



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 11:31 AM UTC

PDB ID : 8RBX / pdb_00008rbx
EMDB ID : EMD-19038
Title : Structure of Integrator-PP2A bound to a paused RNA polymerase II-DSIF-N
ELF-nucleosome complex
Authors : Fianu, I.; Ochmann, M.; Walshe, J.L.; Cramer, P.
Deposited on : 2023-12-05
Resolution : 4.10 Å (reported)
Based on initial models : 7PKS, 6SN1, ., 7OHC

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:

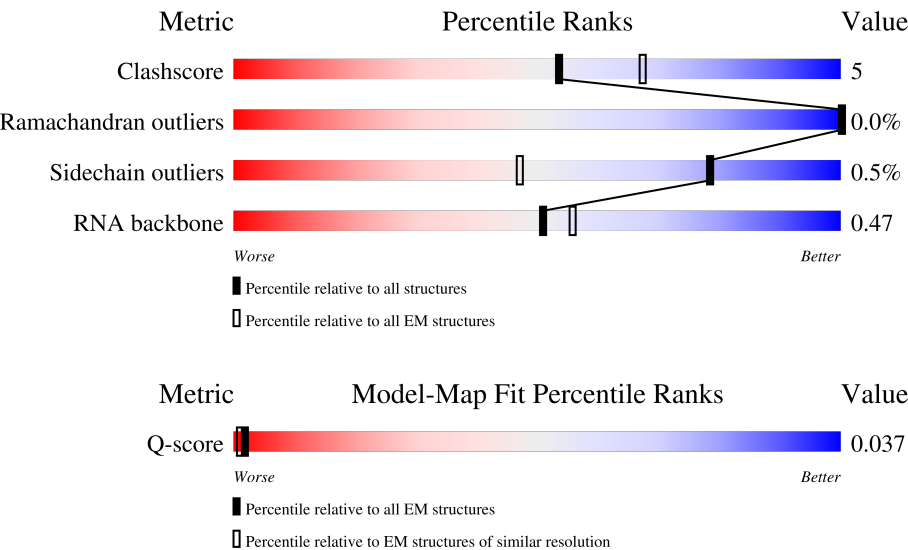
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.10 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	6458 (3.60 - 4.60)

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	1	8	100%
2	A	1970	60%11%29%
2	Y	1970	99%

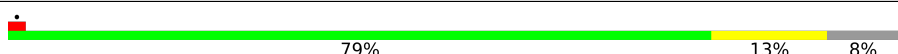
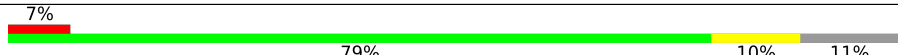
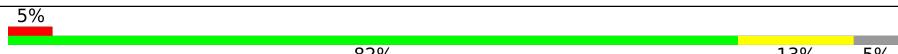
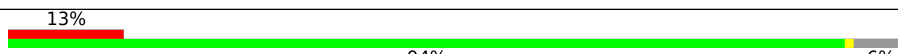
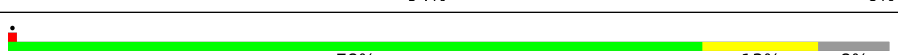
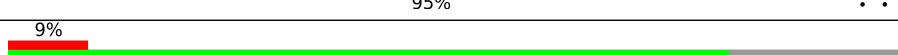
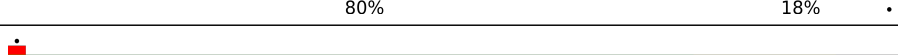
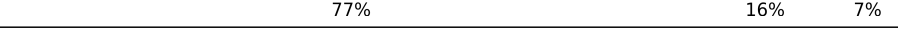
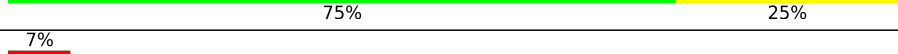
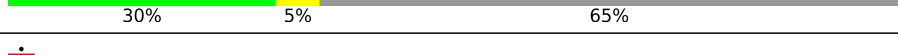
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Mol	Chain	Length	Quality of chain
3	B	1174	
4	C	275	
5	D	142	
6	E	210	
7	F	127	
8	G	172	
9	H	150	
10	I	125	
11	J	67	
12	K	117	
13	L	58	
14	M	135	
14	S	135	
15	N	148	
16	O	103	
16	U	103	
17	P	17	
18	Q	130	
18	V	130	
19	R	126	
19	W	126	
20	T	185	
21	Z	1087	
22	a	2192	
23	b	1204	

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Mol	Chain	Length	Quality of chain
24	d	963	
25	e	1021	
26	f	889	
27	g	964	
28	h	995	
29	i	658	
30	j	710	
31	k	602	
32	m	706	
33	n	518	
34	o	451	
35	p	591	
36	q	311	
37	r	28	
38	u	528	
39	v	613	
40	w	583	
41	x	22	

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 129226 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 UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	8	Total	C	N	O	0	0
			40	24	8	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1391	Total	C	N	O	S	0	0
			11008	6931	1972	2036	69		
2	Y	13	Total	C	N	O		0	0
			95	60	13	22			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
Y	?	-	TYR	deletion	UNP A0A7M4DUC2
Y	?	-	SER	deletion	UNP A0A7M4DUC2
Y	?	-	PRO	deletion	UNP A0A7M4DUC2
Y	?	-	THR	deletion	UNP A0A7M4DUC2
Y	?	-	SER	deletion	UNP A0A7M4DUC2

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	?	-	PRO	deletion	UNP A0A7M4DUC2
Y	?	-	SER	deletion	UNP A0A7M4DUC2
Y	?	-	TYR	deletion	UNP A0A7M4DUC2
Y	?	-	SER	deletion	UNP A0A7M4DUC2
Y	?	-	PRO	deletion	UNP A0A7M4DUC2
Y	?	-	THR	deletion	UNP A0A7M4DUC2
Y	?	-	SER	deletion	UNP A0A7M4DUC2
Y	?	-	PRO	deletion	UNP A0A7M4DUC2
Y	?	-	SER	deletion	UNP A0A7M4DUC2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	1112	Total	C	N	O	S	0	0
			8901	5634	1560	1643	64		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	261	Total	C	N	O	S	0	0
			2096	1314	360	416	6		

- Molecule 5 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	126	Total	C	N	O	S	0	0
			977	612	169	192	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	78	Total	C	N	O	S	0	0
			627	401	106	115	5		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	171	Total	C	N	O	S	0	0
			1316	858	208	242	8		

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	117	Total	C	N	O	S	0	0
			944	584	166	183	11		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	115	Total	C	N	O	S	0	0
			917	592	152	171	2		

- Molecule 13 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	46	Total	C	N	O	S	0	0
			383	238	72	67	6		

- Molecule 14 is a protein called Histone H3.3C.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	90	Total	C	N	O	S	0	0
			729	458	139	130	2		
14	S	91	Total	C	N	O	S	0	0
			732	460	140	130	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	79	LYS	ASN	conflict	UNP Q6NXT2
M	87	SER	ALA	conflict	UNP Q6NXT2
M	90	MET	GLY	conflict	UNP Q6NXT2
S	79	LYS	ASN	conflict	UNP Q6NXT2
S	87	SER	ALA	conflict	UNP Q6NXT2
S	90	MET	GLY	conflict	UNP Q6NXT2

- Molecule 15 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	148	Total	C	N	O	P	0	0
			3050	1446	570	887	147		

- Molecule 16 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	82	Total	C	N	O	S	0	0
			647	409	124	113	1		
16	U	80	Total	C	N	O	S	0	0
			634	398	124	111	1		

- Molecule 17 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	17	Total	C	N	O	P	0	0
			370	163	65	125	17		

- Molecule 18 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	109	Total	C	N	O		0	0
			839	530	165	144			
18	V	106	Total	C	N	O		0	0
			814	515	158	141			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	87	VAL	ILE	engineered mutation	UNP P02262
V	87	VAL	ILE	engineered mutation	UNP P02262

- Molecule 19 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	85	Total	C	N	O	S	0	0
			656	411	119	124	2		
19	W	95	Total	C	N	O	S	0	0
			746	467	136	141	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	SER	ALA	conflict	UNP P06899
R	15	ILE	VAL	conflict	UNP P06899
R	121	SER	ALA	conflict	UNP P06899
W	1	SER	ALA	conflict	UNP P06899
W	15	ILE	VAL	conflict	UNP P06899
W	121	SER	ALA	conflict	UNP P06899

- Molecule 20 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	161	Total	C	N	O	P	0	0
			3277	1556	598	962	161		

- Molecule 21 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	274	Total	C	N	O	S	0	0
			2167	1364	390	403	10		

- Molecule 22 is a protein called Integrator complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	1718	Total	C	N	O	S	0	0
			11692	7328	2134	2180	50		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-1	SER	-	expression tag	UNP Q8N201
a	0	ASN	-	expression tag	UNP Q8N201

- Molecule 23 is a protein called Integrator complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	1051	Total	C	N	O	S	0	0
			7991	5121	1352	1456	62		

- Molecule 24 is a protein called Integrator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	d	820	Total	C	N	O	S	0	0
			6407	4089	1093	1191	34		

- Molecule 25 is a protein called Integrator complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	e	856	Total	C	N	O	S	0	0
			6260	3979	1140	1115	26		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	-1	SER	-	expression tag	UNP Q6P9B9
e	0	ASN	-	expression tag	UNP Q6P9B9

- Molecule 26 is a protein called Integrator complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	f	544	Total	C	N	O	S	0	0
			4137	2653	701	758	25		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	-1	SER	-	expression tag	UNP Q9UL03
f	0	ASN	-	expression tag	UNP Q9UL03

- Molecule 27 is a protein called Integrator complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	g	886	Total	C	N	O	S	0	0
			6722	4259	1166	1257	40		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	-1	SER	-	expression tag	UNP Q9NVH2
g	0	ASN	-	expression tag	UNP Q9NVH2

- Molecule 28 is a protein called Integrator complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	h	887	Total	C	N	O	S	0	0
			6751	4334	1156	1223	38		

- Molecule 29 is a protein called Integrator complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	i	626	Total	C	N	O	S	0	0
			4870	3137	792	908	33		

- Molecule 30 is a protein called Integrator complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	j	668	Total	C	N	O		0	0
			3313	1976	668	669			

- Molecule 31 is a protein called Integrator complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	k	552	Total	C	N	O	S	0	0
			4090	2620	707	735	28		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	-1	SER	-	expression tag	UNP Q5TA45
k	0	ASN	-	expression tag	UNP Q5TA45
k	203	GLN	GLU	engineered mutation	UNP Q5TA45

- Molecule 32 is a protein called Integrator complex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	m	552	Total	C	N	O		0	0
			2864	1714	578	572			

- Molecule 33 is a protein called Integrator complex subunit 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	n	503	Total	C	N	O	0	0
			2484	1478	503	503		

- Molecule 34 is a protein called Integrator complex subunit 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	o	367	Total	C	N	O	0	0
			1824	1090	367	367		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
o	-1	SER	-	expression tag	UNP Q96N11
o	0	ASN	-	expression tag	UNP Q96N11

- Molecule 35 is a protein called Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	p	580	Total	C	N	O	S	0	0
			4431	2821	752	831	27		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p	-1	SER	-	expression tag	UNP P30153
p	0	ASN	-	expression tag	UNP P30153

- Molecule 36 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	q	290	Total	C	N	O	S	0	0
			2322	1467	403	437	15		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	-1	SER	-	expression tag	UNP P67775
q	0	ASN	-	expression tag	UNP P67775
q	88	ASN	ASP	engineered mutation	UNP P67775

- | Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 37 | r | 28 | Total | C | N | O | S | 0 | 0 |
| | | | 250 | 156 | 41 | 52 | 1 | | |

- | Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38 | u | 183 | Total | C | N | O | S | 0 | 0 |
| | | | 1395 | 887 | 238 | 264 | 6 | | |

- | Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 39 | v | 451 | Total | C | N | O | 0 | 0 |
| | | | 2070 | 1132 | 466 | 472 | | |

- | Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 40 | w | 511 | Total | C | N | O | S | 0 | 0 |
| | | | 3825 | 2446 | 650 | 710 | 19 | | |

Chain	Residue	Modelled	Actual	Comment	Reference
w	8	SER	-	expression tag	UNP Q8IXH7
w	9	ASN	-	expression tag	UNP Q8IXH7

- | Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 41 | x | 22 | Total | C | N | O | 0 | 0 |
| | | | 110 | 66 | 22 | 22 | | |

- | Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 42 | A | 2 | Total
2 | Zn
2 | 0 |



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Mol	Chain	Residues	Atoms		AltConf
42	B	1	Total 1	Zn 1	0
42	C	1	Total 1	Zn 1	0
42	I	2	Total 2	Zn 2	0
42	J	1	Total 1	Zn 1	0
42	L	1	Total 1	Zn 1	0
42	k	2	Total 2	Zn 2	0

- Molecule 43 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
43	P	1	Total 1	Mg 1	0

- Molecule 44 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
44	f	1	Total 1	Mn 1	0
44	q	1	Total 1	Mn 1	0

3 Residue-property plots

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

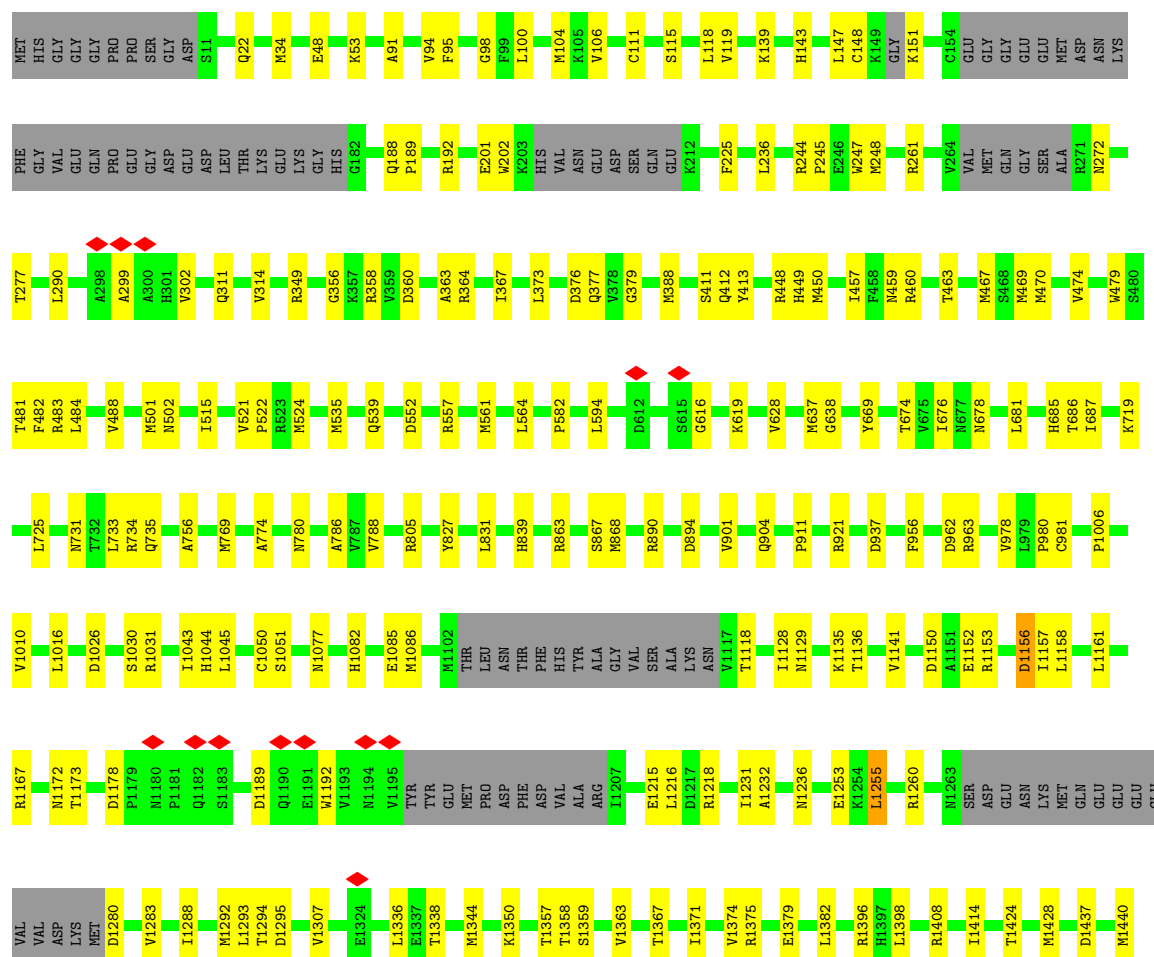
- Molecule 1: UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK

Chain 1:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA-directed RNA polymerase subunit

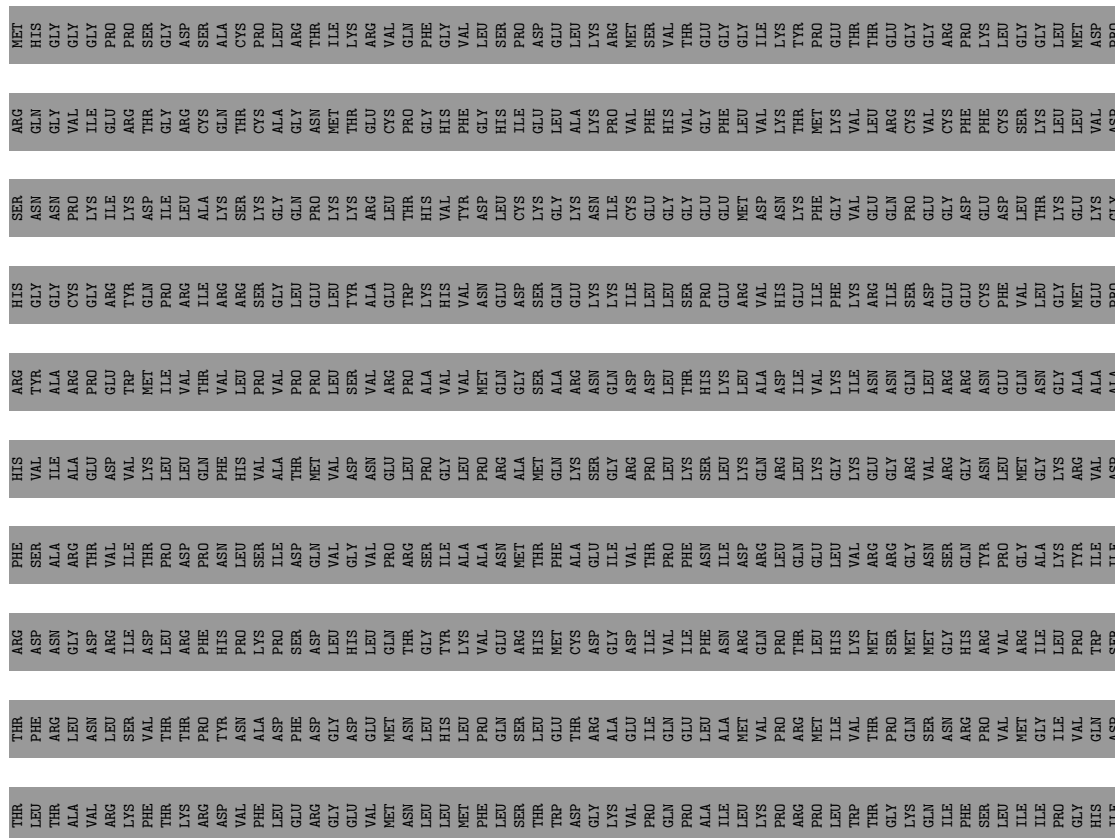
Chain A:  60% 11% 29%





- Molecule 2: DNA-directed RNA polymerase subunit

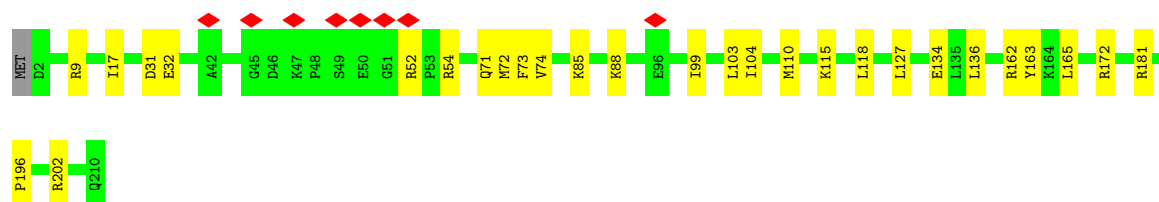
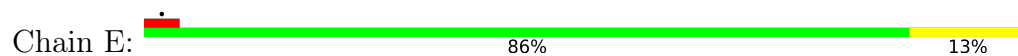
Chain Y: . 99%



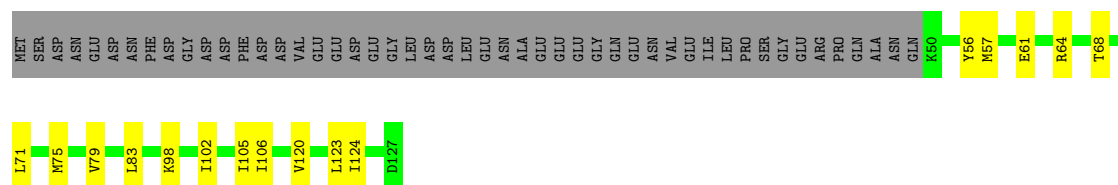




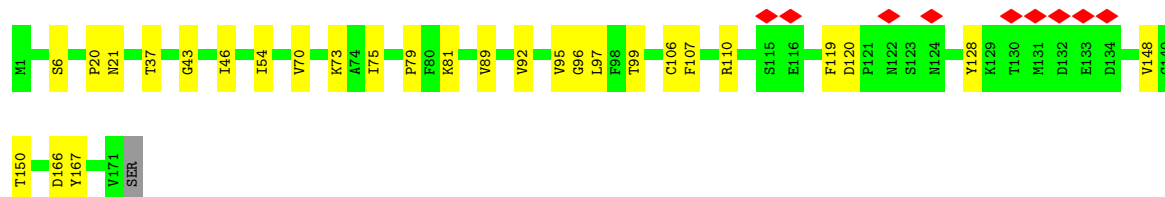
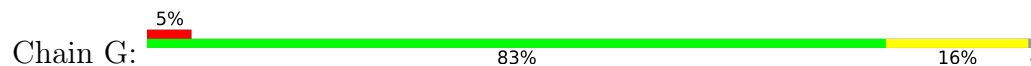
- Molecule 6: DNA-directed RNA polymerase II subunit E



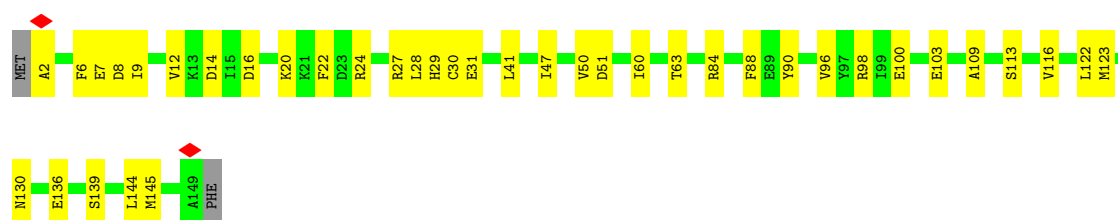
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC2



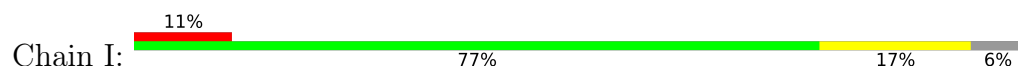
- Molecule 8: DNA-directed RNA polymerase II subunit RPB7

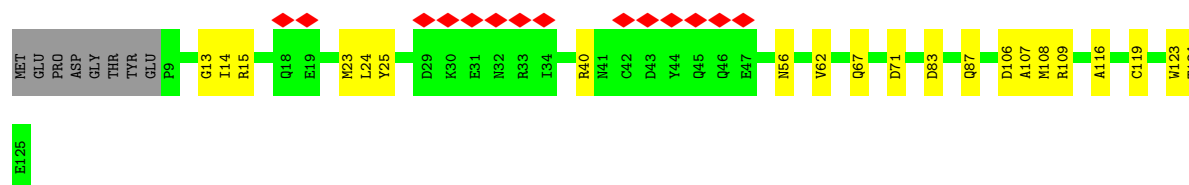


- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3

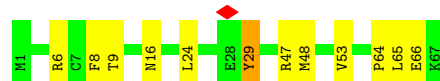
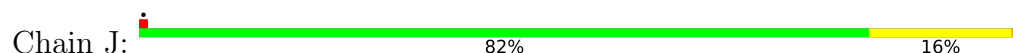


- Molecule 10: DNA-directed RNA polymerase II subunit RPB9

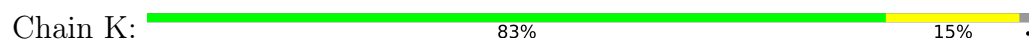




- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



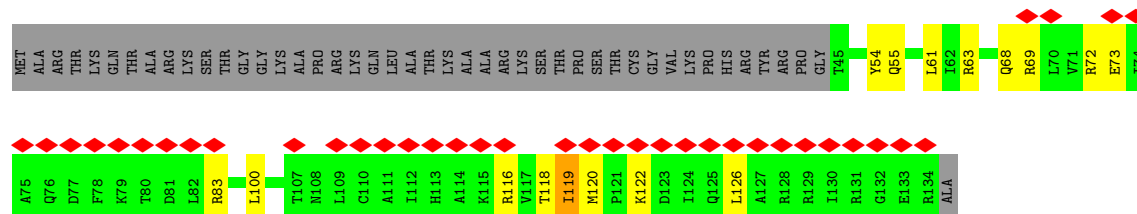
- Molecule 12: DNA-directed RNA polymerase II subunit RPB11-a



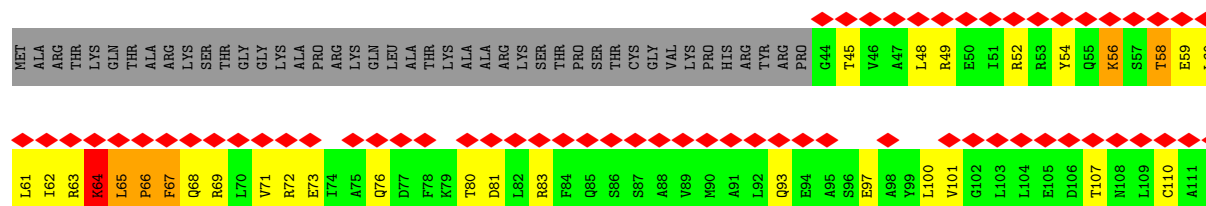
- Molecule 13: RNA polymerase II subunit K

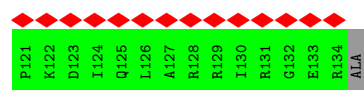


- Molecule 14: Histone H3.3C

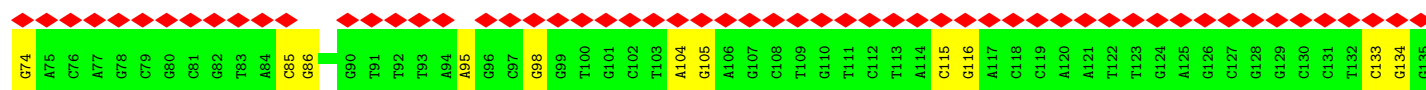
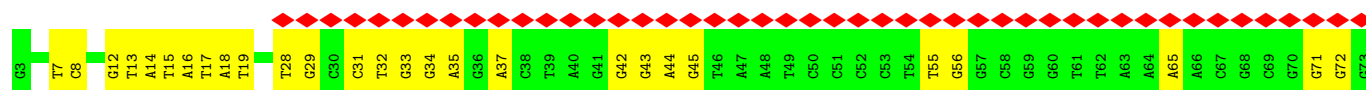
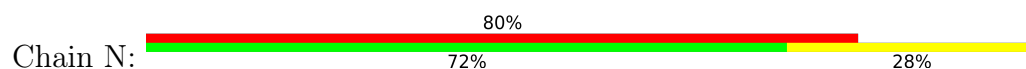


