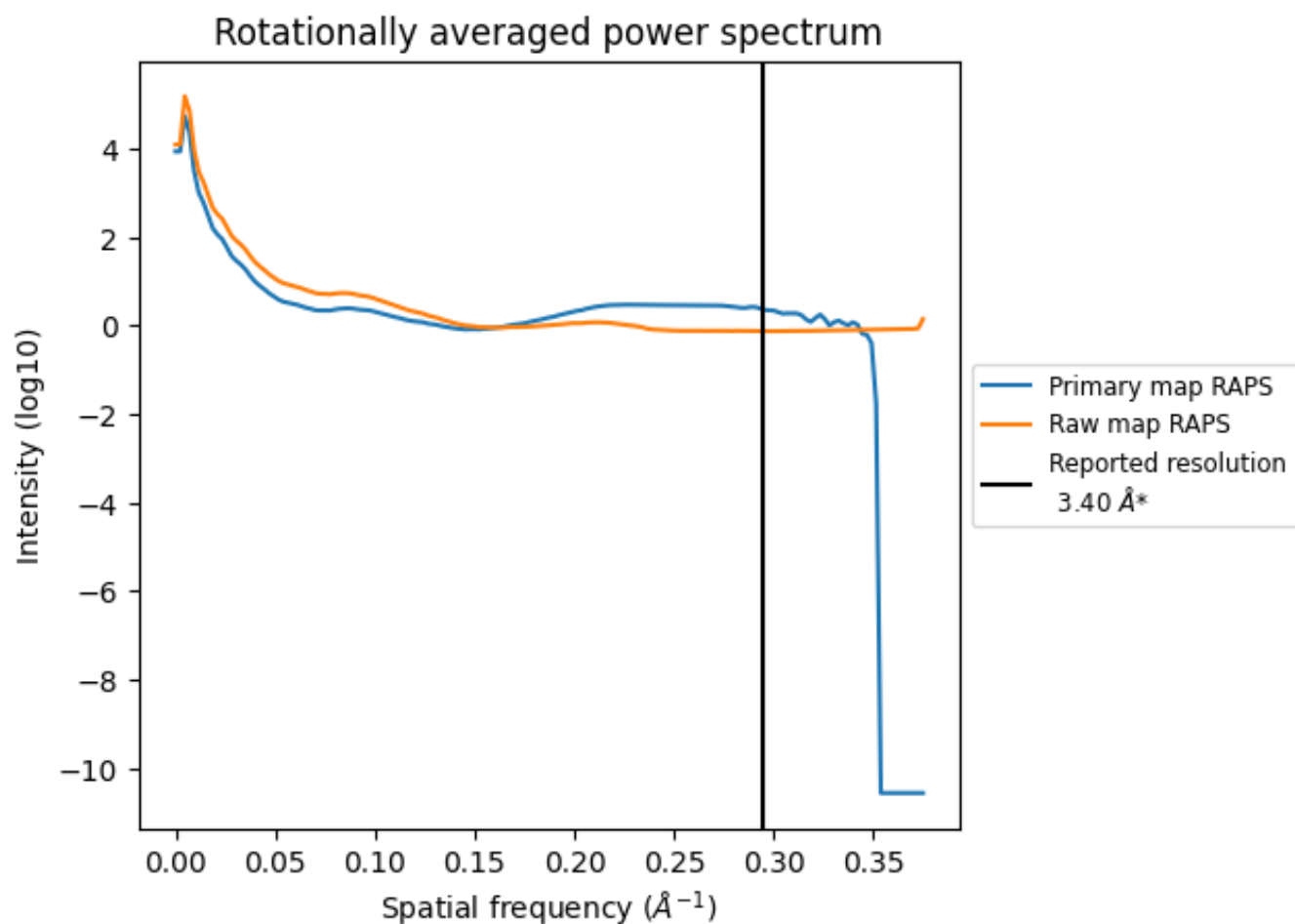
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 931  $\text{nm}^3$ ; this corresponds to an approximate mass of 841 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

