



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 05:57 PM UTC

PDB ID : 9J0N / pdb_00009j0n
EMDB ID : EMD-61058
Title : Paused elongation complex of mammalian RNA polymerase II with nucleosome (PEC2-nuc)
Authors : Naganuma, M.; Kujirai, T.; Ehara, H.; Uejima, T.; Ito, T.; Goto, M.; Aoki, M.; Henmi, M.; Miyamoto-Kohno, S.; Shirouzu, M.; Kurumizaka, H.; Sekine, S.
Deposited on : 2024-08-02
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

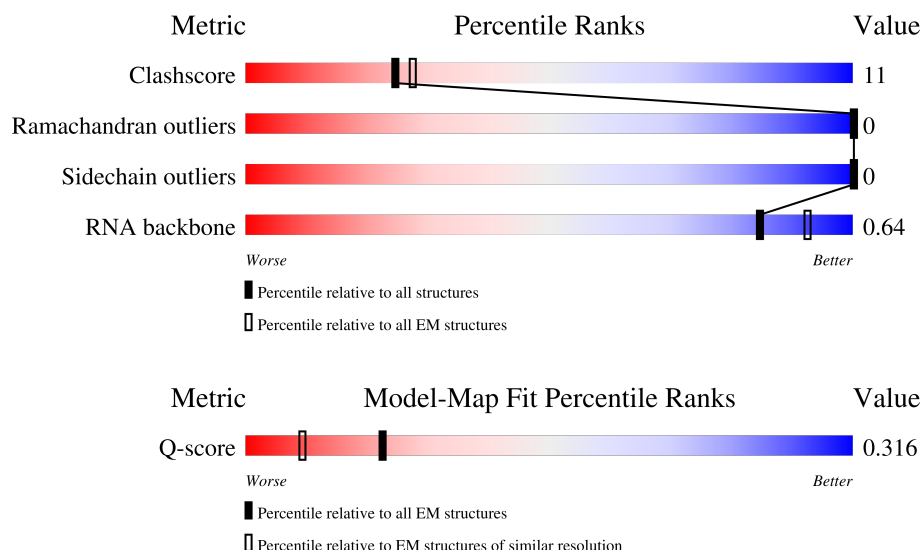
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	A	1970	54% 17% 29%
2	B	1174	75% 20% 5%
3	C	271	75% 20% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	210	
5	F	127	
6	G	172	
7	H	150	
8	I	125	
9	Y	118	
10	Z	1107	
11	N	198	
12	P	42	
13	T	198	
14	D	142	
15	J	67	
16	K	117	
17	L	58	
18	M	301	
19	a	136	
19	e	136	
20	b	103	
20	f	103	
21	c	130	
21	g	130	
22	d	126	
22	h	126	
23	U	528	
24	V	580	

Continued on next page...

Mol	Chain	Length	Quality of chain
25	W	611	30% 64% 25% 11%
26	X	404	7% 91%

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 59666 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 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1394	Total	C	N	O	S	0	0
			11042	6947	1981	2046	68		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1121	Total	C	N	O	S	0	0
			8971	5679	1575	1653	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	258	Total	C	N	O	S	0	0
			2072	1300	356	410	6		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	78	Total	C	N	O	S	0	0
			626	401	106	114	5		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	149	Total	C	N	O	S	0	0
			1197	759	195	238	5		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	116	Total	C	N	O	S	0	0
			942	582	168	181	11		

- Molecule 9 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Y	116	Total	C	N	O	S	0	0
			911	570	159	173	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	0	SER	-	expression tag	UNP P63272

- Molecule 10 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	480	Total	C	N	O	S	0	0
			3837	2439	676	705	17		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	1088	LYS	-	expression tag	UNP O00267
Z	1089	GLU	-	expression tag	UNP O00267
Z	1090	THR	-	expression tag	UNP O00267
Z	1091	ALA	-	expression tag	UNP O00267
Z	1092	ALA	-	expression tag	UNP O00267
Z	1093	ALA	-	expression tag	UNP O00267
Z	1094	LYS	-	expression tag	UNP O00267
Z	1095	PHE	-	expression tag	UNP O00267
Z	1096	GLU	-	expression tag	UNP O00267
Z	1097	ARG	-	expression tag	UNP O00267
Z	1098	GLN	-	expression tag	UNP O00267
Z	1099	HIS	-	expression tag	UNP O00267

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Z	1100	MET	-	expression tag	UNP O00267
Z	1101	ASP	-	expression tag	UNP O00267
Z	1102	SER	-	expression tag	UNP O00267
Z	1103	SER	-	expression tag	UNP O00267
Z	1104	THR	-	expression tag	UNP O00267
Z	1105	SER	-	expression tag	UNP O00267
Z	1106	ALA	-	expression tag	UNP O00267
Z	1107	ALA	-	expression tag	UNP O00267

- Molecule 11 is a DNA chain called Non-template DNA (157-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	156	Total	C	N	O	P	0	0
			3207	1526	559	966	156		

- Molecule 12 is a RNA chain called RNA (5'-R(P*UP*GP*GP*GP*UP*GP*GP*UP*GP*GP*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	12	Total	C	N	O	P	0	0
			261	115	47	87	12		

- Molecule 13 is a DNA chain called Template DNA (168-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	167	Total	C	N	O	P	0	0
			3405	1613	658	968	166		

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	126	Total	C	N	O	S	0	0
			1004	630	170	200	4		

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 16 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 17 is a protein called RPB12.

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

- Molecule 18 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	122	Total	C	N	O	S	0	0
			969	589	181	191	8		

- Molecule 19 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	97	Total	C	N	O	S	0	0
			797	503	155	137	2		
19	e	97	Total	C	N	O	S	0	0
			796	501	155	138	2		

- Molecule 20 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
20	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

- Molecule 21 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	c	103	Total	C	N	O	0	0
			796	502	155	139		
21	g	105	Total	C	N	O	0	0
			810	511	158	141		

- Molecule 22 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	d	95	Total	C	N	O	S	0	0
			746	468	136	140	2		
22	h	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

- Molecule 23 is a protein called Negative elongation factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	187	Total	C	N	O	S	0	0
			1439	912	245	273	9		

- Molecule 24 is a protein called Negative elongation factor B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	542	Total	C	N	O	S	0	0
			4341	2785	736	795	25		

- Molecule 25 is a protein called Negative elongation factor C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	543	Total	C	N	O	S	0	0
			4312	2755	722	811	24		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	591	GLY	-	expression tag	UNP Q8IXH7
W	592	SER	-	expression tag	UNP Q8IXH7
W	593	SER	-	expression tag	UNP Q8IXH7
W	594	GLY	-	expression tag	UNP Q8IXH7
W	595	SER	-	expression tag	UNP Q8IXH7
W	596	SER	-	expression tag	UNP Q8IXH7
W	597	GLY	-	expression tag	UNP Q8IXH7
W	598	LEU	-	expression tag	UNP Q8IXH7
W	599	GLU	-	expression tag	UNP Q8IXH7
W	600	VAL	-	expression tag	UNP Q8IXH7
W	601	LEU	-	expression tag	UNP Q8IXH7
W	602	PHE	-	expression tag	UNP Q8IXH7
W	603	GLN	-	expression tag	UNP Q8IXH7
W	604	GLY	-	expression tag	UNP Q8IXH7
W	605	PRO	-	expression tag	UNP Q8IXH7
W	606	HIS	-	expression tag	UNP Q8IXH7
W	607	HIS	-	expression tag	UNP Q8IXH7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
W	608	HIS	-	expression tag	UNP Q8IXH7
W	609	HIS	-	expression tag	UNP Q8IXH7
W	610	HIS	-	expression tag	UNP Q8IXH7
W	611	HIS	-	expression tag	UNP Q8IXH7

- Molecule 26 is a protein called Negative elongation factor E.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	35	Total	C	N	O	S	0	0
			281	185	48	47	1		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-23	MET	-	initiating methionine	UNP P18615
X	-22	ASP	-	expression tag	UNP P18615
X	-21	TYR	-	expression tag	UNP P18615
X	-20	LYS	-	expression tag	UNP P18615
X	-19	ASP	-	expression tag	UNP P18615
X	-18	ASP	-	expression tag	UNP P18615
X	-17	ASP	-	expression tag	UNP P18615
X	-16	ASP	-	expression tag	UNP P18615
X	-15	LYS	-	expression tag	UNP P18615
X	-14	LEU	-	expression tag	UNP P18615
X	-13	GLU	-	expression tag	UNP P18615
X	-12	VAL	-	expression tag	UNP P18615
X	-11	LEU	-	expression tag	UNP P18615
X	-10	PHE	-	expression tag	UNP P18615
X	-9	GLN	-	expression tag	UNP P18615
X	-8	GLY	-	expression tag	UNP P18615
X	-7	PRO	-	expression tag	UNP P18615
X	-6	GLY	-	expression tag	UNP P18615
X	-5	SER	-	expression tag	UNP P18615
X	-4	SER	-	expression tag	UNP P18615
X	-3	GLY	-	expression tag	UNP P18615
X	-2	SER	-	expression tag	UNP P18615
X	-1	SER	-	expression tag	UNP P18615
X	0	GLY	-	expression tag	UNP P18615

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
27	A	2	Total 2	Zn 2	0
27	B	1	Total 1	Zn 1	0
27	C	1	Total 1	Zn 1	0
27	I	2	Total 2	Zn 2	0
27	Y	1	Total 1	Zn 1	0
27	J	1	Total 1	Zn 1	0
27	L	1	Total 1	Zn 1	0

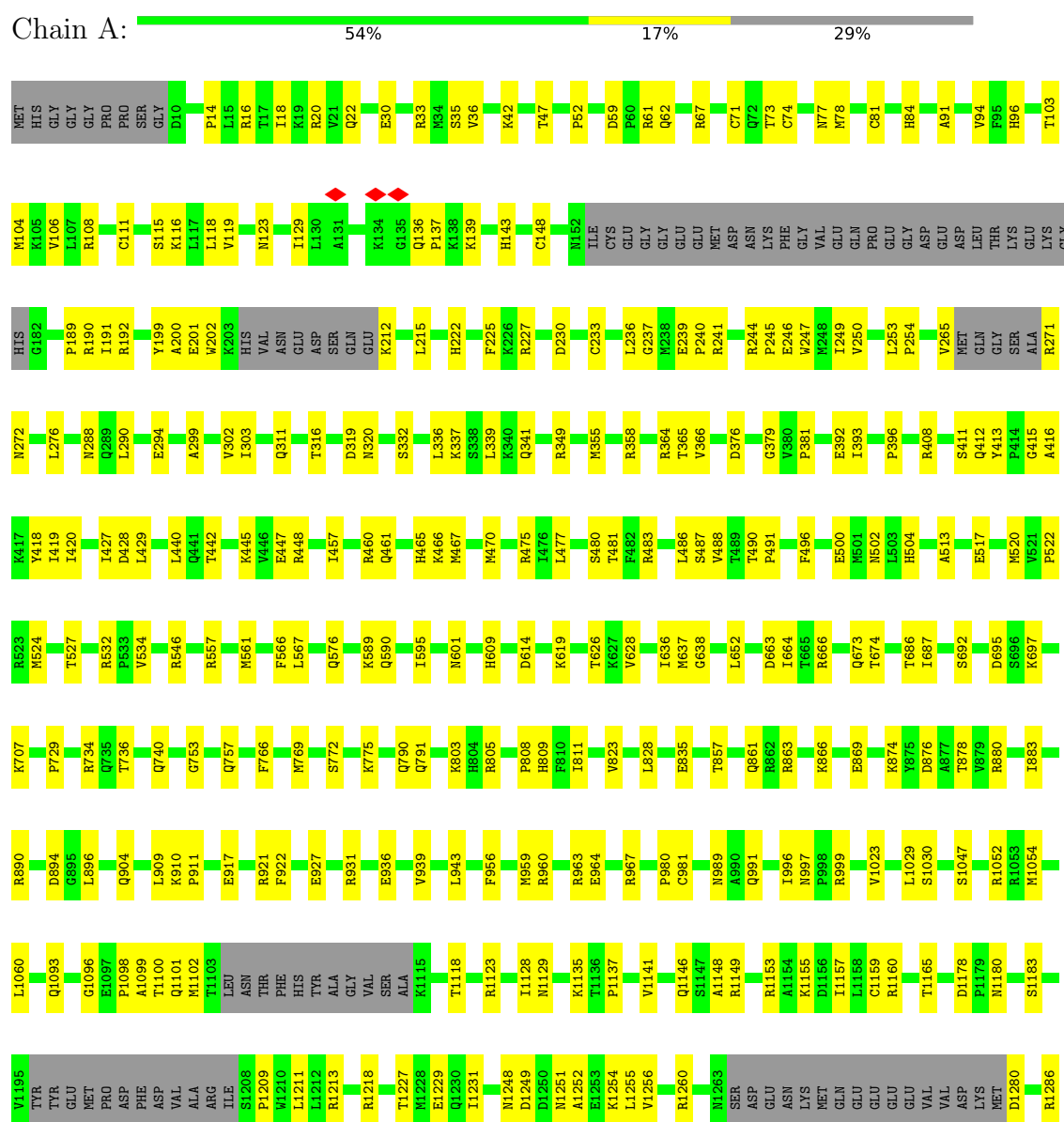
- Molecule 28 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

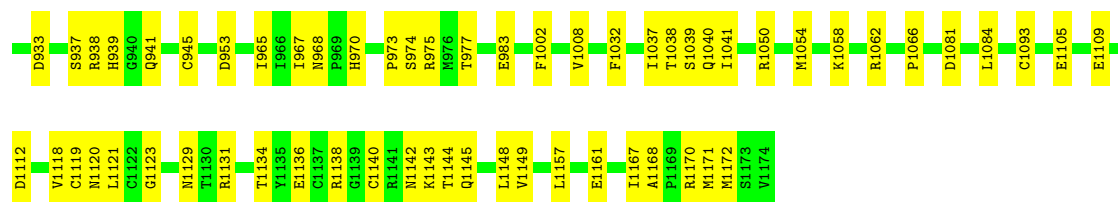
Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total 1	Mg 1	0

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.

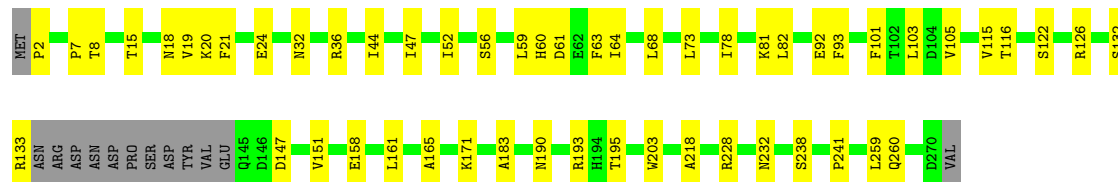
- Molecule 1: DNA-directed RNA polymerase subunit





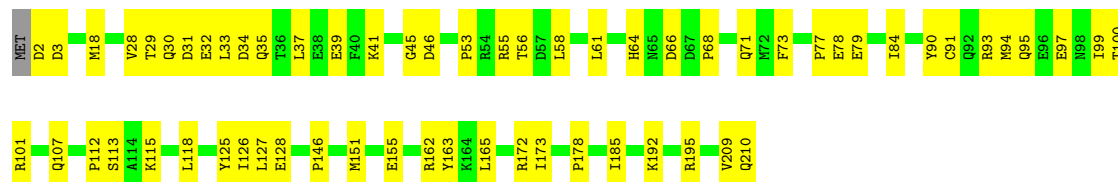
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 75% 20% 5%



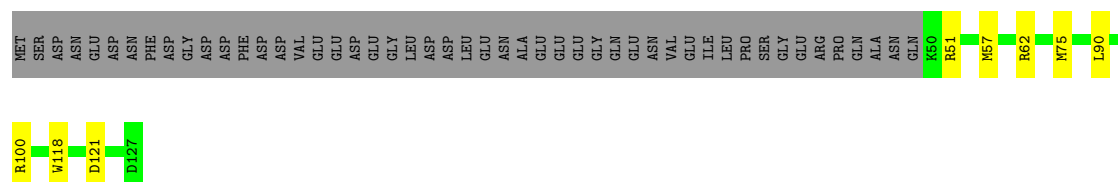
• Molecule 4: DNA-directed RNA polymerase II subunit E

Chain E: 70% 30%



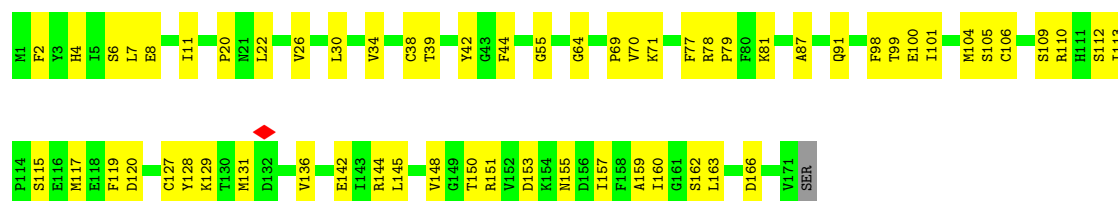
• Molecule 5: DNA-directed RNA polymerase II subunit F

Chain F: 55% 6% 39%



• Molecule 6: DNA-directed RNA polymerase II subunit RPB7

Chain G: 65% 35%



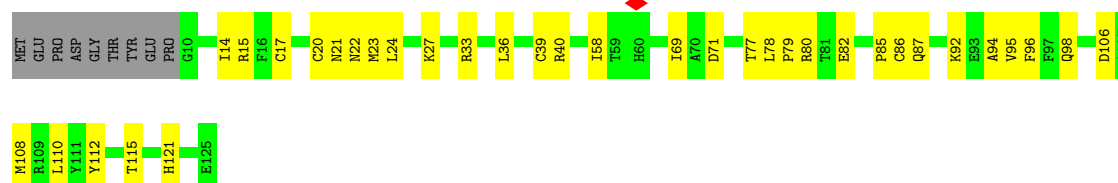
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 



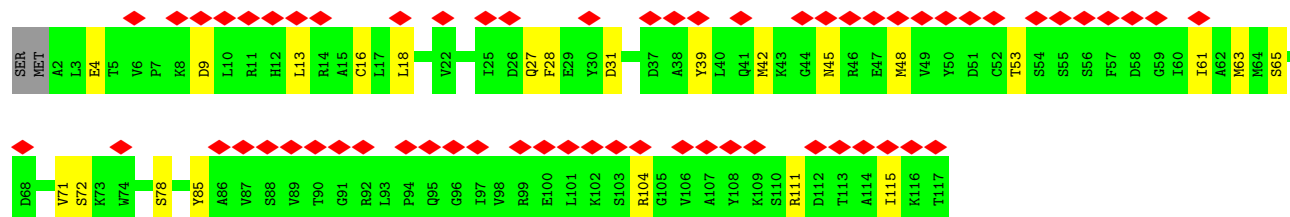
- Molecule 8: DNA-directed RNA polymerase II subunit RPB9

Chain I: 



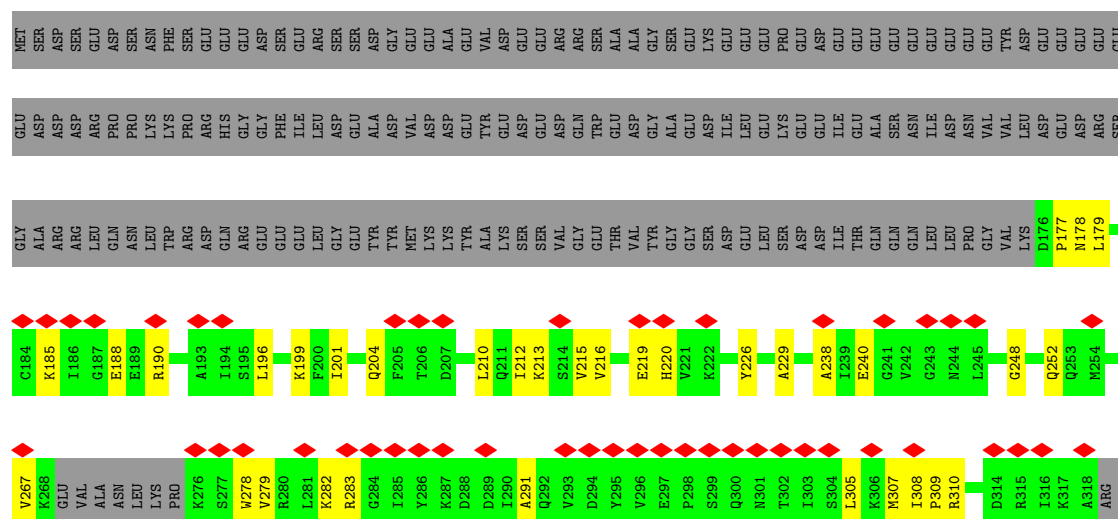
- Molecule 9: Transcription elongation factor SPT4

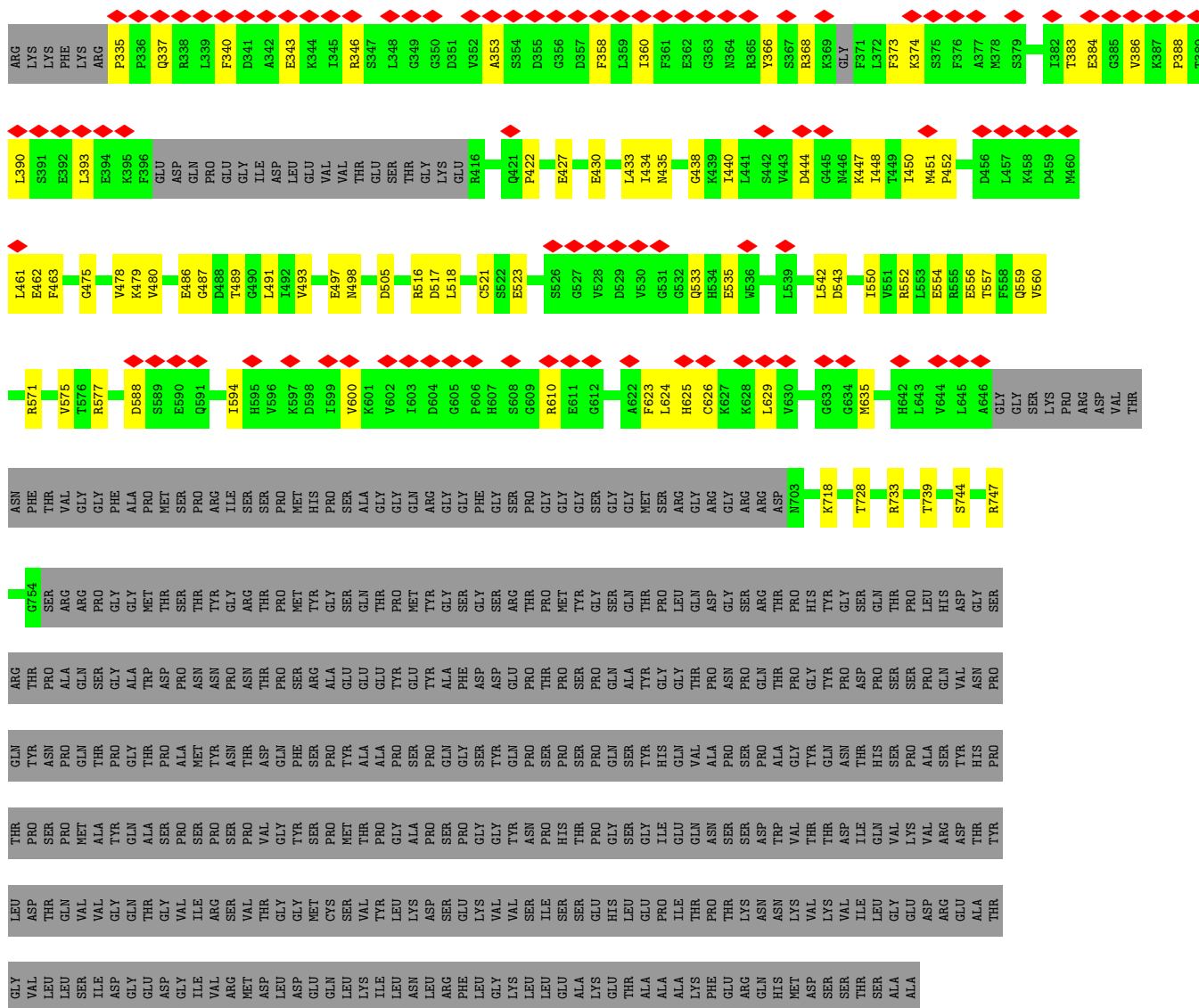
Chain Y: 