- Molecule 14: Histone H3.3C

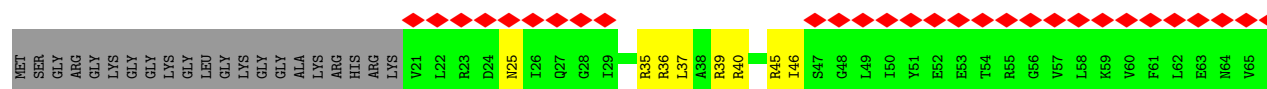




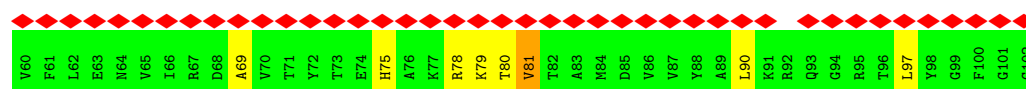
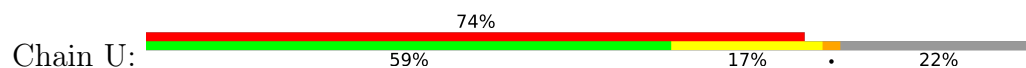
- Molecule 15: non-template DNA



- Molecule 16: Histone H4



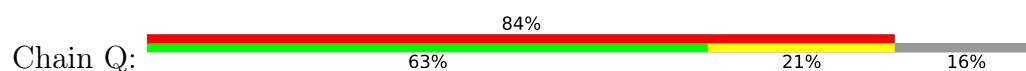
- Molecule 16: Histone H4

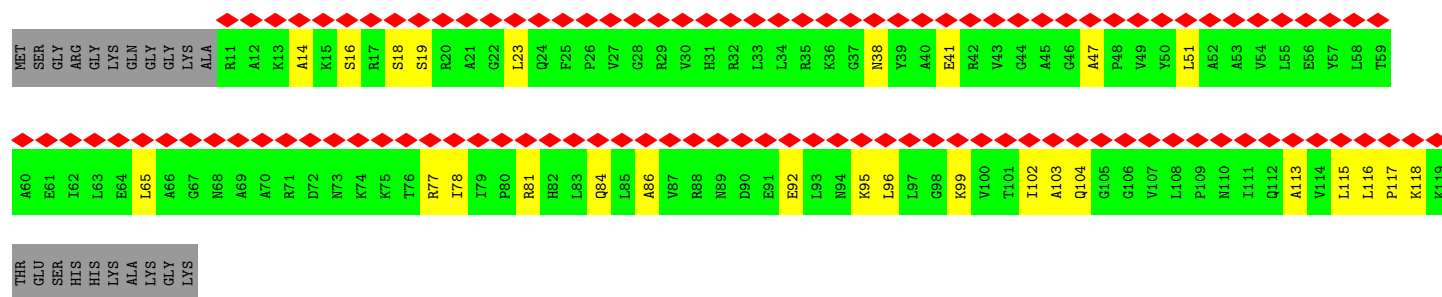


- Molecule 17: RNA

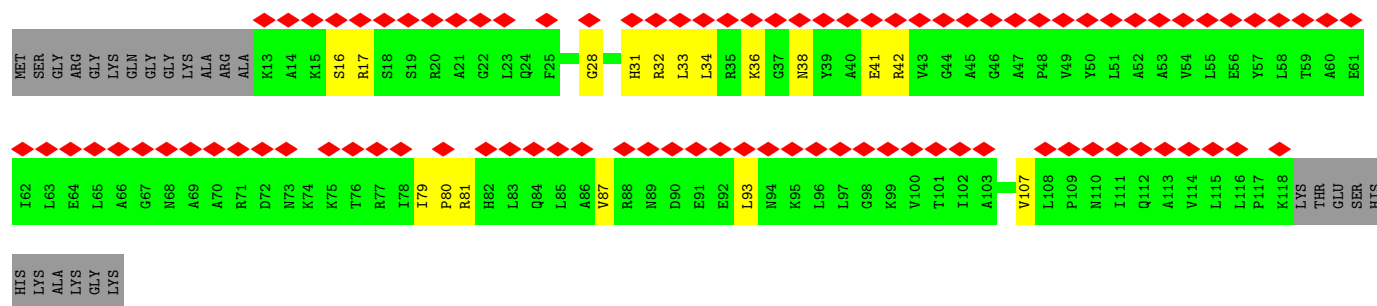


- Molecule 18: Histone H2A type 1

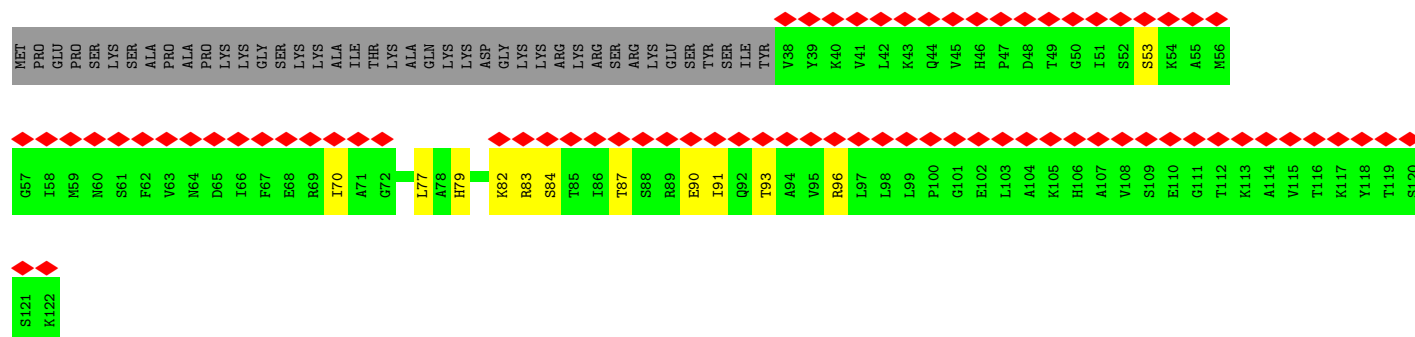




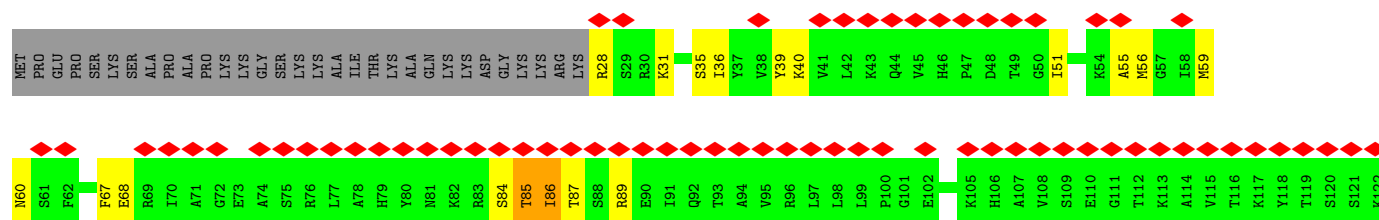
- Molecule 18: Histone H2A type 1



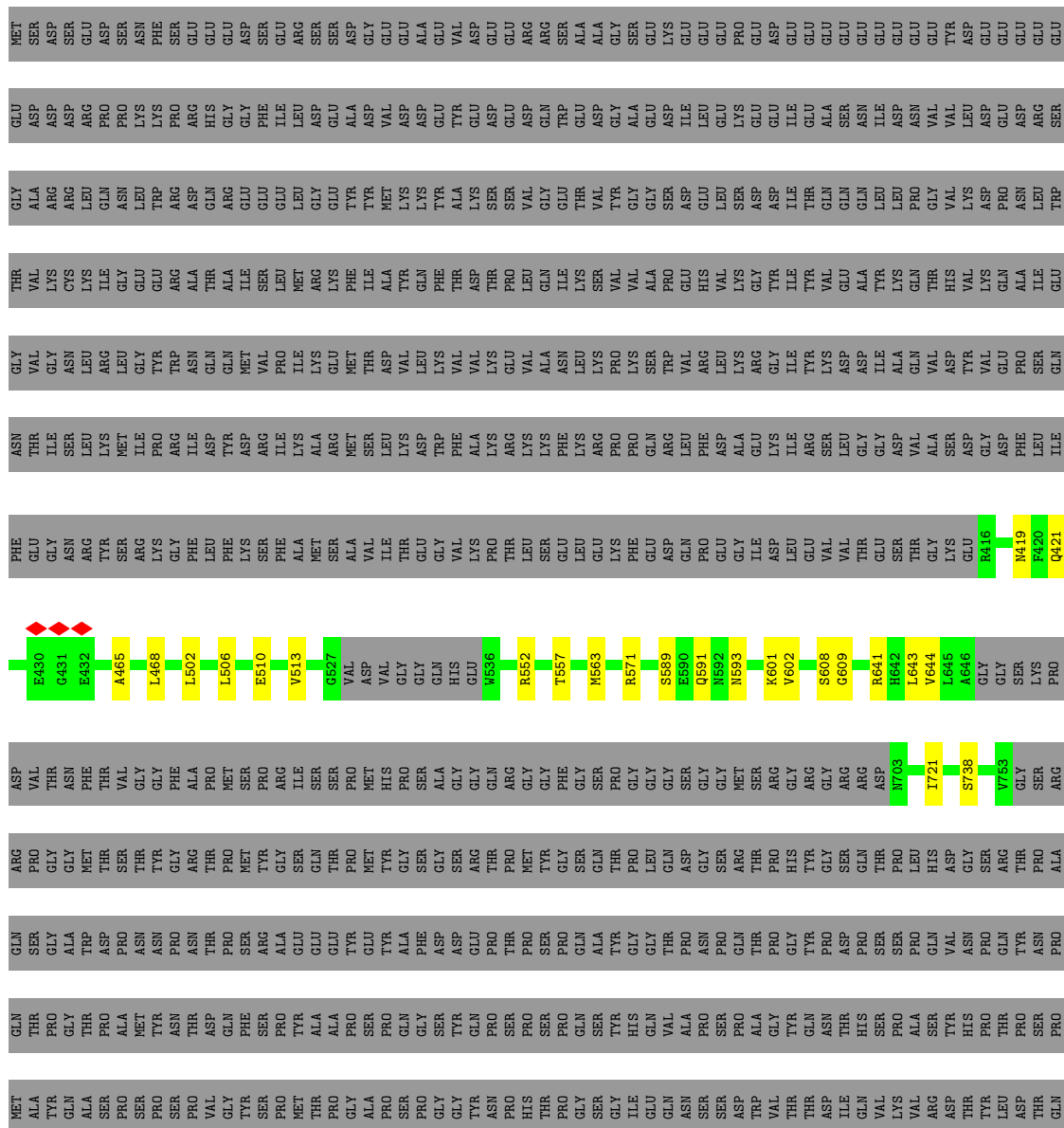
- Molecule 19: Histone H2B type 1-J

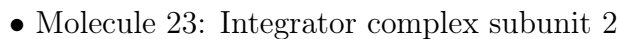


- Molecule 19: Histone H2B type 1-J



- Molecule 20: Template DNA

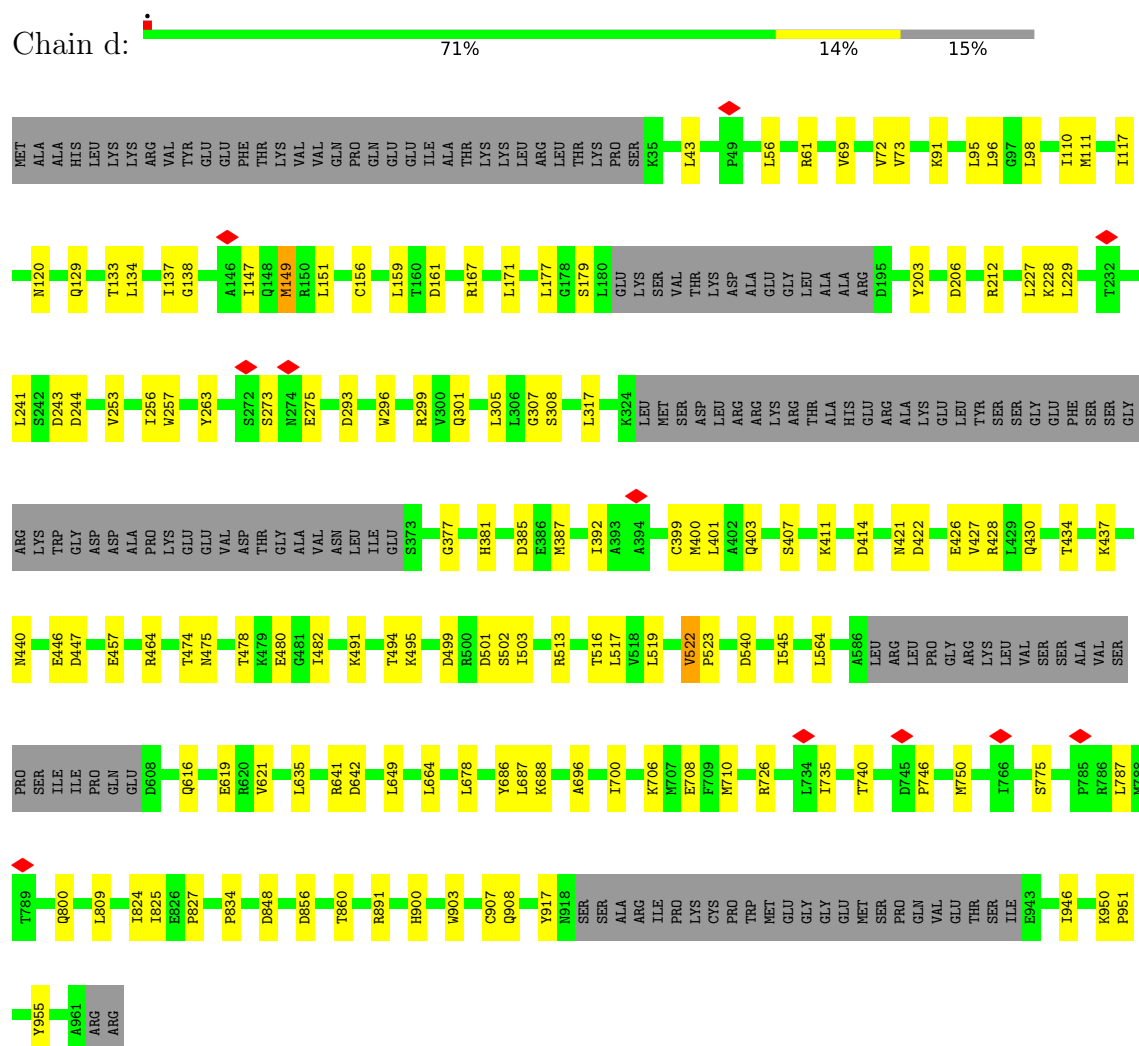




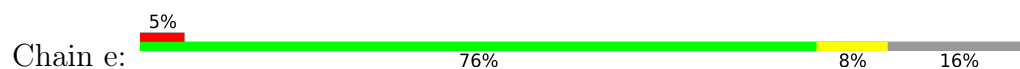
Frequency	Percentage
Daily	75%
Weekly	12%
Monthly	13%



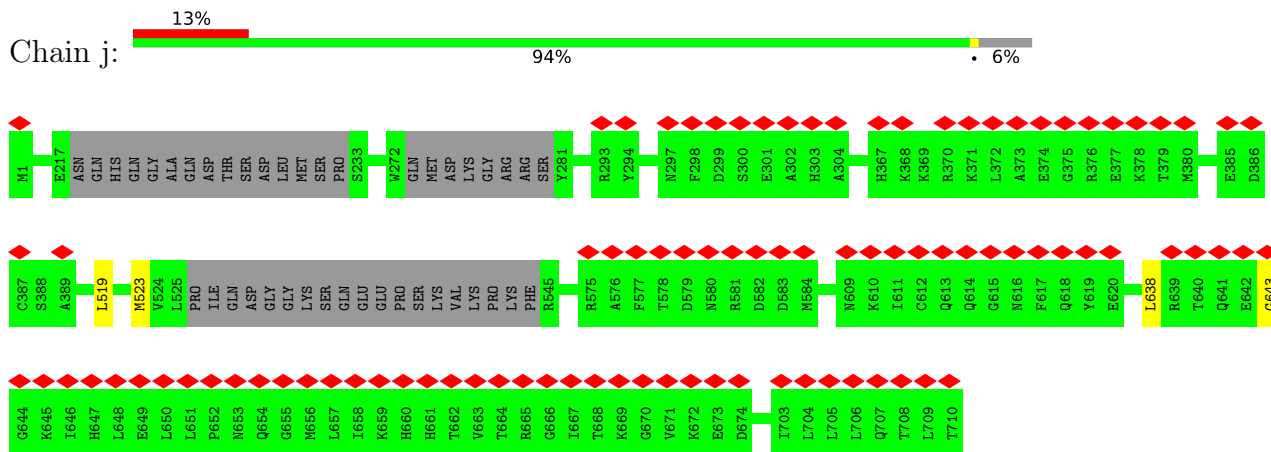
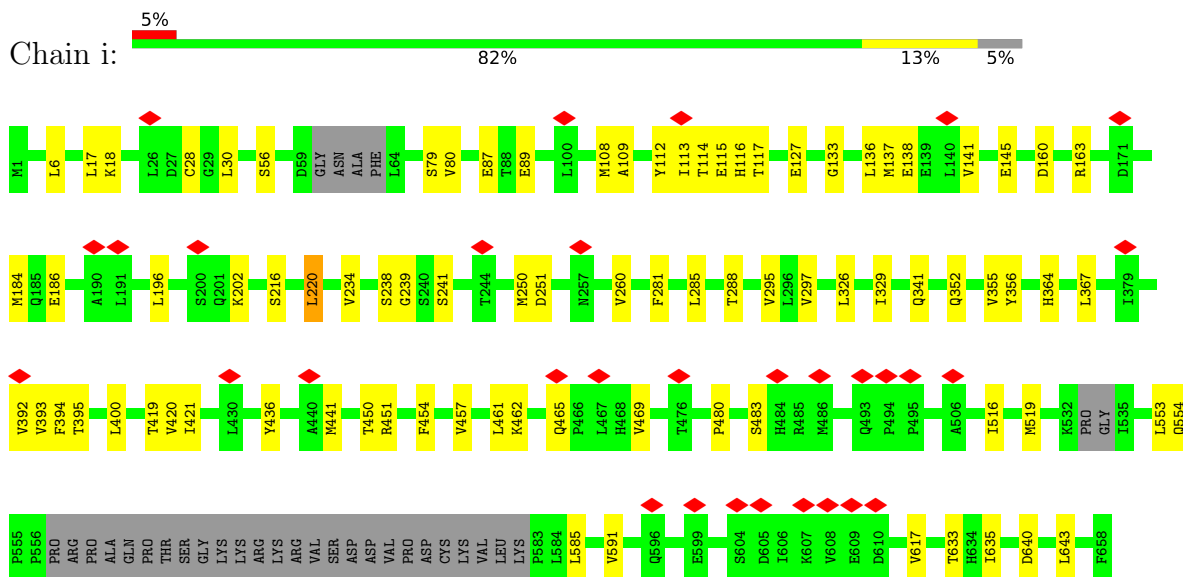
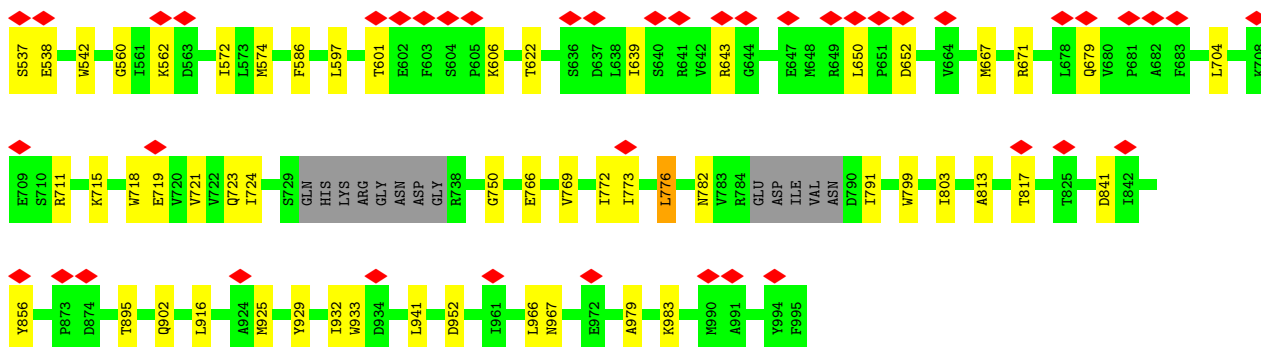
- Molecule 24: Integrator complex subunit 4

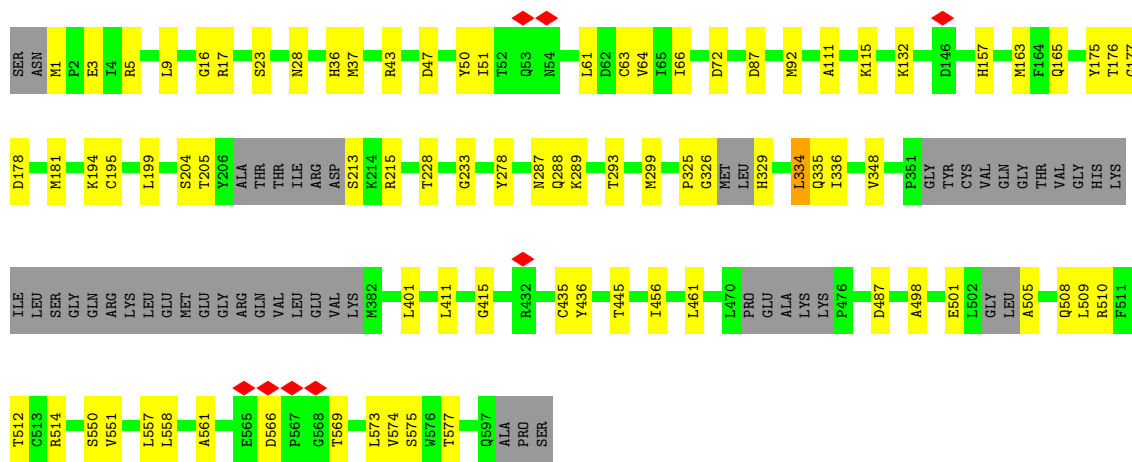


- Molecule 25: Integrator complex subunit 5

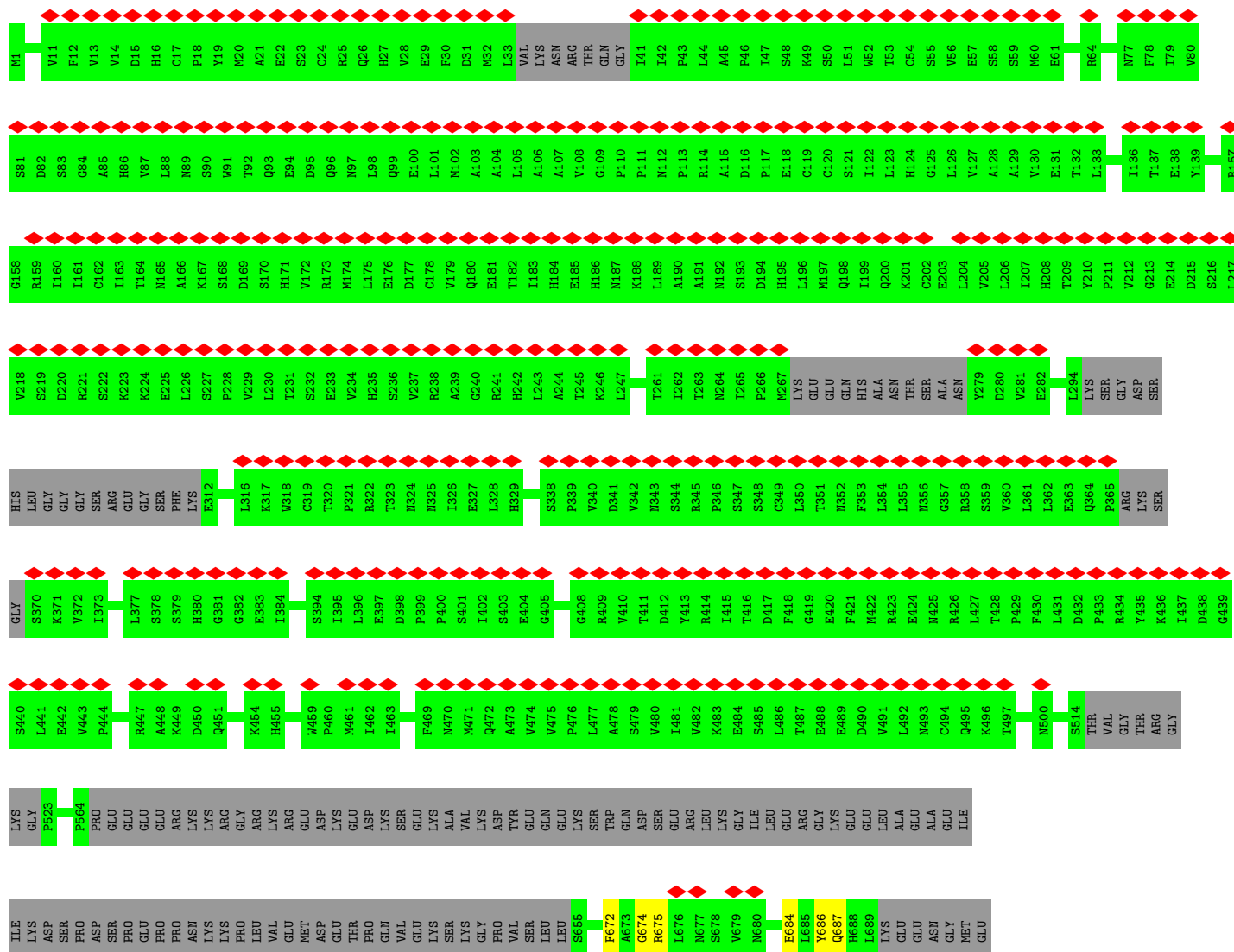
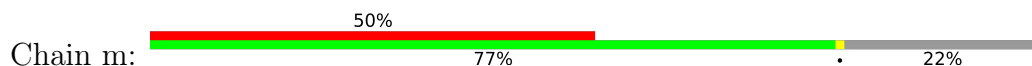






