Full wwPDB EM Validation Report ⓘ

Oct 18, 2021 – 10:52 am BST

PDB ID	:	7OPC
EMDB ID	:	EMD-13015
Title	:	Pol II-CSB-CRL4CSA-UVSSA-SPT6-PAF (Structure 4)
Authors	:	Kokic, G.; Cramer, P.
Deposited on	:	2021-05-31
Resolution	:	3.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

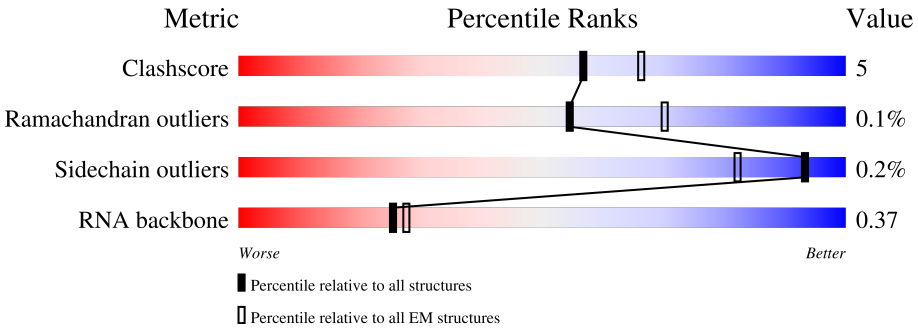
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1970	65% 7% 28%
2	B	1174	6% 89% 7%
3	C	275	87% 7% 5%
4	D	142	14% 73% 15% 10%
5	E	210	91% 9%
6	F	127	5% 61% 35%
7	G	172	10% 73% 24%

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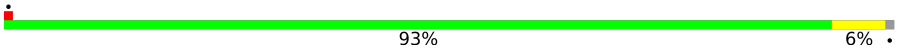
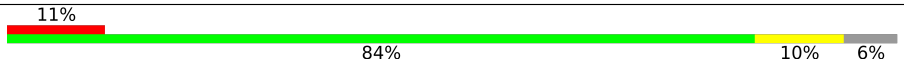
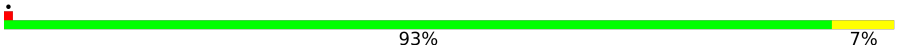
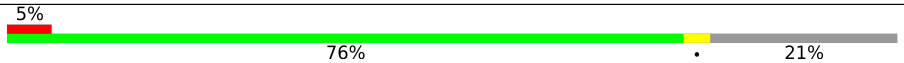
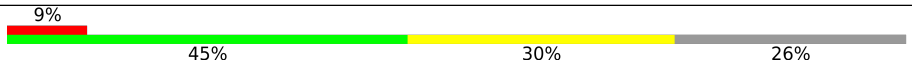
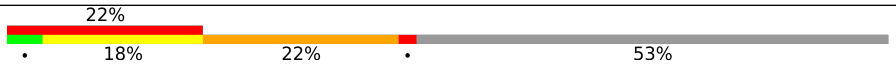
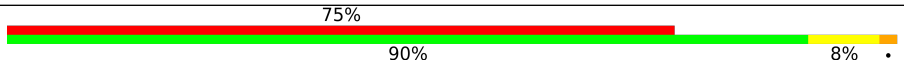
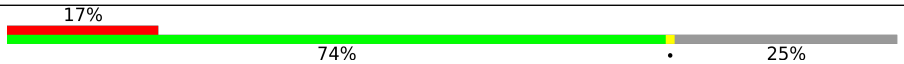
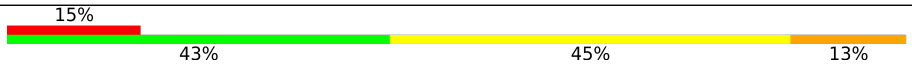
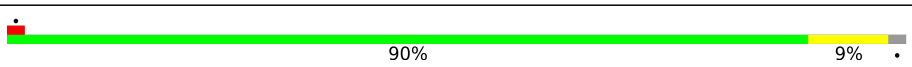
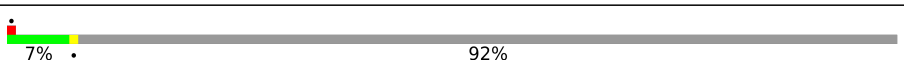
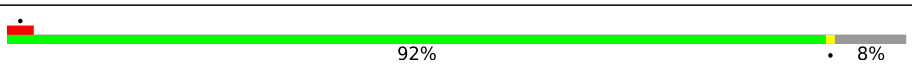
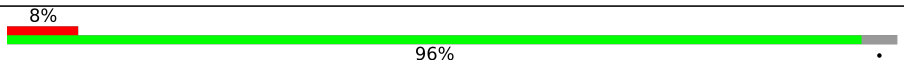
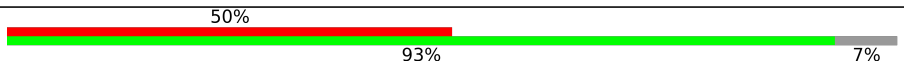
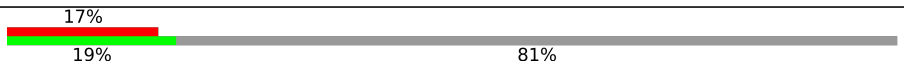
Mol	Chain	Length	Quality of chain
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	1729	
14	N	47	
15	P	45	
16	R	40	
17	S	1179	
18	T	47	
19	U	666	
20	V	531	
21	Y	305	
22	Z	531	
23	a	396	
24	b	1496	
25	c	712	
26	d	1143	
27	e	762	
28	f	108	