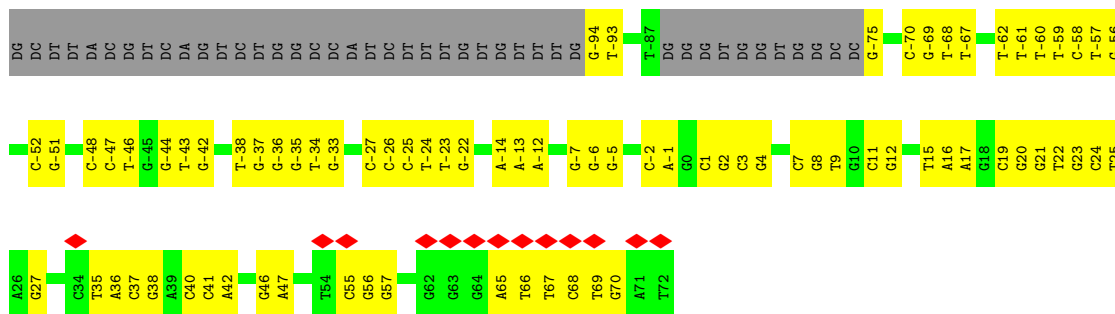
- Molecule 10: Transcription elongation factor SPT5

Chain Z: 





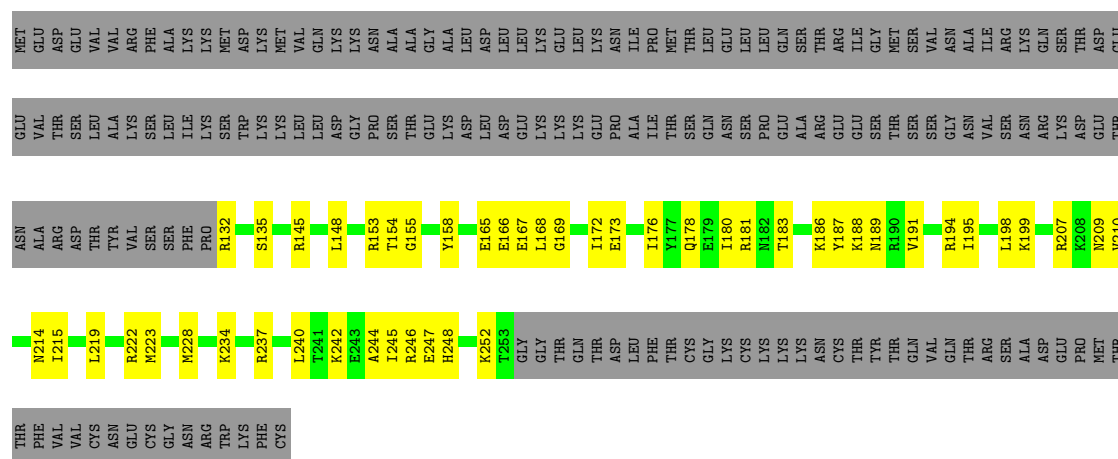
• Molecule 11: Non-template DNA (157-MER)



• Molecule 12: RNA (5'-R(P*UP*GP*GP*GP*UP*GP*GP*UP*GP*GP*CP*C)-3')

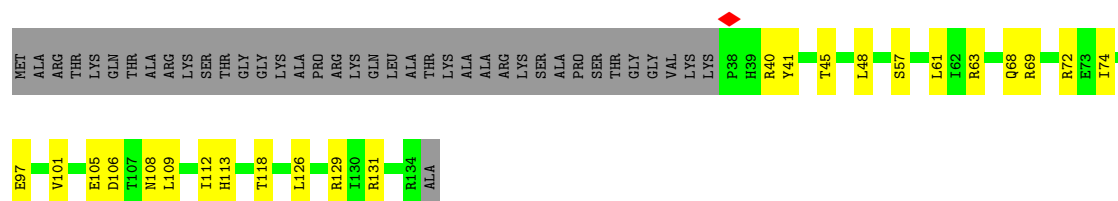


Chain M:  25% 16% 59%

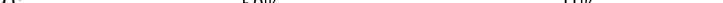


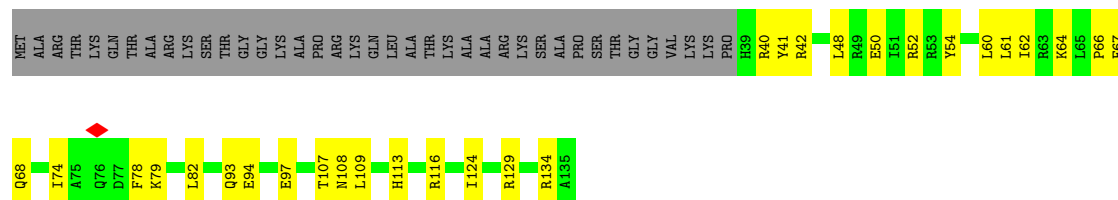
- Molecule 19: Histone H3.3

Chain a: 54% 17% 29%



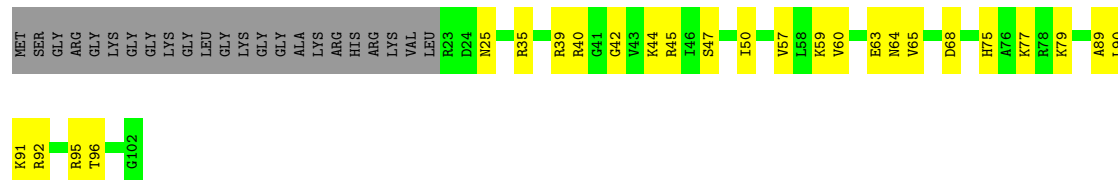
- Molecule 19: Histone H3.3

Chain e:  50% 21% 29%

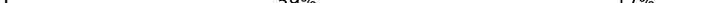


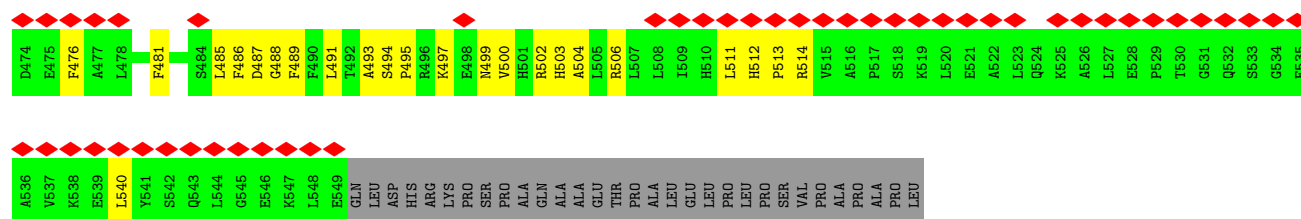
- Molecule 20: Histone H4

Chain b: 53% 24% 22%

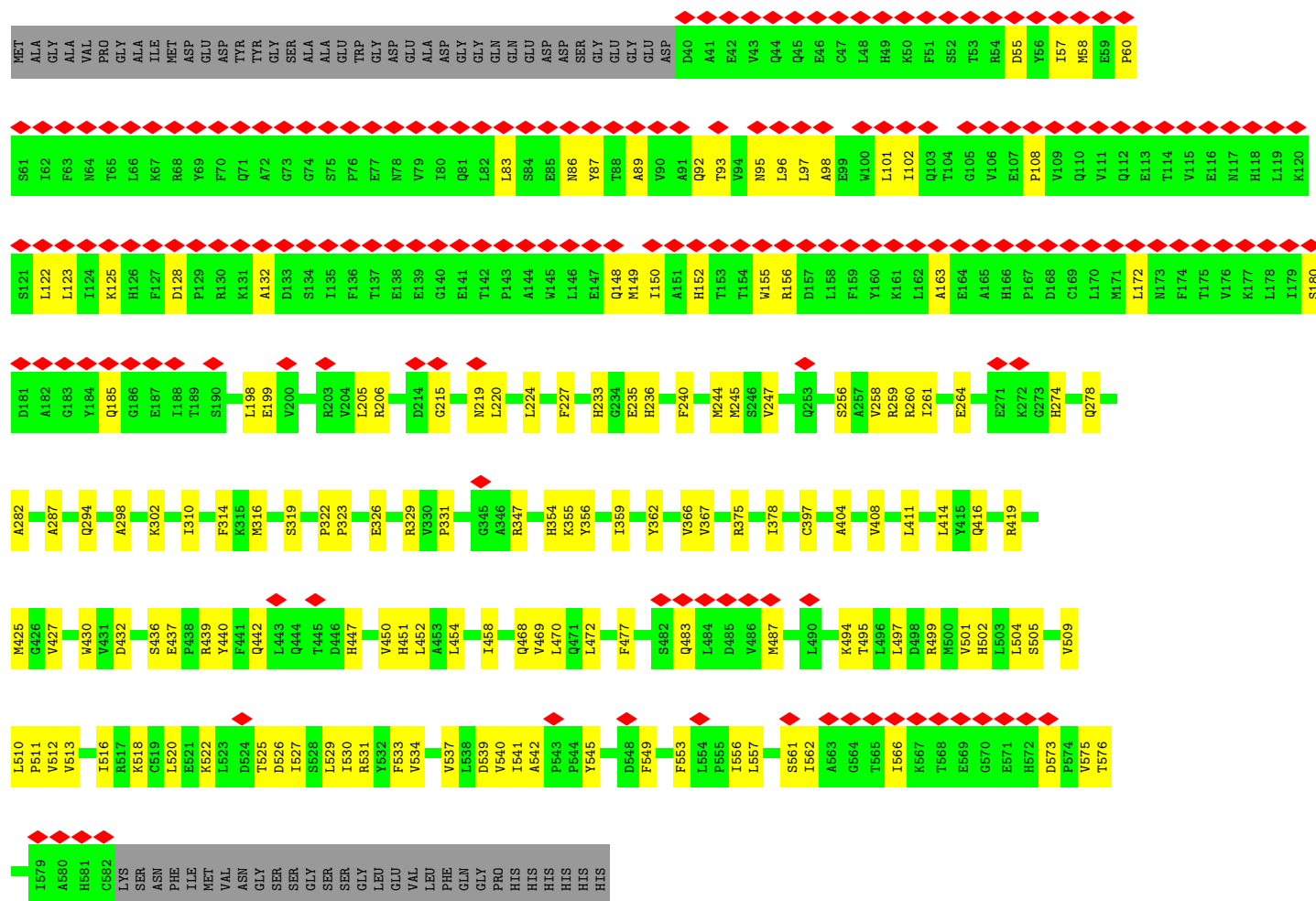


- Molecule 20: Histone H4

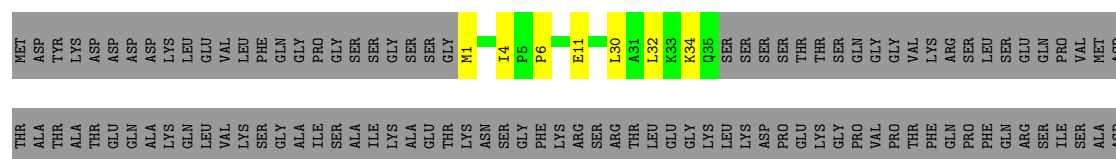
Chain f: 



• Molecule 25: Negative elongation factor C/D



• Molecule 26: Negative elongation factor E



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47563	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.149	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	356.16, 356.16, 356.16	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.484, 1.484, 1.484	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, 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	0.17	0/11240	0.32	0/15169
2	B	0.17	0/9149	0.30	0/12348
3	C	0.20	0/2115	0.33	0/2873
4	E	0.16	0/1751	0.32	0/2366
5	F	0.17	0/636	0.26	0/859
6	G	0.13	0/1382	0.33	0/1874
7	H	0.17	0/1219	0.29	0/1644
8	I	0.11	0/964	0.28	0/1305
9	Y	0.09	0/927	0.26	0/1250
10	Z	0.09	0/3903	0.27	0/5254
11	N	0.16	0/3588	0.36	0/5541
12	P	0.14	0/291	0.20	0/453
13	T	0.17	0/3827	0.35	0/5895
14	D	0.12	0/1017	0.32	0/1368
15	J	0.19	0/542	0.29	0/730
16	K	0.19	0/939	0.28	0/1271
17	L	0.14	0/394	0.35	0/524
18	M	0.12	0/977	0.33	0/1307
19	a	0.13	0/809	0.35	0/1085
19	e	0.12	0/807	0.25	0/1081
20	b	0.12	0/645	0.32	0/862
20	f	0.11	0/626	0.28	0/837
21	c	0.10	0/806	0.26	0/1089
21	g	0.11	0/820	0.30	0/1107
22	d	0.10	0/757	0.29	0/1015
22	h	0.10	0/736	0.27	0/990
23	U	0.11	0/1463	0.30	0/1985
24	V	0.12	0/4424	0.30	0/5975
25	W	0.10	0/4404	0.27	0/5982
26	X	0.10	0/283	0.26	0/372
All	All	0.15	0/61441	0.31	0/84411

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

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	11042	0	11191	242	0
2	B	8971	0	9013	167	0
3	C	2072	0	2019	44	0
4	E	1720	0	1737	44	0
5	F	626	0	657	7	0
6	G	1351	0	1358	50	0
7	H	1197	0	1156	29	0
8	I	942	0	871	28	0
9	Y	911	0	904	20	0
10	Z	3837	0	3895	82	0
11	N	3207	0	1769	65	0
12	P	261	0	130	2	0
13	T	3405	0	1860	62	0
14	D	1004	0	980	37	0
15	J	533	0	553	6	0
16	K	920	0	942	12	0
17	L	388	0	393	11	0
18	M	969	0	981	38	0
19	a	797	0	835	22	0
19	e	796	0	832	26	0
20	b	638	0	676	21	0
20	f	619	0	659	19	0
21	c	796	0	848	20	0
21	g	810	0	866	20	0
22	d	746	0	771	19	0
22	h	725	0	745	15	0
23	U	1439	0	1491	64	0
24	V	4341	0	4435	132	0
25	W	4312	0	4312	122	0
26	X	281	0	330	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	A	2	0	0	0	0
27	B	1	0	0	0	0
27	C	1	0	0	0	0
27	I	2	0	0	0	0
27	J	1	0	0	0	0
27	L	1	0	0	0	0
27	Y	1	0	0	0	0
28	A	1	0	0	0	0
All	All	59666	0	57209	1234	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 11.