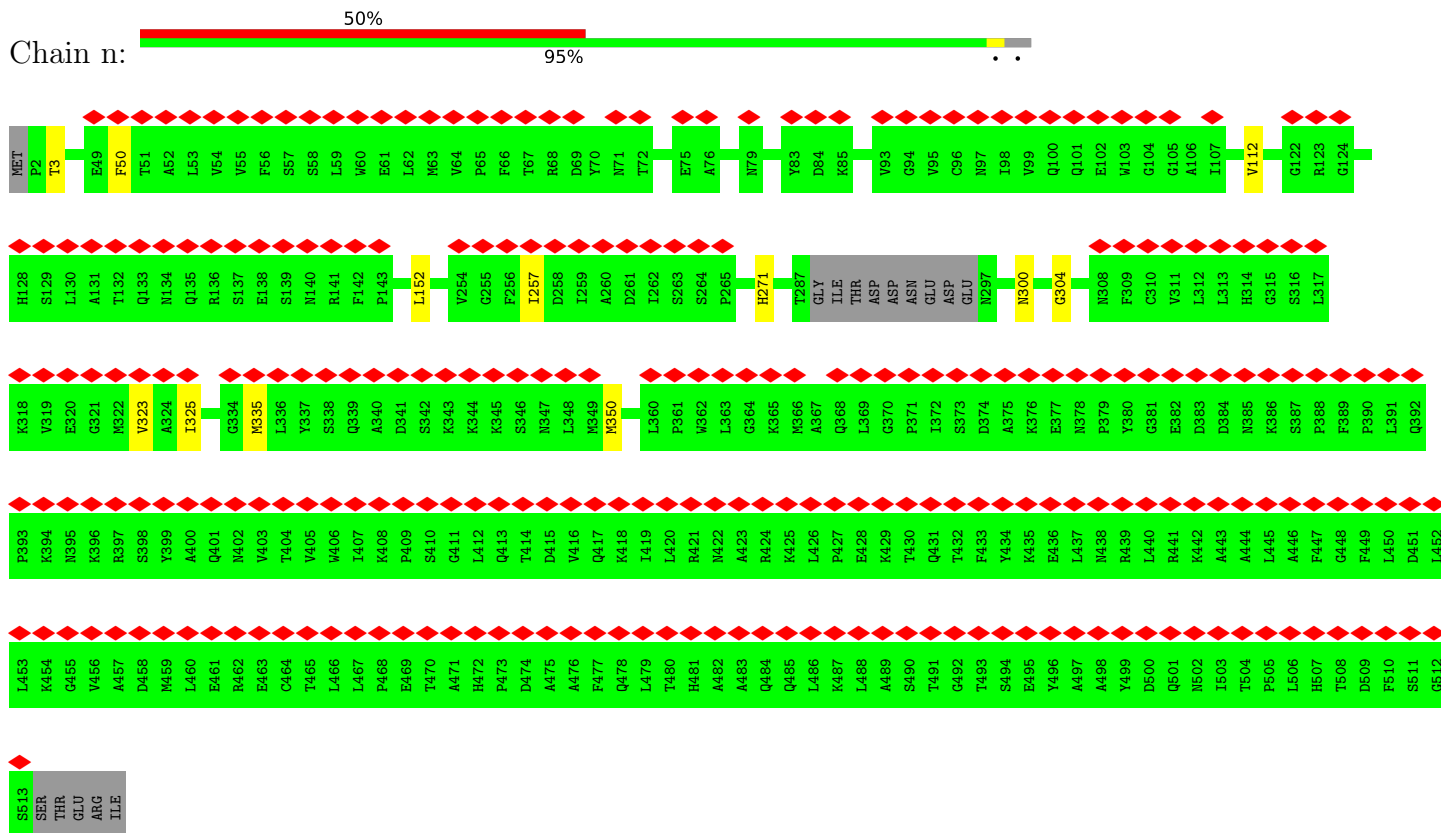


• Molecule 32: Integrator complex subunit 13

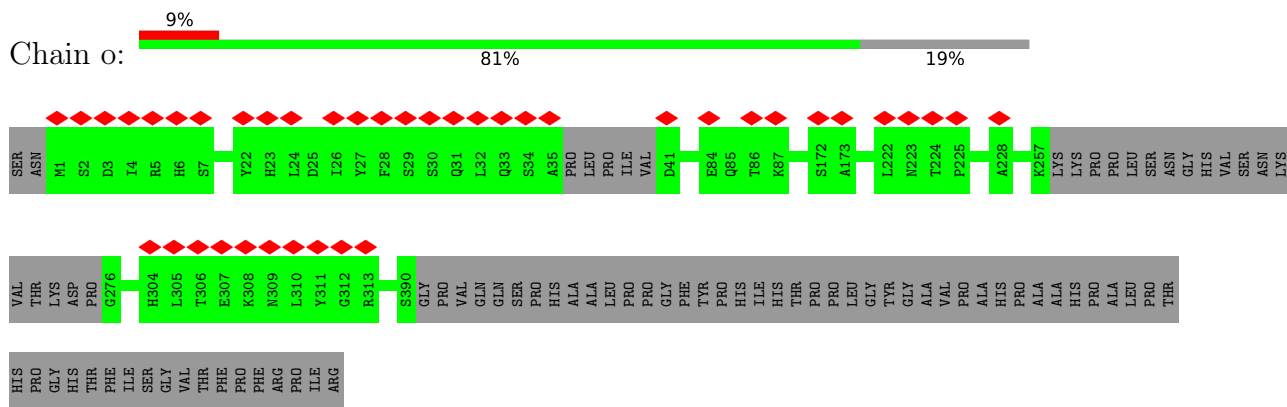


THR
THR
GLU
ASN
GLY
LYS
ALA
SER
ARG
GLN

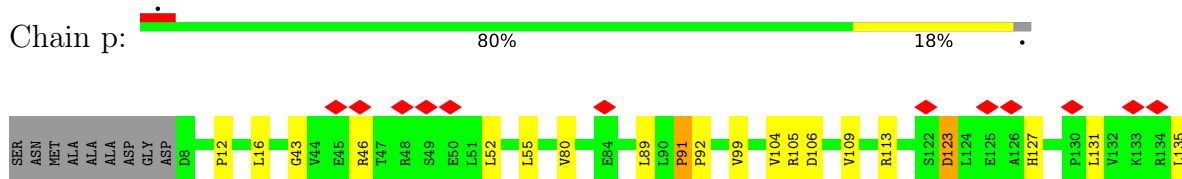
• Molecule 33: Integrator complex subunit 14



• Molecule 34: Integrator complex subunit 15



• Molecule 35: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80717	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.44	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.105	Depositor
Minimum map value	-0.046	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00453	Depositor
Map size ($\text{\AA}$)	525.0, 525.0, 525.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MN, 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	$\# Z > 5$
2	A	0.28	0/11205	0.49	0/15122
2	Y	0.33	0/100	0.38	0/139
3	B	0.28	0/9076	0.46	0/12250
4	C	0.28	0/2139	0.44	0/2906
5	D	0.16	0/990	0.41	0/1335
6	E	0.28	0/1752	0.48	0/2366
7	F	0.29	0/637	0.54	0/859
8	G	0.21	0/1347	0.47	0/1833
9	H	0.29	0/1207	0.57	0/1628
10	I	0.31	0/967	0.64	0/1309
11	J	0.34	0/542	0.48	0/730
12	K	0.32	0/936	0.54	0/1267
13	L	0.35	0/389	0.56	0/517
14	M	0.28	0/736	0.59	0/989
14	S	0.52	0/739	0.94	2/993 (0.2%)
15	N	0.22	0/3425	0.46	0/5290
16	O	0.28	0/654	0.60	0/876
16	U	0.40	0/641	0.69	0/858
17	P	0.25	0/413	0.40	0/644
18	Q	0.20	0/849	0.52	0/1143
18	V	0.26	0/824	0.59	0/1111
19	R	0.20	0/665	0.48	0/893
19	W	0.36	0/757	0.61	0/1015
20	T	0.26	0/3672	0.47	1/5658 (0.0%)
21	Z	0.19	0/2200	0.43	0/2964
22	a	0.25	0/11854	0.50	0/16192
23	b	0.39	0/8131	0.57	0/11076
24	d	0.35	1/6532 (0.0%)	0.56	0/8873
25	e	0.30	0/6398	0.52	1/8718 (0.0%)
26	f	0.30	0/4240	0.52	0/5784
27	g	0.35	0/6832	0.53	0/9268
28	h	0.30	0/6870	0.49	0/9334

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
29	i	0.31	0/4989	0.52	0/6802
30	j	0.12	0/3309	0.38	0/4608
31	k	0.24	0/4179	0.50	0/5679
32	m	0.13	0/2863	0.38	0/3972
33	n	0.11	0/2482	0.35	0/3453
34	o	0.13	0/1821	0.41	0/2538
35	p	0.28	0/4505	0.59	1/6129 (0.0%)
36	q	0.35	0/2378	0.50	0/3228
37	r	0.31	0/255	0.61	0/345
38	u	0.26	0/1419	0.57	0/1930
39	v	0.21	0/1952	0.46	0/2522
40	w	0.23	0/3900	0.52	0/5310
All	All	0.29	1/131771 (0.0%)	0.51	5/180456 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
19	R	1	0
19	W	1	0
All	All	2	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	522	VAL	CA-CB	6.83	1.57	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	S	56	LYS	N-CA-CB	6.65	120.00	110.16
35	p	91	PRO	N-CA-C	6.24	118.31	110.70
25	e	538	LEU	CD1-CG-CD2	-5.70	98.27	110.80
14	S	63	ARG	CB-CA-C	-5.15	102.78	112.00
20	T	9	DC	O5'-P-OP2	5.02	123.07	108.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	R	66	ILE	CB

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Mol	Chain	Res	Type	Atom
19	W	66	ILE	CB

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	1	40	0	12	0	0
2	A	11008	0	11156	140	0
2	Y	95	0	82	0	0
3	B	8901	0	8923	99	0
4	C	2096	0	2040	22	0
5	D	977	0	929	7	0
6	E	1721	0	1737	18	0
7	F	627	0	657	10	0
8	G	1316	0	1288	16	0
9	H	1186	0	1147	27	0
10	I	944	0	868	19	0
11	J	533	0	553	9	0
12	K	917	0	940	13	0
13	L	383	0	382	7	0
14	M	729	0	763	20	0
14	S	732	0	763	37	0
15	N	3050	0	1664	35	0
16	O	647	0	685	17	0
16	U	634	0	665	19	0
17	P	370	0	182	2	0
18	Q	839	0	906	20	0
18	V	814	0	875	15	0
19	R	656	0	677	13	0
19	W	746	0	766	13	0
20	T	3277	0	1805	45	0
21	Z	2167	0	2180	17	0
22	a	11692	0	10122	104	0
23	b	7991	0	8034	93	0
24	d	6407	0	6432	93	0
25	e	6260	0	6070	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	f	4137	0	3989	48	0
27	g	6722	0	6685	86	0
28	h	6751	0	6615	63	0
29	i	4870	0	4849	55	0
30	j	3313	0	1464	2	0
31	k	4090	0	3891	60	0
32	m	2864	0	1380	6	0
33	n	2484	0	1104	6	0
34	o	1824	0	802	0	0
35	p	4431	0	4483	62	0
36	q	2322	0	2215	31	0
37	r	250	0	217	7	0
38	u	1395	0	1434	17	0
39	v	2070	0	921	4	0
40	w	3825	0	3650	37	0
41	x	110	0	24	0	0
42	A	2	0	0	0	0
42	B	1	0	0	0	0
42	C	1	0	0	0	0
42	I	2	0	0	0	0
42	J	1	0	0	0	0
42	L	1	0	0	0	0
42	k	2	0	0	0	0
43	P	1	0	0	0	0
44	f	1	0	0	0	0
44	q	1	0	0	0	0
All	All	129226	0	117026	1270	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 5.