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 64223 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1412	11179	7033	2002	2074	70	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1131	9052	5727	1592	1669	64	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	260	2089	1309	359	415	6	0	0

- Molecule 4 is a protein called RPOL4c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	128	1013	636	172	201	4	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	82	657	418	113	121	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1334	867	216	243	8		

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

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	117	Total	C	N	O	S	0	0
			949	587	169	182	11		

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

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

- Molecule 11 is a protein called RNA_pol_L_2 domain-containing protein.

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

- Molecule 12 is a protein called RNA polymerase II subunit K.

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

- Molecule 13 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	810	Total	C	N	O	S	0	0
			6648	4226	1155	1234	33		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q7KZ85
M	-1	ASN	-	expression tag	UNP Q7KZ85
M	0	ALA	-	expression tag	UNP Q7KZ85

- Molecule 14 is a DNA chain called NTS.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	35	Total	C	N	O	P	0	0
			727	344	142	206	35		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	21	Total	C	N	O	P	0	0
			454	204	89	140	21		

- Molecule 16 is a protein called LEO1 helix.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	R	40	Total	C	N	O	0	0
			160	80	40	40		

- Molecule 17 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	S	890	Total	C	N	O	0	0
			3560	1780	890	890		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	1174	GLU	-	expression tag	UNP Q6PD62
S	1175	ASN	-	expression tag	UNP Q6PD62
S	1176	LEU	-	expression tag	UNP Q6PD62
S	1177	TYR	-	expression tag	UNP Q6PD62
S	1178	PHE	-	expression tag	UNP Q6PD62
S	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 18 is a DNA chain called TS.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	47	Total	C	N	O	P	0	0
			947	453	159	288	47		

- Molecule 19 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	U	104	Total	C	N	O	0	0
			416	208	104	104		

- Molecule 20 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	V	217	Total	C	N	O	0	0
			868	434	217	217		

- Molecule 21 is a protein called WD repeat-containing protein 61.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Y	300	Total	C	N	O	0	0
			1200	600	300	300		

- Molecule 22 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	Z	43	Total	C	N	O	0	0
			172	86	43	43		

- Molecule 23 is a protein called DNA excision repair protein ERCC-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	365	Total	C	N	O	S	0	0
			2849	1775	507	548	19		

- Molecule 24 is a protein called DNA excision repair protein ERCC-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	520	Total	C	N	O	S	0	0
			4261	2746	748	746	21		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-2	SER	-	expression tag	UNP Q03468
b	-1	ASN	-	expression tag	UNP Q03468
b	0	ALA	-	expression tag	UNP Q03468
b	538	ARG	LYS	conflict	UNP Q03468