All (1234) 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)
24:V:317:SER:O	24:V:321:HIS:ND1	2.07	0.87
9:Y:42:MET:HA	9:Y:48:MET:HE2	1.57	0.83
23:U:57:LEU:HD11	23:U:90:VAL:HG23	1.61	0.81
1:A:74:CYS:SG	1:A:84:HIS:CE1	2.74	0.80
7:H:32:SER:HB3	7:H:37:MET:H	1.48	0.79
2:B:268:PRO:HG2	2:B:271:ILE:HD13	1.66	0.78
24:V:219:LEU:HD22	24:V:238:ARG:HG3	1.66	0.77
11:N:-94:DG:H2''	11:N:-93:DT:H5'	1.65	0.77
8:I:82:GLU:O	8:I:92:LYS:NZ	2.18	0.77
1:A:139:LYS:HG2	1:A:143:HIS:CE1	2.20	0.75
2:B:1142:ASN:HD21	2:B:1145:GLN:HB2	1.52	0.75
6:G:11:ILE:HD11	6:G:26:VAL:HG13	1.69	0.75
23:U:4:MET:O	23:U:40:ASN:ND2	2.20	0.74
3:C:47:ILE:HD11	3:C:68:LEU:HB3	1.68	0.73
4:E:68:PRO:O	4:E:71:GLN:NE2	2.20	0.73
19:e:61:LEU:HD22	20:f:36:ARG:HD3	1.70	0.73
1:A:1343:LEU:HD13	1:A:1359:SER:HB2	1.71	0.73
3:C:7:PRO:O	16:K:104:ARG:NH1	2.22	0.73
3:C:47:ILE:HA	3:C:165:ALA:HA	1.70	0.72
2:B:927:ARG:NH1	2:B:1054:MET:SD	2.63	0.72
2:B:256:ILE:HG22	2:B:269:ILE:HG13	1.72	0.72
2:B:407:MET:HE2	2:B:443:GLY:HA3	1.72	0.72
2:B:311:ILE:HG23	2:B:316:VAL:HG13	1.72	0.71
18:M:198:LEU:O	18:M:207:ARG:NH1	2.23	0.71
7:H:17:PRO:O	25:W:347:ARG:NH1	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:GLU:HG2	2:B:127:ASP:HB3	1.72	0.71
25:W:562:ILE:HG23	25:W:566:ILE:HD12	1.70	0.71
1:A:1248:ASN:HD21	1:A:1252:ALA:HB3	1.56	0.71
2:B:953:ASP:OD1	3:C:36:ARG:NH2	2.24	0.71
2:B:222:ARG:HD3	2:B:234:THR:HG22	1.73	0.70
1:A:481:THR:O	1:A:483:ARG:NH1	2.23	0.70
1:A:663:ASP:OD1	1:A:666:ARG:NH2	2.25	0.70
19:a:108:ASN:HD21	21:g:115:LEU:HD11	1.57	0.70
10:Z:440:ILE:HG12	10:Z:450:ILE:HD11	1.74	0.69
25:W:89:ALA:HB1	25:W:92:GLN:HB2	1.75	0.69
1:A:904:GLN:NE2	1:A:981:CYS:O	2.25	0.69
10:Z:309:PRO:HG3	10:Z:340:PHE:HB2	1.75	0.69
24:V:46:SER:HB2	25:W:149:MET:HE2	1.75	0.69
2:B:754:PRO:HB2	2:B:773:PRO:HG2	1.73	0.68
23:U:62:HIS:HD2	25:W:278:GLN:HE21	1.41	0.68
24:V:61:PHE:HB2	25:W:122:LEU:HD13	1.75	0.68
8:I:69:ILE:HG22	8:I:71:ASP:H	1.59	0.68
23:U:75:LEU:HD22	23:U:101:PRO:HG3	1.76	0.68
21:g:63:LEU:HD22	22:h:42:LEU:HD13	1.76	0.68
1:A:74:CYS:SG	1:A:81:CYS:HB2	2.33	0.67
1:A:230:ASP:HB2	1:A:240:PRO:HG3	1.76	0.67
1:A:22:GLN:NE2	1:A:1447:GLU:O	2.28	0.67
4:E:30:GLN:NE2	4:E:34:ASP:OD2	2.27	0.67
11:N:-2:DC:H2'	11:N:-1:DA:C8	2.29	0.67
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.77	0.67
8:I:86:CYS:SG	8:I:121:HIS:ND1	2.62	0.67
24:V:74:LEU:HD21	24:V:112:VAL:HA	1.75	0.67
1:A:1165:THR:HG22	1:A:1297:THR:H	1.60	0.67
6:G:160:ILE:HD11	10:Z:493:VAL:HG22	1.76	0.67
8:I:39:CYS:SG	8:I:40:ARG:N	2.68	0.67
10:Z:610:ARG:HD3	10:Z:629:LEU:HD11	1.77	0.67
14:D:31:THR:HB	14:D:94:LYS:HE2	1.76	0.67
2:B:315:ASN:O	2:B:319:ASN:ND2	2.28	0.66
19:e:50:GLU:OE1	20:f:35:ARG:NH1	2.26	0.66
3:C:92:GLU:CD	3:C:93:PHE:H	2.01	0.66
6:G:38:CYS:HB2	6:G:44:PHE:HD1	1.60	0.66
6:G:39:THR:HG23	6:G:42:TYR:H	1.61	0.66
24:V:390:ASP:HA	24:V:393:LEU:HB2	1.78	0.66
7:H:103:GLU:HG3	7:H:109:ALA:HB2	1.78	0.66
19:a:74:ILE:HD11	20:b:63:GLU:HG3	1.78	0.66
2:B:1032:PHE:O	3:C:32:ASN:ND2	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ARG:NH2	12:P:10:C:O2'	2.29	0.65
14:D:44:ARG:HH12	14:D:57:LEU:HD23	1.61	0.65
19:e:108:ASN:HB2	20:f:43:VAL:HG22	1.77	0.65
1:A:1213:ARG:HH21	1:A:1256:VAL:HG11	1.59	0.65
10:Z:279:VAL:HG12	10:Z:383:THR:HA	1.77	0.65
2:B:265:GLN:HB3	2:B:324:ARG:HD3	1.77	0.65
3:C:193:ARG:NH2	3:C:218:ALA:O	2.30	0.65
1:A:1248:ASN:ND2	1:A:1254:LYS:O	2.29	0.65
4:E:71:GLN:HB2	4:E:99:ILE:HG21	1.78	0.65
1:A:1427:LEU:HD22	1:A:1459:MET:HE1	1.79	0.65
2:B:565:THR:HG21	2:B:580:PRO:HB3	1.79	0.65
19:e:61:LEU:HD13	20:f:36:ARG:HG2	1.79	0.65
25:W:205:LEU:HG	25:W:227:PHE:HE1	1.61	0.65
1:A:1030:SER:HB2	4:E:162:ARG:HE	1.61	0.64
1:A:1155:LYS:NZ	1:A:1159:CYS:SG	2.61	0.64
14:D:43:HIS:CE1	14:D:47:GLN:HE22	2.16	0.64
14:D:87:LEU:HD22	14:D:97:LEU:HD12	1.79	0.64
23:U:167:ARG:NH1	25:W:539:ASP:O	2.29	0.64
24:V:246:HIS:HD1	24:V:254:CYS:HG	1.45	0.64
2:B:761:THR:H	2:B:764:MET:HE3	1.62	0.64
2:B:1144:THR:HG23	2:B:1145:GLN:HG3	1.79	0.64
18:M:155:GLY:HA3	18:M:207:ARG:HH21	1.61	0.64
24:V:106:MET:O	24:V:110:GLN:N	2.30	0.64
8:I:14:ILE:HG23	8:I:23:MET:HE1	1.77	0.64
10:Z:444:ASP:HB2	10:Z:448:ILE:HA	1.78	0.64
2:B:228:SER:O	2:B:405:ARG:NH1	2.31	0.63
2:B:827:GLU:HG2	2:B:871:VAL:HG12	1.78	0.63
9:Y:39:TYR:O	9:Y:104:ARG:NH1	2.31	0.63
3:C:132:SER:O	3:C:133:ARG:NH1	2.31	0.63
7:H:128:ASP:OD1	7:H:131:ASN:ND2	2.31	0.63
24:V:117:MET:HE3	24:V:123:VAL:HG11	1.81	0.63
1:A:265:VAL:HG12	1:A:271:ARG:HH21	1.62	0.63
1:A:546:ARG:HD3	1:A:772:SER:HB3	1.80	0.63
10:Z:478:VAL:HB	10:Z:518:LEU:HD22	1.80	0.63
15:J:65:LEU:O	17:L:23:HIS:ND1	2.32	0.63
25:W:557:LEU:HD13	25:W:575:VAL:HG13	1.80	0.63
1:A:1180:ASN:O	1:A:1183:SER:OG	2.16	0.63
13:T:38:DA:H5''	21:g:44:GLY:HA2	1.80	0.63
24:V:46:SER:OG	25:W:148:GLN:OE1	2.17	0.63
1:A:129:ILE:HD13	1:A:143:HIS:HB3	1.80	0.63
2:B:299:GLU:HA	2:B:302:LYS:HD3	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LEU:HD21	1:A:595:ILE:HG12	1.80	0.63
11:N:17:DA:H4'	19:a:63:ARG:HG2	1.81	0.63
23:U:131:CYS:HB2	23:U:134:SER:HB3	1.81	0.63
1:A:513:ALA:HB2	5:F:90:LEU:HD21	1.80	0.62
1:A:803:LYS:N	2:B:671:GLU:OE2	2.31	0.62
1:A:883:ILE:HD11	1:A:1424:THR:HA	1.81	0.62
2:B:721:ARG:HD2	2:B:975:ARG:HB3	1.81	0.62
2:B:209:ALA:O	2:B:211:LYS:NZ	2.32	0.62
9:Y:27:GLN:NE2	9:Y:31:ASP:OD2	2.32	0.62
14:D:24:LYS:HE3	14:D:24:LYS:HA	1.80	0.62
23:U:177:GLU:HG3	23:U:181:LYS:HE3	1.81	0.62
11:N:-47:DC:H2''	11:N:-46:DT:C5	2.35	0.62
21:g:88:ARG:HB3	21:g:108:LEU:HD11	1.81	0.62
2:B:792:ASP:OD2	2:B:975:ARG:NH2	2.32	0.62
11:N:17:DA:OP1	19:a:69:ARG:NH2	2.33	0.62
19:e:74:ILE:HD11	20:f:63:GLU:HG3	1.80	0.62
23:U:57:LEU:HB3	23:U:93:VAL:HG11	1.80	0.62
25:W:245:MET:HE2	25:W:261:ILE:HB	1.82	0.62
9:Y:13:LEU:HD12	10:Z:190:ARG:HH21	1.63	0.61
3:C:59:LEU:HB2	3:C:64:ILE:HD11	1.81	0.61
10:Z:248:GLY:O	10:Z:252:GLN:NE2	2.34	0.61
2:B:388:TYR:H	2:B:504:THR:HG21	1.65	0.61
8:I:15:ARG:HB3	8:I:24:LEU:HD12	1.82	0.61
19:a:108:ASN:ND2	20:b:42:GLY:O	2.33	0.61
2:B:591:ARG:NH2	2:B:663:GLU:OE2	2.33	0.61
24:V:147:ARG:NH1	24:V:151:GLN:OE1	2.29	0.61
24:V:245:LEU:HD13	24:V:253:ILE:HD13	1.82	0.61
24:V:512:HIS:CG	24:V:513:PRO:HD3	2.35	0.61
1:A:896:LEU:HB2	1:A:1396:ARG:HH21	1.65	0.61
1:A:967:ARG:NH2	1:A:1326:GLY:O	2.32	0.61
5:F:100:ARG:NH2	5:F:121:ASP:O	2.33	0.61
1:A:381:PRO:HB3	1:A:480:SER:HA	1.80	0.61
13:T:-43:DT:H5''	21:c:16:THR:HA	1.82	0.61
7:H:5:LEU:HD22	7:H:134:GLY:HA3	1.83	0.61
13:T:-52:DG:OP2	22:d:39:TYR:OH	2.17	0.61
10:Z:353:ALA:HB3	10:Z:360:ILE:HB	1.83	0.61
1:A:496:PHE:HD2	2:B:791:GLU:HB2	1.66	0.61
11:N:15:DT:H2''	11:N:16:DA:C8	2.36	0.60
25:W:245:MET:HE3	25:W:258:VAL:HG13	1.82	0.60
2:B:789:ASN:HA	2:B:793:SER:HB3	1.83	0.60
19:e:61:LEU:N	19:e:97:GLU:OE2	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:SER:OG	1:A:227:ARG:NH1	2.34	0.60
21:c:65:LEU:HB3	21:c:86:ALA:HB1	1.82	0.60
24:V:138:TYR:HE1	24:V:149:ILE:HG21	1.67	0.60
24:V:427:TYR:O	24:V:431:HIS:ND1	2.31	0.60
2:B:91:ILE:HG22	2:B:126:VAL:HG23	1.82	0.60
11:N:40:DC:H2'	11:N:41:DC:C6	2.36	0.60
19:a:57:SER:OG	20:b:40:ARG:NH2	2.35	0.60
1:A:190:ARG:NH1	1:A:201:GLU:OE2	2.35	0.60
9:Y:28:PHE:HB3	9:Y:42:MET:HE1	1.84	0.60
18:M:153:ARG:NE	18:M:165:GLU:OE2	2.34	0.60
23:U:45:PHE:HZ	23:U:90:VAL:HG21	1.65	0.60
25:W:452:LEU:HB3	25:W:499:ARG:HD2	1.83	0.60
2:B:548:TRP:CD1	2:B:549:SER:H	2.20	0.60
14:D:92:LEU:HA	14:D:121:ARG:HH22	1.67	0.60
24:V:117:MET:HE1	24:V:131:VAL:HG21	1.83	0.60
1:A:1141:VAL:HA	1:A:1357:THR:HG23	1.83	0.59
24:V:147:ARG:HD3	24:V:211:ASN:HB2	1.84	0.59
1:A:96:HIS:HB2	1:A:250:VAL:HG23	1.84	0.59
18:M:148:LEU:HD23	18:M:169:GLY:HA2	1.83	0.59
24:V:394:PRO:HD3	26:X:32:LEU:HD22	1.84	0.59
25:W:497:LEU:HD11	25:W:529:LEU:HB3	1.84	0.59
1:A:136:GLN:NE2	1:A:1423:ASP:OD2	2.33	0.59
1:A:1248:ASN:HD22	1:A:1255:LEU:HA	1.66	0.59
25:W:316:MET:O	25:W:319:SER:OG	2.20	0.59
2:B:677:MET:H	2:B:682:LEU:HD22	1.67	0.59
7:H:2:ALA:O	7:H:84:ARG:NH2	2.35	0.59
11:N:20:DG:H2''	11:N:21:DG:H5''	1.84	0.59
10:Z:626:CYS:HB3	10:Z:629:LEU:HD13	1.85	0.59
18:M:168:LEU:O	18:M:172:ILE:HG13	2.01	0.59
4:E:37:LEU:HG	4:E:41:LYS:HE2	1.83	0.59
19:a:126:LEU:HD22	19:e:113:HIS:CG	2.38	0.59
20:f:68:ASP:OD2	20:f:93:GLN:NE2	2.35	0.59
2:B:391:LYS:O	2:B:392:ARG:NH1	2.36	0.59
10:Z:479:LYS:HG3	10:Z:489:THR:HG22	1.84	0.59
24:V:215:TYR:CZ	24:V:219:LEU:HD11	2.38	0.59
24:V:389:VAL:O	24:V:393:LEU:N	2.36	0.59
6:G:110:ARG:HH22	6:G:115:SER:HA	1.68	0.59
11:N:-24:DT:H2'	11:N:-23:DT:H71	1.85	0.59
23:U:120:ILE:HG12	25:W:206:ARG:HG3	1.83	0.59
1:A:874:LYS:HG3	1:A:880:ARG:HD2	1.84	0.58
3:C:116:THR:HB	3:C:147:ASP:HB2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:429:VAL:HG11	24:V:448:LEU:HD11	1.84	0.58
1:A:517:GLU:OE1	5:F:62:ARG:NH1	2.36	0.58
1:A:959:MET:HE1	1:A:1047:SER:HA	1.83	0.58
3:C:47:ILE:HG22	3:C:165:ALA:HB2	1.84	0.58
2:B:84:TYR:HA	2:B:132:VAL:HA	1.85	0.58
2:B:933:ASP:OD2	2:B:1050:ARG:NH2	2.31	0.58
19:a:129:ARG:HD2	19:e:109:LEU:HD13	1.84	0.58
24:V:512:HIS:CD2	24:V:513:PRO:HD3	2.39	0.58
1:A:253:LEU:HD12	1:A:254:PRO:HD2	1.86	0.58
14:D:34:ASN:O	14:D:68:THR:OG1	2.21	0.58
22:h:38:VAL:HB	22:h:56:MET:HE1	1.86	0.58
11:N:37:DC:H2''	11:N:38:DG:C8	2.38	0.58
24:V:100:SER:HB2	24:V:113:VAL:HG22	1.86	0.58
24:V:243:MET:HA	24:V:243:MET:HE3	1.85	0.58
25:W:440:TYR:HH	25:W:451:HIS:HE2	1.52	0.58
24:V:168:TYR:HB2	24:V:200:VAL:HG11	1.85	0.58
1:A:119:VAL:HG11	1:A:123:ASN:HD22	1.68	0.58
1:A:480:SER:HB3	16:K:2:ASN:HB2	1.85	0.58
11:N:-69:DG:H2'	11:N:-68:DT:C6	2.39	0.58
13:T:87:DA:C8	13:T:87:DA:H5''	2.39	0.58
3:C:259:LEU:HD22	16:K:42:LEU:HD21	1.85	0.57
6:G:142:GLU:OE2	14:D:70:ARG:NH2	2.33	0.57
1:A:1251:ASN:OD1	1:A:1252:ALA:N	2.37	0.57
10:Z:542:LEU:HD23	10:Z:575:VAL:HG11	1.86	0.57
13:T:9:DG:N3	19:e:40:ARG:NH2	2.52	0.57
13:T:74:DA:H2'	13:T:75:DC:C6	2.39	0.57
25:W:150:ILE:O	25:W:156:ARG:NH1	2.37	0.57
3:C:260:GLN:HB2	16:K:91:ILE:HG21	1.85	0.57
6:G:113:ILE:HA	6:G:163:LEU:HD23	1.87	0.57
10:Z:550:ILE:HG12	10:Z:560:VAL:HG22	1.87	0.57
9:Y:45:ASN:HB3	9:Y:48:MET:HG2	1.86	0.57
10:Z:199:LYS:NZ	10:Z:240:GLU:O	2.33	0.57
13:T:-47:DT:H2''	13:T:-46:DC:C5	2.39	0.57
25:W:518:LYS:O	25:W:522:LYS:HB2	2.05	0.57
2:B:222:ARG:HB3	2:B:232:THR:HG21	1.87	0.57
2:B:1131:ARG:NH1	10:Z:535:GLU:OE1	2.36	0.57
18:M:187:TYR:O	18:M:191:VAL:HG23	2.05	0.57
24:V:375:PRO:HB2	26:X:11:GLU:HB3	1.86	0.57
2:B:866:ILE:HG22	2:B:867:ILE:HG13	1.87	0.56
9:Y:61:ILE:N	9:Y:85:TYR:O	2.33	0.56
21:g:63:LEU:HB3	22:h:45:VAL:HG11	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:181:LEU:HD13	24:V:466:THR:HB	1.86	0.56
2:B:67:LEU:HB2	2:B:84:TYR:CE1	2.40	0.56
19:a:48:LEU:HD13	20:b:44:LYS:HZ1	1.70	0.56
1:A:1146:GLN:OE1	1:A:1153:ARG:NH2	2.38	0.56
2:B:549:SER:OG	2:B:577:HIS:NE2	2.34	0.56
10:Z:199:LYS:NZ	10:Z:238:ALA:O	2.34	0.56
24:V:30:ILE:HD11	25:W:57:ILE:HG13	1.88	0.56
25:W:259:ARG:HH22	25:W:326:GLU:HB2	1.70	0.56
1:A:276:LEU:HD21	1:A:339:LEU:HD21	1.86	0.56
2:B:907:VAL:HG22	2:B:921:ILE:HG12	1.87	0.56
1:A:909:LEU:C	1:A:911:PRO:HD3	2.29	0.56
1:A:911:PRO:O	1:A:963:ARG:NH2	2.38	0.56
2:B:236:TRP:HB2	2:B:259:THR:HB	1.88	0.56
4:E:55:ARG:HB2	4:E:78:GLU:HG3	1.86	0.56
8:I:85:PRO:O	8:I:87:GLN:NE2	2.38	0.56
11:N:-38:DT:H2"	11:N:-37:DG:C8	2.40	0.56
18:M:244:ALA:C	18:M:248:HIS:HD1	2.14	0.56
11:N:1:DC:H2"	11:N:2:DG:C8	2.41	0.56
16:K:77:THR:OG1	16:K:81:TYR:O	2.17	0.56
21:c:24:GLN:N	21:c:56:GLU:OE1	2.36	0.56
2:B:327:LYS:NZ	2:B:328:PRO:O	2.38	0.56
7:H:95:LYS:HG3	7:H:140:ARG:HH11	1.69	0.56
20:b:90:LEU:HD22	20:b:95:ARG:HB2	1.87	0.56
24:V:212:VAL:HG13	24:V:256:VAL:HG21	1.88	0.56
18:M:242:LYS:HG3	18:M:246:ARG:HH12	1.71	0.56
1:A:911:PRO:HD2	1:A:963:ARG:HH21	1.70	0.56
2:B:859:ARG:NH2	10:Z:739:THR:O	2.37	0.56
7:H:31:GLU:HG3	25:W:302:LYS:HE2	1.88	0.56
11:N:-2:DC:H2'	11:N:-1:DA:H8	1.70	0.56
18:M:176:ILE:O	18:M:180:ILE:HG12	2.05	0.56
23:U:166:LYS:HG2	25:W:542:ALA:HB2	1.88	0.56
24:V:376:MET:HG3	24:V:411:PHE:HB2	1.87	0.56
1:A:487:SER:OG	1:A:673:GLN:NE2	2.39	0.56
20:f:55:ARG:O	20:f:59:LYS:HG3	2.05	0.56
3:C:78:ILE:HG22	3:C:82:LEU:HG	1.88	0.55
10:Z:533:GLN:O	10:Z:577:ARG:NH1	2.39	0.55
18:M:154:THR:O	18:M:207:ARG:NE	2.40	0.55
1:A:520:MET:HE2	1:A:520:MET:HA	1.87	0.55
1:A:876:ASP:HB3	1:A:878:THR:HG22	1.87	0.55
1:A:1301:ILE:HG22	1:A:1345:ARG:HH21	1.69	0.55
8:I:94:ALA:HA	8:I:115:THR:HG23	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:29:ILE:HG12	23:U:59:GLY:HA3	1.87	0.55
17:L:26:ASN:HD21	17:L:44:MET:HE1	1.71	0.55
23:U:33:LEU:HD22	23:U:38:ILE:HD11	1.88	0.55
1:A:139:LYS:HG2	1:A:143:HIS:HE1	1.67	0.55
1:A:418:TYR:HB2	1:A:447:GLU:HG3	1.88	0.55
1:A:863:ARG:HH22	1:A:1129:ASN:HD21	1.54	0.55
3:C:92:GLU:O	10:Z:718:LYS:NZ	2.38	0.55
21:c:51:LEU:HD13	22:d:70:ILE:HG21	1.88	0.55
24:V:305:LEU:HD22	24:V:314:LEU:HD11	1.87	0.55
3:C:190:ASN:ND2	3:C:195:THR:O	2.32	0.55
10:Z:307:MET:HE1	10:Z:374:LYS:HB3	1.89	0.55
19:e:60:LEU:HD21	19:e:94:GLU:HG2	1.87	0.55
19:e:64:LYS:O	19:e:68:GLN:HG2	2.06	0.55
1:A:358:ARG:NH1	13:T:79:DC:OP1	2.34	0.55
17:L:15:MET:SD	17:L:46:LYS:NZ	2.77	0.55
7:H:95:LYS:HG3	7:H:140:ARG:NH1	2.22	0.55
11:N:2:DG:H2''	11:N:3:DC:H5''	1.89	0.55
21:c:100:VAL:HG22	20:f:96:THR:HB	1.89	0.55
24:V:57:PRO:HG2	24:V:60:GLU:OE1	2.07	0.55
24:V:246:HIS:ND1	24:V:254:CYS:SG	2.75	0.55
25:W:497:LEU:HD22	25:W:533:PHE:HB2	1.88	0.55
1:A:299:ALA:HB3	1:A:302:VAL:HG12	1.89	0.55
2:B:1121:LEU:HD12	2:B:1140:CYS:HB3	1.87	0.55
11:N:-44:DG:OP1	21:g:32:ARG:NH1	2.39	0.55
8:I:78:LEU:O	8:I:80:ARG:NH1	2.40	0.55
9:Y:16:CYS:HA	9:Y:53:THR:HG22	1.88	0.55
13:T:49:DC:H2''	13:T:50:DA:C8	2.42	0.55
24:V:38:GLY:O	25:W:95:ASN:ND2	2.40	0.55
25:W:152:HIS:HB2	25:W:155:TRP:HD1	1.72	0.55
11:N:35:DT:H2''	11:N:36:DA:C8	2.42	0.54
24:V:217:MET:HE3	24:V:217:MET:HA	1.88	0.54
1:A:734:ARG:NH1	8:I:108:MET:SD	2.80	0.54
13:T:42:DC:H2'	13:T:43:DA:C8	2.41	0.54
14:D:23:PRO:O	14:D:27:GLU:N	2.40	0.54
21:c:79:ILE:HG22	21:c:81:ARG:H	1.72	0.54
21:g:54:VAL:HG21	22:h:95:VAL:HG21	1.89	0.54
24:V:493:ALA:O	24:V:497:LYS:N	2.40	0.54
2:B:759:VAL:HG11	2:B:983:GLU:HG3	1.89	0.54
6:G:38:CYS:SG	6:G:39:THR:N	2.81	0.54
11:N:55:DC:H2''	11:N:56:DG:C8	2.42	0.54
11:N:70:DG:H5''	19:e:41:TYR:HA	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:-4:DC:H2''	13:T:-3:DG:C8	2.41	0.54
13:T:61:DA:H2''	13:T:62:DA:H5''	1.88	0.54
24:V:464:LEU:O	24:V:468:ASN:ND2	2.31	0.54
25:W:573:ASP:HB3	25:W:576:THR:HB	1.89	0.54
2:B:565:THR:HA	2:B:610:ARG:HB3	1.90	0.54
2:B:789:ASN:O	2:B:968:ASN:HB2	2.06	0.54
25:W:245:MET:HE3	25:W:258:VAL:HA	1.90	0.54
2:B:937:SER:OG	2:B:938:ARG:N	2.40	0.54
6:G:30:LEU:HD22	6:G:70:VAL:HG21	1.90	0.54
25:W:298:ALA:HB1	25:W:302:LYS:HZ1	1.72	0.54
1:A:22:GLN:HB3	2:B:1170:ARG:HB2	1.90	0.54
21:g:40:SER:OG	21:g:42:ARG:O	2.26	0.54
23:U:4:MET:O	23:U:9:THR:OG1	2.25	0.54
24:V:469:LEU:HB3	24:V:476:PHE:HZ	1.72	0.54
1:A:753:GLY:O	1:A:757:GLN:HG2	2.08	0.54