All (1270) 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)
19:W:56:MET:HA	19:W:59:MET:HE3	1.58	0.85
24:d:56:LEU:HD22	24:d:95:LEU:HD21	1.59	0.85
18:Q:84:GLN:HE21	18:Q:102:ILE:HG22	1.41	0.84
15:N:55:DT:H5'	14:S:83:ARG:HD3	1.64	0.78
20:T:111:DT:H4'	18:V:42:ARG:HA	1.66	0.78
15:N:35:DA:H4'	18:V:16:SER:HA	1.68	0.76
28:h:253:CYS:HG	28:h:281:THR:HG1	1.31	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:d:179:SER:HA	24:d:227:LEU:HD21	1.71	0.73
3:B:927:ARG:NH1	3:B:1054:MET:SD	2.64	0.71
14:M:118:THR:HG22	16:O:45:ARG:HB3	1.73	0.71
14:S:65:LEU:HB3	20:T:90:DA:OP2	1.91	0.70
3:B:593:GLN:HG2	22:a:415:LYS:H	1.57	0.70
3:B:610:ARG:NH1	10:I:71:ASP:OD2	2.24	0.70
24:d:540:ASP:HA	24:d:545:ILE:HD11	1.73	0.69
22:a:1283:LYS:HA	22:a:1286:MET:HE2	1.74	0.69
29:i:138:GLU:HA	29:i:184:MET:HE1	1.73	0.69
3:B:841:ARG:NH2	17:P:-13:G:N7	2.39	0.69
2:A:1218:ARG:HH12	2:A:1253:GLU:HA	1.56	0.69
22:a:1886:ALA:HB2	24:d:516:THR:HG22	1.74	0.69
36:q:88:ASN:HD21	36:q:124:THR:HA	1.58	0.68
9:H:28:LEU:HD21	9:H:50:VAL:HG11	1.75	0.68
14:M:63:ARG:HH21	20:T:59:DA:H4'	1.59	0.67
3:B:854:ILE:HG13	3:B:866:ILE:HD12	1.76	0.67
22:a:2042:LEU:N	22:a:2046:GLU:OE1	2.27	0.67
18:Q:104:GLN:NE2	14:S:97:GLU:OE2	2.26	0.67
14:S:62:ILE:HB	14:S:66:PRO:HG2	1.77	0.67
24:d:834:PRO:HB3	24:d:955:TYR:HB3	1.77	0.67
31:k:165:GLN:NE2	31:k:195:CYS:SG	2.69	0.66
21:Z:557:THR:HA	21:Z:571:ARG:HH22	1.60	0.66
3:B:666:ASP:OD1	3:B:667:THR:N	2.30	0.65
24:d:426:GLU:OE2	24:d:430:GLN:NE2	2.30	0.65
16:U:32:PRO:HA	16:U:35:ARG:HB2	1.79	0.65
18:Q:81:ARG:HB2	14:S:58:THR:HG21	1.79	0.65
19:R:84:SER:HB2	18:V:38:ASN:HB2	1.79	0.65
14:S:100:LEU:HD11	16:U:58:LEU:HD11	1.79	0.65
25:e:970:ILE:HD11	28:h:371:GLN:HG3	1.78	0.65
39:v:39:VAL:HG23	39:v:40:LEU:HG	1.77	0.65
24:d:257:TRP:NE1	24:d:308:SER:OG	2.30	0.65
28:h:639:ILE:HG23	28:h:667:MET:HE1	1.79	0.65
2:A:272:ASN:ND2	20:T:161:DG:N3	2.45	0.65
15:N:74:DG:H3'	14:S:116:ARG:HB2	1.79	0.65
39:v:76:ARG:NH2	40:w:101:LEU:O	2.30	0.64
3:B:565:THR:HG21	3:B:580:PRO:HB3	1.77	0.64
24:d:706:LYS:HB3	24:d:710:MET:HE2	1.78	0.64
3:B:1085:ARG:NH1	20:T:152:DC:OP1	2.29	0.64
4:C:106:ARG:NH1	4:C:158:GLU:OE1	2.31	0.64
27:g:671:MET:HG3	27:g:721:ILE:HG21	1.78	0.64
28:h:471:ASP:OD1	28:h:474:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:h:560:GLY:O	28:h:562:LYS:NZ	2.29	0.64
3:B:1033:THR:HG22	12:K:44:ASN:HD21	1.63	0.64
22:a:1076:VAL:O	22:a:1130:ARG:NH1	2.30	0.64
24:d:688:LYS:NZ	24:d:740:THR:OG1	2.30	0.64
2:A:119:VAL:HG21	2:A:147:LEU:HD11	1.80	0.63
2:A:349:ARG:NH1	3:B:1161:GLU:OE2	2.30	0.63
9:H:2:ALA:O	9:H:84:ARG:NH2	2.31	0.63
21:Z:563:MET:H	31:k:115:LYS:HG3	1.62	0.63
24:d:117:ILE:HD12	24:d:120:ASN:HD21	1.62	0.63
14:S:64:LYS:O	14:S:68:GLN:HB3	1.97	0.63
24:d:91:LYS:NZ	29:i:89:GLU:O	2.30	0.63
31:k:299:MET:SD	31:k:299:MET:N	2.71	0.63
3:B:760:THR:HG23	3:B:764:MET:HE3	1.80	0.63
35:p:91:PRO:HD2	35:p:92:PRO:HD2	1.81	0.63
32:m:684:GLU:O	32:m:687:GLN:NE2	2.31	0.63
19:R:82:LYS:HD2	18:V:36:LYS:HD3	1.81	0.63
21:Z:419:ASN:OD1	21:Z:421:GLN:NE2	2.32	0.63
35:p:123:ASP:O	35:p:127:HIS:ND1	2.32	0.63
2:A:827:TYR:HH	2:A:839:HIS:HE2	1.44	0.63
6:E:110:MET:HE3	6:E:115:LYS:HG2	1.80	0.63
2:A:98:GLY:HA3	2:A:1440:MET:HE3	1.81	0.63
19:R:53:SER:H	20:T:19:DA:H5"	1.63	0.62
35:p:572:ASP:OD2	36:q:110:ARG:NH1	2.33	0.62
3:B:604:ILE:HD11	3:B:613:ARG:HD3	1.81	0.62
27:g:417:VAL:HA	27:g:456:ILE:HD11	1.80	0.62
2:A:582:PRO:HD2	9:H:47:ILE:HD12	1.81	0.62
3:B:379:ARG:HE	10:I:67:GLN:HE22	1.46	0.62
14:S:52:ARG:NH2	20:T:9:DC:H5"	2.14	0.62
28:h:348:ASP:OD2	28:h:359:ARG:NH1	2.33	0.62
18:Q:113:ALA:O	18:Q:118:LYS:NZ	2.33	0.62
22:a:1928:GLN:HE21	22:a:1973:ALA:HB2	1.63	0.62
2:A:1152:GLU:OE1	40:w:531:ARG:NH1	2.33	0.62
3:B:89:GLU:OE2	3:B:143:GLN:NE2	2.32	0.62
35:p:80:VAL:HG21	35:p:89:LEU:HD11	1.80	0.62
22:a:1758:ILE:HD11	22:a:1802:LEU:HD23	1.81	0.61
2:A:388:MET:HA	3:B:1063:ALA:HB2	1.82	0.61
3:B:938:ARG:NH2	3:B:983:GLU:OE2	2.31	0.61
23:b:16:GLN:O	23:b:209:TRP:NE1	2.30	0.61
24:d:457:GLU:OE2	24:d:495:LYS:NZ	2.33	0.61
22:a:1842:PHE:HZ	22:a:2187:GLU:HA	1.65	0.61
38:u:145:ASN:HA	40:w:421:PRO:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:63:THR:O	9:H:84:ARG:NH1	2.33	0.61
26:f:319:ILE:HD11	26:f:322:LEU:HD13	1.82	0.61
40:w:473:LEU:HB3	40:w:500:MET:HE1	1.83	0.61
2:A:363:ALA:HB2	2:A:388:MET:HE1	1.81	0.61
22:a:1713:GLN:O	22:a:1714:ARG:NH1	2.33	0.61
27:g:826:GLN:OE1	27:g:895:ASN:ND2	2.34	0.61
40:w:244:MET:SD	40:w:244:MET:N	2.74	0.61
6:E:52:ARG:HA	6:E:54:ARG:HH21	1.65	0.61
15:N:105:DG:H5''	16:O:79:LYS:HG3	1.82	0.61
2:A:413:TYR:O	2:A:449:HIS:ND1	2.26	0.61
3:B:812:ARG:NH1	20:T:156:DA:OP1	2.34	0.61
28:h:542:TRP:HA	28:h:572:ILE:HD11	1.81	0.61
2:A:481:THR:O	2:A:483:ARG:NH1	2.33	0.61
2:A:863:ARG:NH1	2:A:1129:ASN:OD1	2.34	0.61
4:C:70:LEU:O	11:J:6:ARG:NH1	2.34	0.60
23:b:791:GLU:OE2	23:b:827:ARG:NH2	2.33	0.60
23:b:856:ASP:OD2	23:b:862:ARG:NH2	2.33	0.60
3:B:567:ILE:HD11	3:B:577:HIS:HB2	1.82	0.60
5:D:32:LEU:HD12	5:D:36:GLU:HB3	1.83	0.60
27:g:638:CYS:HB3	27:g:774:THR:HG23	1.83	0.60
3:B:311:ILE:HG23	3:B:316:VAL:HG13	1.82	0.60
24:d:848:ASP:OD2	24:d:891:ARG:NH2	2.34	0.60
26:f:193:ASP:OD1	26:f:193:ASP:N	2.33	0.60
27:g:793:ARG:NH2	37:r:2040:ASN:O	2.34	0.60
39:v:155:ALA:O	39:v:160:GLU:N	2.35	0.60
26:f:587:MET:SD	36:q:249:ASN:ND2	2.74	0.60
2:A:106:VAL:HG23	2:A:236:LEU:HD21	1.84	0.60
24:d:228:LYS:NZ	24:d:229:LEU:O	2.33	0.60
35:p:105:ARG:HH21	35:p:142:THR:HB	1.64	0.60
25:e:922:PRO:O	25:e:926:ASN:ND2	2.34	0.60
15:N:37:DA:N1	20:T:115:DC:N4	2.49	0.60
35:p:99:VAL:HB	35:p:104:VAL:HG11	1.84	0.60
2:A:564:LEU:HD21	2:A:594:LEU:HD13	1.84	0.60
18:Q:47:ALA:HB1	19:R:91:ILE:HG13	1.83	0.60
14:S:56:LYS:NZ	20:T:9:DC:H2'	2.17	0.60
31:k:228:THR:O	31:k:233:GLY:N	2.34	0.60
4:C:175:LYS:NZ	13:L:57:ALA:O	2.35	0.59
9:H:88:PHE:HD2	9:H:144:LEU:HB3	1.65	0.59
31:k:1:MET:SD	31:k:1:MET:N	2.73	0.59
4:C:266:GLU:OE1	12:K:17:LYS:NZ	2.35	0.59
23:b:731:GLU:OE2	27:g:85:LYS:NZ	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:d:111:MET:HE2	24:d:147:ILE:HG22	1.84	0.59
2:A:894:ASP:OD1	2:A:1396:ARG:NH2	2.35	0.59
22:a:1424:SER:HA	22:a:1427:ARG:HH12	1.67	0.59
22:a:1629:VAL:O	22:a:1637:GLN:NE2	2.32	0.59
22:a:1838:LEU:HD11	22:a:2190:MET:HA	1.84	0.59
25:e:994:ARG:NH1	28:h:160:PRO:O	2.35	0.59
3:B:114:ARG:NH1	3:B:191:GLU:OE2	2.35	0.59
23:b:447:GLU:O	23:b:450:GLN:NE2	2.36	0.59
4:C:193:ARG:NH2	4:C:218:ALA:O	2.34	0.59
23:b:232:ASN:OD1	23:b:246:ARG:NH1	2.35	0.59
2:A:360:ASP:OD1	3:B:1062:ARG:NE	2.34	0.59
2:A:1167:ARG:HD2	2:A:1293:LEU:HD12	1.83	0.59
12:K:63:VAL:HG22	12:K:71:ILE:HG22	1.85	0.59
18:Q:81:ARG:HH12	14:S:56:LYS:HA	1.68	0.59
35:p:12:PRO:HA	35:p:16:LEU:HD23	1.85	0.59
40:w:449:PRO:HG2	40:w:452:LEU:HD23	1.85	0.59
24:d:407:SER:O	24:d:411:LYS:NZ	2.33	0.59
2:A:448:ARG:NH1	2:A:449:HIS:O	2.33	0.59
3:B:283:ASP:N	3:B:283:ASP:OD1	2.32	0.59
3:B:602:SER:OG	3:B:620:ARG:NH1	2.36	0.59
5:D:62:MET:O	5:D:66:ASN:ND2	2.35	0.59
22:a:1215:LEU:HA	22:a:1219:LEU:HD23	1.84	0.59
23:b:926:LEU:HG	26:f:563:LEU:HD12	1.85	0.59
28:h:333:LEU:HD11	28:h:362:VAL:HG23	1.84	0.59
29:i:116:HIS:NE2	29:i:186:GLU:OE1	2.36	0.58
31:k:23:SER:OG	31:k:28:ASN:OD1	2.21	0.58
29:i:461:LEU:HD21	29:i:469:VAL:HG21	1.85	0.58
22:a:1706:ARG:NH1	23:b:992:GLU:OE2	2.36	0.58
2:A:261:ARG:HH11	2:A:277:THR:HG22	1.69	0.58
22:a:1147:GLN:NE2	22:a:1207:ASP:OD2	2.37	0.58
23:b:169:GLU:HG3	23:b:210:PHE:HE2	1.69	0.58
31:k:498:ALA:O	31:k:505:ALA:N	2.37	0.58
6:E:104:ILE:HD11	6:E:127:LEU:HD23	1.85	0.58
14:M:54:TYR:HB3	16:O:40:ARG:HG3	1.85	0.58
25:e:133:ILE:HD11	25:e:144:ILE:HD11	1.85	0.58
2:A:911:PRO:O	2:A:963:ARG:NH2	2.35	0.58
2:A:1424:THR:OG1	2:A:1428:MET:SD	2.59	0.58
22:a:1162:MET:HE1	22:a:1193:TRP:HH2	1.68	0.58
22:a:2073:MET:O	22:a:2077:ARG:N	2.34	0.58
18:V:87:VAL:HG22	18:V:93:LEU:HD23	1.85	0.58
22:a:1280:ILE:HG12	22:a:1286:MET:HE1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:d:641:ARG:NH2	24:d:642:ASP:OD1	2.34	0.58
36:q:61:GLN:NE2	36:q:64:ASP:OD2	2.37	0.58
24:d:421:ASN:O	31:k:215:ARG:NH2	2.36	0.57
26:f:271:ARG:NH1	26:f:328:GLU:OE2	2.37	0.57
3:B:200:MET:SD	3:B:385:ARG:NH2	2.77	0.57
23:b:205:ARG:O	23:b:245:ARG:NH2	2.37	0.57
3:B:591:ARG:NH2	3:B:663:GLU:OE1	2.37	0.57
18:Q:84:GLN:NE2	18:Q:103:ALA:O	2.36	0.57
38:u:144:LEU:HD21	40:w:329:ARG:HE	1.68	0.57
9:H:14:ASP:HB2	9:H:29:HIS:HB2	1.85	0.57
36:q:156:THR:HG22	36:q:166:LEU:HD13	1.86	0.57
8:G:79:PRO:HG2	8:G:150:THR:HG23	1.87	0.57
15:N:45:DG:OP1	19:W:89:ARG:NH1	2.38	0.57
2:A:111:CYS:SG	2:A:188:GLN:NE2	2.77	0.57
15:N:35:DA:H3'	18:V:17:ARG:HG3	1.86	0.57
29:i:341:GLN:OE1	29:i:364:HIS:NE2	2.37	0.57
22:a:773:ASN:O	22:a:983:GLN:NE2	2.38	0.57
22:a:1833:CYS:SG	22:a:1834:LYS:N	2.77	0.57
3:B:198:GLU:OE1	3:B:487:SER:OG	2.22	0.57
23:b:26:MET:HE1	23:b:48:CYS:HB3	1.86	0.57
25:e:60:LEU:HD21	25:e:125:VAL:HG22	1.85	0.57
25:e:660:ARG:HH22	25:e:701:ASN:HA	1.70	0.57
5:D:66:ASN:OD1	5:D:70:ARG:NH2	2.38	0.57
2:A:1172:ASN:ND2	2:A:1215:GLU:OE1	2.38	0.57
18:V:80:PRO:HD3	19:W:55:ALA:HB2	1.87	0.56
22:a:1023:LEU:HG	22:a:1026:TYR:HB2	1.87	0.56
11:J:9:THR:OG1	11:J:47:ARG:NH2	2.38	0.56
22:a:1277:GLU:HA	22:a:1280:ILE:HD12	1.86	0.56
23:b:1104:LEU:HB3	23:b:1192:THR:HG21	1.88	0.56
28:h:537:SER:OG	28:h:538:GLU:N	2.38	0.56
31:k:3:GLU:OE1	31:k:445:THR:OG1	2.22	0.56
23:b:734:THR:HG21	27:g:199:PRO:HG2	1.87	0.56
26:f:210:VAL:HG23	26:f:215:MET:HG3	1.87	0.56
35:p:440:ASP:OD2	35:p:477:TRP:NE1	2.30	0.56
2:A:1189:ASP:HB2	2:A:1192:TRP:HE3	1.71	0.56
22:a:1776:VAL:HG21	22:a:1810:ARG:HD3	1.86	0.56
23:b:837:GLN:NE2	23:b:844:ARG:O	2.38	0.56
35:p:255:LYS:O	35:p:255:LYS:NZ	2.35	0.56
15:N:34:DG:H3'	18:V:28:GLY:HA3	1.87	0.56
24:d:523:PRO:HD3	24:d:564:LEU:HD21	1.86	0.56
28:h:586:PHE:HB3	28:h:622:THR:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:148:CYS:O	2:A:151:LYS:N	2.39	0.56
2:A:535:MET:O	2:A:669:TYR:OH	2.20	0.56
26:f:17:ARG:O	28:h:967:ASN:ND2	2.39	0.56
3:B:310:VAL:HG13	3:B:311:ILE:HG13	1.88	0.56
35:p:502:LEU:HD13	35:p:539:ASN:HB3	1.87	0.56
10:I:13:GLY:O	10:I:15:ARG:NH1	2.39	0.56
22:a:1494:LEU:HD21	22:a:1503:ARG:HH22	1.70	0.56
26:f:156:GLU:OE2	26:f:455:TYR:OH	2.24	0.56
27:g:911:LYS:HG3	27:g:917:VAL:HG22	1.86	0.56
29:i:108:MET:HE2	29:i:136:LEU:HB3	1.88	0.56
35:p:432:GLY:HA2	35:p:472:LYS:HD2	1.88	0.56
22:a:1131:MET:HG3	22:a:1162:MET:HG2	1.88	0.55
26:f:389:LEU:HB2	26:f:415:TYR:CE1	2.41	0.55
2:A:552:ASP:OD2	9:H:24:ARG:NH2	2.39	0.55
14:S:52:ARG:NE	20:T:9:DC:OP1	2.39	0.55
22:a:1281:MET:HE3	22:a:1281:MET:H	1.71	0.55
2:A:34:MET:O	3:B:1138:ARG:NH2	2.37	0.55
2:A:678:ASN:HA	2:A:681:LEU:HD23	1.88	0.55
2:A:1216:LEU:HD12	2:A:1255:LEU:HB3	1.88	0.55
22:a:1518:SER:OG	22:a:1522:ARG:NH2	2.40	0.55
22:a:1560:LEU:HD23	22:a:1563:PHE:HE1	1.71	0.55
23:b:350:ILE:HD11	23:b:384:LYS:HD2	1.87	0.55
25:e:177:LEU:HA	25:e:180:TRP:HD1	1.71	0.55
26:f:189:VAL:HG11	26:f:208:TYR:HD1	1.71	0.55
26:f:484:ILE:HG22	26:f:529:VAL:H	1.71	0.55
28:h:652:ASP:OD1	28:h:652:ASP:N	2.38	0.55
38:u:53:LYS:NZ	38:u:85:ASP:OD1	2.34	0.55
24:d:475:ASN:OD1	24:d:513:ARG:NH1	2.37	0.55
27:g:458:MET:HE2	27:g:535:ARG:HH21	1.70	0.55
31:k:50:TYR:O	32:m:674:GLY:N	2.35	0.55
14:S:107:THR:HG22	14:S:119:ILE:HD11	1.88	0.55
28:h:61:PRO:O	28:h:78:ASN:ND2	2.40	0.55
28:h:295:CYS:SG	28:h:296:THR:N	2.76	0.55
28:h:952:ASP:N	28:h:952:ASP:OD1	2.32	0.55
4:C:48:ASP:OD1	4:C:175:LYS:NZ	2.35	0.55
13:L:25:GLU:OE2	13:L:25:GLU:N	2.39	0.55
23:b:133:SER:O	23:b:138:ARG:NH1	2.39	0.55
29:i:79:SER:OG	29:i:80:VAL:N	2.38	0.55
3:B:550:MET:HE1	3:B:574:VAL:HG22	1.89	0.55
4:C:113:ARG:NH1	4:C:114:HIS:O	2.39	0.55
13:L:17:TYR:HB2	13:L:44:MET:HE3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:75:HIS:HB2	19:R:93:THR:HG21	1.88	0.55
26:f:539:GLN:O	26:f:543:ASN:N	2.39	0.55
35:p:219:SER:HA	35:p:222:LEU:HD12	1.89	0.55
40:w:475:LYS:O	40:w:479:THR:OG1	2.22	0.55
2:A:686:THR:OG1	2:A:687:ILE:N	2.40	0.55
4:C:99:VAL:HG21	4:C:127:VAL:HG11	1.88	0.55
10:I:116:ALA:HB3	10:I:119:CYS:HB3	1.89	0.55
24:d:708:GLU:OE1	24:d:726:ARG:NH2	2.35	0.55
27:g:353:TYR:OH	27:g:385:ASP:OD1	2.25	0.55
29:i:297:VAL:HB	29:i:394:PHE:HD1	1.71	0.55
31:k:176:THR:HG21	31:k:401:LEU:HD21	1.89	0.55
23:b:328:LYS:O	23:b:331:THR:OG1	2.24	0.55
36:q:83:MET:HE3	36:q:240:ALA:HB2	1.89	0.55
23:b:46:LEU:HA	23:b:49:LEU:HD12	1.89	0.54
24:d:678:LEU:HD11	24:d:686:TYR:HD1	1.72	0.54
27:g:416:MET:HE2	27:g:430:VAL:HG13	1.89	0.54
22:a:2139:THR:O	22:a:2143:ASN:ND2	2.38	0.54
24:d:317:LEU:HD22	24:d:401:LEU:HD21	1.89	0.54
29:i:393:VAL:HG12	29:i:395:THR:HG23	1.89	0.54
35:p:247:THR:HA	35:p:250:GLN:HG3	1.89	0.54
38:u:79:ILE:HD12	38:u:98:LYS:HA	1.89	0.54
18:V:79:ILE:HG22	18:V:81:ARG:H	1.73	0.54
26:f:439:LEU:HD22	26:f:440:ILE:HD12	1.89	0.54
28:h:643:ARG:NH2	28:h:679:GLN:OE1	2.40	0.54
31:k:289:LYS:O	31:k:293:THR:OG1	2.24	0.54
35:p:113:ARG:NH2	35:p:149:GLY:O	2.40	0.54
2:A:95:PHE:O	2:A:311:GLN:NE2	2.39	0.54
3:B:579:ASP:OD1	3:B:579:ASP:N	2.40	0.54
6:E:85:LYS:HZ1	6:E:88:LYS:HD3	1.73	0.54
24:d:464:ARG:NH1	24:d:499:ASP:OD2	2.40	0.54
25:e:968:ARG:HD3	28:h:371:GLN:HE22	1.70	0.54
4:C:16:ASP:OD1	4:C:16:ASP:N	2.40	0.54
15:N:16:DA:H2''	15:N:17:DT:H5'	1.90	0.54
18:Q:38:ASN:HD21	19:W:84:SER:HA	1.71	0.54
23:b:146:LEU:O	23:b:150:MET:HG2	2.07	0.54
23:b:733:ILE:HD12	27:g:156:GLU:HB3	1.90	0.54
26:f:13:SER:O	26:f:16:GLN:NE2	2.38	0.54
35:p:131:LEU:O	35:p:135:LEU:HB2	2.07	0.54
40:w:486:VAL:HG13	40:w:487:MET:HE2	1.89	0.54
6:E:134:GLU:OE1	6:E:181:ARG:NH2	2.41	0.54
13:L:13:GLN:O	13:L:29:LYS:NZ	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:49:ARG:HE	20:T:8:DT:H4'	1.73	0.54
18:Q:77:ARG:NH1	18:Q:78:ILE:O	2.40	0.54
27:g:184:ILE:HD11	27:g:197:LEU:HB3	1.90	0.54
31:k:63:CYS:SG	31:k:64:VAL:N	2.81	0.54
23:b:169:GLU:HG3	23:b:210:PHE:CE2	2.43	0.54
24:d:253:VAL:HA	24:d:256:ILE:HG22	1.90	0.54
35:p:499:MET:HE1	35:p:536:VAL:HA	1.90	0.54
3:B:228:SER:O	3:B:405:ARG:NE	2.41	0.54
22:a:1691:PRO:HB2	22:a:1742:GLU:HG2	1.89	0.54
3:B:149:ILE:HG22	3:B:435:ILE:HG21	1.90	0.53
24:d:746:PRO:O	24:d:750:MET:HG2	2.08	0.53
31:k:435:CYS:SG	31:k:436:TYR:N	2.80	0.53
35:p:138:GLY:O	35:p:144:ARG:NH1	2.41	0.53
22:a:2149:LEU:HD22	22:a:2183:ILE:HG21	1.90	0.53
23:b:308:GLY:O	23:b:314:ARG:NH2	2.40	0.53
24:d:908:GLN:NE2	27:g:891:GLN:OE1	2.38	0.53
3:B:301:VAL:O	3:B:304:SER:OG	2.27	0.53
27:g:705:LEU:O	27:g:752:TYR:OH	2.26	0.53
28:h:782:ASN:ND2	28:h:791:ILE:O	2.42	0.53
23:b:741:ARG:NH1	23:b:785:GLU:OE2	2.40	0.53
27:g:826:GLN:HE21	27:g:893:LEU:HD12	1.73	0.53
35:p:198:LEU:HB2	35:p:235:LEU:HD21	1.91	0.53
15:N:33:DG:OP2	19:W:28:ARG:NH1	2.32	0.53
22:a:1589:GLN:O	22:a:1610:ARG:NH2	2.40	0.53
29:i:585:LEU:HB3	31:k:509:LEU:HB2	1.89	0.53
31:k:51:ILE:HA	32:m:672:PHE:HB2	1.91	0.53
40:w:269:ALA:HB1	40:w:274:HIS:HB3	1.89	0.53
3:B:430:ASN:HB3	3:B:433:LEU:HB3	1.89	0.53
23:b:588:LEU:HD11	23:b:650:LEU:HD21	1.91	0.53
3:B:124:LEU:HD22	3:B:152:ILE:HD11	1.91	0.53
23:b:22:ALA:HB1	23:b:45:LEU:HD11	1.90	0.53
24:d:478:THR:OG1	24:d:480:GLU:OE1	2.25	0.53
25:e:923:ALA:HB1	25:e:985:LEU:HD21	1.91	0.53
27:g:390:LEU:HD13	27:g:416:MET:HG2	1.90	0.53
2:A:1218:ARG:NH1	2:A:1253:GLU:HA	2.22	0.53
18:V:33:LEU:HD11	19:W:67:PHE:HE2	1.74	0.53
27:g:374:CYS:O	27:g:423:ARG:NH2	2.40	0.53
28:h:412:LYS:NZ	28:h:416:ASP:OD2	2.40	0.53
24:d:414:ASP:OD1	24:d:414:ASP:N	2.41	0.53
24:d:385:ASP:OD1	24:d:387:MET:N	2.41	0.53
22:a:1032:ASP:OD1	22:a:1033:LEU:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:79:GLU:O	23:b:82:ASN:ND2	2.42	0.52
12:K:17:LYS:HE3	12:K:20:THR:HG22	1.91	0.52
35:p:52:LEU:HA	35:p:55:LEU:HD12	1.92	0.52
36:q:121:ARG:NH1	36:q:188:GLU:OE1	2.37	0.52
2:A:687:ILE:HB	2:A:769:MET:HE1	1.91	0.52
3:B:955:PRO:HB2	3:B:1028:LEU:HD13	1.90	0.52
2:A:780:ASN:HA	3:B:976:MET:HE1	1.90	0.52
15:N:136:DC:OP1	18:Q:77:ARG:NH2	2.42	0.52
24:d:900:HIS:CD2	24:d:903:TRP:HE1	2.27	0.52
3:B:67:LEU:HD21	3:B:416:ARG:HG2	1.90	0.52
15:N:115:DC:H2''	15:N:116:DG:N7	2.23	0.52
12:K:51:LEU:HD22	12:K:59:ALA:HB3	1.91	0.52
18:V:31:HIS:HA	18:V:34:LEU:HD12	1.92	0.52
24:d:377:GLY:O	24:d:381:HIS:ND1	2.41	0.52
29:i:585:LEU:HD11	31:k:577:THR:HA	1.92	0.52
33:n:112:VAL:HA	33:n:152:LEU:HA	1.91	0.52
38:u:38:ILE:HA	38:u:41:ILE:HD12	1.90	0.52
39:v:215:TYR:O	39:v:220:GLN:N	2.39	0.52
40:w:517:ARG:HG2	40:w:556:ILE:HD11	1.90	0.52
2:A:1153:ARG:HA	2:A:1156:ASP:HB3	1.91	0.52
31:k:561:ALA:HB3	31:k:573:LEU:HD13	1.91	0.52
14:S:62:ILE:HD12	14:S:66:PRO:HB2	1.92	0.52
22:a:972:LEU:HA	22:a:976:LEU:HD23	1.92	0.52
23:b:496:ILE:HD12	23:b:509:ILE:HG13	1.92	0.52
23:b:517:MET:O	23:b:521:PHE:HB2	2.08	0.52
24:d:206:ASP:O	24:d:212:ARG:NH1	2.41	0.52
25:e:791:GLY:HA2	28:h:409:ARG:HE	1.73	0.52
2:A:373:LEU:HD22	2:A:377:GLN:HB3	1.92	0.52
10:I:25:TYR:HD2	10:I:40:ARG:HH22	1.58	0.52
28:h:291:LEU:O	28:h:296:THR:OG1	2.27	0.52
29:i:400:LEU:O	29:i:436:TYR:OH	2.27	0.52
36:q:141:ASN:HA	36:q:144:LYS:HE3	1.91	0.52
2:A:411:SER:OG	2:A:412:GLN:OE1	2.28	0.52
23:b:422:THR:HG23	23:b:425:GLY:H	1.73	0.52
33:n:257:ILE:O	33:n:323:VAL:N	2.43	0.52
8:G:120:ASP:N	8:G:120:ASP:OD1	2.43	0.51
14:S:76:GLN:HE22	14:S:81:ASP:H	1.58	0.51
22:a:1888:LEU:HD11	22:a:1911:VAL:HG21	1.92	0.51
24:d:678:LEU:HD11	24:d:686:TYR:CD1	2.45	0.51
27:g:435:LEU:HD11	27:g:467:MET:HB2	1.92	0.51
31:k:456:ILE:HG21	31:k:461:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:q:239:ARG:NH1	36:q:242:GLN:OE1	2.33	0.51
2:A:34:MET:HE2	3:B:1124:ILE:HG21	1.92	0.51
22:a:2088:LEU:HA	22:a:2091:LEU:HB2	1.91	0.51
26:f:29:LYS:O	26:f:33:GLU:HG2	2.09	0.51
27:g:699:THR:HG21	27:g:794:TYR:HB3	1.93	0.51
31:k:181:MET:HE3	31:k:401:LEU:HB2	1.92	0.51
2:A:1344:MET:CE	6:E:134:GLU:HA	2.41	0.51
3:B:748:ALA:HB3	3:B:811:TYR:HB2	1.93	0.51
25:e:449:LEU:O	25:e:469:ARG:NH1	2.43	0.51
35:p:538:PHE:HB3	35:p:575:VAL:HG22	1.93	0.51
3:B:1157:LEU:O	3:B:1161:GLU:HG3	2.09	0.51
24:d:161:ASP:O	24:d:167:ARG:NH1	2.39	0.51
23:b:262:LEU:HD22	23:b:265:ARG:HH21	1.75	0.51
2:A:272:ASN:OD1	20:T:161:DG:H1'	2.10	0.51
22:a:2151:CYS:O	22:a:2153:GLU:N	2.43	0.51
28:h:506:SER:HA	28:h:509:ILE:HD12	1.92	0.51
3:B:258:ALA:HB2	3:B:269:ILE:HD13	1.93	0.51
8:G:92:VAL:HG13	8:G:97:LEU:HA	1.93	0.51
22:a:1643:SER:OG	22:a:1644:ARG:N	2.44	0.51
24:d:399:CYS:HB2	24:d:434:THR:HG22	1.92	0.51
35:p:177:ASP:OD1	35:p:177:ASP:N	2.41	0.51
2:A:1453:GLY:O	2:A:1457:ASN:ND2	2.43	0.51
3:B:1119:CYS:HB2	3:B:1137:CYS:SG	2.50	0.51
4:C:183:ALA:HB3	4:C:232:ASN:HB3	1.91	0.51
7:F:79:VAL:HG21	7:F:83:LEU:HD11	1.92	0.51
15:N:16:DA:H2'	15:N:17:DT:H71	1.93	0.51
2:A:1307:VAL:HG13	2:A:1338:THR:HG22	1.93	0.51
21:Z:602:VAL:HG22	21:Z:643:LEU:HD12	1.92	0.51
27:g:555:SER:N	37:r:2057:GLU:OE2	2.44	0.51
8:G:37:THR:OG1	8:G:43:GLY:O	2.26	0.51
9:H:8:ASP:OD1	9:H:9:ILE:N	2.44	0.51
23:b:600:ILE:HA	23:b:603:ILE:HD12	1.92	0.51
24:d:95:LEU:HA	24:d:98:LEU:HD12	1.92	0.51
27:g:520:VAL:HG12	27:g:522:ASN:H	1.76	0.51
2:A:244:ARG:HB2	2:A:247:TRP:CE2	2.46	0.50
3:B:733:MET:HE1	3:B:1054:MET:HE3	1.94	0.50
18:Q:92:GLU:OE1	18:Q:95:LYS:NZ	2.34	0.50
19:R:83:ARG:NH2	20:T:40:DA:OP2	2.44	0.50
24:d:649:LEU:HD11	27:g:245:SER:HA	1.93	0.50
35:p:328:PRO:HA	35:p:331:LYS:HD3	1.92	0.50
2:A:118:LEU:HD23	2:A:148:CYS:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:225:LEU:HD22	3:B:353:VAL:HG21	1.93	0.50
3:B:225:LEU:HB3	3:B:349:PRO:HB2	1.92	0.50
18:Q:65:LEU:HG	18:Q:86:ALA:HB1	1.91	0.50
22:a:475:LYS:HA	22:a:515:PHE:HA	1.92	0.50
22:a:1897:GLN:O	22:a:1901:GLN:HG2	2.11	0.50
23:b:462:GLU:OE2	23:b:464:ALA:N	2.42	0.50
27:g:232:ILE:HG23	27:g:271:LEU:HD22	1.91	0.50
28:h:718:TRP:HE1	28:h:803:ILE:HG22	1.75	0.50
3:B:64:PRO:HB2	3:B:85:LEU:HD11	1.93	0.50
6:E:196:PRO:HA	6:E:202:ARG:HA	1.94	0.50
28:h:512:LEU:HD22	28:h:528:ILE:HG23	1.92	0.50
28:h:813:ALA:O	28:h:817:THR:OG1	2.25	0.50
40:w:219:ASN:O	40:w:223:ASN:N	2.42	0.50
40:w:531:ARG:NH2	40:w:561:SER:O	2.44	0.50
17:P:-11:C:O2'	17:P:-10:U:O2	2.20	0.50
24:d:678:LEU:HD21	24:d:686:TYR:HE1	1.76	0.50
2:A:904:GLN:NE2	2:A:981:CYS:O	2.44	0.50
14:M:55:GLN:NE2	18:V:107:VAL:O	2.45	0.50
22:a:1810:ARG:NH2	22:a:1812:GLU:OE1	2.41	0.50
29:i:141:VAL:O	29:i:145:GLU:HG3	2.12	0.50
35:p:463:THR:HG22	35:p:507:VAL:HG11	1.94	0.50
18:Q:51:LEU:HD21	19:R:70:ILE:HG21	1.94	0.50
24:d:917:TYR:HE2	24:d:946:ILE:HG23	1.77	0.50
35:p:158:VAL:O	35:p:163:LYS:NZ	2.41	0.50
2:A:734:ARG:NH2	10:I:107:ALA:O	2.45	0.50
2:A:1030:SER:OG	6:E:162:ARG:NE	2.45	0.50
9:H:20:LYS:NZ	9:H:22:PHE:O	2.40	0.50
24:d:616:GLN:HA	24:d:619:GLU:HG2	1.92	0.50
27:g:395:VAL:HG22	27:g:437:GLN:NE2	2.26	0.50
29:i:519:MET:SD	29:i:519:MET:N	2.79	0.50
14:M:63:ARG:HG2	15:N:95:DA:H4'	1.93	0.50
22:a:1402:THR:HA	22:a:1405:VAL:HG12	1.94	0.50
24:d:134:LEU:HD13	24:d:137:ILE:HD12	1.94	0.50
26:f:24:TYR:OH	26:f:175:LEU:O	2.28	0.50
27:g:119:ARG:NH1	27:g:154:GLU:OE1	2.44	0.50
28:h:718:TRP:HB2	28:h:799:TRP:HE3	1.77	0.50
2:A:1150:ASP:HB3	2:A:1153:ARG:HG2	1.93	0.50
22:a:1023:LEU:HD23	22:a:1065:ALA:HB2	1.94	0.50
22:a:1208:THR:OG1	22:a:1210:GLU:OE1	2.28	0.50
22:a:2096:GLU:OE2	22:a:2097:GLU:N	2.44	0.50
18:Q:41:GLU:OE2	18:V:41:GLU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:84:ILE:HG23	23:b:184:LEU:HD21	1.94	0.49
25:e:523:LEU:O	25:e:577:ASN:ND2	2.43	0.49
27:g:299:ALA:HB2	27:g:311:MET:HG3	1.93	0.49
15:N:98:DG:N1	20:T:54:DG:O6	2.45	0.49
23:b:865:GLN:HG3	25:e:733:ARG:NH2	2.27	0.49
24:d:775:SER:HB2	24:d:809:LEU:HD11	1.95	0.49
27:g:273:ILE:HD11	27:g:311:MET:HE2	1.94	0.49
27:g:400:ASP:N	27:g:400:ASP:OD1	2.43	0.49
36:q:29:LYS:O	36:q:33:GLU:HG3	2.11	0.49
28:h:895:THR:HG21	28:h:925:MET:HA	1.93	0.49
29:i:420:VAL:HB	29:i:441:MET:HE2	1.94	0.49
36:q:229:ASN:ND2	36:q:255:ASN:OD1	2.46	0.49
8:G:46:ILE:HB	8:G:75:ILE:HB	1.95	0.49
26:f:309:PHE:HB3	26:f:350:VAL:HG12	1.94	0.49
26:f:428:LYS:HE3	26:f:432:ARG:HH12	1.76	0.49
27:g:127:GLY:O	27:g:164:ASN:ND2	2.42	0.49
2:A:1408:ARG:HH22	6:E:172:ARG:HH21	1.59	0.49
3:B:195:ILE:O	3:B:197:GLN:NE2	2.44	0.49
6:E:71:GLN:HB2	6:E:99:ILE:HD12	1.92	0.49
8:G:54:ILE:HG23	8:G:70:VAL:HG22	1.95	0.49
12:K:80:ASP:OD1	12:K:81:TYR:N	2.45	0.49
23:b:462:GLU:OE2	23:b:463:GLU:N	2.46	0.49
24:d:621:VAL:HG11	24:d:664:LEU:HD11	1.93	0.49
3:B:577:HIS:CG	3:B:583:LEU:HD12	2.47	0.49
14:S:119:ILE:HD13	16:U:43:VAL:HG13	1.94	0.49
22:a:1840:HIS:O	22:a:1844:THR:HG23	2.13	0.49
24:d:273:SER:OG	24:d:275:GLU:OE1	2.30	0.49
2:A:358:ARG:HA	3:B:1085:ARG:HA	1.94	0.49
2:A:1118:THR:OG1	2:A:1136:THR:OG1	2.31	0.49
4:C:148:ILE:HD13	11:J:16:ASN:HB3	1.94	0.49
4:C:260:GLN:HB2	12:K:91:ILE:HG21	1.95	0.49
22:a:1626:ASP:OD2	22:a:1637:GLN:NE2	2.46	0.49
24:d:501:ASP:N	24:d:501:ASP:OD1	2.41	0.49
24:d:900:HIS:HD2	24:d:903:TRP:HE1	1.61	0.49
25:e:491:LEU:HD21	25:e:534:LEU:HD11	1.95	0.49
29:i:238:SER:OG	29:i:239:GLY:N	2.45	0.49
31:k:87:ASP:N	31:k:87:ASP:OD1	2.44	0.49
35:p:479:HIS:HA	35:p:483:ILE:HD12	1.94	0.49
3:B:912:ASN:ND2	3:B:914:GLU:OE2	2.45	0.49
18:V:33:LEU:HD11	19:W:67:PHE:CE2	2.47	0.49
26:f:185:GLN:O	26:f:214:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:g:839:SER:OG	27:g:840:LYS:N	2.46	0.49
29:i:326:LEU:HD13	29:i:392:VAL:HB	1.94	0.49
30:j:638:LEU:HA	30:j:643:GLY:HA3	1.94	0.49
31:k:514:ARG:HG2	31:k:573:LEU:HG	1.94	0.49
38:u:143:TYR:OH	40:w:335:ASP:OD1	2.26	0.49
16:U:38:ALA:HB1	16:U:43:VAL:HB	1.95	0.49
25:e:126:GLN:HE22	25:e:192:ILE:HB	1.78	0.49
25:e:985:LEU:O	25:e:989:HIS:ND1	2.45	0.49
26:f:33:GLU:HB2	36:q:211:ILE:HD11	1.94	0.49
27:g:800:GLN:HE22	27:g:845:ARG:H	1.59	0.49
28:h:119:SER:HB3	28:h:139:THR:HG22	1.95	0.49
28:h:933:TRP:HA	28:h:966:LEU:HD11	1.94	0.49
29:i:241:SER:OG	29:i:450:THR:O	2.24	0.49
22:a:1630:VAL:HG12	22:a:1637:GLN:HB3	1.94	0.49
25:e:35:ILE:O	25:e:39:LEU:HB2	2.13	0.49
28:h:671:ARG:NH1	28:h:766:GLU:OE2	2.46	0.49
35:p:394:VAL:HG23	35:p:395:ILE:HG12	1.94	0.49
2:A:299:ALA:HB3	2:A:302:VAL:HG12	1.95	0.48
10:I:83:ASP:N	10:I:83:ASP:OD1	2.46	0.48
14:S:62:ILE:H	14:S:93:GLN:HE22	1.58	0.48
23:b:298:LEU:O	23:b:302:VAL:HG12	2.13	0.48
24:d:399:CYS:SG	24:d:403:GLN:NE2	2.86	0.48
24:d:499:ASP:O	24:d:502:SER:OG	2.22	0.48
35:p:106:ASP:N	35:p:106:ASP:OD1	2.35	0.48
35:p:271:GLN:HG2	35:p:279:THR:HG21	1.95	0.48
2:A:1288:ILE:O	2:A:1292:MET:HG3	2.13	0.48
16:O:72:TYR:HE2	16:O:92:ARG:HD3	1.78	0.48
23:b:18:VAL:HG11	23:b:216:ALA:HB2	1.95	0.48
25:e:227:VAL:HA	25:e:230:ILE:HG22	1.94	0.48
28:h:597:LEU:O	28:h:601:THR:OG1	2.29	0.48
40:w:531:ARG:NE	40:w:565:THR:OG1	2.45	0.48
9:H:88:PHE:CD2	9:H:144:LEU:HB3	2.45	0.48
13:L:56:ASP:OD1	21:Z:738:SER:OG	2.23	0.48
22:a:1856:GLU:OE1	22:a:1903:ASN:ND2	2.47	0.48
2:A:139:LYS:HE3	2:A:143:HIS:CE1	2.48	0.48
14:M:69:ARG:NH2	16:O:25:ASN:OD1	2.46	0.48
14:S:56:LYS:HZ3	20:T:9:DC:H2'	1.78	0.48
21:Z:465:ALA:HA	21:Z:468:LEU:HD12	1.95	0.48
27:g:149:SER:OG	27:g:150:HIS:N	2.45	0.48
35:p:373:LEU:HG	35:p:384:ILE:HG21	1.94	0.48
35:p:429:LEU:HD23	35:p:430:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:827:TYR:OH	2:A:839:HIS:NE2	2.36	0.48
4:C:7:PRO:HB2	12:K:101:LEU:HD13	1.93	0.48
8:G:106:CYS:SG	8:G:107:PHE:N	2.87	0.48
22:a:746:ALA:HB2	22:a:863:GLY:HA2	1.95	0.48
22:a:1776:VAL:O	22:a:1780:THR:OG1	2.28	0.48
23:b:84:ILE:HA	23:b:87:LEU:HD12	1.96	0.48
27:g:239:THR:OG1	27:g:275:ASP:OD2	2.28	0.48
28:h:606:LYS:NZ	28:h:652:ASP:O	2.40	0.48
38:u:6:GLU:OE1	38:u:9:THR:OG1	2.30	0.48
14:S:101:VAL:HG22	16:U:40:ARG:HG3	1.95	0.48
24:d:243:ASP:HA	31:k:194:LYS:NZ	2.28	0.48
25:e:615:LEU:HD21	25:e:650:ALA:HA	1.95	0.48
27:g:675:MET:CE	27:g:679:ARG:HH22	2.26	0.48
31:k:287:ASN:OD1	31:k:288:GLN:N	2.46	0.48
35:p:516:ILE:O	35:p:520:HIS:ND1	2.46	0.48
3:B:794:VAL:HG12	3:B:967:ILE:HG22	1.95	0.48
18:Q:16:SER:O	18:Q:19:SER:OG	2.31	0.48
26:f:25:LEU:HD22	26:f:82:ALA:HB2	1.95	0.48
27:g:827:LEU:HD23	27:g:894:LEU:HD12	1.95	0.48
29:i:239:GLY:HA3	29:i:451:ARG:HE	1.78	0.48
37:r:2048:ASP:N	37:r:2048:ASP:OD1	2.44	0.48
16:U:69:ALA:HB1	16:U:81:VAL:HG11	1.94	0.48
22:a:1526:ALA:O	22:a:1530:SER:OG	2.28	0.48
25:e:833:PRO:HA	25:e:951:ARG:HD2	1.96	0.48
27:g:133:ILE:HG13	27:g:136:ARG:HB2	1.95	0.48
3:B:114:ARG:NH2	3:B:176:GLU:OE2	2.46	0.48
23:b:758:GLN:O	23:b:758:GLN:NE2	2.47	0.48
25:e:531:GLU:HA	25:e:534:LEU:HD13	1.95	0.48
29:i:127:GLU:HA	29:i:196:LEU:HD22	1.96	0.48
35:p:160:SER:HA	35:p:163:LYS:HB2	1.95	0.48
35:p:240:LEU:HA	35:p:243:LEU:HB2	1.96	0.48
15:N:31:DC:H2"	15:N:32:DT:C5	2.49	0.48
21:Z:608:SER:OG	21:Z:609:GLY:N	2.47	0.48
22:a:1079:GLN:OE1	22:a:1130:ARG:NE	2.44	0.48
22:a:2108:LEU:HD11	22:a:2143:ASN:HB3	1.96	0.48
23:b:150:MET:HA	23:b:153:VAL:HG22	1.95	0.48
24:d:392:ILE:HG13	24:d:427:VAL:HG22	1.96	0.48
28:h:711:ARG:O	28:h:715:LYS:HG2	2.14	0.48
2:A:1455:SER:O	2:A:1459:MET:HG3	2.14	0.47
3:B:1142:ASN:HD21	3:B:1145:GLN:HB2	1.79	0.47
23:b:833:VAL:HG11	23:b:853:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:w:431:VAL:HG11	40:w:455:LEU:HD11	1.96	0.47
4:C:154:ARG:HD3	11:J:64:PRO:HD3	1.95	0.47
10:I:14:ILE:HG13	10:I:15:ARG:H	1.79	0.47
14:M:119:ILE:HD12	16:O:46:ILE:HD12	1.96	0.47
23:b:868:HIS:O	23:b:869:ARG:NH1	2.37	0.47
27:g:207:ASP:OD1	27:g:208:ALA:N	2.47	0.47
27:g:282:LYS:HG2	27:g:283:THR:HG23	1.96	0.47
27:g:373:SER:OG	27:g:374:CYS:N	2.47	0.47
35:p:360:ASN:OD1	35:p:364:HIS:ND1	2.47	0.47
40:w:145:TRP:CD1	40:w:146:LEU:HG	2.48	0.47
40:w:442:GLN:NE2	40:w:483:GLN:O	2.47	0.47
2:A:1178:ASP:O	2:A:1260:ARG:NH1	2.37	0.47
15:N:85:DC:H3'	16:O:35:ARG:HH12	1.78	0.47
16:U:26:ILE:HG13	16:U:55:ARG:HD3	1.96	0.47
22:a:1149:GLN:HG3	22:a:1206:VAL:HG11	1.95	0.47
22:a:1842:PHE:CZ	22:a:2187:GLU:HA	2.48	0.47
24:d:687:LEU:HD12	27:g:704:GLU:HG3	1.96	0.47
29:i:285:LEU:HB2	29:i:295:VAL:HG21	1.97	0.47
35:p:487:LEU:O	35:p:490:SER:OG	2.29	0.47
38:u:58:LEU:HD13	40:w:235:GLU:HB2	1.95	0.47
18:Q:115:LEU:HB3	16:U:44:LYS:HZ2	1.78	0.47
24:d:61:ARG:NH2	29:i:87:GLU:OE1	2.48	0.47
24:d:437:LYS:O	24:d:440:ASN:ND2	2.47	0.47
27:g:675:MET:HE3	27:g:679:ARG:HH22	1.79	0.47
29:i:635:ILE:N	31:k:510:ARG:O	2.43	0.47
31:k:17:ARG:NH1	31:k:43:ARG:O	2.46	0.47
40:w:497:LEU:HA	40:w:500:MET:HG2	1.97	0.47
7:F:57:MET:HB2	7:F:123:LEU:HB3	1.97	0.47
13:L:17:TYR:HB3	13:L:44:MET:HB3	1.97	0.47
16:O:73:THR:HG21	16:O:81:VAL:HA	1.97	0.47
22:a:1428:SER:HB2	22:a:1431:LEU:HD12	1.96	0.47
24:d:229:LEU:O	24:d:263:TYR:OH	2.33	0.47
25:e:447:GLN:HE22	28:h:514:HIS:HB2	1.79	0.47
29:i:462:LYS:HA	29:i:465:GLN:OE1	2.13	0.47
20:T:37:DT:H2''	20:T:38:DA:C8	2.48	0.47
23:b:669:LEU:HD11	23:b:676:PRO:HD3	1.97	0.47
23:b:725:ASP:N	23:b:725:ASP:OD1	2.47	0.47
29:i:216:SER:OG	29:i:239:GLY:O	2.33	0.47
35:p:489:MET:SD	35:p:501:THR:OG1	2.63	0.47
36:q:31:LEU:HD11	36:q:102:ALA:HA	1.97	0.47
2:A:450:MET:SD	2:A:474:VAL:HG21	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:73:GLU:OE1	16:O:25:ASN:ND2	2.40	0.47
20:T:148:DC:H2'	20:T:149:DG:C8	2.50	0.47
22:a:2069:ASP:O	22:a:2073:MET:HG3	2.15	0.47
25:e:632:CYS:O	25:e:676:ARG:NH2	2.42	0.47
28:h:916:LEU:HD22	28:h:941:LEU:HD21	1.96	0.47
29:i:352:GLN:HA	29:i:355:VAL:HG22	1.96	0.47
31:k:176:THR:O	31:k:176:THR:OG1	2.30	0.47
31:k:501:GLU:O	31:k:505:ALA:N	2.47	0.47
35:p:43:GLY:HA3	35:p:46:ARG:HH21	1.80	0.47
40:w:562:ILE:O	40:w:565:THR:OG1	2.33	0.47
2:A:460:ARG:HB2	2:A:501:MET:HE2	1.97	0.47
9:H:16:ASP:OD1	9:H:27:ARG:N	2.46	0.47
12:K:111:ASP:O	12:K:115:GLY:N	2.48	0.47
26:f:129:THR:OG1	26:f:130:ASP:N	2.47	0.47
2:A:628:VAL:HA	2:A:638:GLY:HA3	1.96	0.47
2:A:788:VAL:HG21	2:A:831:LEU:HD11	1.96	0.47
6:E:110:MET:HE1	6:E:118:LEU:HD12	1.97	0.47
14:M:61:LEU:HD13	16:O:36:ARG:HD2	1.96	0.47
14:S:76:GLN:HA	14:S:80:THR:HA	1.96	0.47
23:b:259:SER:HB3	27:g:591:ALA:HB1	1.97	0.47
23:b:1186:CYS:O	23:b:1190:GLU:HG3	2.15	0.47
38:u:126:GLU:OE1	38:u:126:GLU:N	2.43	0.47
3:B:677:MET:HB3	3:B:678:THR:HG22	1.97	0.47
10:I:109:ARG:HE	10:I:124:THR:HG21	1.80	0.47
24:d:474:THR:O	24:d:513:ARG:NH2	2.35	0.47
25:e:637:GLU:OE1	25:e:638:ALA:N	2.48	0.47
26:f:32:VAL:HG12	26:f:36:MET:HE2	1.97	0.47
28:h:650:LEU:HD12	28:h:650:LEU:HA	1.79	0.47
3:B:1112:ASP:OD1	3:B:1112:ASP:N	2.47	0.46
8:G:96:GLY:N	21:Z:510:GLU:OE1	2.48	0.46
14:M:83:ARG:NH2	15:N:104:DA:O4'	2.48	0.46
15:N:44:DA:H5'	19:W:85:THR:HG22	1.97	0.46
19:W:36:ILE:HG13	19:W:40:LYS:HE3	1.97	0.46
22:a:1171:VAL:HG11	22:a:1219:LEU:HD21	1.96	0.46
27:g:299:ALA:HB3	27:g:347:LEU:HD21	1.98	0.46
3:B:59:VAL:HG21	3:B:91:ILE:HD13	1.97	0.46
3:B:595:ASP:OD1	3:B:595:ASP:N	2.47	0.46
4:C:76:ASP:N	4:C:76:ASP:OD1	2.48	0.46
7:F:56:TYR:HD1	7:F:124:ILE:HB	1.80	0.46
9:H:28:LEU:N	9:H:41:LEU:O	2.47	0.46
24:d:293:ASP:O	24:d:299:ARG:NH1	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:g:104:VAL:HG21	27:g:133:ILE:HG21	1.97	0.46
27:g:550:LEU:HB3	27:g:559:TYR:HE1	1.80	0.46
30:j:519:LEU:O	30:j:523:MET:N	2.48	0.46
35:p:501:THR:HG21	35:p:528:MET:HE1	1.96	0.46
36:q:239:ARG:NH2	36:q:241:HIS:HB3	2.30	0.46
3:B:193:VAL:HG21	3:B:470:LEU:HD13	1.98	0.46
3:B:754:PRO:HB2	3:B:773:PRO:HG2	1.97	0.46
15:N:14:DA:H2''	15:N:15:DT:H5'	1.97	0.46
22:a:1790:TRP:CE2	22:a:1795:LEU:HD22	2.50	0.46
22:a:1924:ARG:O	22:a:1928:GLN:N	2.41	0.46
22:a:2184:LEU:HA	22:a:2187:GLU:HB2	1.97	0.46
23:b:351:LEU:HD23	23:b:352:PRO:HD2	1.97	0.46
24:d:447:ASP:N	24:d:447:ASP:OD1	2.45	0.46