- Molecule 25 is a protein called UV-stimulated scaffold protein A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	c	141	Total	C	N	O	0	0
			564	282	141	141		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	-2	SER	-	expression tag	UNP Q2YD98
c	-1	ASN	-	expression tag	UNP Q2YD98
c	0	ALA	-	expression tag	UNP Q2YD98

- Molecule 26 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	1096	Total	C	N	O	S	0	0
			7439	4560	1353	1492	34		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-2	SER	-	expression tag	UNP Q16531
d	-1	ASN	-	expression tag	UNP Q16531
d	0	ALA	-	expression tag	UNP Q16531

- Molecule 27 is a protein called Cullin-4A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	e	711	Total	C	N	O	0	0
			2845	1422	711	712		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	-2	SER	-	expression tag	UNP Q13619
e	-1	ASN	-	expression tag	UNP Q13619
e	0	ALA	-	expression tag	UNP Q13619

- Molecule 28 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	f	21	Total 84	C 42	N 21	O 21	0	0

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

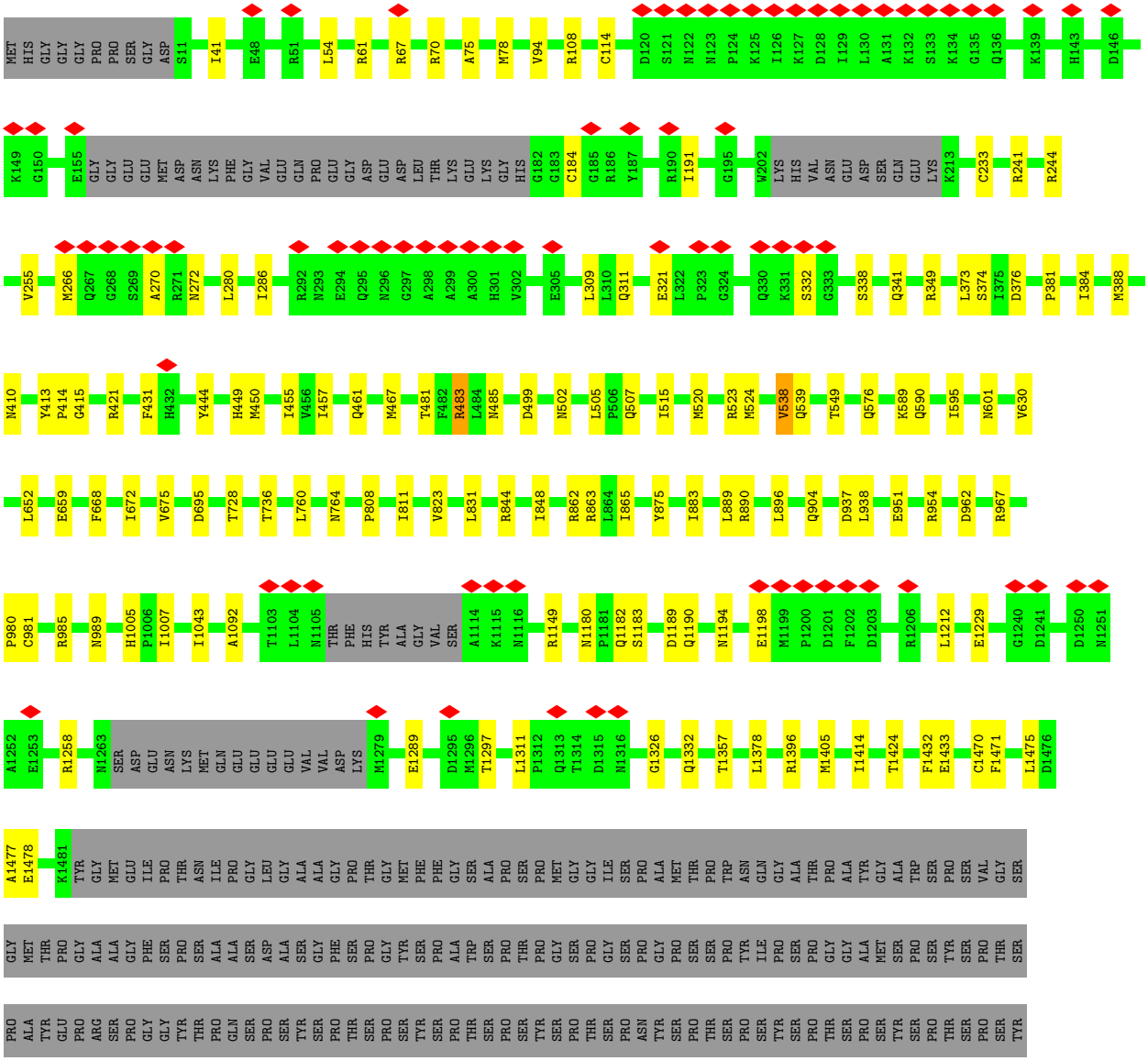
Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total 1	Mg 1	0