2:B:180:ASP:OD2	2:B:184:TYR:OH	2.25	0.54
3:C:59:LEU:HD12	3:C:151:VAL:HG12	1.89	0.54
7:H:37:MET:SD	7:H:127:GLY:HA3	2.48	0.54
11:N:7:DC:H4'	20:b:45:ARG:HE	1.73	0.54
23:U:143:TYR:HE2	25:W:425:MET:HG2	1.73	0.54
25:W:527:ILE:HG23	25:W:561:SER:HB3	1.90	0.54
23:U:89:TRP:HE1	25:W:198:LEU:HB2	1.72	0.54
24:V:370:ILE:HA	24:V:374:LEU:HD13	1.90	0.54
7:H:32:SER:OG	7:H:33:GLU:N	2.39	0.54
10:Z:310:ARG:NH1	10:Z:335:PRO:O	2.41	0.54
10:Z:554:GLU:OE2	10:Z:559:GLN:NE2	2.35	0.54
18:M:234:LYS:HA	18:M:237:ARG:HG2	1.90	0.54
24:V:47:ALA:HB1	25:W:123:LEU:HD11	1.90	0.54
4:E:64:HIS:ND1	4:E:66:ASP:OD1	2.41	0.53
1:A:420:ILE:HB	1:A:445:LYS:HB2	1.90	0.53
2:B:869:LYS:HG2	2:B:892:CYS:HB3	1.89	0.53
6:G:120:ASP:HB2	6:G:127:CYS:HB2	1.90	0.53
10:Z:291:ALA:HB1	10:Z:305:LEU:HB3	1.90	0.53
20:b:91:LYS:HD2	20:b:92:ARG:HH12	1.73	0.53
1:A:364:ARG:HB2	2:B:1084:LEU:HD11	1.90	0.53
1:A:922:PHE:H	1:A:1052:ARG:HD2	1.73	0.53
9:Y:18:LEU:O	9:Y:111:ARG:NH2	2.34	0.53
10:Z:479:LYS:HD3	10:Z:521:CYS:HB2	1.91	0.53
13:T:-54:DA:H2''	13:T:-53:DG:C8	2.43	0.53
21:c:112:GLN:HB2	21:c:115:LEU:HG	1.89	0.53
1:A:364:ARG:NH1	1:A:502:ASN:OD1	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:ARG:O	1:A:561:MET:HG3	2.07	0.53
1:A:823:VAL:HG13	1:A:835:GLU:HB3	1.90	0.53
1:A:1178:ASP:OD1	1:A:1183:SER:OG	2.24	0.53
10:Z:733:ARG:NH1	10:Z:744:SER:OG	2.41	0.53
11:N:27:DG:H5''	20:b:79:LYS:HD2	1.90	0.53
25:W:310:ILE:HG13	25:W:356:TYR:CZ	2.43	0.53
1:A:1453:GLY:O	1:A:1457:ASN:ND2	2.35	0.53
6:G:151:ARG:HB2	10:Z:491:LEU:HD21	1.90	0.53
13:T:-65:DT:H2''	13:T:-64:DC:C5	2.43	0.53
14:D:45:LYS:HE2	14:D:61:PHE:HE2	1.74	0.53
22:d:83:ARG:NH1	22:d:85:THR:O	2.42	0.53
21:g:60:ALA:O	21:g:63:LEU:N	2.42	0.53
24:V:426:LEU:HB3	24:V:461:PHE:CE1	2.43	0.53
3:C:56:SER:HB2	3:C:158:GLU:H	1.74	0.53
4:E:94:MET:SD	4:E:99:ILE:HG13	2.49	0.53
6:G:30:LEU:O	6:G:34:VAL:HG22	2.09	0.53
13:T:35:DC:H2''	13:T:36:DC:C5	2.43	0.53
19:e:129:ARG:HA	19:e:134:ARG:HB3	1.90	0.53
23:U:96:ILE:HG13	23:U:107:ASN:O	2.07	0.53
23:U:105:SER:HB2	25:W:287:ALA:HB2	1.91	0.53
23:U:110:LEU:HD22	23:U:117:VAL:HG11	1.91	0.53
1:A:118:LEU:HD12	1:A:148:CYS:HB3	1.90	0.53
4:E:28:VAL:HG11	4:E:33:LEU:HD13	1.90	0.53
13:T:-69:DA:C8	13:T:-69:DA:H5'	2.44	0.53
22:d:95:VAL:HG13	22:d:99:LEU:HD13	1.91	0.53
24:V:367:VAL:HG21	26:X:4:ILE:HA	1.90	0.53
25:W:260:ARG:O	25:W:264:GLU:HG2	2.08	0.53
23:U:166:LYS:NZ	25:W:541:ILE:O	2.41	0.53
24:V:469:LEU:HD23	24:V:472:LEU:HD12	1.91	0.53
1:A:337:LYS:HG3	1:A:341:GLN:HB2	1.89	0.53
1:A:614:ASP:HA	1:A:619:LYS:HG3	1.90	0.53
2:B:82:PRO:HB3	2:B:134:LYS:HE2	1.91	0.53
9:Y:4:GLU:O	9:Y:27:GLN:NE2	2.42	0.53
11:N:-7:DG:H2''	11:N:-6:DG:C8	2.44	0.53
14:D:22:PHE:HB3	14:D:26:PHE:HD2	1.75	0.53
25:W:322:PRO:O	25:W:375:ARG:NH1	2.42	0.53
1:A:244:ARG:HB3	1:A:247:TRP:CD2	2.44	0.52
1:A:805:ARG:NH1	8:I:77:THR:OG1	2.42	0.52
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.39	0.52
11:N:9:DT:O2	19:a:40:ARG:NH2	2.42	0.52
24:V:54:HIS:HA	25:W:128:ASP:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:487:ASP:HA	24:V:491:LEU:HB2	1.91	0.52
25:W:545:TYR:HB3	25:W:549:PHE:HD2	1.73	0.52
14:D:107:THR:HG23	14:D:110:GLU:H	1.73	0.52
21:c:100:VAL:HG11	20:f:98:TYR:CZ	2.44	0.52
23:U:58:LEU:HD22	25:W:235:GLU:HG2	1.90	0.52
10:Z:450:ILE:O	10:Z:451:MET:HE2	2.10	0.52
23:U:54:LEU:HD21	23:U:89:TRP:HB3	1.90	0.52
23:U:65:ARG:HH12	25:W:294:GLN:HG3	1.74	0.52
23:U:105:SER:OG	25:W:282:ALA:O	2.22	0.52
1:A:244:ARG:HD2	1:A:245:PRO:HD2	1.91	0.52
1:A:857:THR:HG21	1:A:1100:THR:HA	1.91	0.52
10:Z:447:LYS:NZ	10:Z:462:GLU:OE1	2.41	0.52
13:T:81:DC:H2'	13:T:82:DC:C6	2.44	0.52
18:M:242:LYS:NZ	18:M:246:ARG:HH22	2.08	0.52
24:V:70:ARG:NH1	24:V:108:SER:O	2.39	0.52
2:B:44:LEU:HD23	2:B:155:MET:HE3	1.92	0.52
1:A:1137:PRO:HB2	1:A:1341:VAL:HG13	1.91	0.52
3:C:2:PRO:HB3	16:K:54:PRO:HD2	1.91	0.52
4:E:172:ARG:NH1	4:E:210:GLN:OE1	2.43	0.52
1:A:192:ARG:NH1	1:A:201:GLU:OE1	2.42	0.52
13:T:33:DC:H2''	13:T:34:DA:C8	2.44	0.52
1:A:863:ARG:NH1	1:A:1129:ASN:OD1	2.43	0.52
20:b:35:ARG:O	20:b:39:ARG:HG2	2.09	0.52
1:A:18:ILE:HD11	2:B:1149:VAL:HG11	1.92	0.52
1:A:734:ARG:NH2	8:I:98:GLN:OE1	2.35	0.52
2:B:580:PRO:HB2	2:B:605:ARG:HE	1.75	0.52
7:H:90:TYR:CE2	7:H:92:MET:HE3	2.45	0.52
24:V:418:GLN:HB2	24:V:421:ALA:HB3	1.91	0.52
25:W:437:GLU:HG2	25:W:439:ARG:H	1.74	0.52
4:E:2:ASP:OD1	4:E:3:ASP:N	2.43	0.52
10:Z:440:ILE:HG23	10:Z:450:ILE:HG13	1.92	0.52
10:Z:600:VAL:HG13	10:Z:624:LEU:HD21	1.92	0.52
11:N:-43:DT:H5''	21:g:16:THR:HA	1.91	0.52
1:A:1248:ASN:OD1	1:A:1249:ASP:N	2.43	0.51
4:E:55:ARG:NH1	4:E:107:GLN:OE1	2.43	0.51
10:Z:282:LYS:HG3	10:Z:283:ARG:HG2	1.91	0.51
10:Z:623:PHE:HB3	10:Z:635:MET:HE3	1.90	0.51
2:B:1157:LEU:O	2:B:1161:GLU:HG3	2.10	0.51
18:M:244:ALA:O	18:M:248:HIS:ND1	2.36	0.51
24:V:502:ARG:HG3	24:V:540:LEU:HD11	1.93	0.51
2:B:82:PRO:HB3	2:B:134:LYS:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:42:ASP:HB2	7:H:121:LEU:HB3	1.92	0.51
18:M:209:ASN:HB2	18:M:214:ASN:HB2	1.92	0.51
21:c:30:VAL:HG22	22:d:67:PHE:HE1	1.76	0.51
24:V:165:LEU:HD22	24:V:222:LEU:HD21	1.92	0.51
24:V:281:ARG:NE	24:V:284:GLN:OE1	2.43	0.51
6:G:109:SER:O	6:G:112:SER:OG	2.23	0.51
8:I:85:PRO:HB3	8:I:92:LYS:HA	1.93	0.51
19:a:109:LEU:HD23	19:a:112:ILE:HD11	1.91	0.51
24:V:52:ASP:CG	25:W:60:PRO:HB2	2.35	0.51
4:E:73:PHE:HD2	4:E:94:MET:HE1	1.75	0.51
6:G:129:LYS:HD3	6:G:136:VAL:HG22	1.91	0.51
1:A:67:ARG:HH21	1:A:78:MET:HG2	1.76	0.51
1:A:392:GLU:OE1	1:A:448:ARG:NE	2.38	0.51
2:B:905:ASP:OD1	2:B:924:ARG:NH1	2.43	0.51
2:B:1112:ASP:OD1	2:B:1112:ASP:N	2.44	0.51
23:U:147:ASN:HB2	25:W:367:VAL:HG21	1.91	0.51
1:A:396:PRO:HD3	1:A:442:THR:HG23	1.92	0.51
3:C:15:THR:OG1	3:C:18:ASN:OD1	2.29	0.51
3:C:59:LEU:HD13	3:C:63:PHE:CE2	2.46	0.51
10:Z:543:ASP:N	10:Z:543:ASP:OD1	2.44	0.51
14:D:63:LYS:HA	14:D:66:ASN:HD21	1.74	0.51
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.92	0.51
1:A:1306:LYS:HE2	1:A:1308:TYR:HE1	1.74	0.51
13:T:90:DC:H1'	13:T:91:DA:N7	2.26	0.51
23:U:93:VAL:O	23:U:96:ILE:HG22	2.11	0.51
24:V:53:LEU:HD22	25:W:132:ALA:HA	1.92	0.51
1:A:332:SER:OG	13:T:87:DA:OP2	2.27	0.51
6:G:104:MET:HG3	6:G:157:ILE:HG13	1.93	0.51
11:N:68:DC:H2'	11:N:69:DT:C6	2.46	0.51
21:c:63:LEU:HD13	22:d:42:LEU:HB2	1.92	0.51
24:V:470:ALA:HA	24:V:511:LEU:HD11	1.93	0.51
25:W:442:GLN:HE22	25:W:483:GLN:HG3	1.76	0.51
1:A:419:ILE:HG23	1:A:427:ILE:HB	1.93	0.50
1:A:790:GLN:NE2	1:A:791:GLN:O	2.44	0.50
1:A:1481:LYS:HA	6:G:20:PRO:HA	1.93	0.50
3:C:101:PHE:CE2	3:C:122:SER:HB3	2.46	0.50
4:E:79:GLU:H	4:E:79:GLU:CD	2.19	0.50
6:G:81:LYS:O	14:D:17:ALA:N	2.37	0.50
25:W:470:LEU:HD13	25:W:512:VAL:HG22	1.93	0.50
1:A:320:ASN:ND2	1:A:336:LEU:O	2.44	0.50
4:E:118:LEU:HD11	4:E:127:LEU:HG	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:96:VAL:HA	7:H:116:VAL:HA	1.93	0.50
24:V:8:LEU:HD12	25:W:96:LEU:HD21	1.94	0.50
11:N:-5:DG:H5''	19:e:42:ARG:HH21	1.76	0.50
16:K:99:SER:O	16:K:102:GLU:HG3	2.10	0.50
1:A:736:THR:O	1:A:740:GLN:NE2	2.44	0.50
9:Y:71:VAL:HG13	10:Z:264:LEU:HD11	1.92	0.50
10:Z:196:LEU:HD13	10:Z:215:VAL:HG21	1.93	0.50
10:Z:497:GLU:HG2	10:Z:498:ASN:H	1.76	0.50
10:Z:554:GLU:OE1	10:Z:557:THR:OG1	2.29	0.50
17:L:28:ILE:HD13	17:L:34:ILE:HD13	1.93	0.50
19:e:54:TYR:HD2	20:f:39:ARG:HB2	1.77	0.50
2:B:84:TYR:CD2	2:B:86:LEU:HD23	2.47	0.50
25:W:408:VAL:HG22	25:W:450:VAL:HG21	1.93	0.50
1:A:566:PHE:HB3	1:A:674:THR:HG22	1.94	0.50
4:E:93:ARG:NH1	4:E:97:GLU:OE2	2.44	0.50
14:D:48:ASN:HB3	14:D:57:LEU:HD11	1.92	0.50
23:U:38:ILE:HA	23:U:41:ILE:HD12	1.94	0.50
24:V:354:MET:HE3	24:V:359:VAL:O	2.11	0.50
11:N:-62:DT:H2'	11:N:-61:DT:H71	1.94	0.50
11:N:-23:DT:H2''	11:N:-22:DG:H8	1.77	0.50
1:A:1099:ALA:HA	1:A:1102:MET:SD	2.52	0.49
1:A:1353:ASP:O	1:A:1357:THR:OG1	2.24	0.49
13:T:-16:DT:H2''	13:T:-15:DA:N7	2.27	0.49
23:U:111:GLU:HA	23:U:118:GLN:HG2	1.93	0.49
25:W:447:HIS:HE1	25:W:487:MET:HE1	1.77	0.49
25:W:534:VAL:HG13	25:W:553:PHE:HZ	1.76	0.49
2:B:317:ALA:O	2:B:321:ILE:HG12	2.13	0.49
25:W:526:ASP:HB3	25:W:529:LEU:HG	1.94	0.49
1:A:244:ARG:NE	1:A:246:GLU:OE1	2.43	0.49
10:Z:212:ILE:HG23	10:Z:229:ALA:HB2	1.94	0.49
10:Z:450:ILE:HG22	10:Z:463:PHE:H	1.77	0.49
19:a:69:ARG:HB3	20:b:25:ASN:ND2	2.27	0.49
8:I:110:LEU:HB2	8:I:112:TYR:HE1	1.76	0.49
11:N:46:DG:H2''	11:N:47:DA:N7	2.27	0.49
1:A:769:MET:HE3	2:B:970:HIS:CD2	2.48	0.49
1:A:1405:MET:HG2	1:A:1414:ILE:HD11	1.95	0.49
2:B:1129:ASN:HB2	2:B:1134:THR:HG22	1.94	0.49
11:N:7:DC:H2''	11:N:8:DG:C8	2.48	0.49
11:N:55:DC:H2''	11:N:56:DG:N7	2.27	0.49
25:W:55:ASP:HA	25:W:86:ASN:O	2.13	0.49
2:B:295:PRO:HA	2:B:298:MET:HG2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:165:LEU:O	24:V:169:ILE:HG12	2.12	0.49
1:A:1288:ILE:HG13	1:A:1289:GLU:N	2.28	0.49
13:T:-69:DA:H5'	13:T:-69:DA:H8	1.77	0.49
24:V:436:ARG:HA	24:V:472:LEU:HD21	1.94	0.49
25:W:427:VAL:HG23	25:W:458:ILE:HD11	1.95	0.49
4:E:163:TYR:HB2	4:E:165:LEU:HD22	1.95	0.49
6:G:150:THR:HA	6:G:159:ALA:HA	1.95	0.49
6:G:151:ARG:NH1	6:G:153:ASP:OD2	2.45	0.49
10:Z:450:ILE:HG23	10:Z:452:PRO:HD3	1.94	0.49
21:g:112:GLN:HB2	21:g:115:LEU:HG	1.95	0.49
1:A:1337:GLU:OE2	18:M:252:LYS:NZ	2.45	0.49
3:C:81:LYS:HZ3	3:C:126:ARG:HH22	1.61	0.49
14:D:93:HIS:HB3	14:D:96:GLU:OE1	2.13	0.49
18:M:132:ARG:N	18:M:167:GLU:OE2	2.46	0.49
1:A:861:GLN:HG3	1:A:1096:GLY:HA3	1.95	0.49
10:Z:178:ASN:N	10:Z:229:ALA:O	2.46	0.49
11:N:-58:DC:H2''	11:N:-57:DT:C5	2.48	0.49
24:V:473:ALA:HB1	24:V:514:ARG:HG3	1.94	0.49
3:C:52:ILE:HD12	3:C:61:ASP:HB3	1.95	0.48
4:E:55:ARG:O	4:E:56:THR:OG1	2.31	0.48
6:G:4:HIS:HB3	14:D:30:GLU:HB3	1.95	0.48
6:G:166:ASP:N	6:G:166:ASP:OD1	2.45	0.48
23:U:110:LEU:HD12	25:W:247:VAL:HG11	1.95	0.48
2:B:439:ILE:HG13	2:B:440:ILE:N	2.28	0.48
10:Z:199:LYS:HD3	10:Z:210:LEU:HD21	1.95	0.48
10:Z:625:HIS:HA	10:Z:635:MET:HA	1.94	0.48
21:c:87:ILE:HD12	21:c:102:ILE:HD11	1.95	0.48
22:d:88:SER:O	22:d:92:GLN:HG2	2.12	0.48
24:V:186:ASN:ND2	24:V:189:SER:OG	2.46	0.48
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.94	0.48
20:b:64:ASN:OD1	20:b:65:VAL:N	2.45	0.48
22:d:65:ASP:OD2	22:d:69:ARG:NH2	2.45	0.48
23:U:38:ILE:HG23	23:U:78:ILE:HD12	1.94	0.48
24:V:34:GLN:HG2	25:W:58:MET:HE1	1.94	0.48
2:B:157:ARG:NH1	2:B:180:ASP:O	2.45	0.48
4:E:41:LYS:HB3	4:E:46:ASP:HB2	1.95	0.48
6:G:81:LYS:HG3	6:G:148:VAL:HA	1.94	0.48
8:I:87:GLN:HG2	8:I:121:HIS:HE1	1.78	0.48
25:W:477:PHE:HZ	25:W:525:THR:HG23	1.77	0.48
1:A:809:HIS:HE1	2:B:697:GLU:HG3	1.77	0.48
7:H:14:ASP:HB3	7:H:29:HIS:HB2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:GLN:HG3	13:T:78:DC:H2''	1.95	0.48
1:A:1372:GLU:HG2	4:E:146:PRO:HG3	1.95	0.48
13:T:36:DC:H2''	13:T:37:DC:C5	2.48	0.48
18:M:237:ARG:HA	18:M:240:LEU:HG	1.96	0.48
23:U:138:PRO:HD2	23:U:141:CYS:SG	2.53	0.48
1:A:408:ARG:HH21	1:A:412:GLN:HB3	1.79	0.48
1:A:500:GLU:OE2	2:B:1058:LYS:HD3	2.14	0.48
1:A:808:PRO:HB2	2:B:675:LEU:HD12	1.95	0.48
2:B:851:ASP:HB2	17:L:15:MET:HE3	1.96	0.48
10:Z:480:VAL:O	10:Z:487:GLY:N	2.44	0.48
13:T:76:DG:H2'	13:T:77:DG:H8	1.77	0.48
20:b:91:LYS:HA	20:b:96:THR:HG22	1.95	0.48
25:W:531:ARG:HA	25:W:566:ILE:HD11	1.95	0.48
10:Z:521:CYS:HB3	10:Z:523:GLU:OE1	2.14	0.48
14:D:36:GLU:HG3	14:D:39:MET:HE2	1.94	0.48
20:b:75:HIS:ND1	22:d:77:LEU:HD12	2.28	0.48
19:e:54:TYR:CE2	20:f:36:ARG:HG3	2.48	0.48
1:A:1054:MET:HE1	1:A:1060:LEU:HD12	1.96	0.48
6:G:117:MET:HE3	6:G:128:TYR:HB3	1.96	0.48
11:N:-57:DT:H2''	11:N:-56:DG:C8	2.49	0.48
13:T:-38:DC:H2''	13:T:-37:DG:C8	2.49	0.48
13:T:10:DC:H2'	13:T:11:DG:C8	2.48	0.48
19:a:106:ASP:OD2	19:a:131:ARG:NE	2.46	0.48
24:V:487:ASP:OD1	24:V:488:GLY:N	2.47	0.48
2:B:710:ILE:HA	2:B:764:MET:HE2	1.95	0.48
2:B:1118:VAL:HG21	2:B:1171:MET:HB3	1.96	0.48
8:I:96:PHE:HD2	8:I:110:LEU:HD22	1.78	0.48
10:Z:552:ARG:HB2	10:Z:559:GLN:HB2	1.95	0.48
23:U:57:LEU:HD13	23:U:93:VAL:HB	1.96	0.48
23:U:116:ASN:ND2	25:W:199:GLU:OE2	2.47	0.48
24:V:5:LEU:HB2	24:V:12:ASN:HB3	1.96	0.48
24:V:275:VAL:HG21	24:V:314:LEU:HD23	1.95	0.48
6:G:151:ARG:HH22	10:Z:505:ASP:HB2	1.79	0.47
8:I:27:LYS:N	8:I:36:LEU:O	2.47	0.47
13:T:-36:DT:H2''	13:T:-35:DA:N7	2.29	0.47
23:U:167:ARG:HB2	25:W:540:VAL:HA	1.96	0.47
1:A:686:THR:HG21	2:B:1040:GLN:O	2.14	0.47
6:G:87:ALA:HB2	6:G:101:ILE:HG13	1.95	0.47
7:H:106:THR:OG1	7:H:107:GLU:OE1	2.28	0.47
19:e:61:LEU:HD12	20:f:37:LEU:HD23	1.96	0.47
1:A:1218:ARG:HG2	18:M:237:ARG:HH12	1.77	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1062:ARG:NH1	2:B:1081:ASP:O	2.47	0.47
10:Z:430:GLU:HA	10:Z:434:ILE:HD12	1.97	0.47
11:N:-36:DG:H2''	11:N:-35:DG:N7	2.28	0.47
24:V:58:ARG:H	25:W:60:PRO:HD3	1.79	0.47
25:W:314:PHE:HA	25:W:359:ILE:HD11	1.96	0.47
1:A:18:ILE:HD12	2:B:1171:MET:HG3	1.97	0.47
1:A:104:MET:O	1:A:108:ARG:HG3	2.14	0.47
6:G:110:ARG:HG2	6:G:119:PHE:CZ	2.50	0.47
23:U:24:TRP:CZ3	25:W:274:HIS:HB3	2.49	0.47
24:V:57:PRO:HA	25:W:60:PRO:HG3	1.95	0.47
24:V:212:VAL:HG11	24:V:256:VAL:HG11	1.96	0.47
2:B:625:LEU:HD13	2:B:675:LEU:HD21	1.97	0.47
4:E:94:MET:HE2	4:E:94:MET:HA	1.95	0.47
6:G:44:PHE:CZ	14:D:60:VAL:HG11	2.50	0.47
7:H:28:LEU:HD21	7:H:50:VAL:HG21	1.95	0.47
13:T:91:DA:H1'	13:T:92:DC:H5'	1.96	0.47
14:D:14:GLU:HG3	14:D:15:GLU:HG2	1.96	0.47
16:K:63:VAL:HG22	16:K:71:ILE:HG22	1.96	0.47
1:A:890:ARG:HH21	1:A:1023:VAL:HA	1.78	0.47
2:B:134:LYS:HG3	2:B:138:GLU:HB3	1.95	0.47
2:B:388:TYR:CD1	2:B:505:LEU:HD21	2.50	0.47
2:B:623:ARG:NH2	2:B:670:GLU:OE2	2.41	0.47
2:B:846:ASP:OD1	2:B:846:ASP:N	2.46	0.47
10:Z:177:PRO:HG3	10:Z:213:LYS:HG3	1.96	0.47
13:T:-37:DG:H2''	13:T:-36:DT:C6	2.49	0.47
13:T:73:DA:H2'	13:T:74:DA:C8	2.49	0.47
24:V:86:ALA:HA	24:V:89:ARG:NE	2.30	0.47
25:W:163:ALA:HA	25:W:172:LEU:HD13	1.97	0.47
25:W:452:LEU:HD12	25:W:495:THR:HG22	1.96	0.47
1:A:863:ARG:HG2	1:A:1432:PHE:HZ	1.79	0.47
6:G:78:ARG:HH12	14:D:23:PRO:HG2	1.80	0.47
10:Z:368:ARG:HB3	10:Z:373:PHE:CD2	2.50	0.47
11:N:67:DT:H2''	11:N:68:DC:C6	2.49	0.47
13:T:90:DC:H1'	13:T:91:DA:C8	2.50	0.47
19:e:64:LYS:HA	19:e:93:GLN:HE22	1.80	0.47
23:U:41:ILE:HA	23:U:44:CYS:SG	2.55	0.47
24:V:236:THR:OG1	24:V:308:PRO:HD2	2.14	0.47
24:V:290:VAL:HG11	24:V:298:LEU:HG	1.97	0.47
1:A:413:TYR:O	1:A:415:GLY:N	2.47	0.47
2:B:627:ILE:HD11	2:B:663:GLU:HB2	1.96	0.47
6:G:131:MET:HE3	6:G:131:MET:HA	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:D:126:GLU:O	14:D:129:GLN:HG3	2.14	0.47
23:U:57:LEU:O	23:U:60:THR:OG1	2.31	0.47
1:A:349:ARG:HA	1:A:349:ARG:HD3	1.75	0.47
1:A:729:PRO:HG3	18:M:247:GLU:HB3	1.96	0.47
1:A:1118:THR:O	1:A:1123:ARG:HB2	2.15	0.47
2:B:626:LEU:HD23	2:B:662:VAL:HG12	1.97	0.47
4:E:97:GLU:OE1	4:E:97:GLU:N	2.48	0.47
7:H:72:ASP:OD1	7:H:72:ASP:N	2.46	0.47
8:I:20:CYS:SG	8:I:22:ASN:ND2	2.84	0.47
8:I:106:ASP:N	8:I:106:ASP:OD1	2.47	0.47
9:Y:9:ASP:OD1	9:Y:9:ASP:N	2.47	0.47
10:Z:516:ARG:NH2	10:Z:517:ASP:OD1	2.48	0.47
21:g:16:THR:O	21:g:19:SER:OG	2.28	0.47
25:W:180:SER:HA	25:W:185:GLN:HB3	1.97	0.47