24:d:735:ILE:HD12	24:d:800:GLN:HB2	1.97	0.46
26:f:220:LEU:O	26:f:224:VAL:HG23	2.15	0.46
27:g:472:MET:HE3	27:g:508:GLU:HB3	1.96	0.46
27:g:819:ILE:O	27:g:929:LYS:N	2.42	0.46
2:A:1358:THR:OG1	2:A:1359:SER:N	2.47	0.46
3:B:449:ALA:HB1	20:T:158:DC:H5''	1.97	0.46
6:E:73:PHE:O	6:E:103:LEU:N	2.45	0.46
11:J:66:GLU:N	11:J:66:GLU:OE1	2.49	0.46
14:M:100:LEU:HD11	16:O:37:LEU:HD13	1.97	0.46
23:b:599:TYR:CZ	23:b:603:ILE:HD11	2.50	0.46
24:d:241:LEU:HD23	24:d:241:LEU:HA	1.75	0.46
27:g:535:ARG:HD2	37:r:2041:TRP:CZ2	2.50	0.46
29:i:633:THR:N	31:k:508:GLN:O	2.49	0.46
8:G:21:ASN:OD1	8:G:21:ASN:N	2.46	0.46
15:N:65:DA:H2'	16:U:32:PRO:HG2	1.98	0.46
23:b:1190:GLU:O	23:b:1194:ILE:HD12	2.14	0.46
24:d:307:GLY:O	24:d:400:MET:HG3	2.16	0.46
28:h:512:LEU:HD13	28:h:532:LEU:HG	1.98	0.46
29:i:364:HIS:HA	29:i:367:LEU:HB2	1.98	0.46
31:k:16:GLY:HA2	31:k:72:ASP:HB2	1.97	0.46
35:p:144:ARG:HH21	35:p:178:THR:HG21	1.80	0.46
2:A:467:MET:SD	2:A:467:MET:N	2.88	0.46
3:B:1029:TYR:HA	3:B:1036:LYS:HA	1.98	0.46
22:a:2059:THR:OG1	22:a:2062:ASP:OD2	2.25	0.46
23:b:263:LYS:O	23:b:267:MET:HG3	2.15	0.46
28:h:458:MET:HE3	28:h:458:MET:HB2	1.82	0.46
35:p:386:SER:O	35:p:426:TYR:OH	2.30	0.46
2:A:557:ARG:O	2:A:561:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:87:THR:OG1	19:R:90:GLU:OE1	2.25	0.46
25:e:500:HIS:HB3	28:h:495:VAL:HG21	1.98	0.46
29:i:113:ILE:O	29:i:117:THR:OG1	2.27	0.46
31:k:566:ASP:OD2	31:k:569:THR:OG1	2.32	0.46
2:A:364:ARG:NH1	2:A:502:ASN:OD1	2.45	0.46
9:H:96:VAL:HB	9:H:116:VAL:HG22	1.96	0.46
11:J:65:LEU:HD12	11:J:65:LEU:HA	1.82	0.46
31:k:550:SER:OG	31:k:551:VAL:N	2.47	0.46
35:p:113:ARG:HG2	35:p:153:VAL:HG21	1.97	0.46
3:B:187:ILE:HG13	3:B:448:LEU:HB3	1.98	0.46
4:C:103:LEU:HB3	4:C:161:LEU:HG	1.98	0.46
20:T:35:DC:H2"	20:T:36:DG:N7	2.31	0.46
35:p:455:VAL:HG12	35:p:457:ALA:H	1.81	0.46
35:p:531:ASP:O	35:p:537:ARG:NH1	2.45	0.46
40:w:476:LEU:HA	40:w:476:LEU:HD23	1.84	0.46
2:A:98:GLY:HA3	2:A:1440:MET:CE	2.45	0.46
22:a:1422:VAL:HB	22:a:1463:MET:HE1	1.98	0.46
22:a:1915:LEU:HA	22:a:1918:LEU:HD12	1.96	0.46
23:b:710:LEU:HD23	23:b:710:LEU:HA	1.80	0.46
23:b:1066:ILE:HD11	23:b:1112:ARG:HD3	1.98	0.46
31:k:512:THR:HA	31:k:575:SER:HA	1.98	0.46
35:p:106:ASP:HA	35:p:109:VAL:HG12	1.97	0.46
36:q:94:VAL:O	36:q:98:THR:OG1	2.28	0.46
2:A:479:TRP:H	2:A:483:ARG:HH22	1.64	0.45
2:A:1157:ILE:O	2:A:1161:LEU:HB2	2.16	0.45
3:B:298:MET:HE3	3:B:298:MET:HB3	1.65	0.45
14:S:67:PHE:O	14:S:71:VAL:HG22	2.16	0.45
22:a:1154:TRP:HA	22:a:1201:PRO:HB3	1.98	0.45
27:g:239:THR:HG21	27:g:275:ASP:HB2	1.98	0.45
27:g:745:GLU:O	27:g:749:MET:HG2	2.16	0.45
27:g:824:ASN:N	27:g:824:ASN:OD1	2.47	0.45
31:k:66:ILE:HB	31:k:92:MET:HB3	1.98	0.45
22:a:1891:ARG:NH2	22:a:1907:CYS:SG	2.90	0.45
31:k:175:TYR:CZ	31:k:177:GLY:HA2	2.51	0.45
2:A:1026:ASP:O	2:A:1031:ARG:NH2	2.49	0.45
2:A:1141:VAL:HB	2:A:1336:LEU:HB2	1.98	0.45
3:B:331:THR:OG1	3:B:333:GLU:OE2	2.32	0.45
16:U:58:LEU:HD23	16:U:58:LEU:HA	1.83	0.45
22:a:1549:ILE:HG22	22:a:1556:LEU:HD21	1.98	0.45
23:b:1046:ILE:HD12	23:b:1083:VAL:HG11	1.99	0.45
25:e:219:HIS:HB2	25:e:223:PHE:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:u:35:ALA:O	38:u:39:ASP:HB2	2.16	0.45
2:A:674:THR:O	2:A:678:ASN:ND2	2.45	0.45
2:A:1231:ILE:HD12	2:A:1231:ILE:H	1.80	0.45
20:T:138:DA:H1'	20:T:139:DC:H5'	1.98	0.45
22:a:1365:PHE:HE2	22:a:1409:LEU:HB3	1.81	0.45
22:a:2152:GLN:NE2	22:a:2187:GLU:OE2	2.49	0.45
26:f:186:LEU:HA	26:f:214:ARG:HH12	1.80	0.45
36:q:25:GLU:OE1	36:q:25:GLU:N	2.45	0.45
40:w:299:MET:HE1	40:w:305:LEU:HA	1.99	0.45
7:F:71:LEU:O	7:F:75:MET:HE3	2.17	0.45
16:O:71:THR:HG23	19:R:96:ARG:HD3	1.99	0.45
16:U:75:HIS:HD1	19:W:89:ARG:HG2	1.81	0.45
23:b:549:THR:OG1	23:b:550:GLY:N	2.45	0.45
24:d:243:ASP:HA	31:k:194:LYS:HZ3	1.80	0.45
24:d:641:ARG:HH22	27:g:283:THR:HG22	1.81	0.45
25:e:496:PHE:O	25:e:500:HIS:HB2	2.15	0.45
26:f:390:LEU:O	26:f:394:ASP:HB2	2.16	0.45
31:k:512:THR:HG21	31:k:573:LEU:HD23	1.98	0.45
2:A:539:GLN:HA	2:A:774:ALA:HB1	1.99	0.45
2:A:1173:THR:HG23	10:I:56:ASN:HB3	1.98	0.45
8:G:6:SER:HA	8:G:73:LYS:HA	1.97	0.45
14:S:56:LYS:HE3	20:T:9:DC:P	2.56	0.45
21:Z:593:ASN:ND2	31:k:335:GLN:HA	2.31	0.45
24:d:149:MET:H	24:d:149:MET:HG2	1.50	0.45
24:d:491:LYS:O	24:d:494:THR:OG1	2.26	0.45
24:d:621:VAL:HA	24:d:635:LEU:HD21	1.99	0.45
24:d:856:ASP:O	24:d:860:THR:OG1	2.23	0.45
25:e:344:LEU:O	25:e:348:SER:N	2.43	0.45
29:i:160:ASP:HA	29:i:163:ARG:HG2	1.99	0.45
3:B:330:VAL:H	3:B:334:LYS:NZ	2.15	0.45
9:H:116:VAL:HB	9:H:123:MET:HE2	1.98	0.45
18:Q:14:ALA:HA	20:T:31:DT:H5'	1.99	0.45
22:a:1059:ASP:HB3	22:a:1062:THR:HG23	1.99	0.45
23:b:711:LEU:HD12	23:b:711:LEU:HA	1.78	0.45
28:h:841:ASP:OD1	28:h:856:TYR:OH	2.24	0.45
29:i:6:LEU:HG	29:i:87:GLU:O	2.16	0.45
35:p:251:ALA:HA	35:p:254:ASP:HB2	1.99	0.45
3:B:393:LEU:HD12	3:B:532:ILE:HG12	1.98	0.45
3:B:1127:ILE:HB	3:B:1136:GLU:HG3	1.98	0.45
10:I:14:ILE:C	10:I:15:ARG:HD3	2.42	0.45
14:M:126:LEU:HD11	14:S:110:CYS:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1628:GLU:HB2	22:a:1631:SER:HB3	1.99	0.45
22:a:1878:LEU:HD11	22:a:1922:VAL:HA	1.98	0.45
22:a:2171:MET:HE3	22:a:2171:MET:HB3	1.93	0.45
26:f:121:GLU:N	26:f:165:ASP:OD2	2.41	0.45
27:g:369:ASN:OD1	27:g:418:LYS:NZ	2.31	0.45
2:A:364:ARG:HB2	3:B:1084:LEU:HD11	1.99	0.45
2:A:463:THR:OG1	3:B:1090:GLU:OE2	2.29	0.45
2:A:470:MET:HE3	2:A:521:VAL:HG22	1.99	0.45
2:A:921:ARG:HG3	2:A:956:PHE:CG	2.52	0.45
16:U:44:LYS:HE3	16:U:44:LYS:HB2	1.77	0.45
22:a:1686:GLU:OE2	22:a:1688:ARG:NH2	2.50	0.45
23:b:1111:CYS:HB3	23:b:1199:MET:HE1	1.99	0.45
25:e:410:LEU:O	25:e:413:THR:OG1	2.31	0.45
26:f:129:THR:HG23	26:f:172:VAL:HG12	1.99	0.45
26:f:484:ILE:HG21	26:f:529:VAL:HG22	1.99	0.45
28:h:769:VAL:O	28:h:773:ILE:HG13	2.16	0.45
2:A:367:ILE:HG22	2:A:482:PHE:HB2	1.99	0.45
2:A:1474:LEU:O	7:F:105:ILE:N	2.42	0.45
4:C:86:ARG:NH2	4:C:172:GLU:OE2	2.39	0.45
16:O:75:HIS:ND1	19:R:77:LEU:HB3	2.32	0.45
16:U:55:ARG:O	16:U:59:LYS:HG2	2.16	0.45
22:a:1220:LYS:O	22:a:1224:ILE:HG22	2.16	0.45
22:a:1380:GLN:HG2	27:g:395:VAL:HG21	1.99	0.45
22:a:1744:GLU:HG3	22:a:1795:LEU:HD12	1.98	0.45
2:A:379:GLY:HA3	2:A:483:ARG:HB2	1.99	0.44
8:G:81:LYS:HG3	8:G:148:VAL:HG13	1.99	0.44
20:T:147:DT:H2'	20:T:148:DC:C6	2.52	0.44
24:d:134:LEU:HD12	24:d:151:LEU:HD21	1.99	0.44
27:g:391:GLU:O	27:g:395:VAL:HG23	2.17	0.44
28:h:386:ALA:O	28:h:390:VAL:HG23	2.16	0.44
29:i:281:PHE:HD1	29:i:421:ILE:HG21	1.83	0.44
3:B:907:VAL:HG13	3:B:921:ILE:HG12	2.00	0.44
14:M:116:ARG:HH21	20:T:70:DG:H3'	1.81	0.44
15:N:7:DT:H2''	15:N:8:DC:H5'	1.98	0.44
20:T:31:DT:H2''	20:T:32:DG:H8	1.82	0.44
23:b:1101:MET:HE3	23:b:1101:MET:HB3	1.80	0.44
24:d:950:LYS:HD3	24:d:951:PRO:HD2	1.99	0.44
27:g:193:LEU:O	27:g:197:LEU:HB2	2.17	0.44
29:i:18:LYS:HE2	29:i:18:LYS:HB3	1.74	0.44
31:k:558:LEU:HG	31:k:574:VAL:HG22	1.99	0.44
9:H:6:PHE:HB3	9:H:60:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:72:ARG:NH2	14:S:73:GLU:OE2	2.46	0.44
20:T:97:DA:H2''	20:T:98:DG:N7	2.33	0.44
22:a:1738:LEU:HD12	22:a:1738:LEU:HA	1.85	0.44
23:b:726:ASP:OD1	23:b:726:ASP:N	2.47	0.44
25:e:989:HIS:HA	25:e:992:LEU:HD12	1.99	0.44
31:k:5:ARG:HD2	32:m:675:ARG:HD3	2.00	0.44
35:p:12:PRO:O	35:p:16:LEU:HB2	2.17	0.44
2:A:225:PHE:HB3	2:A:245:PRO:HB2	1.99	0.44
6:E:17:ILE:HG21	6:E:74:VAL:HG11	1.98	0.44
9:H:7:GLU:OE1	9:H:8:ASP:N	2.50	0.44
15:N:65:DA:H3'	16:U:32:PRO:HD2	2.00	0.44
18:Q:18:SER:HB3	18:Q:23:LEU:HB2	2.00	0.44
14:S:48:LEU:HB2	16:U:44:LYS:HZ3	1.82	0.44
14:S:61:LEU:HD11	16:U:36:ARG:HE	1.81	0.44
22:a:1071:SER:HB2	22:a:1123:ILE:HD11	2.00	0.44
22:a:1946:ARG:NH2	22:a:1987:ASP:OD1	2.51	0.44
24:d:825:ILE:HD11	24:d:891:ARG:HH12	1.83	0.44
26:f:314:CYS:O	26:f:346:THR:OG1	2.34	0.44
31:k:213:SER:O	31:k:213:SER:OG	2.32	0.44
2:A:48:GLU:HG2	2:A:53:LYS:HB2	2.00	0.44
3:B:110:PRO:HG2	3:B:163:LEU:HD11	2.00	0.44
3:B:509:VAL:HG11	3:B:524:LYS:HD2	1.99	0.44
3:B:1105:GLU:O	3:B:1110:ALA:N	2.46	0.44
23:b:445:THR:OG1	23:b:448:GLN:OE1	2.30	0.44
23:b:479:MET:HA	23:b:482:LEU:HD12	2.00	0.44
28:h:327:SER:O	28:h:331:ILE:HG22	2.18	0.44
20:T:138:DA:H2''	20:T:139:DC:H2'	2.00	0.44
23:b:947:LEU:HD11	23:b:1021:PRO:HG2	2.00	0.44
24:d:482:ILE:HD12	24:d:517:LEU:HD23	2.00	0.44
25:e:677:LEU:O	25:e:680:THR:OG1	2.31	0.44
29:i:635:ILE:O	31:k:512:THR:N	2.51	0.44
31:k:87:ASP:HA	31:k:132:LYS:HD3	1.99	0.44
33:n:325:ILE:HA	33:n:335:MET:HA	2.00	0.44
36:q:114:LEU:HD21	36:q:157:ALA:HB2	2.00	0.44
40:w:319:SER:C	40:w:320:MET:HE2	2.42	0.44
2:A:484:LEU:HD22	2:A:488:VAL:HG21	1.99	0.44
2:A:733:LEU:HD23	10:I:108:MET:H	1.82	0.44
8:G:89:VAL:HG13	8:G:99:THR:HG22	2.00	0.44
15:N:18:DA:H2'	15:N:19:DT:H71	2.00	0.44
20:T:47:DT:H2''	20:T:48:DA:C8	2.52	0.44
24:d:138:GLY:HA3	24:d:177:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:h:574:MET:HE3	28:h:574:MET:HB2	1.85	0.44
31:k:205:THR:O	31:k:205:THR:OG1	2.36	0.44
36:q:237:VAL:HB	36:q:256:VAL:HG22	2.00	0.44
6:E:72:MET:HE2	6:E:72:MET:HB3	1.85	0.44
11:J:8:PHE:CE2	11:J:48:MET:HE1	2.53	0.44
15:N:71:DG:H2''	15:N:72:DG:C8	2.53	0.44
23:b:1093:GLN:NE2	23:b:1182:ASP:OD1	2.51	0.44
27:g:535:ARG:NH2	37:r:2039:GLU:OE2	2.50	0.44
28:h:929:TYR:HA	28:h:932:ILE:HD12	2.00	0.44
3:B:379:ARG:HE	10:I:67:GLN:NE2	2.12	0.44
15:N:148:DG:OP1	14:S:45:THR:HG21	2.18	0.44
20:T:34:DT:H6	20:T:34:DT:H2'	1.70	0.44
16:U:90:LEU:HD22	16:U:97:LEU:HD12	1.99	0.44
22:a:1188:ALA:O	22:a:1192:ILE:HG22	2.18	0.44
29:i:56:SER:O	29:i:56:SER:OG	2.35	0.44
2:A:756:ALA:HB2	2:A:786:ALA:HB2	2.00	0.43
2:A:1016:LEU:HD23	2:A:1045:LEU:HD21	2.00	0.43
3:B:604:ILE:HG21	3:B:668:LEU:HB3	2.00	0.43
14:S:48:LEU:HB2	16:U:44:LYS:NZ	2.33	0.43
25:e:51:SER:N	25:e:54:GLU:OE1	2.44	0.43
27:g:192:ASP:OD1	27:g:192:ASP:N	2.47	0.43
27:g:215:ARG:NH1	27:g:252:GLN:OE1	2.50	0.43
28:h:108:LEU:HD12	28:h:108:LEU:HA	1.87	0.43
28:h:456:VAL:HG21	28:h:481:MET:HG3	1.99	0.43
28:h:529:LEU:HA	28:h:529:LEU:HD23	1.73	0.43
29:i:220:LEU:H	29:i:220:LEU:HG	1.45	0.43
40:w:393:VAL:HG21	40:w:423:VAL:HG11	2.00	0.43
2:A:459:ASN:HB2	2:A:469:MET:HE3	2.00	0.43
2:A:1232:ALA:O	2:A:1236:ASN:ND2	2.51	0.43
2:A:1280:ASP:HB3	2:A:1283:VAL:HG22	1.99	0.43
14:M:118:THR:OG1	20:T:70:DG:O5'	2.32	0.43
15:N:133:DC:H2''	15:N:134:DG:N7	2.34	0.43
24:d:133:THR:O	24:d:137:ILE:HG13	2.18	0.43
26:f:172:VAL:HG21	26:f:192:ASP:CG	2.44	0.43
27:g:68:LEU:HD23	27:g:68:LEU:HA	1.82	0.43
27:g:379:LEU:O	27:g:383:GLU:HG3	2.18	0.43
29:i:519:MET:HE2	29:i:554:GLN:HE22	1.83	0.43
33:n:3:THR:N	33:n:50:PHE:O	2.51	0.43
40:w:123:LEU:O	40:w:126:HIS:ND1	2.51	0.43
2:A:867:SER:OG	2:A:868:MET:N	2.51	0.43
3:B:579:ASP:OD2	3:B:582:GLN:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:73:LEU:O	4:C:238:SER:OG	2.34	0.43
5:D:74:PHE:HB2	5:D:80:ILE:HD11	2.00	0.43
9:H:136:GLU:OE2	9:H:139:SER:HB3	2.18	0.43
20:T:97:DA:H2"	20:T:98:DG:C8	2.53	0.43
22:a:1275:THR:O	22:a:1279:ASN:ND2	2.51	0.43
22:a:1663:LEU:O	22:a:1667:GLN:CB	2.65	0.43
23:b:1083:VAL:HG23	26:f:486:VAL:HG21	2.00	0.43
24:d:446:GLU:N	24:d:446:GLU:OE1	2.51	0.43
25:e:525:ARG:O	25:e:573:ARG:NH1	2.51	0.43
26:f:484:ILE:H	26:f:528:GLN:HB2	1.83	0.43
36:q:254:ARG:NH1	36:q:284:TYR:OH	2.52	0.43
2:A:91:ALA:HB3	2:A:290:LEU:HD23	2.01	0.43
2:A:637:MET:HB3	9:H:122:LEU:HD21	2.00	0.43
23:b:146:LEU:HD23	23:b:192:LEU:HD21	1.99	0.43
23:b:743:MET:HE3	27:g:271:LEU:HD13	2.00	0.43
27:g:611:LEU:H	27:g:611:LEU:HG	1.43	0.43
32:m:672:PHE:HZ	32:m:675:ARG:HH21	1.65	0.43
35:p:397:ILE:HD13	35:p:433:GLN:HB2	2.00	0.43
40:w:361:ALA:O	40:w:365:SER:OG	2.30	0.43
2:A:100:LEU:O	2:A:104:MET:HG2	2.18	0.43
2:A:1437:ASP:N	2:A:1437:ASP:OD1	2.50	0.43
4:C:34:ILE:HD11	12:K:98:LEU:HD11	2.01	0.43
9:H:130:ASN:OD1	9:H:130:ASN:N	2.51	0.43
23:b:1125:LEU:HA	23:b:1125:LEU:HD23	1.81	0.43
24:d:824:ILE:HG23	24:d:827:PRO:HD2	2.00	0.43
26:f:269:TYR:HB2	26:f:328:GLU:HG2	2.01	0.43
28:h:711:ARG:O	28:h:715:LYS:NZ	2.52	0.43
31:k:199:LEU:HD11	31:k:411:LEU:HB2	1.99	0.43
31:k:325:PRO:O	31:k:329:HIS:N	2.52	0.43
38:u:137:LEU:HD23	40:w:464:LEU:HD21	2.00	0.43
2:A:937:ASP:OD1	2:A:937:ASP:N	2.49	0.43
7:F:64:ARG:O	7:F:68:THR:HG23	2.18	0.43
14:S:54:TYR:HB3	16:U:40:ARG:HB3	2.01	0.43
20:T:3:DC:H2"	20:T:4:DA:C8	2.53	0.43
22:a:2111:MET:HG3	22:a:2150:LEU:HD13	1.99	0.43
29:i:288:THR:HG21	29:i:419:THR:HG22	2.00	0.43
29:i:329:ILE:HB	29:i:395:THR:HG22	2.00	0.43
38:u:141:CYS:HB3	38:u:149:LEU:HD13	1.99	0.43
40:w:312:VAL:O	40:w:316:MET:HB2	2.19	0.43
2:A:245:PRO:HA	2:A:248:MET:HE1	2.00	0.43
2:A:1481:LYS:HA	8:G:20:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:9:ARG:HD2	6:E:136:LEU:HD21	2.01	0.43
9:H:12:VAL:HA	9:H:30:CYS:HA	2.01	0.43
19:R:79:HIS:ND1	19:W:68:GLU:OE2	2.49	0.43
22:a:2080:ILE:HD12	22:a:2084:PHE:HE1	1.84	0.43
25:e:206:ASP:OD1	25:e:207:ALA:N	2.51	0.43
26:f:58:PRO:HG3	26:f:90:GLN:NE2	2.34	0.43
27:g:376:GLU:HB2	27:g:379:LEU:HD23	1.99	0.43
27:g:598:HIS:HA	27:g:601:ILE:HG22	2.00	0.43
28:h:719:GLU:CD	28:h:723:GLN:HE22	2.27	0.43
33:n:271:HIS:O	33:n:350:MET:N	2.44	0.43
38:u:107:ASN:ND2	38:u:109:GLU:O	2.51	0.43
2:A:1218:ARG:NH1	2:A:1255:LEU:HD21	2.33	0.43
3:B:561:ILE:HG22	3:B:576:ILE:HD13	2.00	0.43
5:D:41:LEU:HB3	5:D:65:LEU:HD13	2.01	0.43
8:G:166:ASP:OD2	8:G:167:TYR:HD1	2.02	0.43
13:L:39:CYS:SG	13:L:41:TYR:HB2	2.59	0.43
15:N:12:DG:H2'	15:N:13:DT:H71	2.00	0.43
24:d:499:ASP:O	24:d:503:ILE:HD12	2.19	0.43
25:e:921:PRO:HD3	25:e:949:PHE:CZ	2.54	0.43
26:f:110:ASN:OD1	26:f:116:ASN:ND2	2.52	0.43
27:g:22:ALA:HB1	27:g:60:LEU:HD22	2.00	0.43
27:g:705:LEU:HD23	27:g:705:LEU:HA	1.88	0.43
27:g:879:GLN:OE1	27:g:890:THR:OG1	2.25	0.43
28:h:155:VAL:O	28:h:158:SER:OG	2.33	0.43
28:h:250:CYS:SG	28:h:251:GLN:N	2.91	0.43
29:i:591:VAL:HG13	29:i:617:VAL:HB	2.00	0.43
35:p:260:ARG:HA	35:p:263:VAL:HG22	2.01	0.43
35:p:455:VAL:HG13	36:q:71:ILE:HD13	2.00	0.43
40:w:557:LEU:HD12	40:w:557:LEU:HA	1.90	0.43
2:A:685:HIS:NE2	2:A:769:MET:HE2	2.33	0.43
2:A:1135:LYS:HD2	2:A:1135:LYS:HA	1.74	0.43
6:E:163:TYR:HB2	6:E:165:LEU:HD22	2.00	0.43
31:k:111:ALA:O	31:k:115:LYS:N	2.52	0.43
31:k:487:ASP:N	31:k:487:ASP:OD1	2.52	0.43
2:A:115:SER:O	2:A:115:SER:OG	2.36	0.43
2:A:1375:ARG:NH1	2:A:1379:GLU:OE1	2.51	0.43
3:B:57:ARG:O	3:B:61:ASP:HB3	2.18	0.43
7:F:98:LYS:HB2	7:F:98:LYS:HE2	1.82	0.43
15:N:34:DG:OP1	18:V:32:ARG:HB2	2.19	0.43
18:Q:116:LEU:HD12	18:Q:117:PRO:HD2	2.01	0.43
21:Z:601:LYS:HB2	21:Z:644:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1287:ALA:HA	22:a:1290:VAL:HG12	1.99	0.43
26:f:9:ASP:HB3	26:f:14:MET:HE2	2.01	0.43
28:h:721:VAL:HG11	28:h:776:LEU:HD21	2.00	0.43
31:k:557:LEU:N	31:k:575:SER:O	2.35	0.43
2:A:1082:HIS:O	2:A:1085:GLU:HG3	2.19	0.42
2:A:1128:ILE:HD12	2:A:1414:ILE:HD12	2.00	0.42
2:A:1363:VAL:O	2:A:1367:THR:HG23	2.19	0.42
2:A:1476:ASP:HB3	2:A:1479:LYS:HB2	2.01	0.42
11:J:24:LEU:HD22	11:J:29:TYR:HD2	1.84	0.42
14:M:122:LYS:HA	14:M:122:LYS:HD2	1.86	0.42
19:R:83:ARG:NH1	19:R:90:GLU:OE2	2.52	0.42
23:b:47:PRO:HG3	23:b:180:VAL:HG13	2.01	0.42
24:d:430:GLN:O	24:d:434:THR:HG23	2.19	0.42
25:e:51:SER:O	25:e:55:HIS:ND1	2.45	0.42
31:k:326:GLY:O	31:k:329:HIS:N	2.52	0.42
8:G:110:ARG:HH11	8:G:119:PHE:HB2	1.84	0.42
20:T:66:DG:H2"	20:T:67:DT:C5	2.54	0.42
22:a:2164:LEU:HD23	22:a:2164:LEU:HA	1.83	0.42
23:b:202:LEU:HD23	23:b:202:LEU:HA	1.88	0.42
24:d:907:CYS:SG	27:g:828:ALA:HB1	2.59	0.42
25:e:174:ASN:O	25:e:178:GLN:HG2	2.18	0.42
25:e:811:ALA:O	25:e:815:THR:HG22	2.19	0.42
36:q:276:MET:HB2	36:q:286:PHE:CE2	2.54	0.42
2:A:719:LYS:HB3	2:A:725:LEU:HB2	2.01	0.42
2:A:962:ASP:HB3	2:A:1043:ILE:HG23	2.01	0.42
3:B:256:ILE:HD11	3:B:373:LEU:HD21	2.01	0.42
20:T:133:DT:H2"	20:T:134:DA:C8	2.54	0.42
27:g:797:GLN:HA	37:r:2051:ASN:HD21	1.84	0.42
4:C:249:LEU:HD13	12:K:102:GLU:HA	2.01	0.42
9:H:96:VAL:HA	9:H:116:VAL:HA	2.01	0.42
20:T:23:DC:H2"	20:T:24:DG:C8	2.55	0.42
21:Z:502:LEU:HD22	21:Z:513:VAL:HG12	2.01	0.42
22:a:544:VAL:O	22:a:548:SER:N	2.53	0.42
24:d:96:LEU:HD23	24:d:96:LEU:HA	1.91	0.42
24:d:156:CYS:HA	24:d:159:LEU:HD12	2.02	0.42
25:e:125:VAL:O	25:e:129:LEU:HG	2.19	0.42
25:e:225:TRP:H	25:e:225:TRP:CD1	2.37	0.42
26:f:584:ILE:HD11	36:q:251:CYS:HB3	2.00	0.42
27:g:681:LEU:HD23	27:g:681:LEU:HA	1.73	0.42
35:p:453:ASP:O	35:p:459:ARG:NH1	2.51	0.42
3:B:161:CYS:SG	3:B:162:LEU:N	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:103:GLU:HB3	9:H:109:ALA:HB2	2.02	0.42
20:T:123:DA:H5'	19:W:31:LYS:HB2	2.00	0.42
24:d:129:GLN:O	24:d:133:THR:HG23	2.20	0.42
27:g:505:LEU:HB3	27:g:508:GLU:HB2	2.01	0.42
27:g:541:MET:HE3	27:g:541:MET:HB2	1.90	0.42
35:p:299:ARG:NH1	35:p:336:ASP:OD2	2.53	0.42
40:w:351:ASP:O	40:w:355:LYS:HG2	2.20	0.42
2:A:118:LEU:HG	2:A:151:LYS:HB2	2.00	0.42
3:B:756:LYS:O	3:B:777:ASN:ND2	2.48	0.42
3:B:773:PRO:HG3	11:J:53:VAL:HG21	2.00	0.42
3:B:779:ILE:O	3:B:964:ASP:N	2.44	0.42
7:F:61:GLU:OE2	7:F:106:ILE:HG21	2.19	0.42
9:H:90:TYR:CD2	9:H:145:MET:HE2	2.55	0.42
9:H:100:GLU:O	9:H:113:SER:N	2.46	0.42
19:W:35:SER:OG	19:W:60:ASN:HB2	2.19	0.42
29:i:114:THR:OG1	29:i:115:GLU:OE1	2.33	0.42
29:i:133:GLY:O	29:i:137:MET:HG3	2.18	0.42
33:n:300:ASN:O	33:n:304:GLY:N	2.53	0.42
2:A:676:ILE:HD13	2:A:676:ILE:HA	1.90	0.42
20:T:57:DT:H2''	20:T:58:DA:N7	2.35	0.42
22:a:1490:ALA:HB2	22:a:1522:ARG:HD2	2.02	0.42
23:b:616:ASN:O	23:b:620:THR:HG23	2.20	0.42
23:b:1045:LEU:HG	23:b:1057:ALA:HB2	2.01	0.42
26:f:431:VAL:HA	26:f:434:MET:HG3	2.00	0.42
27:g:667:ILE:HD12	27:g:667:ILE:HA	1.75	0.42
28:h:447:CYS:SG	28:h:456:VAL:HG23	2.59	0.42
28:h:724:ILE:HA	28:h:750:GLY:HA3	2.02	0.42
31:k:204:SER:O	31:k:415:GLY:HA3	2.20	0.42
36:q:86:TYR:OH	36:q:114:LEU:O	2.31	0.42
40:w:158:LEU:O	40:w:162:LEU:HG	2.19	0.42
40:w:374:LYS:HB3	40:w:374:LYS:HE2	1.69	0.42
40:w:495:THR:O	40:w:499:ARG:HG2	2.20	0.42
2:A:524:MET:HE1	3:B:1097:HIS:CE1	2.55	0.42
22:a:1120:LEU:HA	22:a:1123:ILE:HD12	2.01	0.42
22:a:1878:LEU:HD13	22:a:1878:LEU:HA	1.86	0.42
23:b:246:ARG:O	23:b:250:LEU:HD12	2.19	0.42
23:b:1188:CYS:O	23:b:1192:THR:HG23	2.19	0.42
26:f:62:ILE:HG12	26:f:98:LEU:HD12	2.01	0.42
35:p:586:LEU:HD23	35:p:586:LEU:HA	1.91	0.42
36:q:263:PRO:HB2	36:q:291:PRO:HD3	2.00	0.42
38:u:178:LEU:HD13	38:u:178:LEU:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:71:ASP:OD1	10:I:71:ASP:N	2.51	0.42
14:S:66:PRO:O	14:S:69:ARG:N	2.52	0.42
21:Z:589:SER:O	21:Z:591:GLN:NE2	2.52	0.42
26:f:78:LYS:NZ	36:q:204:ASP:OD2	2.40	0.42
26:f:352:VAL:O	26:f:355:SER:OG	2.38	0.42
29:i:250:MET:HG3	29:i:251:ASP:N	2.34	0.42
31:k:47:ASP:HB2	32:m:686:TYR:CZ	2.55	0.42
40:w:497:LEU:O	40:w:501:VAL:HG23	2.19	0.42
2:A:376:ASP:HB3	2:A:522:PRO:HD3	2.02	0.42
2:A:1141:VAL:HA	2:A:1357:THR:HG23	2.01	0.42
2:A:1484:MET:SD	2:A:1484:MET:N	2.93	0.42
6:E:31:ASP:OD1	6:E:32:GLU:N	2.52	0.42
14:M:68:GLN:O	14:M:72:ARG:HG2	2.20	0.42
15:N:43:DG:H2"	15:N:44:DA:N7	2.35	0.42
23:b:1038:CYS:HA	23:b:1041:PHE:CE2	2.55	0.42
24:d:642:ASP:OD2	27:g:285:HIS:NE2	2.45	0.42
26:f:106:THR:HG23	26:f:108:ILE:HG12	2.02	0.42
27:g:481:SER:OG	27:g:482:ALA:N	2.53	0.42
29:i:356:TYR:O	31:k:278:TYR:OH	2.35	0.42
29:i:454:PHE:HA	29:i:457:VAL:HG12	2.01	0.42
35:p:217:GLN:HB2	35:p:220:VAL:HG23	2.01	0.42
35:p:492:ASP:O	35:p:498:ARG:NH1	2.49	0.42
2:A:261:ARG:HD2	2:A:277:THR:HG22	2.01	0.41
2:A:356:GLY:O	3:B:1085:ARG:NH2	2.51	0.41
2:A:1077:ASN:HB3	7:F:56:TYR:CE2	2.54	0.41
2:A:1086:MET:HE3	2:A:1086:MET:HB3	1.91	0.41
3:B:677:MET:SD	3:B:700:PRO:HB3	2.60	0.41
14:M:122:LYS:HG3	14:S:113:HIS:NE2	2.35	0.41
21:Z:591:GLN:HG3	31:k:348:VAL:HG11	2.02	0.41
22:a:1907:CYS:O	22:a:1911:VAL:HG13	2.20	0.41
23:b:1097:TYR:HA	23:b:1185:LEU:HD22	2.01	0.41
24:d:696:ALA:O	24:d:700:ILE:HG22	2.19	0.41
25:e:181:MET:O	25:e:187:ARG:NH2	2.38	0.41
26:f:172:VAL:HG23	26:f:209:SER:HA	2.02	0.41
2:A:731:ASN:HB2	2:A:735:GLN:HB2	2.01	0.41
3:B:553:LEU:HG	3:B:575:GLY:H	1.85	0.41
3:B:566:LYS:HA	3:B:576:ILE:HG22	2.02	0.41
3:B:688:ALA:O	3:B:690:CYS:N	2.51	0.41
5:D:126:GLU:O	5:D:130:ILE:HG12	2.20	0.41
10:I:87:GLN:HE22	10:I:123:TRP:CD1	2.38	0.41
15:N:28:DT:H2"	15:N:29:DG:N7	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1043:ARG:HD3	22:a:1075:PRO:HG3	2.01	0.41
23:b:80:ALA:O	23:b:83:SER:OG	2.37	0.41
28:h:902:GLN:H	28:h:902:GLN:HG2	1.68	0.41
29:i:202:LYS:HE3	29:i:202:LYS:HB3	1.89	0.41
2:A:457:ILE:HD11	2:A:515:ILE:HD12	2.02	0.41
2:A:1006:PRO:O	2:A:1010:VAL:HG23	2.20	0.41
2:A:1128:ILE:HD13	2:A:1128:ILE:HA	1.92	0.41
2:A:1294:THR:OG1	2:A:1295:ASP:OD1	2.37	0.41
14:M:118:THR:C	14:M:119:ILE:HG13	2.43	0.41
15:N:42:DG:H2'	15:N:43:DG:C8	2.55	0.41
20:T:151:DC:H2'	20:T:152:DC:C6	2.55	0.41
22:a:1382:ALA:O	22:a:1386:GLU:HG3	2.20	0.41
23:b:684:MET:O	23:b:826:ARG:NH2	2.53	0.41
23:b:703:LEU:HB3	23:b:706:LEU:HB3	2.02	0.41
24:d:159:LEU:HD22	24:d:203:TYR:CZ	2.55	0.41
29:i:516:ILE:HD11	29:i:553:LEU:HG	2.02	0.41
3:B:626:LEU:HG	3:B:698:ILE:HG13	2.02	0.41
14:S:66:PRO:C	14:S:68:GLN:N	2.79	0.41
21:Z:589:SER:OG	21:Z:641:ARG:O	2.29	0.41
21:Z:593:ASN:HD21	31:k:335:GLN:HA	1.85	0.41
22:a:1895:ASN:O	22:a:1899:PHE:HB2	2.20	0.41
23:b:527:THR:OG1	23:b:528:GLU:N	2.53	0.41
27:g:770:SER:H	27:g:773:HIS:HD2	1.67	0.41
28:h:704:LEU:HD11	28:h:772:ILE:HD11	2.02	0.41
29:i:30:LEU:HD13	29:i:109:ALA:HB2	2.02	0.41
2:A:901:VAL:HG22	2:A:978:VAL:HG12	2.01	0.41
2:A:904:GLN:OE1	2:A:1044:HIS:NE2	2.49	0.41
16:O:75:HIS:CE1	19:R:77:LEU:HB3	2.54	0.41
29:i:109:ALA:HA	29:i:112:TYR:HD2	1.86	0.41
31:k:61:LEU:HD23	31:k:61:LEU:HA	1.89	0.41
40:w:245:MET:SD	40:w:245:MET:N	2.94	0.41
2:A:189:PRO:HB3	2:A:202:TRP:CD2	2.56	0.41
22:a:1545:LEU:O	22:a:1549:ILE:HG23	2.20	0.41
23:b:450:GLN:HA	23:b:453:VAL:HG22	2.02	0.41
23:b:1038:CYS:O	23:b:1042:ILE:HG12	2.20	0.41
24:d:73:VAL:HG21	24:d:110:ILE:HD12	2.02	0.41
27:g:389:GLY:O	27:g:393:LEU:HD23	2.20	0.41
28:h:719:GLU:OE1	28:h:723:GLN:NE2	2.47	0.41
29:i:516:ILE:HG21	31:k:456:ILE:HD11	2.03	0.41
36:q:39:LEU:HA	36:q:42:GLU:HG3	2.02	0.41
37:r:2038:GLU:CD	37:r:2038:GLU:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:139:LYS:HE3	2:A:143:HIS:HE1	1.85	0.41
2:A:1371:ILE:HA	2:A:1374:VAL:HG12	2.03	0.41
10:I:23:MET:HE3	10:I:24:LEU:H	1.86	0.41
10:I:87:GLN:HE22	10:I:123:TRP:CG	2.39	0.41
18:Q:96:LEU:O	18:Q:99:LYS:NZ	2.54	0.41
22:a:1915:LEU:HB3	22:a:1962:PHE:CZ	2.56	0.41
23:b:1093:GLN:NE2	23:b:1135:ASP:OD1	2.54	0.41
27:g:563:ASN:O	27:g:567:GLU:HG2	2.20	0.41
28:h:151:ILE:HG23	28:h:259:ALA:HB2	2.01	0.41
28:h:455:TYR:HA	28:h:458:MET:HG2	2.03	0.41
29:i:28:CYS:O	29:i:109:ALA:HB3	2.21	0.41
31:k:163:MET:HE2	31:k:176:THR:HB	2.02	0.41
35:p:189:LEU:O	35:p:193:ALA:N	2.53	0.41
35:p:414:ASP:O	35:p:420:ARG:NH1	2.53	0.41
36:q:198:LEU:HD12	36:q:198:LEU:HA	1.83	0.41
2:A:192:ARG:NH2	2:A:201:GLU:OE2	2.54	0.41
2:A:616:GLY:O	2:A:619:LYS:NZ	2.48	0.41
2:A:805:ARG:NH2	3:B:671:GLU:O	2.51	0.41
3:B:603:MET:HB3	3:B:603:MET:HE3	1.76	0.41
10:I:25:TYR:HD2	10:I:40:ARG:NH2	2.17	0.41
12:K:42:LEU:HD23	12:K:45:ILE:HD11	2.02	0.41
15:N:141:DG:H2''	15:N:142:DG:C8	2.56	0.41
21:Z:506:LEU:HD21	21:Z:552:ARG:HH21	1.86	0.41
22:a:1508:LEU:HD11	22:a:1548:LEU:HG	2.03	0.41
25:e:216:SER:HA	25:e:223:PHE:CG	2.55	0.41
29:i:234:VAL:HG22	29:i:260:VAL:HG22	2.01	0.41
2:A:94:VAL:HG21	2:A:314:VAL:HG21	2.01	0.41
3:B:270:ILE:HD12	3:B:308:ALA:HB2	2.03	0.41
6:E:118:LEU:HA	6:E:118:LEU:HD23	1.90	0.41
9:H:31:GLU:OE1	38:u:16:LYS:NZ	2.52	0.41
9:H:116:VAL:O	9:H:123:MET:N	2.50	0.41
14:M:72:ARG:NH1	20:T:50:DC:OP2	2.54	0.41
14:M:118:THR:HG1	20:T:70:DG:C5'	2.31	0.41
15:N:86:DG:P	16:O:39:ARG:HH22	2.44	0.41
16:O:80:THR:HG21	20:T:49:DG:H5''	2.03	0.41
20:T:156:DA:H2'	20:T:157:DC:C6	2.56	0.41
23:b:794:THR:OG1	23:b:831:MET:HE3	2.21	0.41
24:d:171:LEU:HD23	24:d:171:LEU:HA	1.86	0.41
24:d:422:ASP:HB3	24:d:428:ARG:HG2	2.03	0.41
24:d:787:LEU:HD23	24:d:787:LEU:HA	1.83	0.41
25:e:437:ARG:O	25:e:441:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:g:201:LEU:HD21	27:g:217:LEU:HD23	2.03	0.41
27:g:460:LEU:HD12	27:g:463:LEU:HD22	2.02	0.41
28:h:979:ALA:O	28:h:983:LYS:HB2	2.20	0.41
35:p:123:ASP:OD1	35:p:127:HIS:HE1	2.04	0.41
35:p:266:LYS:HA	35:p:266:LYS:HD2	1.93	0.41
2:A:901:VAL:HA	2:A:980:PRO:HA	2.03	0.41
2:A:1382:LEU:HB3	2:A:1398:LEU:HD22	2.02	0.41
3:B:127:ASP:OD1	3:B:127:ASP:N	2.50	0.41
3:B:526:LEU:HD23	3:B:526:LEU:HA	1.88	0.41
14:S:72:ARG:NH2	14:S:76:GLN:HG3	2.35	0.41
23:b:350:ILE:HA	23:b:350:ILE:HD12	1.66	0.41
23:b:480:LEU:HD12	23:b:480:LEU:HA	1.91	0.41
25:e:950:LEU:HD23	25:e:950:LEU:HA	1.94	0.41
26:f:43:PRO:O	26:f:46:ARG:HG2	2.21	0.41
29:i:480:PRO:O	29:i:483:SER:OG	2.39	0.41
4:C:58:VAL:H	4:C:58:VAL:HG22	1.63	0.40
9:H:98:ARG:NH2	9:H:100:GLU:HG3	2.37	0.40
10:I:106:ASP:OD1	10:I:106:ASP:N	2.54	0.40
14:S:66:PRO:HB2	14:S:67:PHE:H	1.69	0.40
22:a:1541:ILE:HD13	22:a:1563:PHE:HE2	1.86	0.40
22:a:1620:ASP:OD2	27:g:228:THR:OG1	2.32	0.40
23:b:412:LEU:HD23	23:b:412:LEU:HA	1.76	0.40
24:d:296:TRP:CD1	24:d:387:MET:HE2	2.56	0.40
26:f:405:THR:O	26:f:409:ARG:HG3	2.21	0.40
29:i:115:GLU:OE1	29:i:115:GLU:N	2.54	0.40
40:w:425:MET:SD	40:w:425:MET:N	2.83	0.40
3:B:1078:ARG:N	20:T:154:DC:OP1	2.52	0.40
4:C:4:ALA:HB1	12:K:97:GLU:HB2	2.03	0.40
8:G:95:VAL:O	8:G:128:TYR:OH	2.33	0.40
14:S:64:LYS:O	14:S:65:LEU:C	2.63	0.40
22:a:2069:ASP:O	22:a:2072:GLU:HG3	2.22	0.40
23:b:78:VAL:HG23	23:b:81:VAL:HG23	2.04	0.40
23:b:843:VAL:HG23	23:b:845:GLN:H	1.86	0.40
26:f:173:LEU:HA	26:f:210:VAL:HG13	2.03	0.40
26:f:395:ASP:O	26:f:399:VAL:HB	2.21	0.40
31:k:157:HIS:ND1	31:k:178:ASP:HB3	2.36	0.40
35:p:151:PHE:CE2	35:p:170:PHE:HB2	2.57	0.40
35:p:362:ILE:HG12	35:p:399:GLN:HG2	2.03	0.40
36:q:89:ARG:HB3	36:q:266:CYS:SG	2.61	0.40
36:q:223:ASP:OD1	36:q:223:ASP:N	2.52	0.40
2:A:1050:CYS:SG	2:A:1051:SER:N	2.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2181:LEU:HD23	22:a:2181:LEU:HA	1.93	0.40
23:b:305:LEU:HD12	23:b:305:LEU:HA	1.76	0.40
24:d:43:LEU:HD12	24:d:43:LEU:HA	1.88	0.40
25:e:784:VAL:HG12	28:h:408:LEU:HD11	2.04	0.40
29:i:640:ASP:HB3	29:i:643:LEU:HB3	2.02	0.40
31:k:334:LEU:C	31:k:336:ILE:H	2.29	0.40
35:p:336:ASP:OD1	35:p:337:ALA:N	2.55	0.40
36:q:204:ASP:OD1	36:q:205:ASP:N	2.55	0.40
2:A:22:GLN:N	3:B:1170:ARG:O	2.49	0.40
2:A:890:ARG:HD3	2:A:890:ARG:HA	1.97	0.40
14:S:56:LYS:HZ1	20:T:9:DC:H2'	1.84	0.40
23:b:47:PRO:HG3	23:b:180:VAL:HG22	2.02	0.40
23:b:801:LEU:HD11	23:b:867:VAL:HG12	2.03	0.40
23:b:1129:GLY:HA2	23:b:1189:ILE:HD13	2.03	0.40
24:d:69:VAL:HA	24:d:72:VAL:HG22	2.04	0.40
24:d:301:GLN:O	24:d:305:LEU:HG	2.21	0.40
25:e:924:LEU:HD23	25:e:924:LEU:HA	1.91	0.40
38:u:110:LEU:HD22	38:u:113:GLN:HE22	1.86	0.40
3:B:629:GLU:HB2	3:B:634:LEU:HD21	2.03	0.40
5:D:59:GLU:OE1	5:D:59:GLU:N	2.53	0.40
7:F:102:ILE:HB	7:F:120:VAL:HG11	2.03	0.40
15:N:55:DT:H2''	15:N:56:DG:H8	1.87	0.40
21:Z:721:ILE:HD13	21:Z:721:ILE:HA	1.95	0.40
22:a:969:CYS:SG	22:a:970:GLU:N	2.95	0.40
23:b:52:MET:HA	27:g:645:PRO:HG2	2.03	0.40
23:b:496:ILE:HG23	23:b:509:ILE:HG13	2.02	0.40
24:d:519:LEU:HA	24:d:522:VAL:HG23	2.04	0.40
25:e:918:SER:O	25:e:918:SER:OG	2.39	0.40
27:g:308:LYS:O	27:g:312:LEU:HB2	2.22	0.40
27:g:495:THR:O	27:g:499:VAL:HG23	2.21	0.40
35:p:155:TYR:CZ	35:p:196:LEU:HD12	2.57	0.40
36:q:206:ARG:NH2	36:q:209:TRP:O	2.54	0.40
38:u:33:LEU:HD21	38:u:56:LEU:HD23	2.04	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	
2	A	1375/1970 (70%)	1322 (96%)	53 (4%)	0	100	100
2	Y	11/1970 (1%)	11 (100%)	0	0	100	100
3	B	1096/1174 (93%)	1063 (97%)	33 (3%)	0	100	100
4	C	257/275 (94%)	249 (97%)	8 (3%)	0	100	100
5	D	124/142 (87%)	120 (97%)	4 (3%)	0	100	100
6	E	207/210 (99%)	201 (97%)	6 (3%)	0	100	100
7	F	76/127 (60%)	73 (96%)	3 (4%)	0	100	100
8	G	169/172 (98%)	158 (94%)	11 (6%)	0	100	100
9	H	146/150 (97%)	139 (95%)	7 (5%)	0	100	100
10	I	115/125 (92%)	111 (96%)	4 (4%)	0	100	100
11	J	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
12	K	113/117 (97%)	109 (96%)	4 (4%)	0	100	100
13	L	44/58 (76%)	40 (91%)	4 (9%)	0	100	100
14	M	88/135 (65%)	83 (94%)	5 (6%)	0	100	100
14	S	89/135 (66%)	77 (86%)	8 (9%)	4 (4%)	2	19
16	O	80/103 (78%)	78 (98%)	2 (2%)	0	100	100
16	U	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
18	Q	107/130 (82%)	105 (98%)	2 (2%)	0	100	100
18	V	104/130 (80%)	99 (95%)	5 (5%)	0	100	100
19	R	83/126 (66%)	80 (96%)	3 (4%)	0	100	100
19	W	93/126 (74%)	85 (91%)	7 (8%)	1 (1%)	11	44
21	Z	268/1087 (25%)	248 (92%)	20 (8%)	0	100	100
22	a	1676/2192 (76%)	1612 (96%)	64 (4%)	0	100	100
23	b	1033/1204 (86%)	979 (95%)	54 (5%)	0	100	100
24	d	810/963 (84%)	778 (96%)	32 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	e	834/1021 (82%)	799 (96%)	35 (4%)	0	100	100
26	f	530/889 (60%)	507 (96%)	23 (4%)	0	100	100
27	g	876/964 (91%)	835 (95%)	41 (5%)	0	100	100
28	h	865/995 (87%)	840 (97%)	25 (3%)	0	100	100
29	i	618/658 (94%)	581 (94%)	37 (6%)	0	100	100
30	j	660/710 (93%)	627 (95%)	33 (5%)	0	100	100
31	k	540/602 (90%)	488 (90%)	52 (10%)	0	100	100
32	m	538/706 (76%)	505 (94%)	33 (6%)	0	100	100
33	n	499/518 (96%)	448 (90%)	51 (10%)	0	100	100
34	o	361/451 (80%)	337 (93%)	24 (7%)	0	100	100
35	p	578/591 (98%)	554 (96%)	24 (4%)	0	100	100
36	q	288/311 (93%)	275 (96%)	13 (4%)	0	100	100
37	r	26/28 (93%)	24 (92%)	2 (8%)	0	100	100
38	u	181/528 (34%)	174 (96%)	7 (4%)	0	100	100
39	v	400/613 (65%)	371 (93%)	29 (7%)	0	100	100
40	w	501/583 (86%)	479 (96%)	22 (4%)	0	100	100
All	All	16602/23159 (72%)	15805 (95%)	792 (5%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	S	64	LYS
14	S	66	PRO
14	S	67	PHE
19	W	86	ILE
14	S	116	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	1223/1749 (70%)	1219 (100%)	4 (0%)	86	85
2	Y	13/1749 (1%)	13 (100%)	0	100	100
3	B	978/1027 (95%)	976 (100%)	2 (0%)	87	87
4	C	238/252 (94%)	238 (100%)	0	100	100
5	D	101/126 (80%)	101 (100%)	0	100	100
6	E	191/192 (100%)	191 (100%)	0	100	100
7	F	68/111 (61%)	68 (100%)	0	100	100
8	G	141/153 (92%)	141 (100%)	0	100	100
9	H	129/131 (98%)	128 (99%)	1 (1%)	73	77
10	I	104/112 (93%)	103 (99%)	1 (1%)	68	76
11	J	56/56 (100%)	55 (98%)	1 (2%)	51	67
12	K	103/106 (97%)	103 (100%)	0	100	100
13	L	42/55 (76%)	42 (100%)	0	100	100
14	M	77/113 (68%)	75 (97%)	2 (3%)	40	61
14	S	76/113 (67%)	69 (91%)	7 (9%)	8	29
16	O	66/79 (84%)	66 (100%)	0	100	100
16	U	64/79 (81%)	59 (92%)	5 (8%)	11	34
18	Q	85/99 (86%)	85 (100%)	0	100	100
18	V	83/99 (84%)	83 (100%)	0	100	100
19	R	71/107 (66%)	71 (100%)	0	100	100
19	W	81/107 (76%)	76 (94%)	5 (6%)	16	41
21	Z	240/940 (26%)	240 (100%)	0	100	100
22	a	955/1909 (50%)	951 (100%)	4 (0%)	84	83
23	b	870/1072 (81%)	866 (100%)	4 (0%)	81	82
24	d	703/845 (83%)	701 (100%)	2 (0%)	86	85
25	e	617/814 (76%)	614 (100%)	3 (0%)	81	82
26	f	438/798 (55%)	435 (99%)	3 (1%)	76	79
27	g	723/842 (86%)	718 (99%)	5 (1%)	76	79
28	h	701/896 (78%)	699 (100%)	2 (0%)	86	85
29	i	555/600 (92%)	553 (100%)	2 (0%)	84	83
31	k	405/522 (78%)	401 (99%)	4 (1%)	68	76
32	m	32/639 (5%)	32 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	p	485/514 (94%)	483 (100%)	2 (0%)	84	83
36	q	251/276 (91%)	251 (100%)	0	100	100
37	r	28/28 (100%)	28 (100%)	0	100	100
38	u	154/451 (34%)	153 (99%)	1 (1%)	78	80
39	v	59/515 (12%)	57 (97%)	2 (3%)	32	55
40	w	387/511 (76%)	386 (100%)	1 (0%)	86	85
All	All	11593/18787 (62%)	11530 (100%)	63 (0%)	78	82