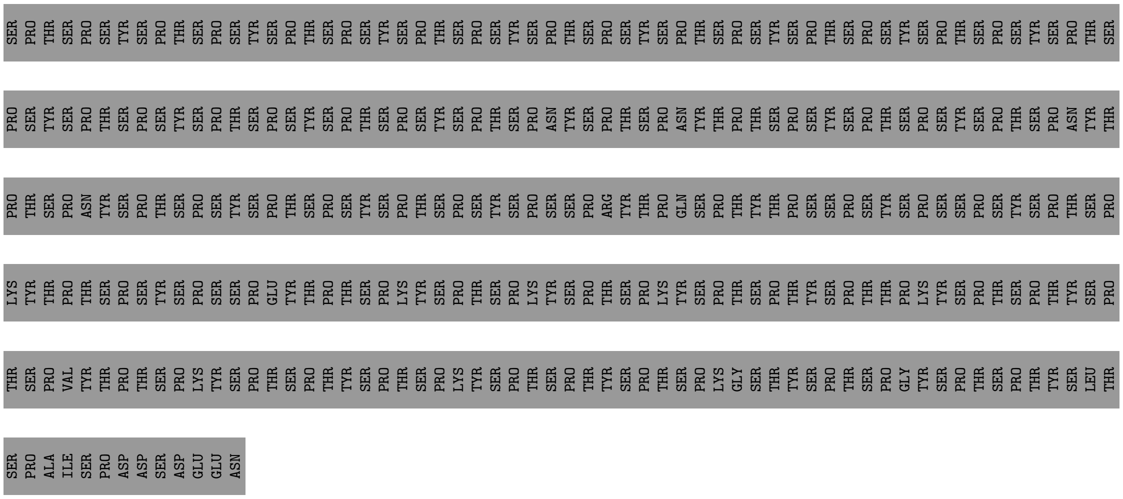
3 Residue-property plots (i)