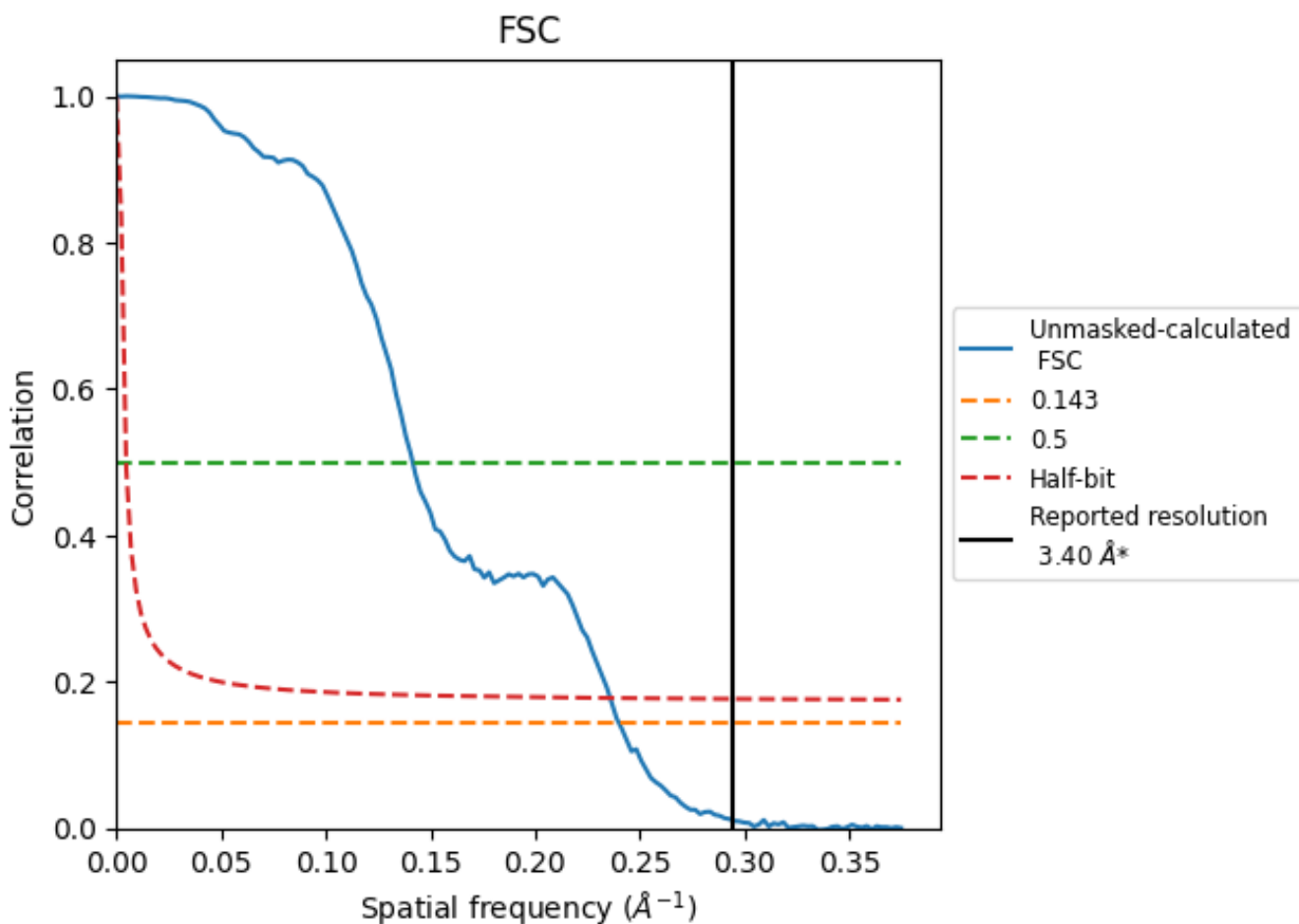


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.16	7.07	4.24

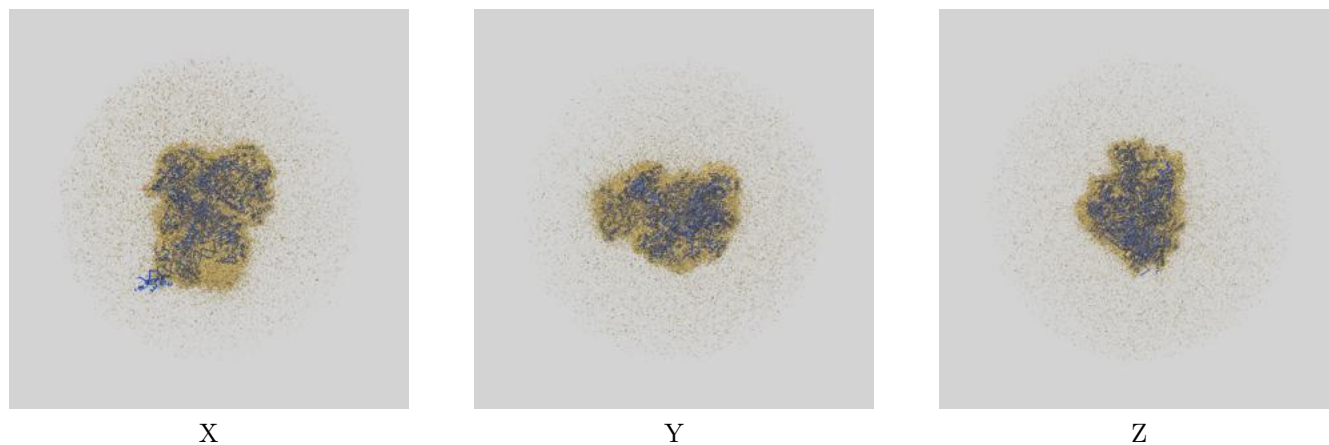
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.16 differs from the reported value 3.4 by more than 10 %