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	1156	ASP
2	A	1158	LEU
2	A	1255	LEU
2	A	1350	LYS
3	B	298	MET
3	B	388	TYR
9	H	51	ASP
10	I	62	VAL
11	J	29	TYR
14	M	119	ILE
14	M	120	MET
14	S	58	THR
14	S	59	GLU
14	S	60	LEU
14	S	64	LYS
14	S	65	LEU
14	S	115	LYS
14	S	117	VAL
16	U	43	VAL
16	U	78	ARG
16	U	79	LYS
16	U	80	THR
16	U	81	VAL
19	W	39	TYR
19	W	51	ILE
19	W	85	THR
19	W	86	ILE
19	W	87	THR
22	a	1302	GLN

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Mol	Chain	Res	Type
22	a	1303	THR
22	a	1905	LEU
22	a	2105	SER
23	b	256	MET
23	b	345	LEU
23	b	347	LEU
23	b	350	ILE
24	d	149	MET
24	d	244	ASP
25	e	149	ILE
25	e	151	LEU
25	e	152	MET
26	f	215	MET
26	f	627	MET
26	f	628	ILE
27	g	235	LEU
27	g	470	ASP
27	g	609	THR
27	g	611	LEU
27	g	637	THR
28	h	256	LEU
28	h	776	LEU
29	i	17	LEU
29	i	220	LEU
31	k	9	LEU
31	k	36	HIS
31	k	37	MET
31	k	334	LEU
35	p	123	ASP
35	p	245	MET
38	u	109	GLU
39	v	40	LEU
39	v	41	LEU
40	w	341	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	136	GLN
2	A	387	ASN
2	A	711	GLN
2	A	723	ASN