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

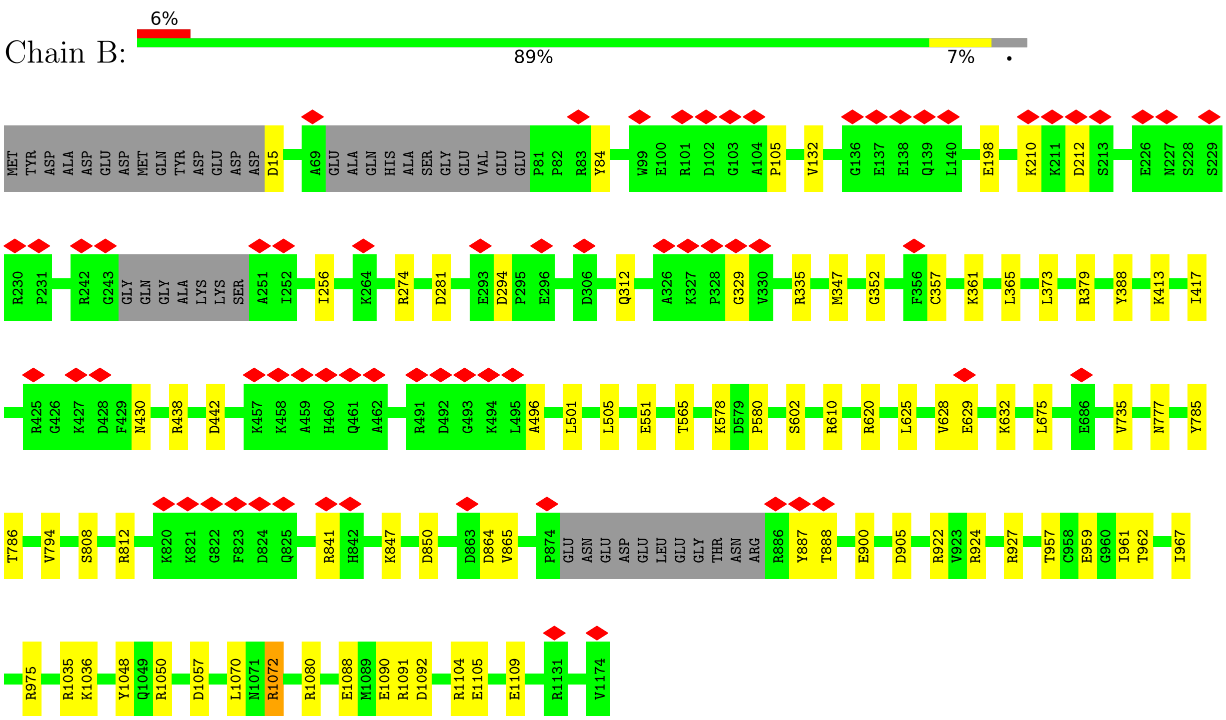
• Molecule 1: DNA-directed RNA polymerase II subunit RPB1

Chain A:

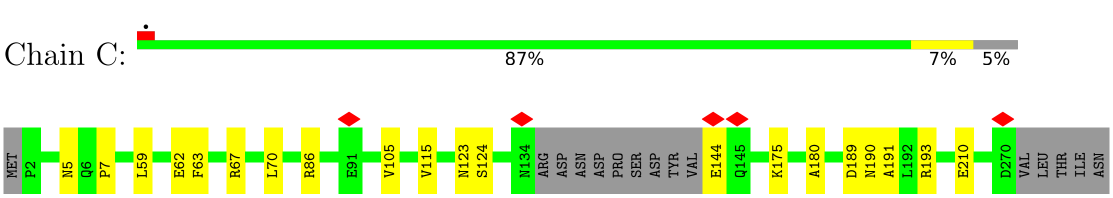




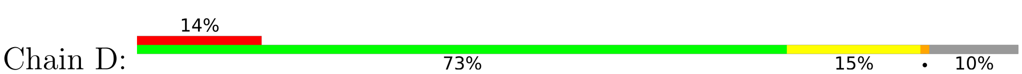
• Molecule 2: DNA-directed RNA polymerase subunit beta

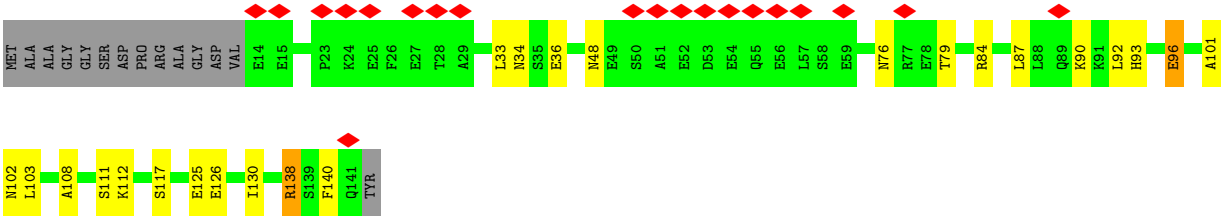


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

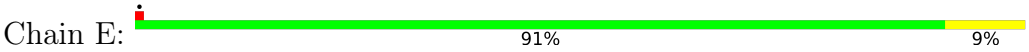


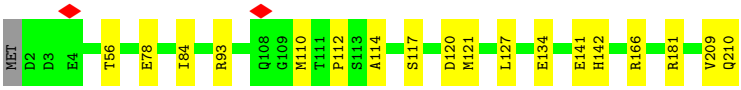
• Molecule 4: RPOL4c domain-containing protein