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

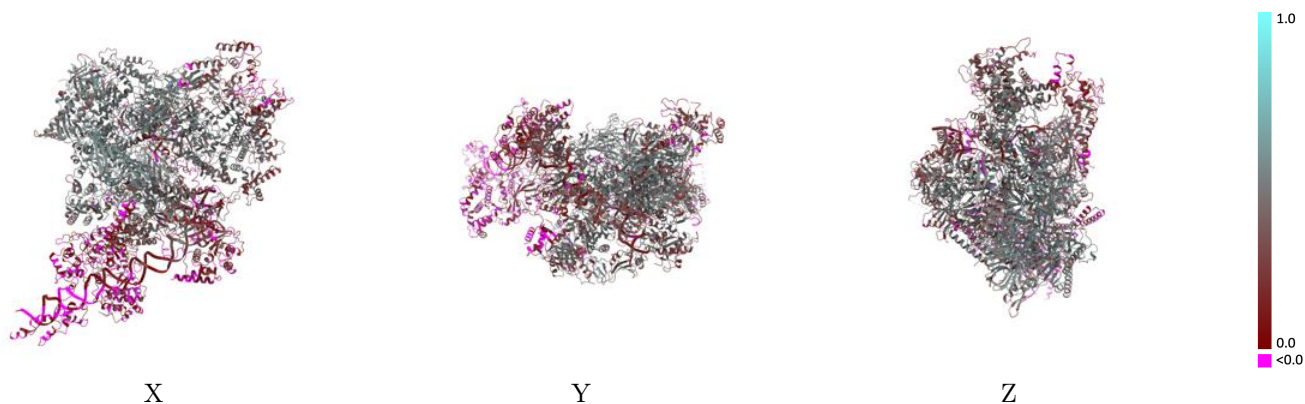
This section contains information regarding the fit between EMDB map EMD-35722 and PDB model 8IUH. Per-residue inclusion information can be found in section 3 on page 11.

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



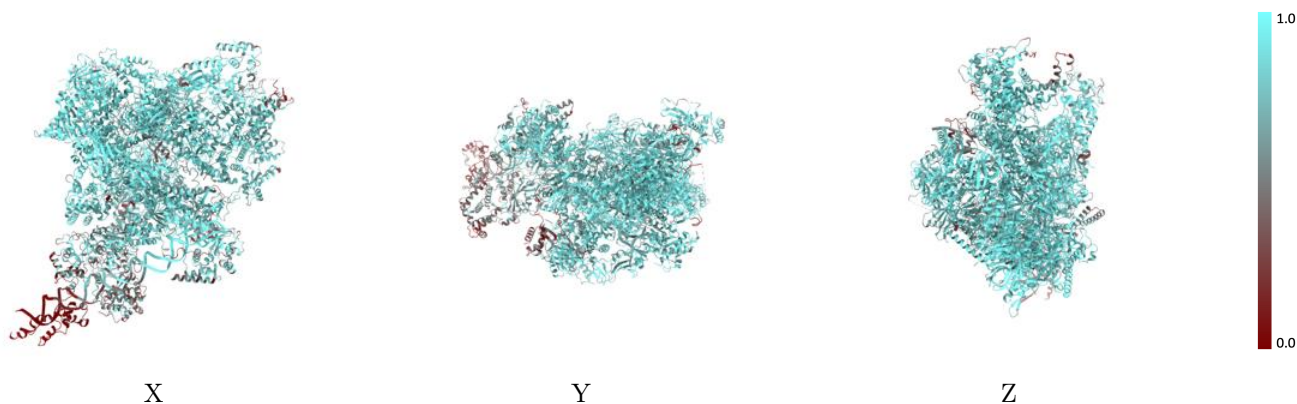
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