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Mol	Chain	Res	Type
2	A	765	ASN
2	A	792	ASN
2	A	884	ASN
3	B	312	GLN
3	B	500	GLN
3	B	525	ASN
3	B	649	ASN
3	B	1040	GLN
3	B	1049	GLN
4	C	25	ASN
4	C	66	HIS
4	C	83	GLN
4	C	265	HIS
5	D	38	HIS
6	E	210	GLN
8	G	53	ASN
8	G	60	GLN
10	I	18	GLN
10	I	41	ASN
10	I	98	GLN
12	K	44	ASN
14	M	55	GLN
18	Q	38	ASN
18	Q	84	GLN
19	R	44	GLN
16	U	27	GLN
18	V	38	ASN
18	V	104	GLN
21	Z	466	GLN
21	Z	607	HIS
21	Z	703	ASN
22	a	1061	GLN
22	a	1278	GLN
22	a	1279	ASN
22	a	1288	HIS
22	a	1667	GLN
22	a	1944	ASN
22	a	2058	GLN
22	a	2154	HIS
22	a	2170	GLN
22	a	2176	GLN
23	b	151	ASN

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Mol	Chain	Res	Type
23	b	285	HIS
23	b	325	GLN
23	b	413	GLN
23	b	450	GLN
23	b	580	GLN
23	b	601	ASN
23	b	695	GLN
23	b	748	ASN
23	b	1003	GLN
23	b	1151	GLN
23	b	1152	GLN
24	d	84	ASN
24	d	120	ASN
24	d	221	GLN
24	d	403	GLN
24	d	568	HIS
24	d	733	GLN
24	d	773	GLN
24	d	873	GLN
24	d	900	HIS
25	e	126	GLN
25	e	127	GLN
25	e	598	HIS
25	e	785	HIS
26	f	70	HIS
26	f	90	GLN
26	f	110	ASN
26	f	116	ASN
26	f	533	ASN
27	g	88	GLN
27	g	236	HIS
27	g	406	GLN
27	g	437	GLN
27	g	515	GLN
27	g	853	ASN
27	g	884	HIS
28	h	113	ASN
28	h	411	ASN
28	h	445	ASN
28	h	527	GLN
28	h	609	GLN
28	h	744	GLN

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Mol	Chain	Res	Type
28	h	781	HIS
28	h	831	ASN
28	h	879	GLN
28	h	922	HIS
29	i	9	HIS
29	i	15	ASN
29	i	37	ASN
29	i	105	HIS
29	i	142	ASN
29	i	284	ASN
29	i	294	ASN
29	i	554	GLN
29	i	627	GLN
31	k	70	HIS
31	k	73	HIS
31	k	304	HIS
31	k	434	ASN
31	k	544	GLN
35	p	72	GLN
35	p	237	GLN
35	p	392	ASN
35	p	433	GLN
35	p	494	ASN
35	p	535	ASN
35	p	571	GLN
36	q	88	ASN
36	q	141	ASN
36	q	179	HIS
37	r	2047	GLN
37	r	2051	ASN
39	v	63	GLN
40	w	219	ASN
40	w	266	GLN
40	w	350	GLN
40	w	373	ASN
40	w	394	HIS
40	w	395	ASN

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	P	16/17 (94%)	4 (25%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
17	P	-16	U
17	P	-15	G
17	P	-14	U
17	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 13 ligands modelled in this entry, 13 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 ⓘ

There are no chain breaks in this entry.

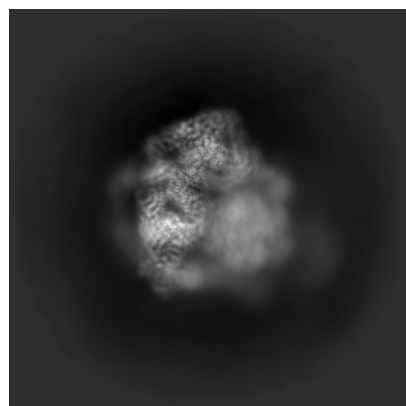
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19038. These allow visual inspection of the internal detail of the map and identification of artifacts.

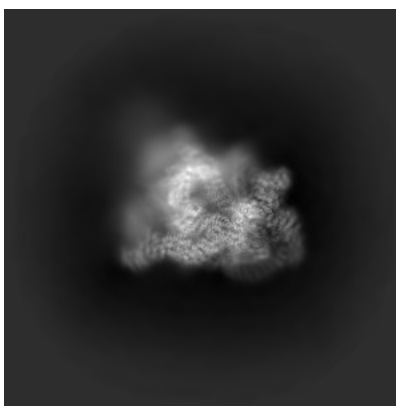
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

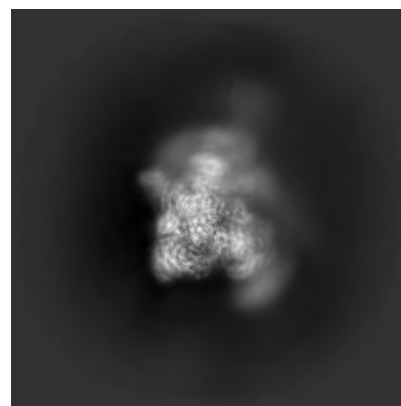
6.1.1 Primary map



X

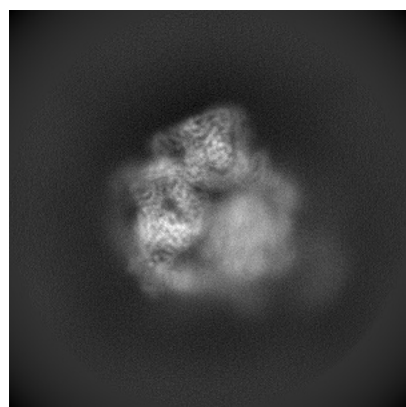


Y

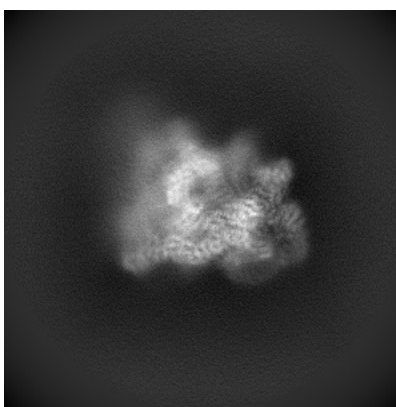


Z

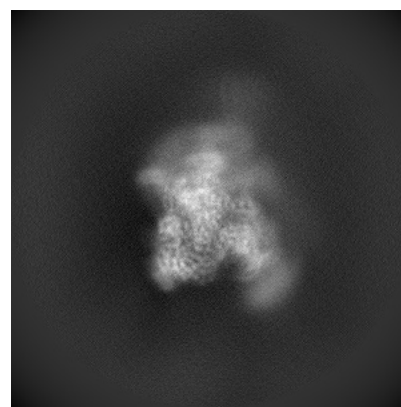
6.1.2 Raw map



X



Y

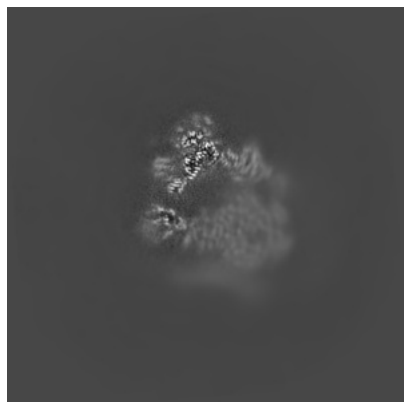


Z

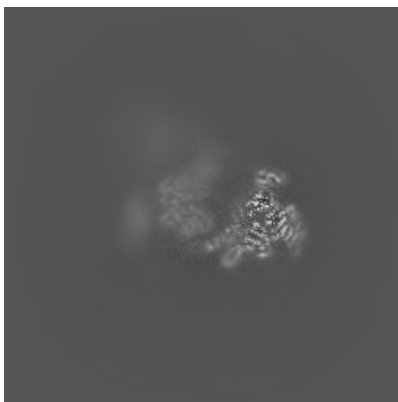
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

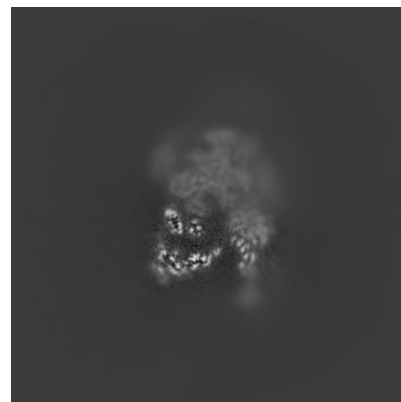
6.2.1 Primary map



X Index: 250

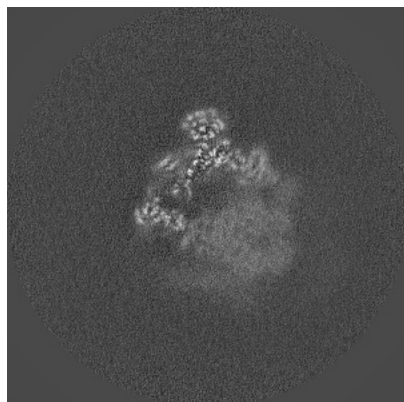


Y Index: 250



Z Index: 250

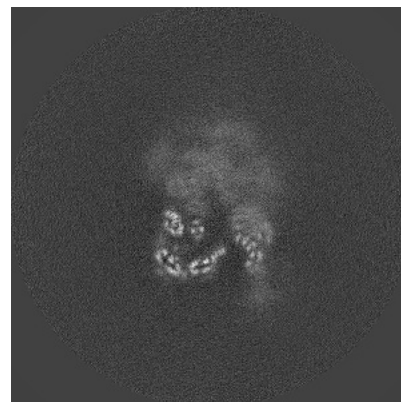
6.2.2 Raw map



X Index: 250



Y Index: 250

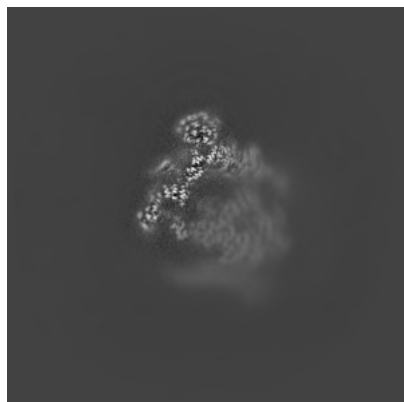


Z Index: 250

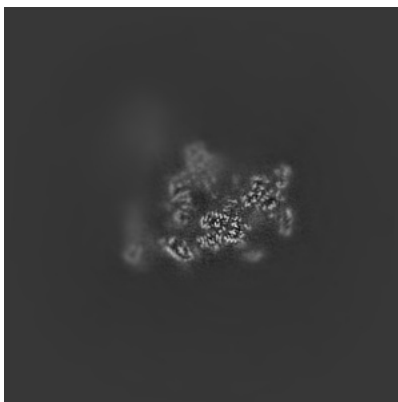
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

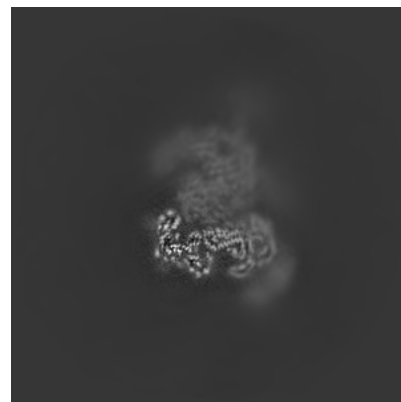
6.3.1 Primary map



X Index: 240

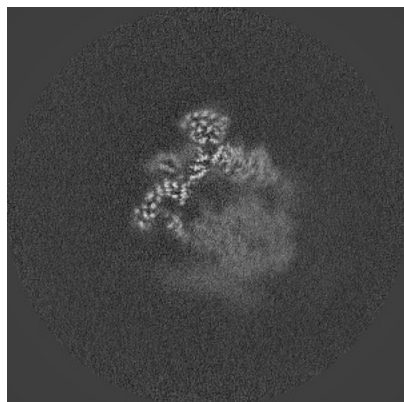


Y Index: 221

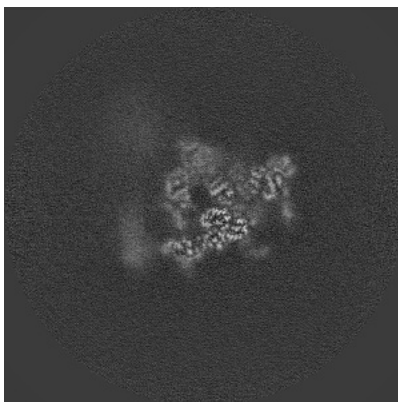


Z Index: 230

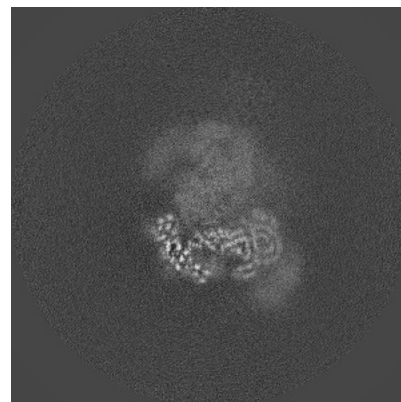
6.3.2 Raw map



X Index: 244



Y Index: 220

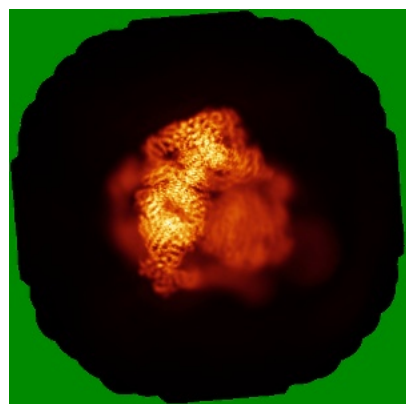


Z Index: 228

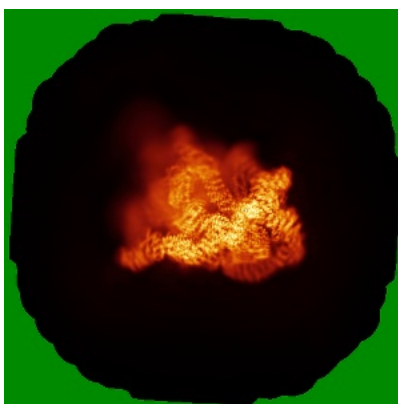
The images above show the largest variance slices of the map in three orthogonal directions.

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

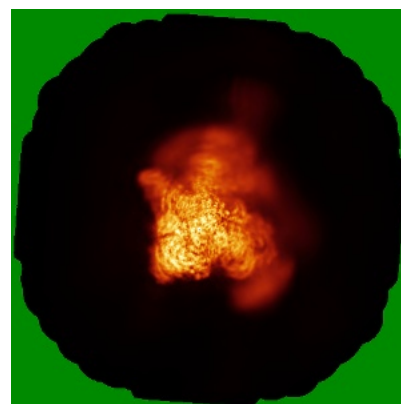
6.4.1 Primary map



X

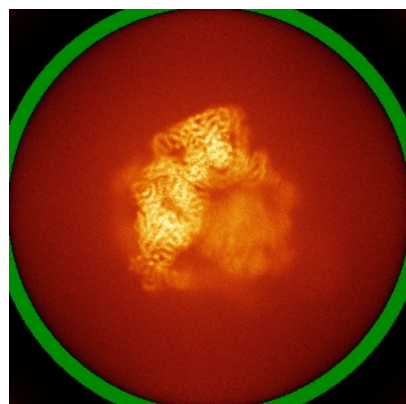


Y

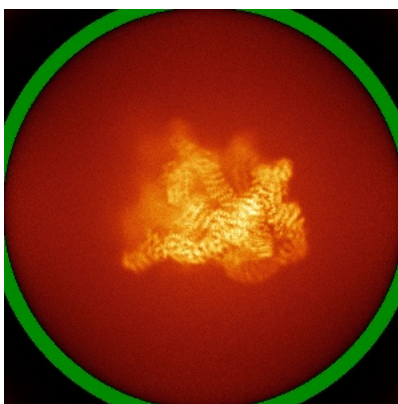


Z

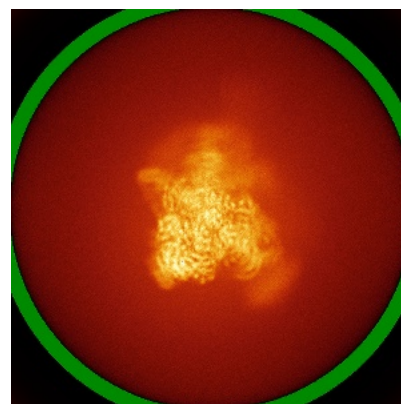
6.4.2 Raw map



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.