25:W:240:PHE:O	25:W:244:MET:HG2	2.15	0.47
25:W:502:HIS:O	25:W:505:SER:OG	2.28	0.47
26:X:1:MET:SD	26:X:1:MET:N	2.83	0.47
1:A:77:ASN:OD1	1:A:78:MET:N	2.41	0.47
1:A:111:CYS:N	1:A:116:LYS:O	2.43	0.47
1:A:465:HIS:CD2	1:A:467:MET:HB2	2.50	0.47
23:U:114:ASN:HB3	23:U:117:VAL:HB	1.96	0.47
24:V:416:GLN:C	24:V:452:PHE:HB2	2.39	0.47
24:V:486:PHE:HE1	24:V:504:ALA:HB1	1.80	0.47
1:A:192:ARG:NH2	1:A:199:TYR:OH	2.48	0.46
1:A:1370:GLY:HA2	4:E:178:PRO:HD2	1.96	0.46
13:T:-43:DT:OP2	21:c:17:ARG:NE	2.48	0.46
1:A:419:ILE:HD11	1:A:440:LEU:HB3	1.97	0.46
2:B:42:GLN:HG2	2:B:43:GLN:N	2.29	0.46
2:B:573:TRP:HZ2	2:B:576:ILE:HD11	1.80	0.46
2:B:702:MET:HA	2:B:702:MET:HE3	1.97	0.46
2:B:1105:GLU:HA	2:B:1109:GLU:HB2	1.97	0.46
13:T:5:DC:H2"	13:T:6:DC:C5	2.50	0.46
21:c:50:TYR:CD1	22:d:111:GLY:HA3	2.50	0.46
23:U:88:PRO:HA	23:U:91:LEU:HD12	1.97	0.46
25:W:57:ILE:HD13	25:W:87:TYR:CD1	2.50	0.46
1:A:828:LEU:HD11	2:B:1008:VAL:HG21	1.97	0.46
2:B:748:ALA:HB3	2:B:811:TYR:HB2	1.96	0.46
3:C:171:LYS:HE3	16:K:10:PHE:HB3	1.96	0.46
4:E:29:THR:OG1	4:E:31:ASP:OD1	2.25	0.46
18:M:242:LYS:O	18:M:245:ILE:HG22	2.16	0.46
24:V:1:MET:HG3	24:V:2:PHE:CD1	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:98:ALA:O	25:W:102:ILE:HG12	2.14	0.46
1:A:1157:ILE:HD13	1:A:1160:ARG:NH1	2.30	0.46
1:A:1442:ALA:HA	1:A:1447:GLU:HG3	1.97	0.46
2:B:83:ARG:HG3	2:B:133:ILE:HG23	1.98	0.46
2:B:411:LEU:HD11	2:B:435:ILE:HG23	1.96	0.46
6:G:100:GLU:HA	6:G:105:SER:HA	1.97	0.46
10:Z:358:PHE:CD1	10:Z:368:ARG:HB2	2.50	0.46
22:d:36:ILE:O	22:d:40:LYS:HG2	2.15	0.46
25:W:122:LEU:HA	25:W:125:LYS:HZ3	1.79	0.46
1:A:20:ARG:NH2	2:B:1172:MET:HG3	2.30	0.46
1:A:917:GLU:OE2	1:A:921:ARG:NH1	2.49	0.46
1:A:997:ASN:O	1:A:999:ARG:N	2.45	0.46
23:U:116:ASN:OD1	23:U:117:VAL:N	2.48	0.46
25:W:531:ARG:HG2	25:W:566:ILE:HG12	1.96	0.46
2:B:1172:MET:HE2	2:B:1172:MET:HA	1.98	0.46
6:G:38:CYS:HB2	6:G:44:PHE:CD1	2.46	0.46
10:Z:278:TRP:CD2	10:Z:388:PRO:HG3	2.51	0.46
11:N:-14:DA:H2''	11:N:-13:DA:C8	2.50	0.46
25:W:354:HIS:CE1	25:W:355:LYS:HG3	2.51	0.46
4:E:45:GLY:HA3	4:E:53:PRO:HD3	1.98	0.46
11:N:-34:DT:H2''	11:N:-33:DG:C8	2.51	0.46
13:T:63:DA:H2''	13:T:64:DA:H2'	1.97	0.46
17:L:47:LYS:HB3	17:L:47:LYS:HE2	1.71	0.46
21:c:16:THR:HG23	21:c:19:SER:H	1.81	0.46
25:W:469:VAL:O	25:W:472:LEU:HG	2.14	0.46
1:A:30:GLU:HA	1:A:33:ARG:HG2	1.98	0.46
1:A:686:THR:OG1	1:A:687:ILE:N	2.48	0.46
1:A:1029:LEU:HD23	4:E:162:ARG:HG2	1.98	0.46
2:B:67:LEU:HD13	2:B:420:GLN:NE2	2.30	0.46
4:E:79:GLU:OE1	4:E:79:GLU:N	2.35	0.46
9:Y:65:SER:N	10:Z:213:LYS:O	2.34	0.46
11:N:56:DG:H2''	11:N:57:DG:N7	2.30	0.46
19:e:79:LYS:HB2	19:e:82:LEU:HD11	1.97	0.46
24:V:150:TRP:HE1	24:V:160:GLU:HG3	1.81	0.46
24:V:203:ARG:O	24:V:207:MET:HG2	2.16	0.46
24:V:445:LEU:HD13	24:V:485:LEU:HD13	1.98	0.46
10:Z:427:GLU:OE2	10:Z:435:ASN:ND2	2.46	0.46
17:L:27:GLU:H	17:L:37:ARG:NH2	2.14	0.46
25:W:163:ALA:HA	25:W:172:LEU:HB3	1.98	0.46
1:A:42:LYS:O	1:A:288:ASN:ND2	2.42	0.46
10:Z:343:GLU:OE1	10:Z:346:ARG:NH2	2.42	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:19:DC:H2''	11:N:20:DG:H8	1.80	0.46
1:A:139:LYS:CG	1:A:143:HIS:HE1	2.28	0.45
1:A:894:ASP:OD2	1:A:1396:ARG:NH2	2.49	0.45
14:D:124:ASP:OD1	14:D:125:GLU:N	2.48	0.45
19:e:78:PHE:O	19:e:79:LYS:HD3	2.16	0.45
24:V:194:THR:HA	24:V:197:GLN:HB2	1.96	0.45
1:A:47:THR:HA	1:A:52:PRO:HA	1.98	0.45
6:G:6:SER:C	6:G:7:LEU:HD12	2.41	0.45
6:G:112:SER:O	6:G:163:LEU:HB3	2.16	0.45
13:T:-3:DG:OP1	19:a:118:THR:N	2.31	0.45
25:W:362:TYR:CD1	25:W:366:VAL:HG21	2.52	0.45
2:B:436:LYS:O	2:B:439:ILE:HG12	2.16	0.45
13:T:-14:DA:H2''	13:T:-13:DA:C8	2.51	0.45
22:d:43:LYS:HA	22:d:43:LYS:HD3	1.80	0.45
23:U:116:ASN:HD21	25:W:198:LEU:HD11	1.82	0.45
1:A:1400:LEU:O	1:A:1404:THR:HG23	2.16	0.45
2:B:84:TYR:HD2	2:B:86:LEU:HD23	1.81	0.45
2:B:133:ILE:HA	2:B:138:GLU:O	2.16	0.45
8:I:78:LEU:HD23	8:I:79:PRO:HD2	1.99	0.45
13:T:30:DT:OP1	22:d:29:SER:N	2.50	0.45
18:M:178:GLN:HA	18:M:181:ARG:NH1	2.31	0.45
24:V:445:LEU:HD22	24:V:485:LEU:HD22	1.98	0.45
1:A:576:GLN:O	1:A:590:GLN:NE2	2.49	0.45
13:T:24:DA:H2''	13:T:25:DG:H5'	1.98	0.45
14:D:76:ASN:O	14:D:79:THR:OG1	2.29	0.45
19:a:61:LEU:N	19:a:97:GLU:OE2	2.49	0.45
24:V:438:LYS:HE3	24:V:481:PHE:HB2	1.97	0.45
25:W:504:LEU:HG	25:W:509:VAL:HG13	1.98	0.45
7:H:8:ASP:OD2	7:H:32:SER:OG	2.20	0.45
9:Y:65:SER:HB3	10:Z:213:LYS:HA	1.99	0.45
11:N:41:DC:H2'	11:N:42:DA:C8	2.52	0.45
17:L:26:ASN:ND2	17:L:36:CYS:SG	2.90	0.45
18:M:219:LEU:HA	18:M:222:ARG:HG2	1.98	0.45
20:b:77:LYS:HA	20:b:77:LYS:HD3	1.82	0.45
22:h:96:ARG:HA	22:h:104:ALA:HB1	1.98	0.45
23:U:49:SER:O	23:U:53:LYS:HG3	2.16	0.45
2:B:282:ARG:HH21	8:I:21:ASN:HA	1.82	0.45
13:T:62:DA:H2''	13:T:63:DA:H8	1.82	0.45
13:T:63:DA:H1'	13:T:64:DA:H5'	1.99	0.45
14:D:41:LEU:HA	14:D:44:ARG:HG2	1.97	0.45
1:A:199:TYR:HB3	1:A:215:LEU:HA	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:SER:HB2	10:Z:733:ARG:HH11	1.81	0.45
10:Z:179:LEU:HD21	10:Z:226:TYR:HB3	1.98	0.45
1:A:364:ARG:NE	1:A:500:GLU:OE1	2.47	0.45
2:B:203:ASN:O	2:B:571:GLY:HA3	2.16	0.45
7:H:15:ILE:HG13	7:H:16:ASP:H	1.81	0.45
8:I:17:CYS:HB3	8:I:22:ASN:H	1.81	0.45
11:N:7:DC:H5''	20:b:47:SER:HA	1.99	0.45
13:T:-10:DC:H2''	13:T:-9:DA:C8	2.52	0.45
13:T:16:DA:H1'	13:T:17:DA:N7	2.32	0.45
21:c:115:LEU:HB3	20:f:44:LYS:HD2	1.99	0.45
1:A:664:ILE:HD12	1:A:664:ILE:H	1.82	0.45
1:A:866:LYS:HD2	1:A:866:LYS:HA	1.78	0.45
2:B:859:ARG:NH1	2:B:860:VAL:O	2.49	0.45
2:B:1040:GLN:HG2	3:C:203:TRP:CZ2	2.52	0.45
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.99	0.45
4:E:91:CYS:O	4:E:95:GLN:HG3	2.16	0.45
6:G:55:GLY:HA3	6:G:69:PRO:HG2	1.98	0.45
11:N:-69:DG:H2'	11:N:-68:DT:H6	1.81	0.45
13:T:87:DA:H2''	13:T:88:DA:N7	2.32	0.45
18:M:178:GLN:CD	18:M:181:ARG:HH12	2.24	0.45
20:f:67:ARG:HH12	22:h:97:LEU:HA	1.82	0.45
24:V:456:ALA:HB1	24:V:489:PHE:HE1	1.81	0.45
1:A:393:ILE:HD13	1:A:445:LYS:HG2	1.99	0.44
1:A:1227:THR:O	1:A:1231:ILE:HG13	2.17	0.44
2:B:235:ILE:HG13	2:B:348:LEU:HD12	1.99	0.44
2:B:295:PRO:HD2	2:B:296:GLU:OE1	2.16	0.44
3:C:133:ARG:HA	3:C:133:ARG:HD3	1.73	0.44
6:G:91:GLN:HB3	6:G:98:PHE:HB2	1.98	0.44
11:N:65:DA:H2''	11:N:66:DT:H72	1.98	0.44
1:A:355:MET:HE3	1:A:1431:SER:OG	2.17	0.44
1:A:927:GLU:OE2	1:A:931:ARG:NH2	2.51	0.44
2:B:1040:GLN:HG2	3:C:203:TRP:CH2	2.51	0.44
6:G:148:VAL:O	10:Z:475:GLY:HA3	2.17	0.44
7:H:112:LEU:HB2	7:H:132:LEU:HD12	1.99	0.44
1:A:488:VAL:O	1:A:491:PRO:HD2	2.17	0.44
6:G:8:GLU:OE1	6:G:71:LYS:HG2	2.18	0.44
18:M:245:ILE:HD12	18:M:248:HIS:HB2	1.99	0.44
24:V:73:LEU:HA	25:W:101:LEU:HD21	1.99	0.44
25:W:89:ALA:O	25:W:93:THR:HG22	2.17	0.44
2:B:342:VAL:HG23	2:B:346:GLU:HG3	2.00	0.44
3:C:73:LEU:O	3:C:238:SER:OG	2.25	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:110:ARG:HA	6:G:113:ILE:HD12	2.00	0.44
13:T:8:DC:H2''	13:T:9:DG:C8	2.52	0.44
23:U:89:TRP:CZ3	25:W:236:HIS:HD2	2.36	0.44
1:A:428:ASP:OD1	1:A:429:LEU:N	2.50	0.44
1:A:922:PHE:HD1	1:A:1052:ARG:HA	1.83	0.44
2:B:1148:LEU:HD23	2:B:1148:LEU:H	1.82	0.44
5:F:57:MET:HE2	5:F:62:ARG:HA	2.00	0.44
7:H:71:ASP:N	7:H:71:ASP:OD1	2.51	0.44
10:Z:185:LYS:HB3	10:Z:188:GLU:HB2	1.98	0.44
21:g:26:PRO:HG2	21:g:29:ARG:HB3	2.00	0.44
23:U:178:LEU:HD23	23:U:181:LYS:HD2	1.99	0.44
24:V:46:SER:O	24:V:49:PRO:HD2	2.18	0.44
24:V:121:PRO:O	24:V:148:GLN:NE2	2.50	0.44
24:V:372:ARG:C	24:V:375:PRO:HD2	2.42	0.44
1:A:36:VAL:HG23	2:B:1138:ARG:HH22	1.82	0.44
1:A:467:MET:HG2	1:A:534:VAL:HG21	2.00	0.44
1:A:1311:LEU:HG	1:A:1334:TRP:CZ3	2.52	0.44
3:C:19:VAL:HG12	3:C:21:PHE:HD1	1.82	0.44
13:T:-8:DC:H2''	13:T:-7:DG:C8	2.53	0.44
24:V:433:THR:HG23	24:V:441:LEU:HD21	2.00	0.44
25:W:526:ASP:OD1	25:W:527:ILE:N	2.51	0.44
26:X:30:LEU:O	26:X:34:LYS:HB2	2.18	0.44
1:A:191:ILE:HA	1:A:200:ALA:HA	2.00	0.44
1:A:416:ALA:HA	1:A:448:ARG:HA	2.00	0.44
1:A:1416:ARG:NH2	13:T:73:DA:H1'	2.32	0.44
2:B:85:LEU:HB2	2:B:131:THR:HB	1.99	0.44
2:B:137:GLU:HG2	2:B:139:GLN:HE22	1.81	0.44
2:B:848:LEU:HD13	2:B:852:GLY:HA2	2.00	0.44
4:E:84:ILE:HD11	4:E:113:SER:HB2	2.00	0.44
5:F:51:ARG:HD2	5:F:118:TRP:NE1	2.32	0.44
15:J:14:VAL:HG11	15:J:48:MET:HG2	2.00	0.44
19:a:69:ARG:NH1	20:b:25:ASN:OD1	2.50	0.44
24:V:60:GLU:OE1	24:V:60:GLU:N	2.50	0.44
24:V:77:VAL:HG12	24:V:119:HIS:HD1	1.82	0.44
25:W:432:ASP:O	25:W:436:SER:OG	2.30	0.44
1:A:496:PHE:CD2	2:B:791:GLU:HB2	2.48	0.44
1:A:960:ARG:O	1:A:964:GLU:HG2	2.17	0.44
1:A:1146:GLN:HG2	1:A:1149:ARG:NH1	2.32	0.44
1:A:1148:ALA:HB1	1:A:1333:GLU:HB3	2.00	0.44
2:B:910:THR:OG1	2:B:911:LEU:N	2.50	0.44
2:B:1037:ILE:HG22	2:B:1039:SER:H	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:-55:DG:H2''	13:T:-54:DA:C8	2.52	0.44
23:U:110:LEU:HD13	23:U:121:LEU:HD11	2.00	0.44
24:V:426:LEU:HD22	24:V:461:PHE:CE2	2.53	0.44
24:V:469:LEU:HB3	24:V:476:PHE:CZ	2.52	0.44
10:Z:438:GLY:HA3	10:Z:452:PRO:HB2	2.00	0.44
20:b:57:VAL:HA	20:b:60:VAL:HG12	1.99	0.44
24:V:81:ALA:HB2	24:V:93:LEU:HD11	2.00	0.44
24:V:193:LYS:HG3	24:V:196:ARG:NH2	2.32	0.44
24:V:431:HIS:O	24:V:434:LYS:HG2	2.18	0.44
25:W:468:GLN:OE1	25:W:468:GLN:N	2.48	0.44
25:W:531:ARG:HG2	25:W:566:ILE:CG1	2.47	0.44
1:A:91:ALA:HB3	1:A:290:LEU:HD23	2.00	0.43
1:A:1155:LYS:HG3	18:M:246:ARG:HH21	1.83	0.43
10:Z:422:PRO:HA	10:Z:440:ILE:HB	2.00	0.43
10:Z:588:ASP:HB3	10:Z:594:ILE:HD13	1.99	0.43
13:T:81:DC:H2'	13:T:82:DC:H6	1.82	0.43
14:D:60:VAL:HA	14:D:63:LYS:HD2	2.00	0.43
19:e:66:PRO:HB3	20:f:28:GLY:HA3	2.00	0.43
24:V:1:MET:HE2	24:V:1:MET:HA	1.99	0.43
24:V:311:ILE:HD11	24:V:348:GLY:HA3	2.00	0.43
24:V:333:ARG:NH1	26:X:6:PRO:O	2.43	0.43
1:A:379:GLY:HA2	1:A:475:ARG:O	2.18	0.43
1:A:496:PHE:HB2	2:B:791:GLU:O	2.18	0.43
1:A:1135:LYS:HD2	1:A:1135:LYS:HA	1.66	0.43
3:C:20:LYS:HE2	3:C:232:ASN:ND2	2.33	0.43
13:T:-57:DC:H2''	13:T:-56:DC:C5	2.52	0.43
14:D:73:ARG:HG3	14:D:104:CYS:SG	2.59	0.43
15:J:67:LYS:HB3	17:L:23:HIS:HB2	1.99	0.43
24:V:219:LEU:HB3	24:V:238:ARG:HE	1.83	0.43
24:V:242:LEU:HD23	24:V:263:THR:HG21	2.00	0.43
2:B:344:GLN:NE2	2:B:355:ASP:O	2.51	0.43
2:B:474:THR:HG23	2:B:477:SER:H	1.83	0.43
2:B:757:PRO:HB2	2:B:760:THR:HG22	2.00	0.43
2:B:796:MET:HE2	2:B:945:CYS:HB2	2.01	0.43
2:B:845:TYR:HA	2:B:865:VAL:HG11	1.99	0.43
2:B:1119:CYS:SG	2:B:1120:ASN:N	2.91	0.43
4:E:58:LEU:HD23	4:E:58:LEU:H	1.83	0.43
5:F:75:MET:HE1	6:G:64:GLY:H	1.84	0.43
10:Z:728:THR:O	10:Z:747:ARG:NH1	2.51	0.43
11:N:-27:DC:H2''	11:N:-26:DC:C5	2.54	0.43
14:D:44:ARG:HH11	14:D:44:ARG:HG3	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:M:135:SER:HA	18:M:145:ARG:HH12	1.83	0.43
18:M:153:ARG:NH2	18:M:166:GLU:OE2	2.51	0.43
22:d:59:MET:O	22:d:63:VAL:HG23	2.17	0.43
21:g:32:ARG:HH22	22:h:32:GLU:CD	2.26	0.43
23:U:65:ARG:HH12	25:W:294:GLN:CG	2.31	0.43
24:V:85:LYS:HD2	24:V:85:LYS:HA	1.73	0.43
24:V:332:PRO:HG3	24:V:378:MET:SD	2.58	0.43
25:W:220:LEU:O	25:W:224:LEU:HB2	2.18	0.43
25:W:450:VAL:O	25:W:454:LEU:HG	2.19	0.43
1:A:14:PRO:HD2	1:A:16:ARG:HH12	1.83	0.43
1:A:36:VAL:HG21	1:A:73:THR:HG21	1.99	0.43
2:B:850:ASP:OD1	2:B:850:ASP:N	2.51	0.43
15:J:48:MET:HE2	15:J:48:MET:HB2	1.77	0.43
19:a:101:VAL:O	19:a:105:GLU:OE1	2.37	0.43
21:g:25:PHE:HZ	21:g:59:THR:HG21	1.84	0.43
24:V:2:PHE:O	24:V:12:ASN:ND2	2.49	0.43
1:A:233:CYS:HA	1:A:236:LEU:HB3	2.00	0.43
1:A:1098:PRO:HA	1:A:1101:GLN:NE2	2.34	0.43
2:B:399:LEU:HB3	2:B:453:TRP:CZ2	2.53	0.43
2:B:808:SER:OG	2:B:1050:ARG:NH1	2.51	0.43
3:C:24:GLU:OE2	3:C:228:ARG:NE	2.52	0.43
13:T:-3:DG:C8	13:T:-3:DG:H5'	2.53	0.43
14:D:63:LYS:HA	14:D:66:ASN:ND2	2.33	0.43
14:D:65:LEU:HA	14:D:68:THR:HG22	2.00	0.43
19:a:113:HIS:CE1	19:e:116:ARG:HH22	2.36	0.43
19:e:107:THR:OG1	19:e:124:ILE:HG12	2.18	0.43
25:W:510:LEU:HB2	25:W:511:PRO:HD3	2.00	0.43
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.99	0.43
1:A:707:LYS:HE2	1:A:707:LYS:HB3	1.87	0.43
1:A:769:MET:HE2	2:B:973:PRO:HG3	2.00	0.43
3:C:103:LEU:HB3	3:C:161:LEU:HG	2.00	0.43
3:C:105:VAL:HG11	3:C:115:VAL:HG22	2.00	0.43
4:E:101:ARG:HA	4:E:126:ILE:O	2.18	0.43
10:Z:366:TYR:HB2	10:Z:373:PHE:O	2.18	0.43
18:M:183:THR:OG1	18:M:188:LYS:NZ	2.52	0.43
23:U:62:HIS:CD2	25:W:278:GLN:HE21	2.29	0.43
24:V:44:LEU:O	24:V:48:LEU:HG	2.18	0.43
1:A:139:LYS:CG	1:A:143:HIS:CE1	2.96	0.43
1:A:863:ARG:HG2	1:A:1432:PHE:CZ	2.54	0.43
1:A:1372:GLU:OE2	4:E:195:ARG:NH1	2.52	0.43
2:B:155:MET:HB2	2:B:185:PHE:CE1	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1062:ARG:NH2	2:B:1066:PRO:O	2.40	0.43
2:B:1168:ALA:HB1	2:B:1170:ARG:HE	1.84	0.43
6:G:44:PHE:HZ	14:D:60:VAL:HG11	1.84	0.43
8:I:82:GLU:HB3	8:I:92:LYS:NZ	2.33	0.43
11:N:-59:DT:H1'	11:N:-58:DC:H5'	1.99	0.43
11:N:11:DC:H2''	11:N:12:DG:C8	2.53	0.43
13:T:-67:DA:H2''	13:T:-66:DA:C8	2.53	0.43
23:U:23:LEU:HD12	25:W:233:HIS:HD1	1.83	0.43
24:V:70:ARG:HG3	24:V:112:VAL:CG2	2.48	0.43
24:V:128:LEU:HA	24:V:131:VAL:HG22	2.01	0.43
24:V:422:CYS:O	24:V:426:LEU:HG	2.18	0.43
25:W:526:ASP:H	25:W:529:LEU:HD12	1.83	0.43
1:A:244:ARG:HB3	1:A:247:TRP:CE3	2.54	0.43
1:A:365:THR:HG22	1:A:366:VAL:N	2.34	0.43
1:A:1093:GLN:HE22	2:B:1093:CYS:HA	1.83	0.43
1:A:1440:MET:SD	2:B:1167:ILE:HD11	2.59	0.43
1:A:1450:PRO:HB2	1:A:1452:LYS:HG2	2.00	0.43
2:B:715:ASP:OD1	2:B:716:HIS:ND1	2.52	0.43
2:B:1123:GLY:H	2:B:1170:ARG:HD2	1.83	0.43
2:B:1170:ARG:HB3	2:B:1172:MET:HE3	2.01	0.43
11:N:-26:DC:H2''	11:N:-25:DC:C5	2.53	0.43
1:A:189:PRO:HB3	1:A:202:TRP:CE3	2.54	0.43
1:A:687:ILE:HD11	1:A:766:PHE:CZ	2.53	0.43
2:B:319:ASN:HD21	2:B:336:ILE:HD11	1.82	0.43
2:B:826:GLU:H	2:B:872:THR:HG22	1.83	0.43
6:G:2:PHE:CD2	14:D:37:VAL:HG21	2.54	0.43
22:d:33:SER:HB2	22:d:60:ASN:ND2	2.34	0.43
23:U:123:GLU:OE2	23:U:124:LEU:HG	2.19	0.43
24:V:494:SER:OG	24:V:495:PRO:HD3	2.19	0.43
25:W:260:ARG:NE	25:W:264:GLU:OE2	2.40	0.43
25:W:411:LEU:HD12	25:W:414:LEU:HD23	2.00	0.43
1:A:94:VAL:HG13	1:A:311:GLN:CD	2.43	0.43
1:A:589:LYS:HZ2	1:A:637:MET:HA	1.84	0.43
1:A:609:HIS:HA	1:A:626:THR:HG21	2.01	0.43
1:A:695:ASP:C	1:A:697:LYS:H	2.27	0.43
16:K:85:GLU:HA	16:K:88:THR:HG22	2.01	0.43
18:M:228:MET:SD	18:M:228:MET:N	2.91	0.43
25:W:516:ILE:HG13	25:W:533:PHE:CZ	2.54	0.43
2:B:790:GLN:HA	2:B:968:ASN:ND2	2.34	0.42
9:Y:72:SER:HB2	9:Y:78:SER:HA	2.01	0.42
18:M:186:LYS:HA	18:M:189:ASN:HD21	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:M:194:ARG:NH2	18:M:223:MET:O	2.52	0.42
23:U:153:ALA:HB2	25:W:256:SER:HB3	2.01	0.42
25:W:329:ARG:NH2	25:W:366:VAL:O	2.52	0.42
1:A:1316:ASN:OD1	1:A:1317:LYS:N	2.52	0.42
2:B:773:PRO:HG3	15:J:53:VAL:HG11	2.02	0.42
2:B:1038:THR:HA	3:C:195:THR:HA	2.01	0.42
2:B:1136:GLU:HA	2:B:1143:LYS:HA	2.00	0.42
11:N:4:DG:H5'	11:N:4:DG:C8	2.55	0.42
21:c:63:LEU:HD22	22:d:42:LEU:HD13	2.01	0.42
22:d:36:ILE:HG13	22:d:37:TYR:N	2.34	0.42
1:A:222:HIS:HB2	1:A:249:ILE:HD11	2.01	0.42
1:A:692:SER:O	1:A:828:LEU:HD22	2.19	0.42
2:B:110:PRO:HG2	2:B:163:LEU:HD13	2.01	0.42
3:C:7:PRO:HD2	16:K:100:LEU:HD23	2.02	0.42
4:E:61:LEU:HD11	4:E:71:GLN:HB3	2.01	0.42
21:c:115:LEU:HD13	20:f:44:LYS:HB2	2.01	0.42