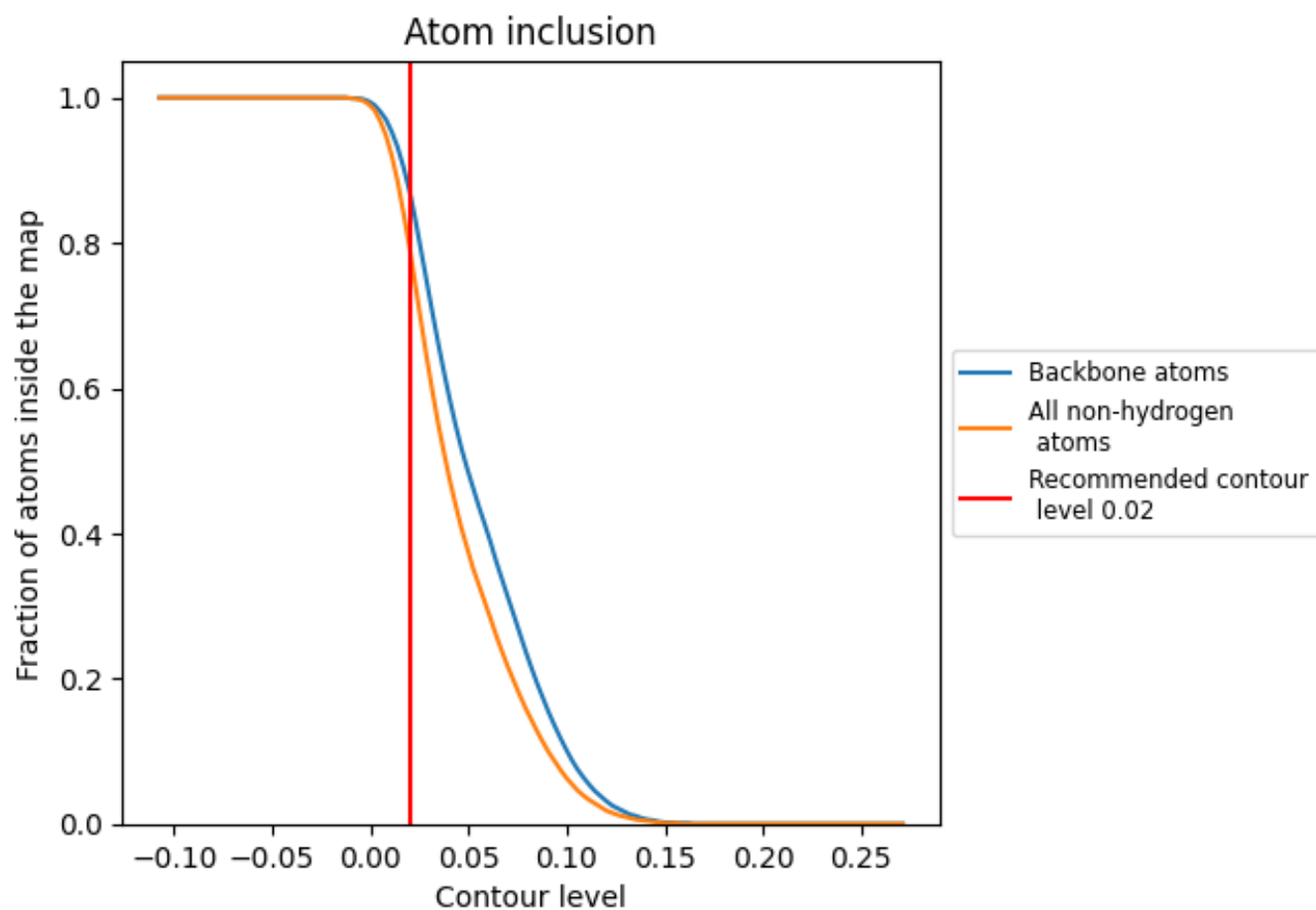
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).





















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 79% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7920	 0.3410
1	 0.4990	 0.0360
3	 0.5890	 0.1040
4	 0.4030	 0.0500
A	 0.8950	 0.4600
B	 0.9140	 0.4830
C	 0.9040	 0.4850
D	 0.7710	 0.2470
E	 0.8480	 0.3780
F	 0.9270	 0.4910
G	 0.8450	 0.3380
H	 0.8590	 0.4510
I	 0.6760	 0.2470
J	 0.9340	 0.5060
K	 0.8920	 0.4660
L	 0.8840	 0.4070
M	 0.8080	 0.3730
N	 0.7700	 0.3590
O	 0.8160	 0.3640
P	 0.6880	 0.2380
Q	 0.7570	 0.2920
U	 0.8210	 0.2440
V	 0.7790	 0.2980
W	 0.6760	 0.1300
X	 0.6490	 0.1050
Y	 0.6490	 0.1450