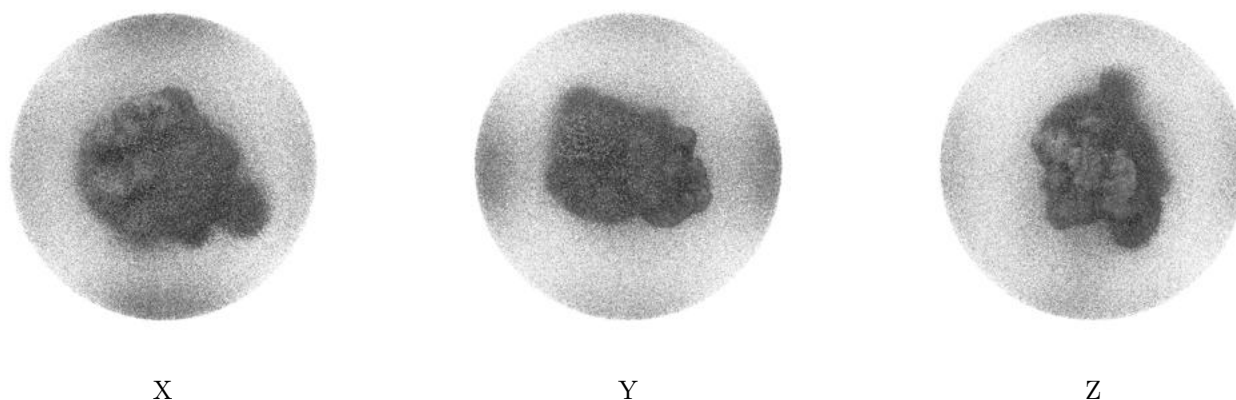
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00453. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

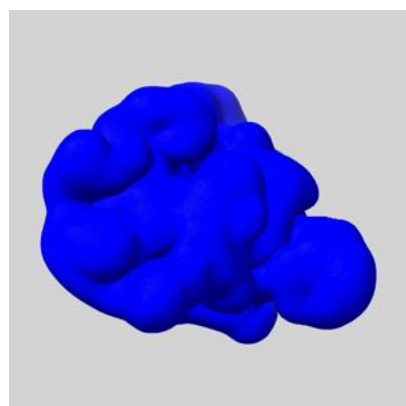
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

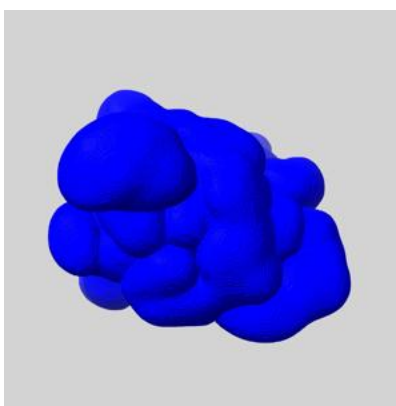
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

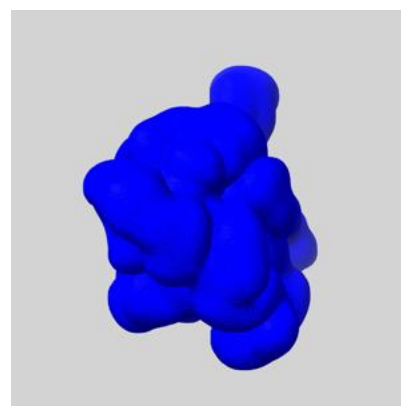
6.6.1 emd_19038_msk_1.map [i](#)



X



Y

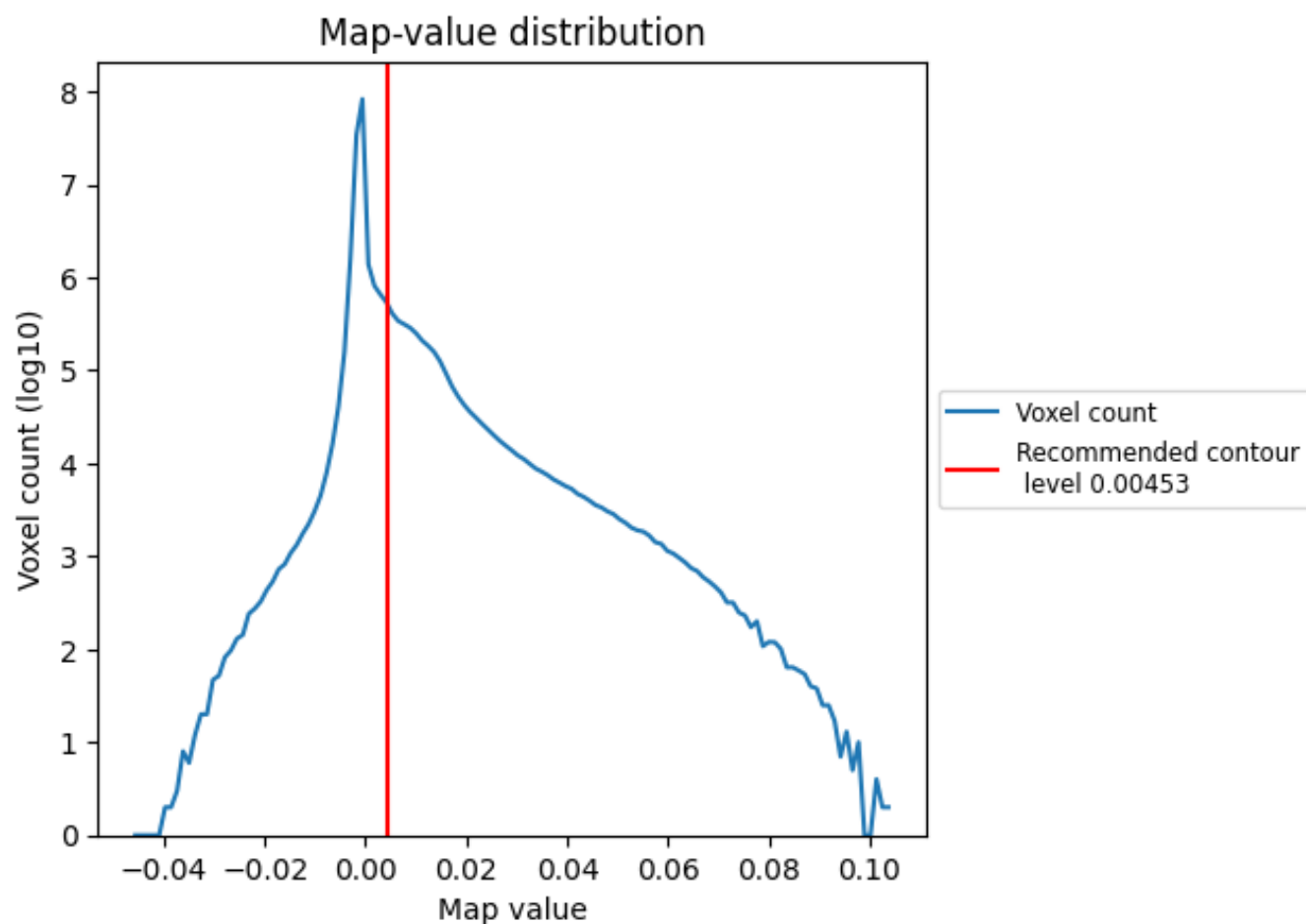


Z

7 Map analysis [i](#)

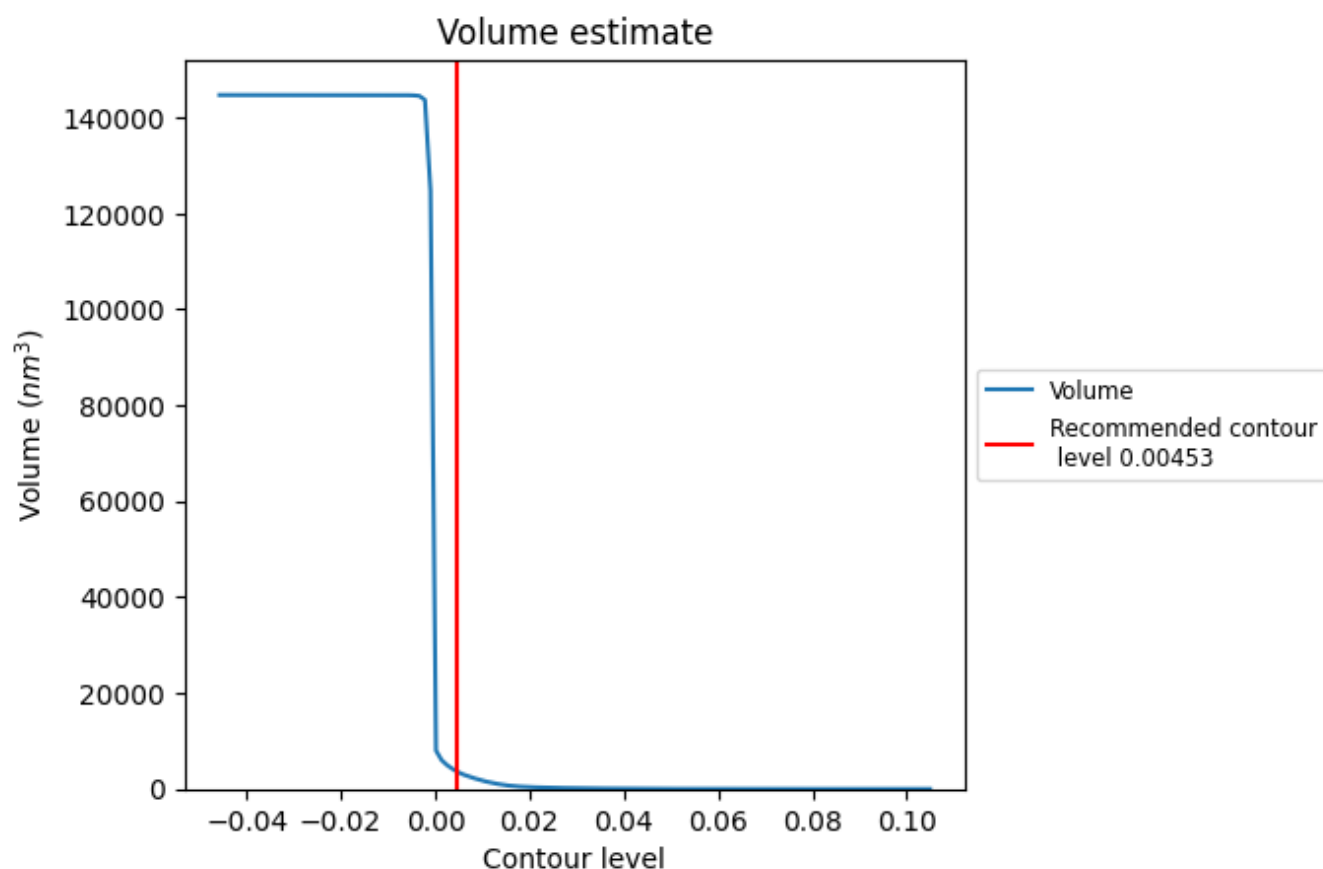
This section contains the results of statistical analysis of the map.

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.

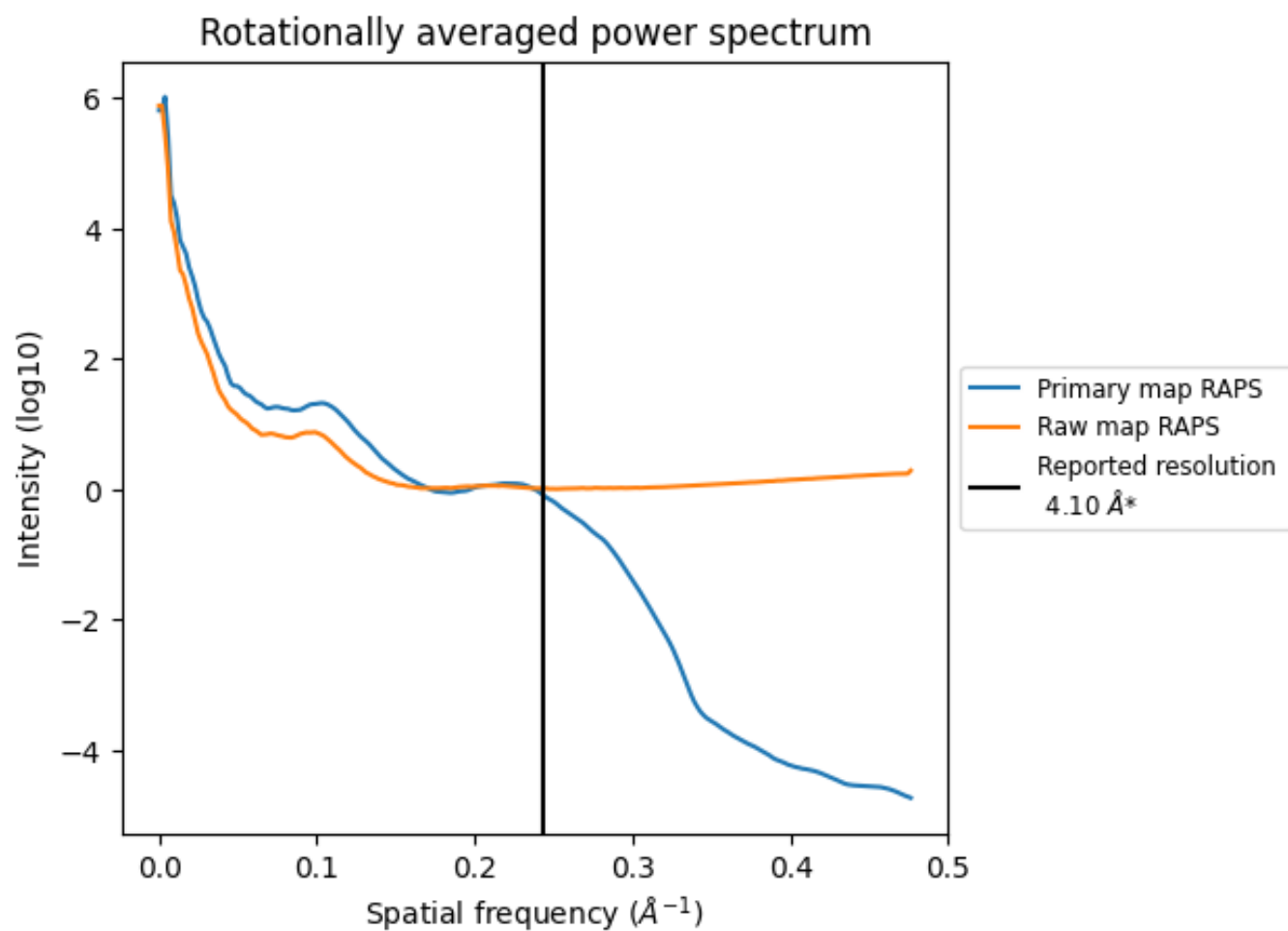
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3701 nm^3 ; this corresponds to an approximate mass of 3343 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

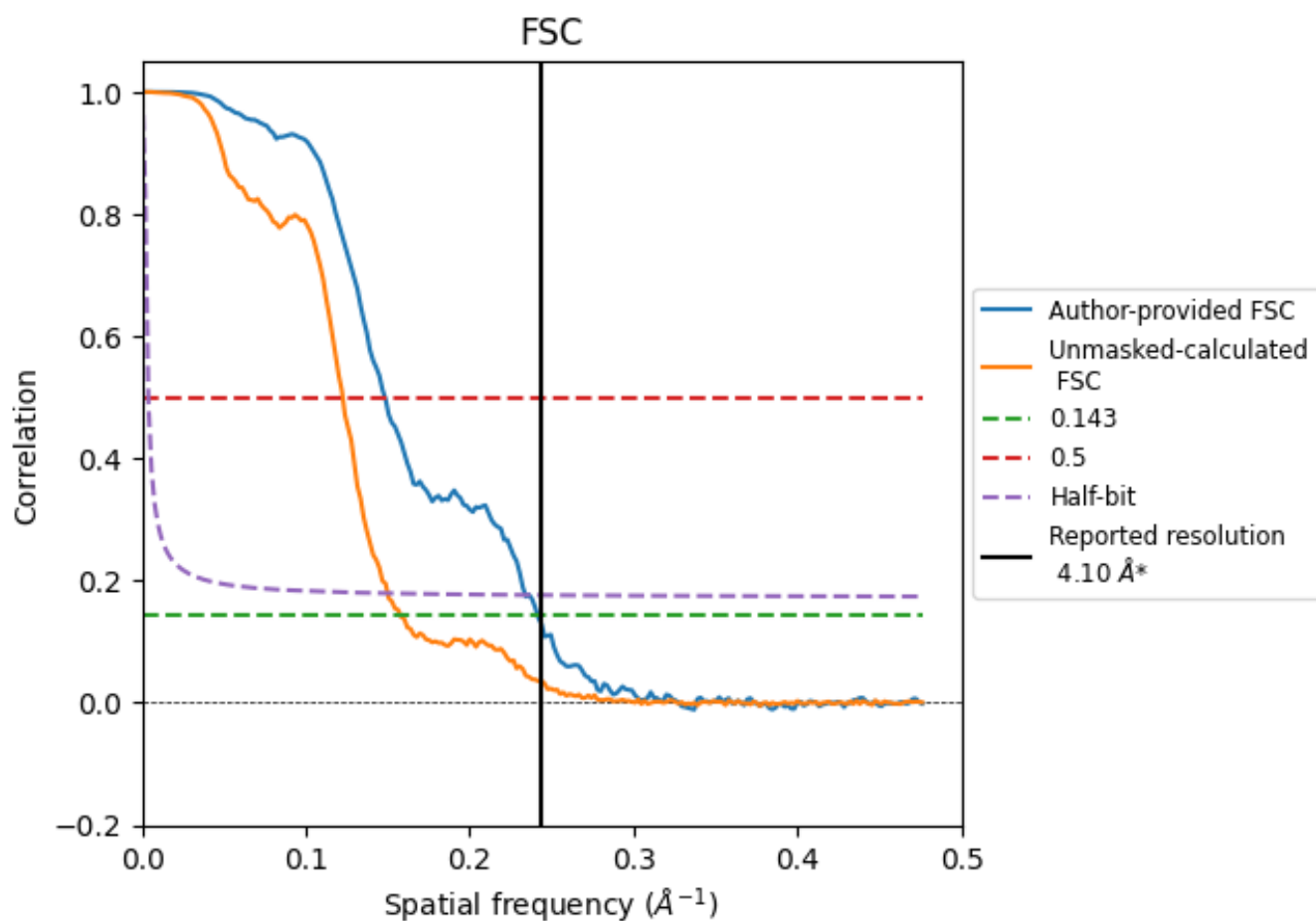


*Reported resolution corresponds to spatial frequency of $0.244 \text{ \AA}^{-1}$

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 0.244 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

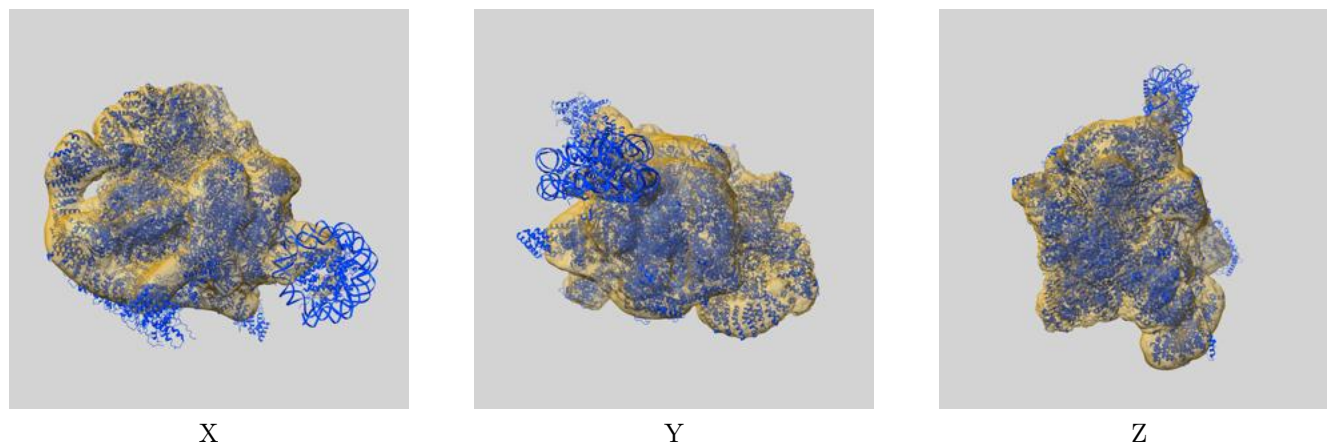
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.14	6.75	4.28
Unmasked-calculated*	6.34	8.17	6.68

*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 6.34 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

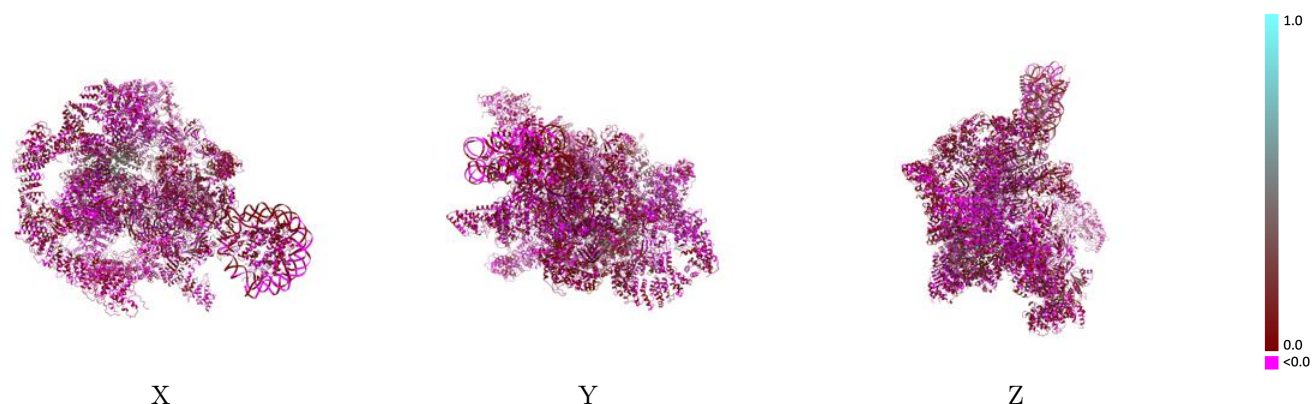
This section contains information regarding the fit between EMDB map EMD-19038 and PDB model 8RBX. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



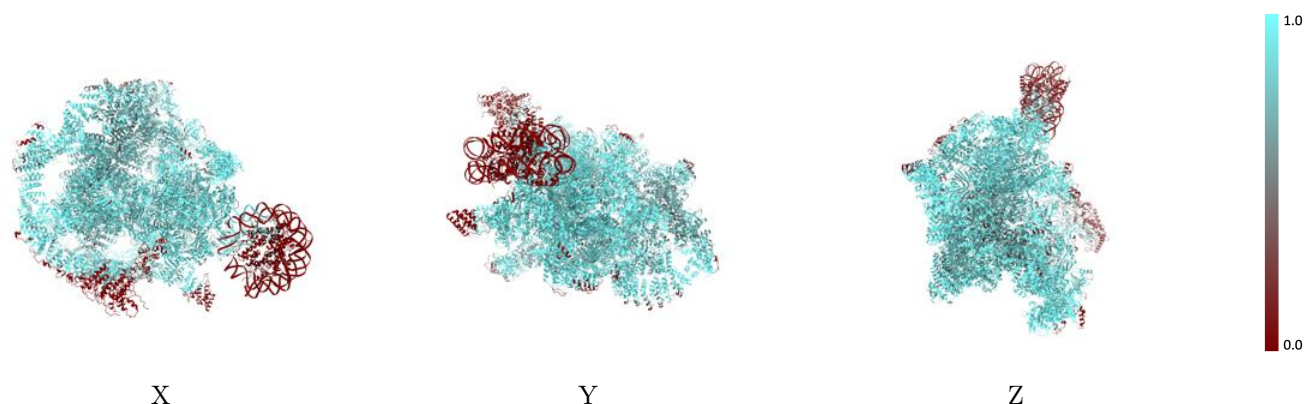
The images above show the 3D surface view of the map at the recommended contour level 0.00453 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



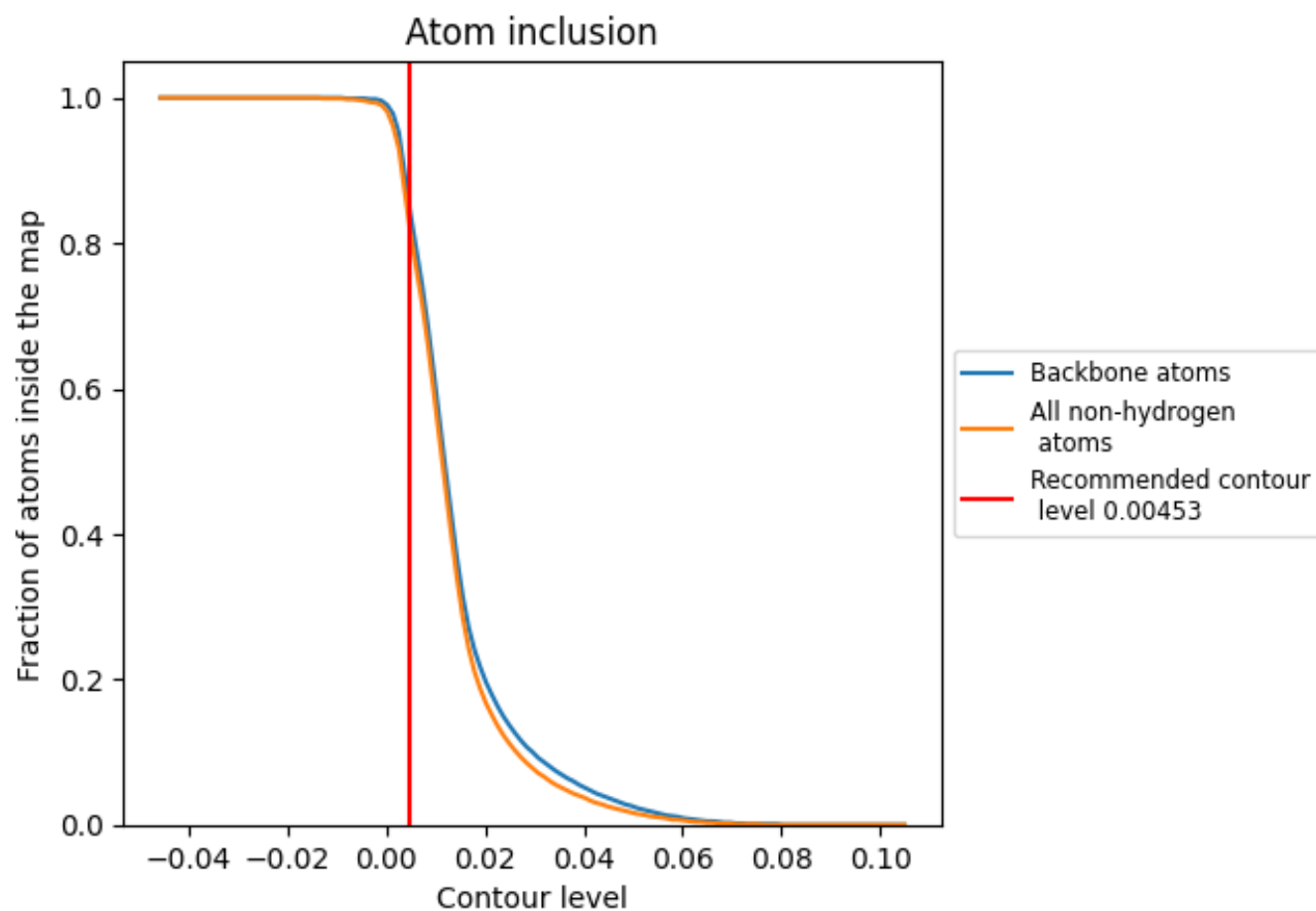
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00453).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 83% 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 (0.00453) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8330	 0.0370
1	 1.0000	 0.1450
A	 0.9910	 0.0430
B	 0.9940	 0.0130
C	 0.9620	 0.0280
D	 0.8820	 0.0530
E	 0.9570	 0.0570
F	 0.9980	 0.0880
G	 0.9380	 0.0570
H	 0.9780	 0.0640
I	 0.8810	 0.0390
J	 0.9620	 0.0310
K	 0.9780	 0.0280
L	 0.9160	 0.0240
M	 0.5350	 0.0490
N	 0.2030	 0.0260
O	 0.3660	 0.0120
P	 1.0000	 0.0260
Q	 0.0000	 0.0270
R	 0.1090	 0.0500
S	 0.0740	 0.0420
T	 0.3020	 0.0350
U	 0.0590	 -0.0090
V	 0.1290	 0.0070
W	 0.2780	 0.0300
Y	 0.9680	 0.3810
Z	 0.9830	 0.0240
a	 0.8430	 0.0360
b	 0.8860	 0.0940
d	 0.9250	 0.0240
e	 0.8810	 0.0130
f	 0.9450	 0.0270
g	 0.8950	 0.0990
h	 0.8590	 0.0010
i	 0.9110	 -0.0080



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Chain	Atom inclusion	Q-score
j	 0.8610	 0.0450
k	 0.9750	 0.0380
m	 0.3720	 0.0090
n	 0.4800	 0.0090
o	 0.8850	 0.0530
p	 0.9320	 0.0720
q	 0.9130	 -0.0130
r	 0.8650	 0.0140
u	 0.7800	 0.0340
v	 0.9490	 0.0730
w	 0.9240	 0.0540
x	 0.9180	 0.0330