22:d:100:PRO:HD2	22:d:103:LEU:HD12	2.00	0.42
22:h:113:LYS:O	22:h:117:LYS:HG2	2.20	0.42
23:U:139:LEU:HB2	25:W:331:PRO:HG3	2.02	0.42
24:V:462:LEU:HB3	24:V:503:HIS:CG	2.55	0.42
1:A:1378:LEU:HD12	1:A:1378:LEU:HA	1.90	0.42
2:B:573:TRP:CZ2	2:B:576:ILE:HD11	2.54	0.42
2:B:795:ILE:O	2:B:965:ILE:HA	2.19	0.42
10:Z:556:GLU:HB2	10:Z:571:ARG:HH12	1.84	0.42
19:e:48:LEU:O	19:e:52:ARG:HG3	2.20	0.42
24:V:318:THR:HA	24:V:341:LEU:HD13	2.01	0.42
25:W:375:ARG:HD2	25:W:378:ILE:HD11	2.01	0.42
25:W:397:CYS:HA	25:W:430:TRP:CZ2	2.54	0.42
1:A:30:GLU:HA	1:A:33:ARG:HE	1.84	0.42
1:A:527:THR:HG22	1:A:532:ARG:O	2.19	0.42
4:E:151:MET:HE3	4:E:192:LYS:HB2	2.01	0.42
13:T:-23:DC:H2''	13:T:-22:DA:H8	1.84	0.42
17:L:17:TYR:CE1	17:L:46:LYS:HG2	2.55	0.42
23:U:93:VAL:HA	23:U:96:ILE:HG22	2.00	0.42
23:U:123:GLU:HG2	25:W:206:ARG:HD2	2.00	0.42
4:E:18:MET:HE3	4:E:32:GLU:HG3	2.02	0.42
4:E:77:PRO:HG3	4:E:90:TYR:HE2	1.84	0.42
4:E:128:GLU:OE1	4:E:128:GLU:N	2.52	0.42
1:A:35:SER:OG	1:A:36:VAL:N	2.51	0.42
1:A:294:GLU:HB3	1:A:303:ILE:HD12	2.02	0.42
1:A:869:GLU:OE2	1:A:1455:SER:OG	2.30	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:991:GLN:HA	1:A:996:ILE:HG12	2.01	0.42
4:E:29:THR:N	4:E:32:GLU:OE2	2.46	0.42
7:H:27:ARG:HD2	7:H:40:ILE:HG23	2.02	0.42
11:N:-6:DG:H2''	11:N:-5:DG:N7	2.35	0.42
14:D:23:PRO:HB2	14:D:25:GLU:HG2	2.02	0.42
18:M:215:ILE:HG13	18:M:219:LEU:HD23	2.02	0.42
25:W:520:LEU:HD22	25:W:530:ILE:HG21	2.01	0.42
3:C:8:THR:OG1	3:C:24:GLU:HB2	2.20	0.42
6:G:99:THR:N	6:G:106:CYS:O	2.51	0.42
7:H:14:ASP:OD1	7:H:15:ILE:N	2.51	0.42
8:I:58:ILE:HD12	8:I:58:ILE:H	1.83	0.42
16:K:88:THR:O	16:K:92:THR:HG23	2.20	0.42
22:h:41:VAL:O	22:h:44:GLN:HG2	2.20	0.42
25:W:123:LEU:HD22	25:W:155:TRP:CZ3	2.54	0.42
1:A:202:TRP:HD1	1:A:212:LYS:HB2	1.85	0.42
2:B:1123:GLY:HA3	2:B:1171:MET:H	1.85	0.42
3:C:78:ILE:HD11	3:C:126:ARG:HD2	2.00	0.42
7:H:147:LYS:HE3	7:H:147:LYS:HB2	1.79	0.42
20:b:47:SER:HB3	20:b:50:ILE:HG12	2.02	0.42
24:V:51:LEU:HD13	24:V:61:PHE:CE1	2.54	0.42
1:A:1227:THR:HG23	1:A:1229:GLU:HG2	2.01	0.42
2:B:603:MET:HG3	2:B:614:ILE:HG12	2.01	0.42
2:B:744:MET:HE2	2:B:744:MET:HB2	1.98	0.42
3:C:44:ILE:HD11	3:C:238:SER:HB3	2.02	0.42
7:H:55:LYS:HE2	7:H:55:LYS:HB3	1.90	0.42
11:N:-48:DC:H2''	11:N:-47:DC:C5	2.55	0.42
13:T:-50:DC:H2''	13:T:-49:DG:C8	2.55	0.42
24:V:215:TYR:CE2	24:V:253:ILE:HG23	2.55	0.42
24:V:262:PHE:HD2	24:V:286:PHE:HB2	1.85	0.42
25:W:494:LYS:HA	25:W:497:LEU:HD12	2.00	0.42
1:A:775:LYS:HD2	2:B:974:SER:HB3	2.02	0.41
1:A:956:PHE:O	1:A:959:MET:HB2	2.19	0.41
1:A:1128:ILE:HG23	1:A:1414:ILE:HG13	2.02	0.41
2:B:168:ASP:OD1	2:B:169:ARG:N	2.53	0.41
11:N:69:DT:H2''	11:N:70:DG:H8	1.84	0.41
13:T:30:DT:H2'	13:T:31:DT:H71	2.02	0.41
13:T:64:DA:H2''	13:T:65:DA:C8	2.55	0.41
17:L:27:GLU:H	17:L:37:ARG:HH22	1.68	0.41
23:U:178:LEU:HD13	25:W:450:VAL:HG23	2.01	0.41
1:A:1288:ILE:O	1:A:1292:MET:HG3	2.20	0.41
1:A:1303:GLN:O	1:A:1340:GLY:HA3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:783:ALA:HB2	2:B:1041:ILE:HG23	2.02	0.41
5:F:90:LEU:HD23	5:F:90:LEU:HA	1.90	0.41
6:G:38:CYS:HB3	6:G:155:ASN:O	2.20	0.41
9:Y:61:ILE:HG22	9:Y:63:MET:SD	2.60	0.41
10:Z:480:VAL:HG12	10:Z:486:GLU:HA	2.02	0.41
11:N:22:DT:H2''	11:N:23:DG:H5''	2.02	0.41
15:J:3:ILE:HD12	15:J:4:PRO:HD2	2.02	0.41
24:V:193:LYS:O	24:V:197:GLN:N	2.48	0.41
25:W:215:GLY:HA3	25:W:219:ASN:HB2	2.02	0.41
1:A:103:THR:HG23	1:A:225:PHE:HE2	1.86	0.41
1:A:136:GLN:HE22	1:A:1423:ASP:CG	2.27	0.41
1:A:466:LYS:HE3	1:A:524:MET:HE1	2.01	0.41
1:A:520:MET:HB3	1:A:522:PRO:HD2	2.02	0.41
1:A:1209:PRO:HB3	8:I:33:ARG:HH11	1.86	0.41
1:A:1368:VAL:HG12	1:A:1369:LEU:HG	2.02	0.41
3:C:81:LYS:HZ3	3:C:126:ARG:NH2	2.17	0.41
10:Z:383:THR:OG1	10:Z:384:GLU:OE1	2.37	0.41
10:Z:390:LEU:HD23	10:Z:393:LEU:HD12	2.01	0.41
22:h:73:GLU:HA	22:h:76:ARG:HD2	2.02	0.41
23:U:35:ALA:HB2	23:U:71:MET:HE1	2.02	0.41
24:V:250:VAL:HG11	24:V:253:ILE:HD12	2.02	0.41
24:V:403:TYR:CD2	24:V:439:ASN:HB3	2.56	0.41
24:V:444:LEU:HD23	24:V:444:LEU:HA	1.90	0.41
25:W:83:LEU:HA	25:W:86:ASN:HB2	2.01	0.41
25:W:501:VAL:HG22	25:W:537:VAL:HG23	2.01	0.41
1:A:775:LYS:HA	1:A:775:LYS:HD3	1.91	0.41
2:B:591:ARG:HD3	2:B:603:MET:HE1	2.02	0.41
6:G:22:LEU:O	6:G:26:VAL:HG23	2.20	0.41
10:Z:308:ILE:HG21	10:Z:337:GLN:HB3	2.03	0.41
11:N:-52:DC:H2''	11:N:-51:DG:H8	1.85	0.41
20:f:89:ALA:O	20:f:93:GLN:HG2	2.20	0.41
24:V:48:LEU:HB3	24:V:58:ARG:NH2	2.36	0.41
24:V:213:LYS:HA	24:V:213:LYS:HD3	1.87	0.41
24:V:274:PHE:HA	24:V:320:ARG:NH2	2.35	0.41
24:V:497:LYS:HB3	24:V:499:ASN:OD1	2.20	0.41
1:A:1211:LEU:HD23	1:A:1260:ARG:HH12	1.85	0.41
2:B:17:ILE:O	2:B:19:PRO:HD3	2.21	0.41
2:B:267:VAL:HG23	2:B:320:PHE:HE2	1.84	0.41
2:B:700:PRO:HB2	2:B:1002:PHE:CD2	2.55	0.41
2:B:759:VAL:HG13	2:B:759:VAL:O	2.21	0.41
3:C:44:ILE:HD11	3:C:238:SER:CB	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:82:GLU:HB3	8:I:92:LYS:HZ2	1.85	0.41
18:M:153:ARG:HG3	18:M:158:TYR:CZ	2.56	0.41
19:a:74:ILE:HD12	20:b:59:LYS:HD2	2.02	0.41
23:U:37:VAL:O	23:U:41:ILE:HG13	2.21	0.41
23:U:110:LEU:HD23	23:U:110:LEU:HA	1.93	0.41
23:U:167:ARG:NH1	25:W:539:ASP:OD1	2.53	0.41
24:V:172:LYS:HD2	24:V:187:PHE:CE1	2.55	0.41
24:V:427:TYR:CD2	24:V:430:LEU:HD12	2.55	0.41
25:W:93:THR:O	25:W:97:LEU:HG	2.21	0.41
1:A:909:LEU:O	1:A:910:LYS:HG2	2.20	0.41
1:A:1286:ARG:O	1:A:1289:GLU:HG3	2.21	0.41
1:A:1311:LEU:HD22	1:A:1332:GLN:HG2	2.03	0.41
2:B:861:SER:HA	2:B:901:THR:HA	2.02	0.41
9:Y:61:ILE:HG12	10:Z:216:VAL:HG13	2.01	0.41
9:Y:115:ILE:HB	10:Z:267:VAL:HG12	2.03	0.41
11:N:-42:DG:OP1	21:g:20:ARG:NH2	2.53	0.41
19:a:41:TYR:HD2	19:a:45:THR:HG21	1.85	0.41
23:U:45:PHE:HE2	23:U:85:ASP:HB2	1.85	0.41
24:V:110:GLN:N	24:V:111:PRO:HD2	2.36	0.41
24:V:274:PHE:HA	24:V:320:ARG:HH21	1.86	0.41
24:V:433:THR:HA	24:V:441:LEU:HD11	2.03	0.41
1:A:71:CYS:HB3	1:A:74:CYS:O	2.21	0.41
1:A:601:ASN:ND2	1:A:989:ASN:OD1	2.49	0.41
2:B:364:PHE:CD2	2:B:368:MET:HE3	2.56	0.41
10:Z:624:LEU:O	10:Z:635:MET:HG3	2.21	0.41
21:g:41:GLU:HB2	22:h:84:SER:HB3	2.02	0.41
21:g:64:GLU:HG3	22:h:45:VAL:HG13	2.02	0.41
24:V:58:ARG:HA	24:V:61:PHE:CE1	2.55	0.41
24:V:324:GLU:O	24:V:328:GLN:HG2	2.21	0.41
25:W:102:ILE:HD12	25:W:108:PRO:HG3	2.03	0.41
1:A:457:ILE:HB	1:A:504:HIS:HB2	2.03	0.41
1:A:652:LEU:HD12	1:A:652:LEU:HA	1.93	0.41
1:A:927:GLU:HG3	1:A:943:LEU:HD11	2.02	0.41
2:B:63:PRO:HA	2:B:64:PRO:HD3	1.95	0.41
4:E:112:PRO:O	4:E:115:LYS:HB2	2.20	0.41
6:G:113:ILE:HG23	6:G:117:MET:HE2	2.03	0.41
11:N:-75:DG:C8	11:N:-75:DG:H5'	2.56	0.41
11:N:-68:DT:H2'	11:N:-67:DT:C6	2.55	0.41
11:N:-44:DG:H2'	11:N:-43:DT:H71	2.03	0.41
11:N:7:DC:H2''	11:N:8:DG:H8	1.85	0.41
14:D:33:LEU:HA	14:D:102:ASN:HD21	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:M:172:ILE:O	18:M:176:ILE:HG12	2.21	0.41
24:V:219:LEU:HD13	24:V:238:ARG:HE	1.86	0.41
1:A:59:ASP:OD2	1:A:61:ARG:HB2	2.21	0.41
1:A:106:VAL:HG22	1:A:236:LEU:HD21	2.03	0.41
1:A:486:LEU:HD21	2:B:790:GLN:HB2	2.03	0.41
1:A:1451:MET:HE1	1:A:1460:LEU:HD23	2.03	0.41
2:B:18:THR:HG22	2:B:637:LYS:HG3	2.02	0.41
2:B:59:VAL:HG23	2:B:408:PHE:CZ	2.56	0.41
2:B:941:GLN:HE21	2:B:977:THR:HG21	1.86	0.41
4:E:185:ILE:HD12	4:E:209:VAL:HG21	2.03	0.41
6:G:106:CYS:SG	6:G:159:ALA:HB3	2.61	0.41
7:H:96:VAL:HG23	7:H:115:TYR:O	2.21	0.41
10:Z:219:GLU:HG2	10:Z:220:HIS:N	2.35	0.41
11:N:-70:DC:H2''	11:N:-69:DG:C8	2.55	0.41
19:a:118:THR:OG1	20:b:45:ARG:HG2	2.21	0.41
21:c:71:ARG:NH2	21:c:75:LYS:O	2.48	0.41
19:e:62:ILE:HG21	19:e:67:PHE:HD1	1.86	0.41
23:U:161:LYS:HE2	23:U:161:LYS:HB3	1.87	0.41
24:V:89:ARG:O	24:V:93:LEU:HG	2.21	0.41
24:V:503:HIS:CE1	24:V:506:ARG:HH12	2.39	0.41
1:A:1362:ILE:HG22	1:A:1411:LEU:HD11	2.02	0.41
1:A:1411:LEU:HD23	1:A:1411:LEU:HA	1.86	0.41
2:B:19:PRO:C	2:B:21:LEU:H	2.29	0.41
2:B:271:ILE:H	2:B:271:ILE:HD12	1.86	0.41
2:B:794:VAL:HG12	2:B:967:ILE:HG22	2.02	0.41
4:E:173:ILE:O	4:E:209:VAL:HA	2.21	0.41
10:Z:201:ILE:O	10:Z:204:GLN:HG2	2.21	0.41
13:T:-26:DT:H6	13:T:-26:DT:H2'	1.73	0.41
18:M:195:ILE:O	18:M:199:LYS:HG2	2.21	0.41
23:U:126:GLU:O	23:U:130:GLU:HG3	2.22	0.41
24:V:138:TYR:CE1	24:V:156:LEU:HD21	2.56	0.41
24:V:231:ASN:HB3	24:V:234:TYR:CE2	2.56	0.41
1:A:191:ILE:HG22	1:A:200:ALA:HB2	2.03	0.40
1:A:477:LEU:HB3	1:A:483:ARG:HH21	1.87	0.40
1:A:1416:ARG:HB3	1:A:1433:GLU:OE1	2.20	0.40
2:B:298:MET:O	2:B:301:VAL:HG22	2.21	0.40
2:B:818:GLU:OE2	2:B:917:LYS:HB2	2.21	0.40
4:E:35:GLN:HB2	4:E:39:GLU:HG3	2.01	0.40
6:G:144:ARG:HH21	14:D:103:LEU:HB3	1.85	0.40
11:N:-13:DA:H2''	11:N:-12:DA:H8	1.86	0.40
11:N:68:DC:H3'	11:N:69:DT:H71	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:-44:DA:H3'	21:c:28:GLY:HA3	2.02	0.40
20:f:75:HIS:CD2	22:h:93:THR:HG21	2.57	0.40
21:g:63:LEU:HD12	22:h:41:VAL:HG12	2.03	0.40
21:g:79:ILE:HG22	21:g:82:HIS:CE1	2.56	0.40
23:U:168:LYS:HG2	23:U:169:PRO:HD2	2.03	0.40
1:A:811:ILE:HD11	8:I:79:PRO:HA	2.02	0.40
1:A:1422:GLN:HG3	1:A:1424:THR:HG23	2.03	0.40
2:B:230:ARG:HD2	2:B:231:PRO:HD2	2.04	0.40
3:C:60:HIS:O	3:C:64:ILE:HG12	2.21	0.40
4:E:151:MET:HB3	4:E:155:GLU:HG3	2.03	0.40
6:G:148:VAL:HG11	6:G:162:SER:HB2	2.03	0.40
7:H:38:ASP:N	7:H:38:ASP:OD1	2.53	0.40
11:N:1:DC:H2''	11:N:2:DG:H8	1.86	0.40
11:N:24:DC:H2''	11:N:25:DT:C6	2.56	0.40
13:T:59:DA:H2''	13:T:60:DA:C8	2.56	0.40
14:D:66:ASN:OD1	14:D:67:TYR:N	2.54	0.40
18:M:145:ARG:NE	18:M:173:GLU:OE1	2.55	0.40
20:b:68:ASP:HB2	20:b:89:ALA:HB1	2.03	0.40
21:c:83:LEU:HD11	22:d:59:MET:HE2	2.04	0.40
23:U:148:ALA:HA	25:W:367:VAL:HG13	2.02	0.40
25:W:322:PRO:HA	25:W:323:PRO:HD3	1.93	0.40
25:W:416:GLN:OE1	25:W:419:ARG:NH1	2.54	0.40
1:A:62:GLN:HG2	1:A:84:HIS:O	2.21	0.40
1:A:137:PRO:HB3	1:A:237:GLY:O	2.21	0.40
1:A:239:GLU:OE2	1:A:241:ARG:NH1	2.54	0.40
1:A:316:THR:HA	1:A:319:ASP:O	2.21	0.40
1:A:337:LYS:HE3	1:A:337:LYS:HB2	1.96	0.40
1:A:636:ILE:HD11	7:H:95:LYS:NZ	2.37	0.40
1:A:1280:ASP:OD1	1:A:1280:ASP:N	2.50	0.40
9:Y:13:LEU:HD12	10:Z:190:ARG:NH2	2.34	0.40
18:M:207:ARG:HA	18:M:210:VAL:HG12	2.03	0.40
19:a:68:GLN:HG2	19:a:72:ARG:HE	1.85	0.40
22:h:101:GLY:O	22:h:105:LYS:HG2	2.21	0.40
24:V:39:VAL:HA	25:W:95:ASN:OD1	2.22	0.40
24:V:77:VAL:HG13	24:V:93:LEU:HD22	2.02	0.40
25:W:278:GLN:H	25:W:278:GLN:CD	2.27	0.40
1:A:490:THR:HB	1:A:491:PRO:HD3	2.04	0.40
2:B:420:GLN:HA	2:B:423:ILE:HG12	2.04	0.40
4:E:100:THR:HA	4:E:125:TYR:HD1	1.86	0.40
6:G:77:PHE:CD1	6:G:79:PRO:HD3	2.56	0.40
9:Y:61:ILE:HG23	10:Z:216:VAL:HG22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:-60:DT:H2''	11:N:-59:DT:C6	2.56	0.40
11:N:70:DG:OP1	19:e:42:ARG:N	2.53	0.40
13:T:31:DT:H2'	13:T:32:DA:C8	2.56	0.40
13:T:54:DG:H2''	13:T:55:DA:C8	2.56	0.40
1:A:272:ASN:ND2	12:P:1:G:H21	2.20	0.40
1:A:467:MET:O	1:A:470:MET:HE3	2.22	0.40
1:A:936:GLU:HA	1:A:939:VAL:HG22	2.04	0.40
2:B:438:ARG:NE	13:T:89:DA:OP1	2.55	0.40
6:G:99:THR:HG21	6:G:145:LEU:HD22	2.02	0.40
8:I:95:VAL:HG13	8:I:115:THR:CG2	2.52	0.40
10:Z:279:VAL:HA	10:Z:386:VAL:HG21	2.03	0.40
10:Z:433:LEU:HD13	10:Z:461:LEU:HD13	2.04	0.40
10:Z:450:ILE:C	10:Z:452:PRO:HD3	2.46	0.40
14:D:47:GLN:O	14:D:51:ALA:N	2.48	0.40
18:M:186:LYS:HA	18:M:189:ASN:ND2	2.37	0.40
20:f:67:ARG:HD2	20:f:67:ARG:C	2.47	0.40
23:U:142:GLN:OE1	25:W:468:GLN:NE2	2.55	0.40
24:V:462:LEU:HD11	24:V:500:VAL:HG22	2.04	0.40
25:W:404:ALA:O	25:W:408:VAL:HG23	2.22	0.40
25:W:513:VAL:HG13	25:W:556:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1380/1970 (70%)	1314 (95%)	66 (5%)	0	100	100
2	B	1111/1174 (95%)	1044 (94%)	67 (6%)	0	100	100
3	C	254/271 (94%)	239 (94%)	15 (6%)	0	100	100
4	E	207/210 (99%)	202 (98%)	5 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	76/127 (60%)	74 (97%)	2 (3%)	0	100	100
6	G	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
7	H	147/150 (98%)	140 (95%)	7 (5%)	0	100	100
8	I	114/125 (91%)	107 (94%)	7 (6%)	0	100	100
9	Y	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
10	Z	468/1107 (42%)	448 (96%)	20 (4%)	0	100	100
14	D	124/142 (87%)	120 (97%)	4 (3%)	0	100	100
15	J	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
16	K	113/117 (97%)	113 (100%)	0	0	100	100
17	L	44/58 (76%)	41 (93%)	3 (7%)	0	100	100
18	M	120/301 (40%)	115 (96%)	5 (4%)	0	100	100
19	a	95/136 (70%)	95 (100%)	0	0	100	100
19	e	95/136 (70%)	93 (98%)	2 (2%)	0	100	100
20	b	78/103 (76%)	74 (95%)	4 (5%)	0	100	100
20	f	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
21	c	101/130 (78%)	101 (100%)	0	0	100	100
21	g	103/130 (79%)	100 (97%)	3 (3%)	0	100	100
22	d	93/126 (74%)	91 (98%)	2 (2%)	0	100	100
22	h	91/126 (72%)	89 (98%)	2 (2%)	0	100	100
23	U	185/528 (35%)	182 (98%)	3 (2%)	0	100	100
24	V	538/580 (93%)	525 (98%)	13 (2%)	0	100	100
25	W	541/611 (88%)	525 (97%)	16 (3%)	0	100	100
26	X	33/404 (8%)	33 (100%)	0	0	100	100
All	All	6535/9222 (71%)	6274 (96%)	261 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1228/1749 (70%)	1228 (100%)	0	100	100
2	B	985/1027 (96%)	985 (100%)	0	100	100
3	C	235/248 (95%)	235 (100%)	0	100	100
4	E	191/192 (100%)	191 (100%)	0	100	100
5	F	68/111 (61%)	68 (100%)	0	100	100
6	G	152/153 (99%)	152 (100%)	0	100	100
7	H	130/131 (99%)	130 (100%)	0	100	100
8	I	104/112 (93%)	104 (100%)	0	100	100
9	Y	102/104 (98%)	102 (100%)	0	100	100
10	Z	423/955 (44%)	423 (100%)	0	100	100
14	D	109/126 (86%)	109 (100%)	0	100	100
15	J	56/56 (100%)	56 (100%)	0	100	100
16	K	104/106 (98%)	104 (100%)	0	100	100
17	L	43/55 (78%)	43 (100%)	0	100	100
18	M	105/266 (40%)	105 (100%)	0	100	100
19	a	83/110 (76%)	83 (100%)	0	100	100
19	e	82/110 (74%)	82 (100%)	0	100	100
20	b	65/79 (82%)	65 (100%)	0	100	100
20	f	63/79 (80%)	63 (100%)	0	100	100
21	c	82/100 (82%)	82 (100%)	0	100	100
21	g	83/100 (83%)	83 (100%)	0	100	100
22	d	81/105 (77%)	81 (100%)	0	100	100
22	h	79/105 (75%)	79 (100%)	0	100	100
23	U	161/451 (36%)	161 (100%)	0	100	100
24	V	485/515 (94%)	485 (100%)	0	100	100
25	W	480/530 (91%)	480 (100%)	0	100	100
26	X	31/351 (9%)	31 (100%)	0	100	100
All	All	5810/8026 (72%)	5810 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	A	143	HIS
1	A	721	HIS
1	A	792	ASN
1	A	825	ASN
1	A	995	HIS
1	A	1093	GLN
1	A	1190	GLN
1	A	1291	ASN
1	A	1332	GLN
1	A	1384	HIS
2	B	139	GLN
2	B	254	GLN
2	B	319	ASN
2	B	420	GLN
2	B	642	GLN
2	B	1009	GLN
2	B	1133	HIS
3	C	25	ASN
3	C	114	HIS
4	E	95	GLN
4	E	116	GLN
4	E	189	GLN
6	G	28	GLN
10	Z	220	HIS
10	Z	292	GLN
10	Z	607	HIS
14	D	47	GLN
16	K	40	HIS
19	a	76	GLN
19	a	108	ASN
21	c	24	GLN
21	c	68	ASN
22	d	60	ASN
22	d	81	ASN
22	d	106	HIS
19	e	76	GLN
23	U	62	HIS
23	U	107	ASN
24	V	202	GLN
25	W	49	HIS
25	W	223	ASN
25	W	242	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	W	253	GLN
25	W	263	GLN
25	W	354	HIS
25	W	447	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	P	11/42 (26%)	1 (9%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	P	11	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

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.

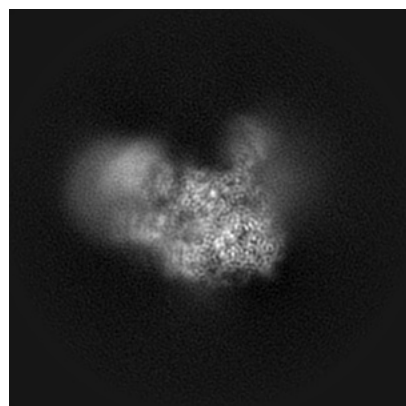
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61058. These allow visual inspection of the internal detail of the map and identification of artifacts.

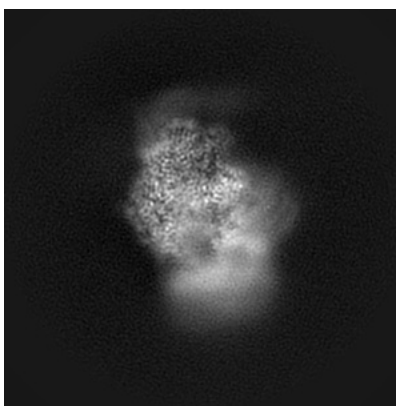
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

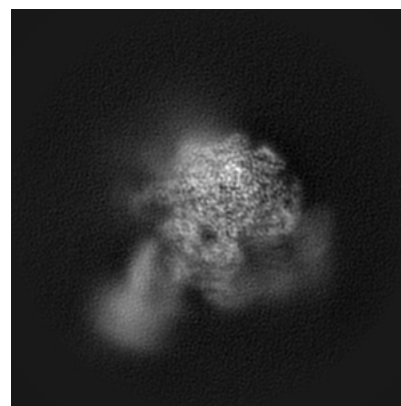
6.1.1 Primary map



X

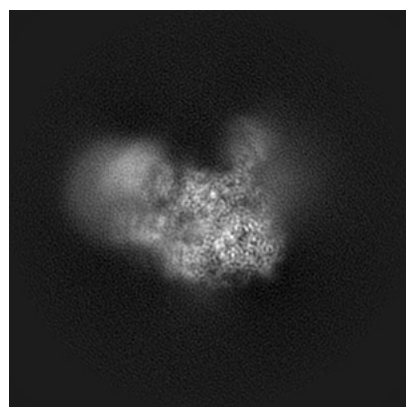


Y

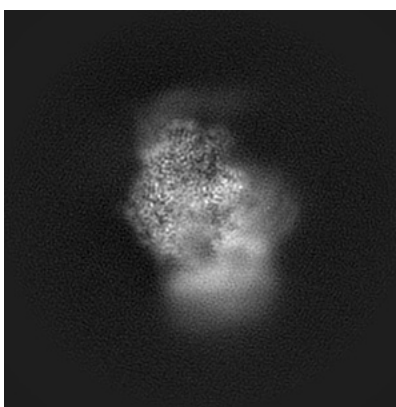


Z

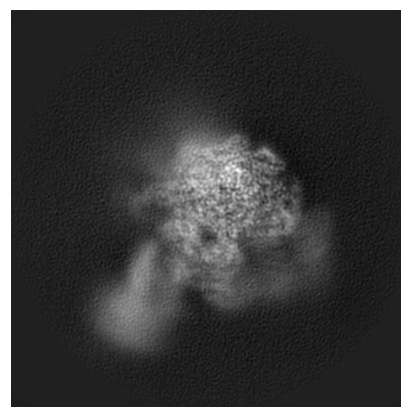
6.1.2 Raw map



X



Y

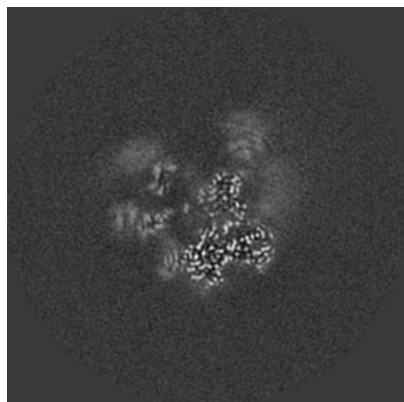


Z

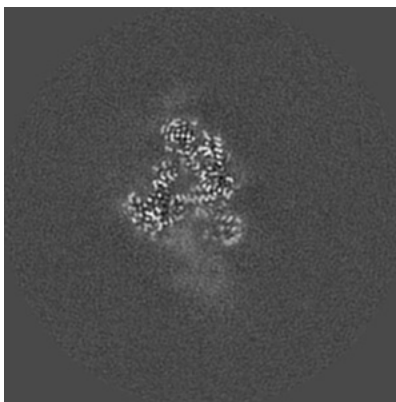
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

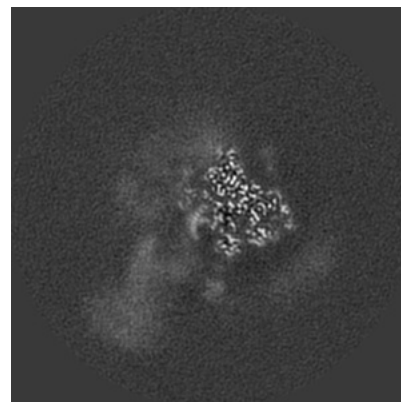
6.2.1 Primary map



X Index: 120

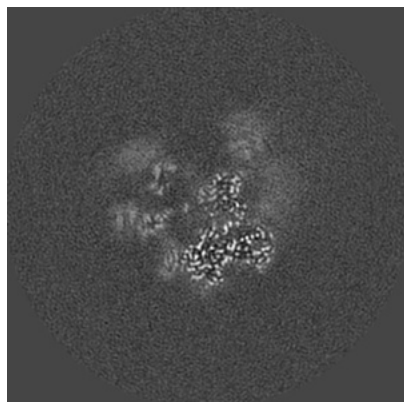


Y Index: 120

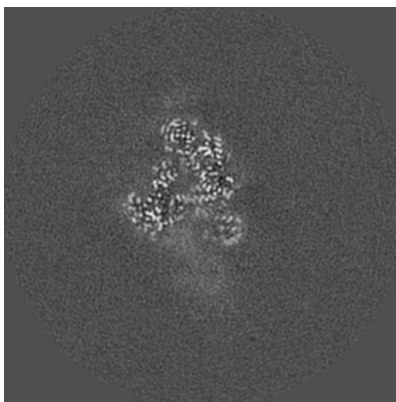


Z Index: 120

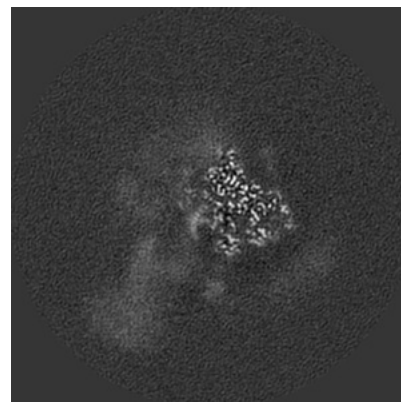
6.2.2 Raw map



X Index: 120



Y Index: 120

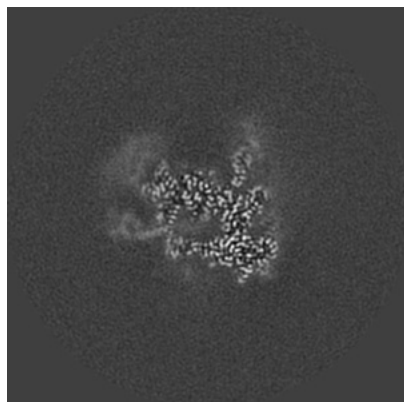


Z Index: 120

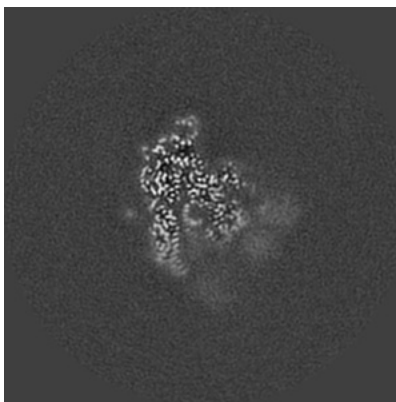
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

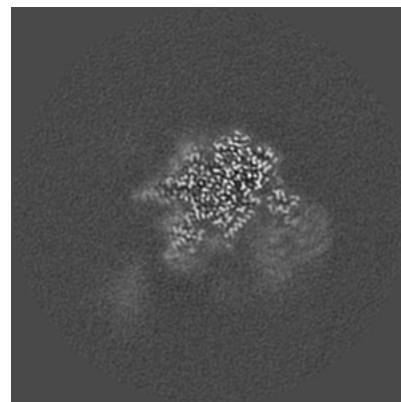
6.3.1 Primary map



X Index: 130

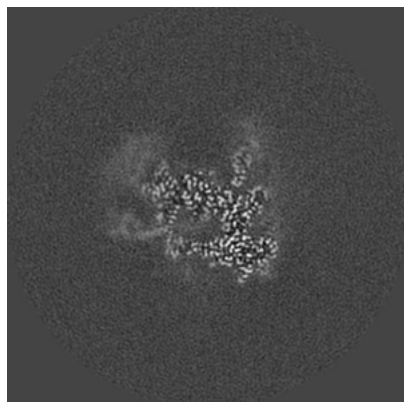


Y Index: 134

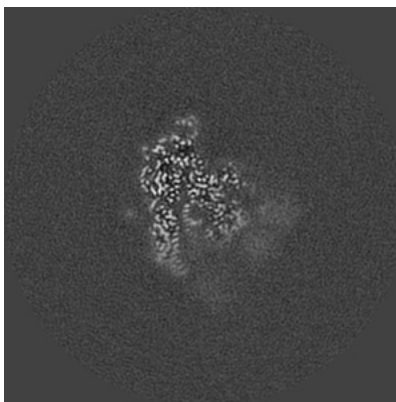


Z Index: 97

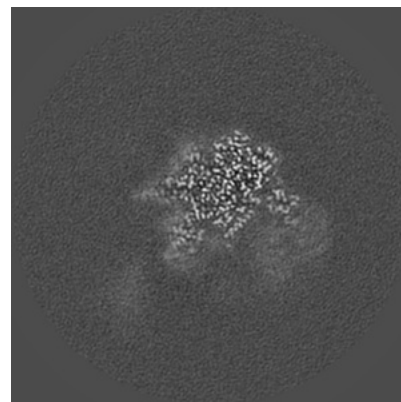
6.3.2 Raw map



X Index: 130



Y Index: 134

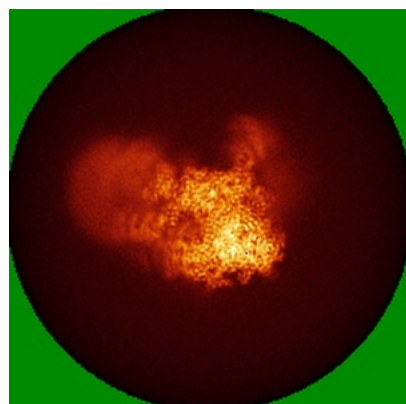


Z Index: 97

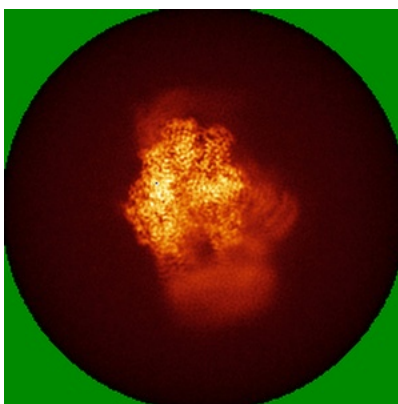
The images above show the largest variance slices of the map in three orthogonal directions.

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

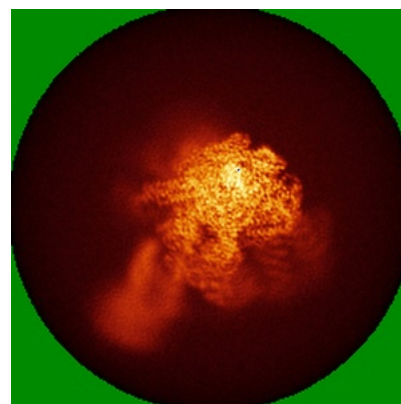
6.4.1 Primary map



X

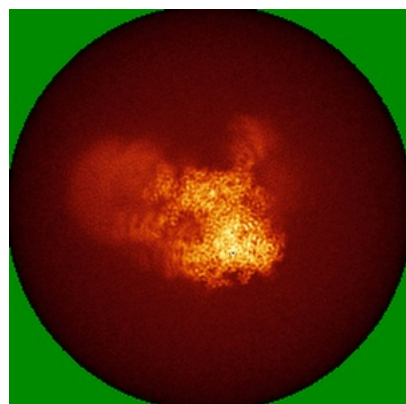


Y

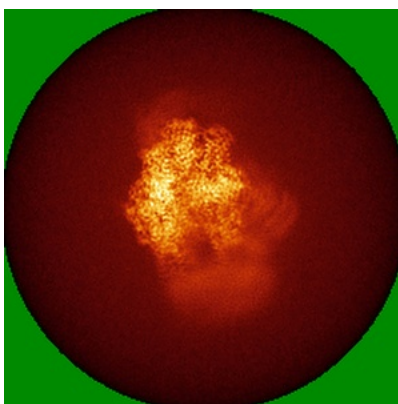


Z

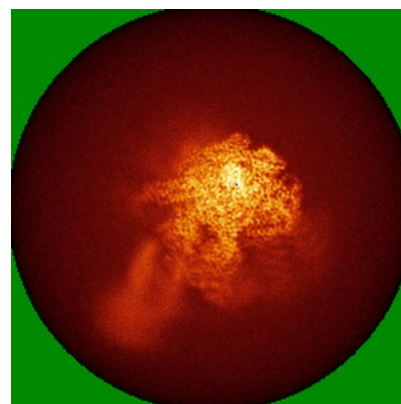
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

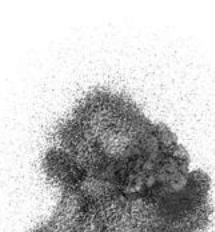
6.5.2 Raw map



X



Y



Z

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.

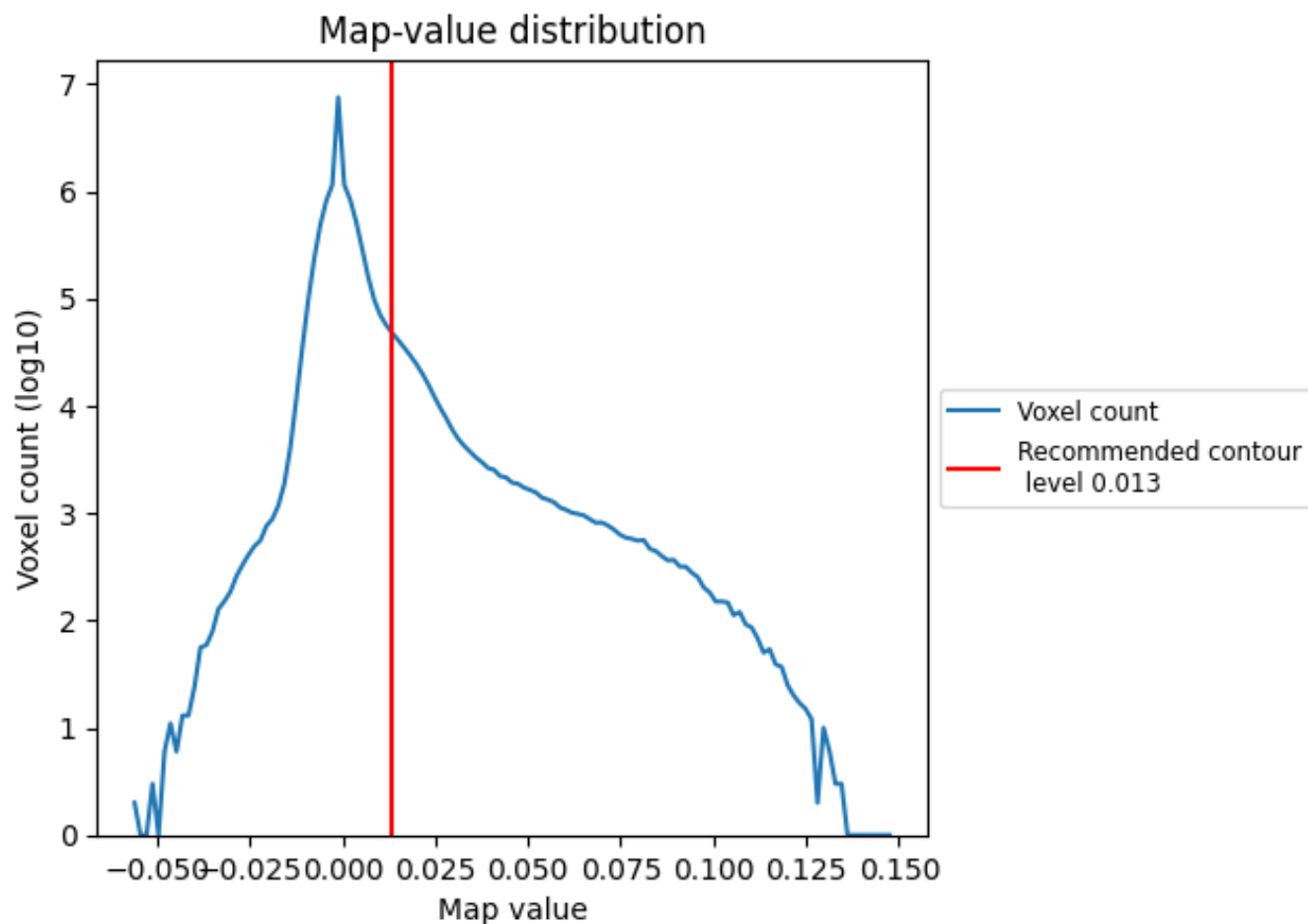
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

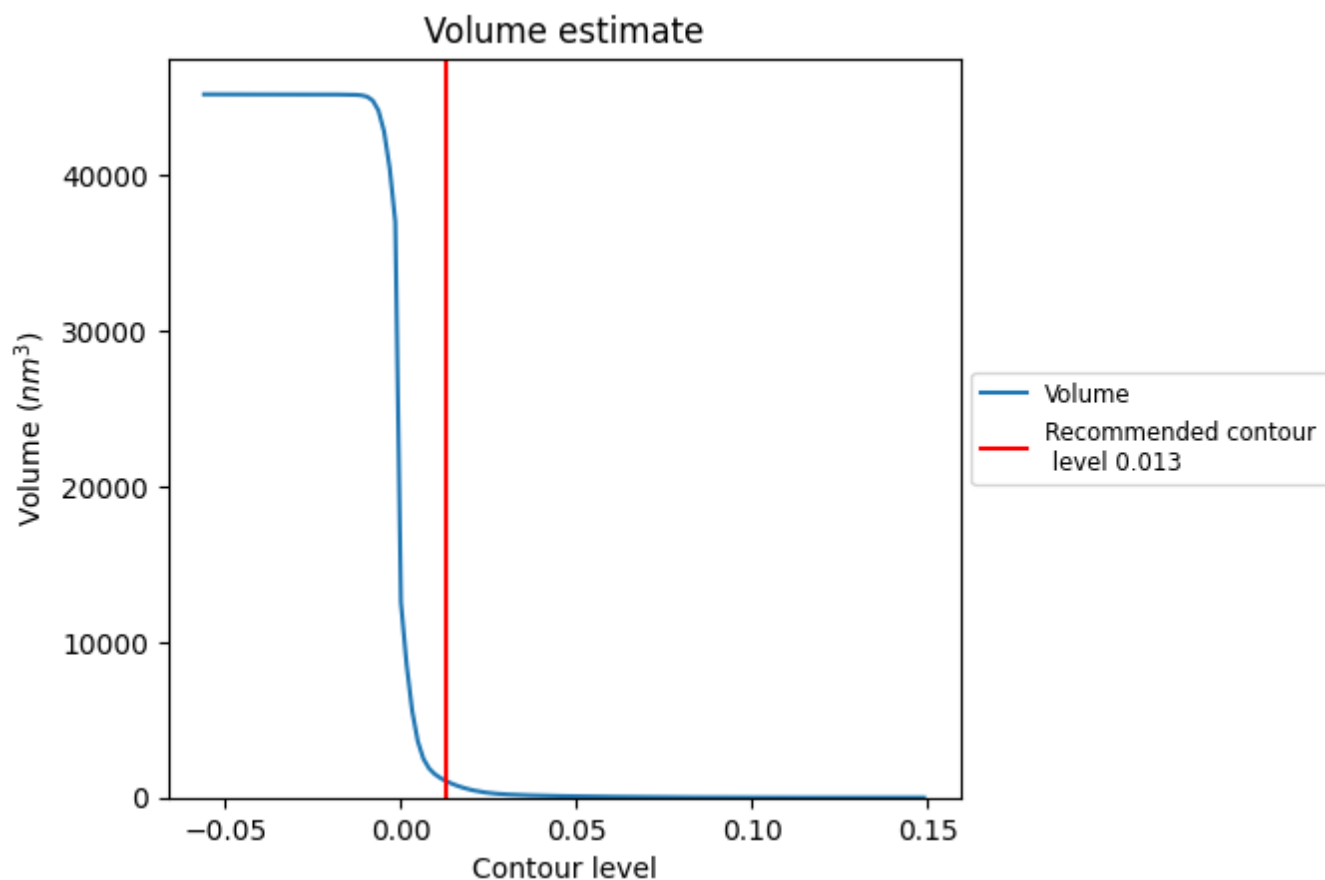
This section contains the results of statistical analysis of the map.

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.

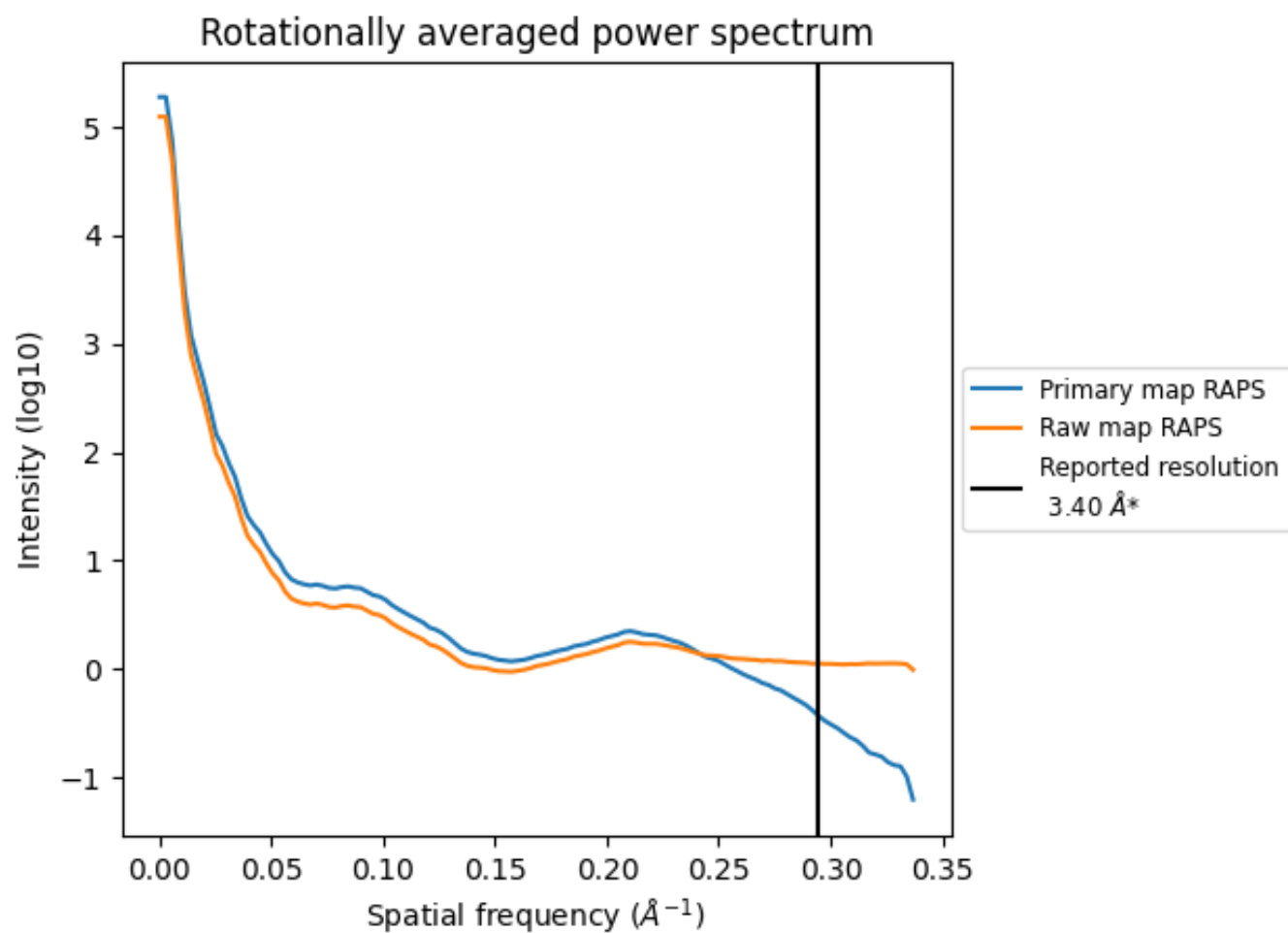
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1050 nm³; this corresponds to an approximate mass of 948 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

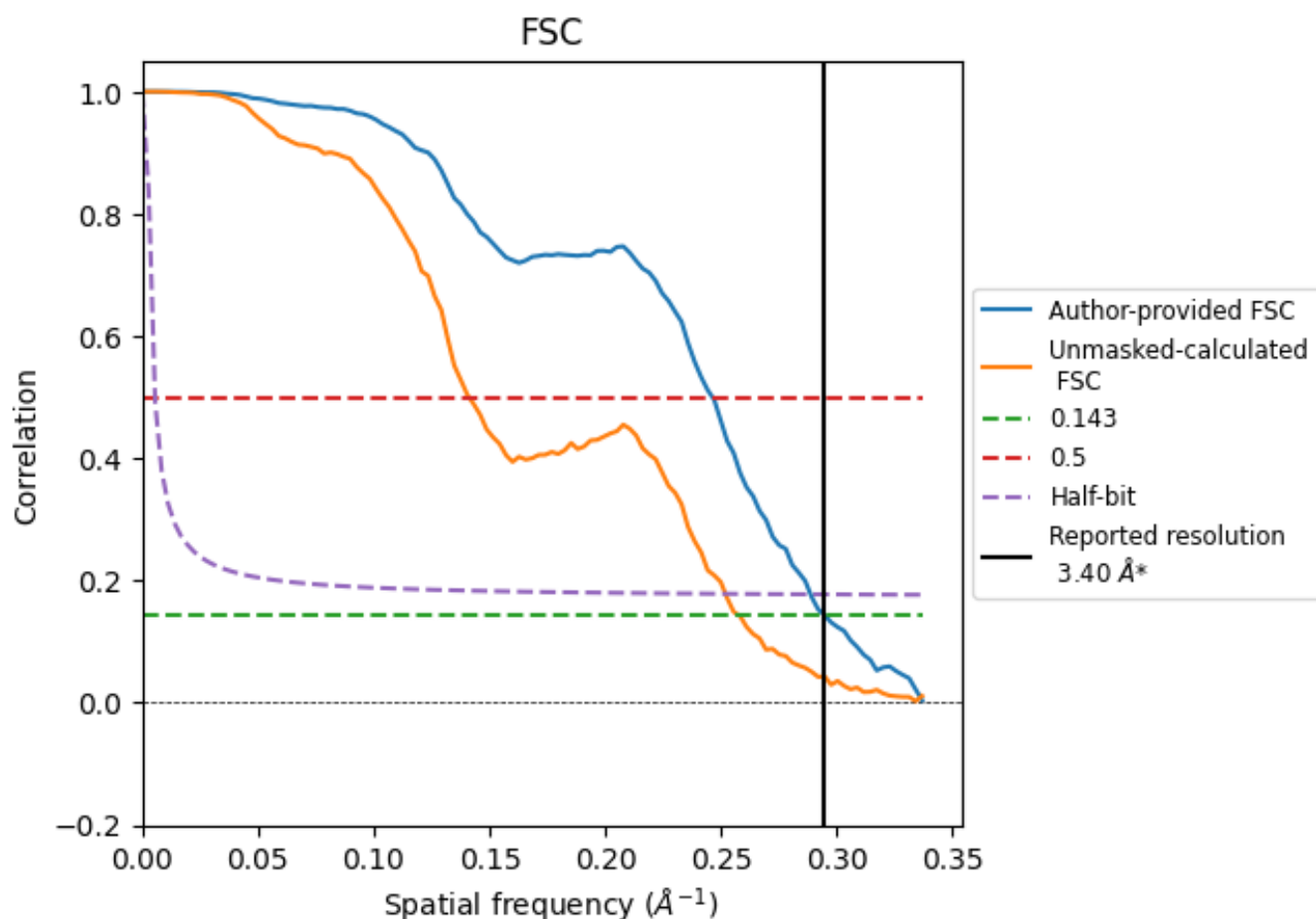


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

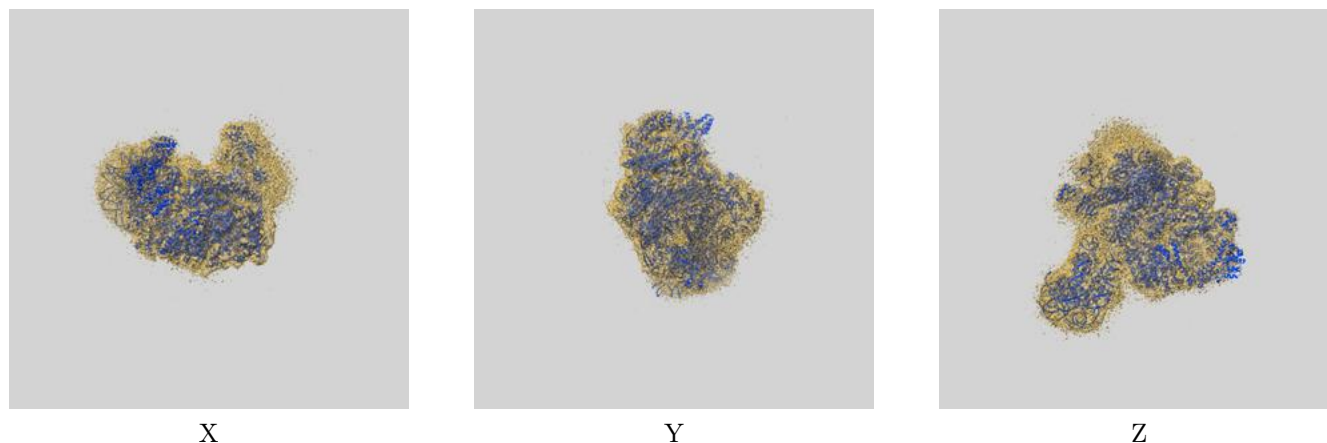
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	4.06	3.46
Unmasked-calculated*	3.88	7.09	3.97

*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 3.88 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

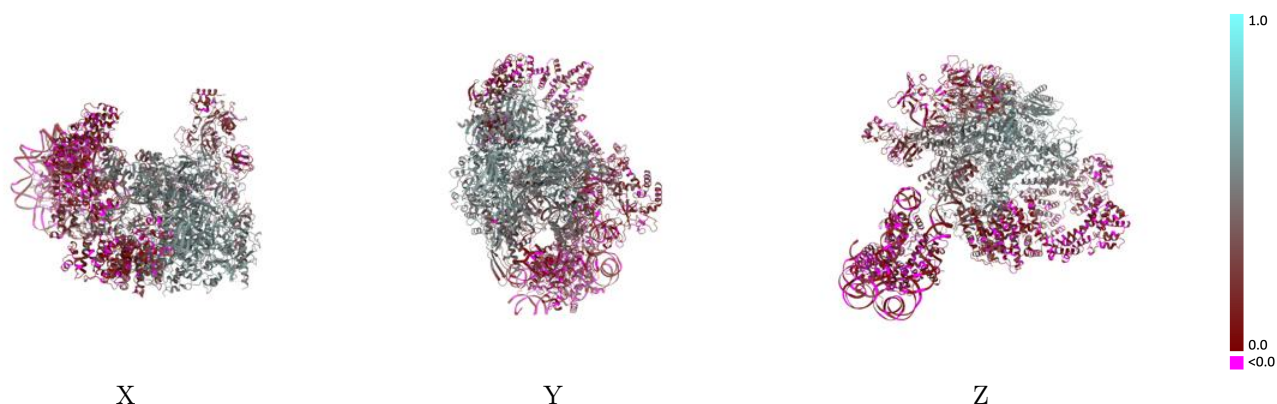
This section contains information regarding the fit between EMDB map EMD-61058 and PDB model 9J0N. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



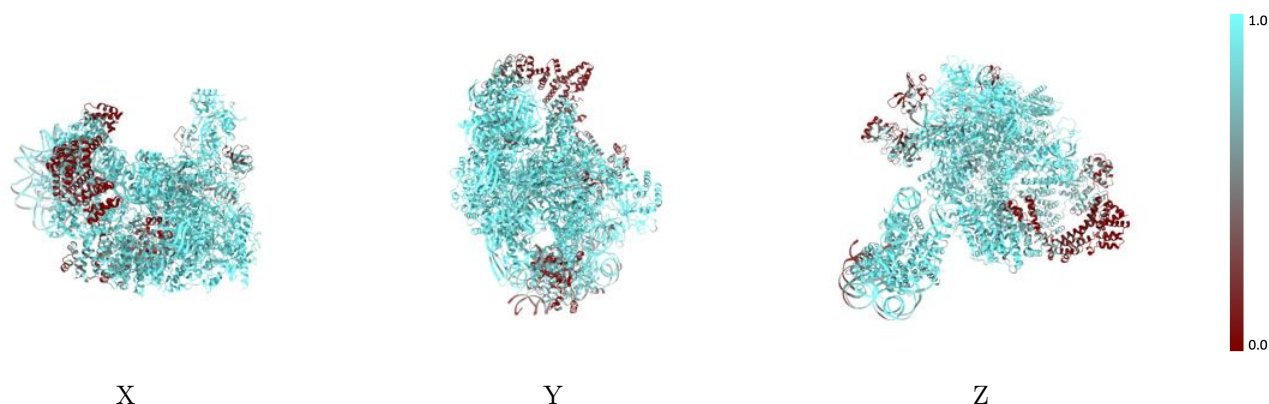
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



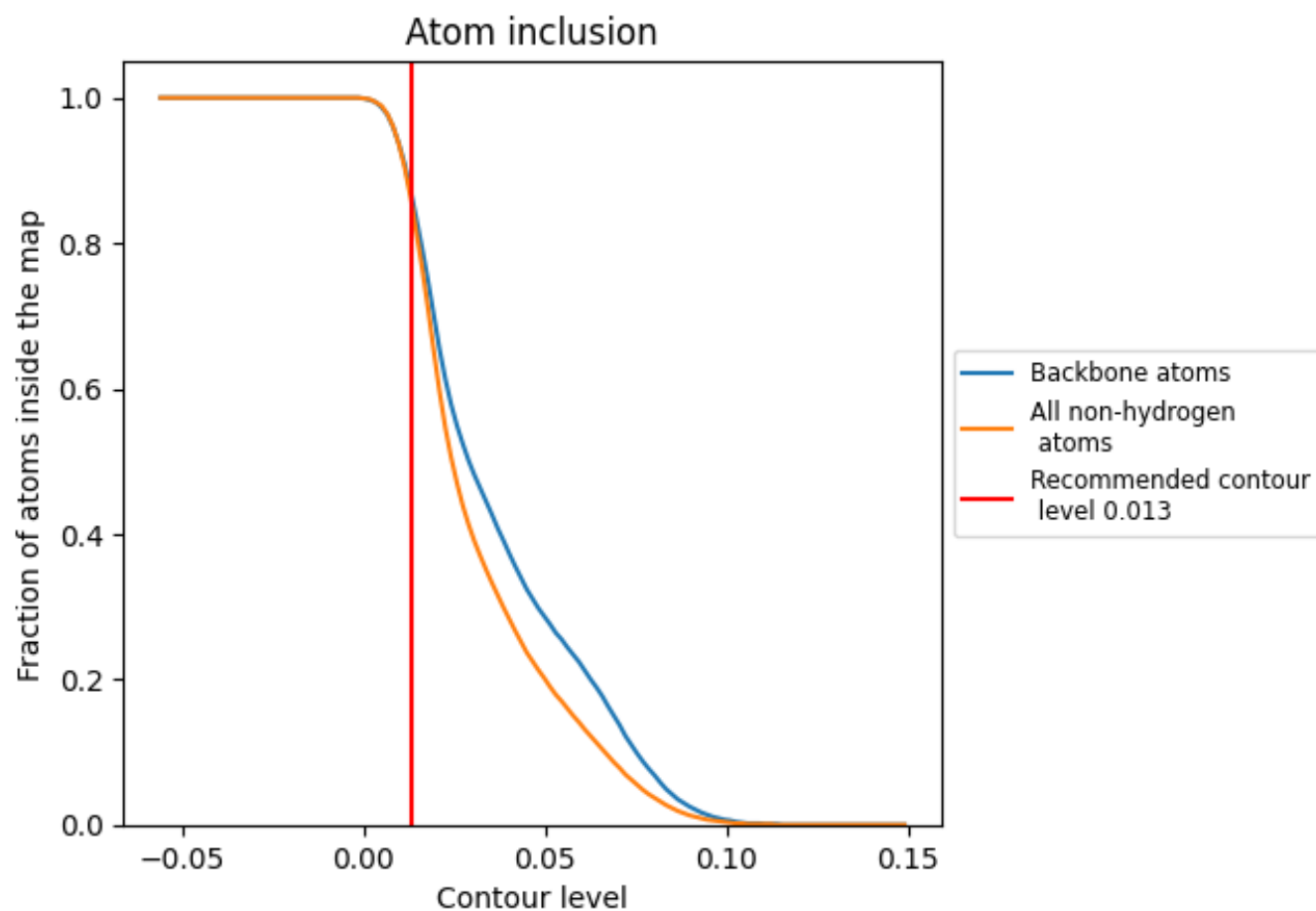
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8600	 0.3160
A	 0.9810	 0.4880
B	 0.9860	 0.4900
C	 0.9940	 0.5290
D	 0.9500	 0.2200
E	 0.9770	 0.4660
F	 0.9950	 0.5280
G	 0.9850	 0.3000
H	 0.9880	 0.5240
I	 0.9650	 0.3810
J	 0.9750	 0.5280
K	 0.9950	 0.5260
L	 0.9840	 0.4120
M	 0.9410	 0.2780
N	 0.8400	 0.1090
P	 1.0000	 0.4780
T	 0.8330	 0.1420
U	 0.5100	 0.1570
V	 0.5860	 0.1400
W	 0.5980	 0.1600
X	 0.9470	 0.1960
Y	 0.4020	 0.1790
Z	 0.6160	 0.1920
a	 0.9690	 0.1250
b	 0.9820	 0.1030
c	 0.8570	 0.0880
d	 0.8710	 0.0860
e	 0.9270	 0.1050
f	 0.9730	 0.0870
g	 0.9540	 0.1210
h	 0.9620	 0.1140