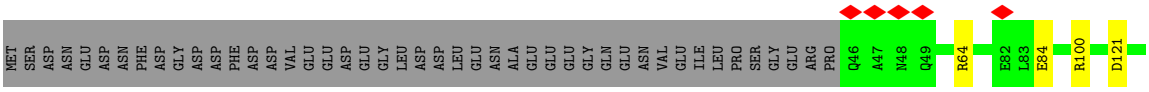


• Molecule 5: DNA-directed RNA polymerase II subunit E

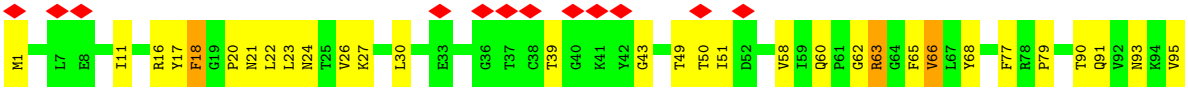


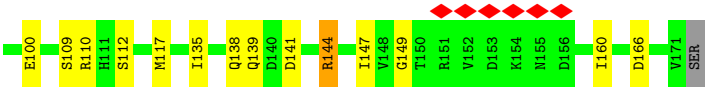


• Molecule 6: DNA-directed RNA polymerase II subunit F

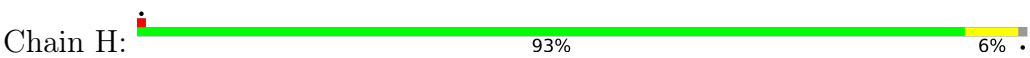


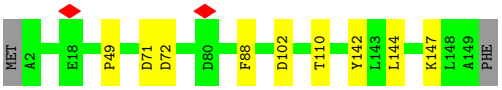
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7



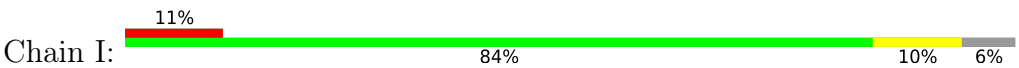


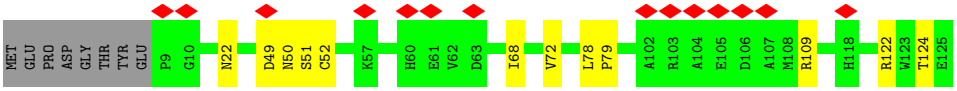
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



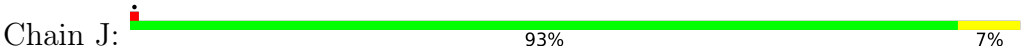


• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

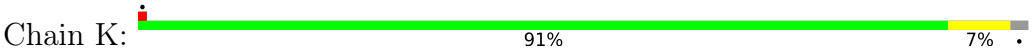


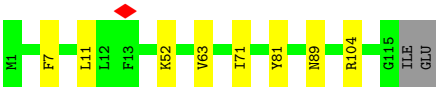


• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

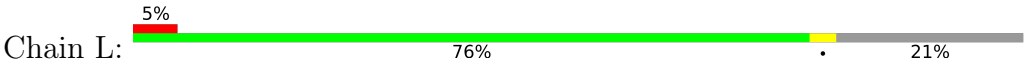


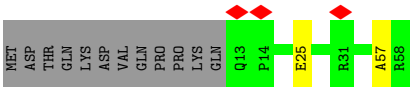
• Molecule 11: RNA_pol_L_2 domain-containing protein



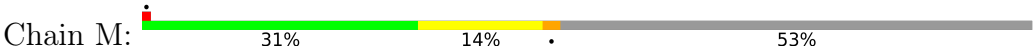


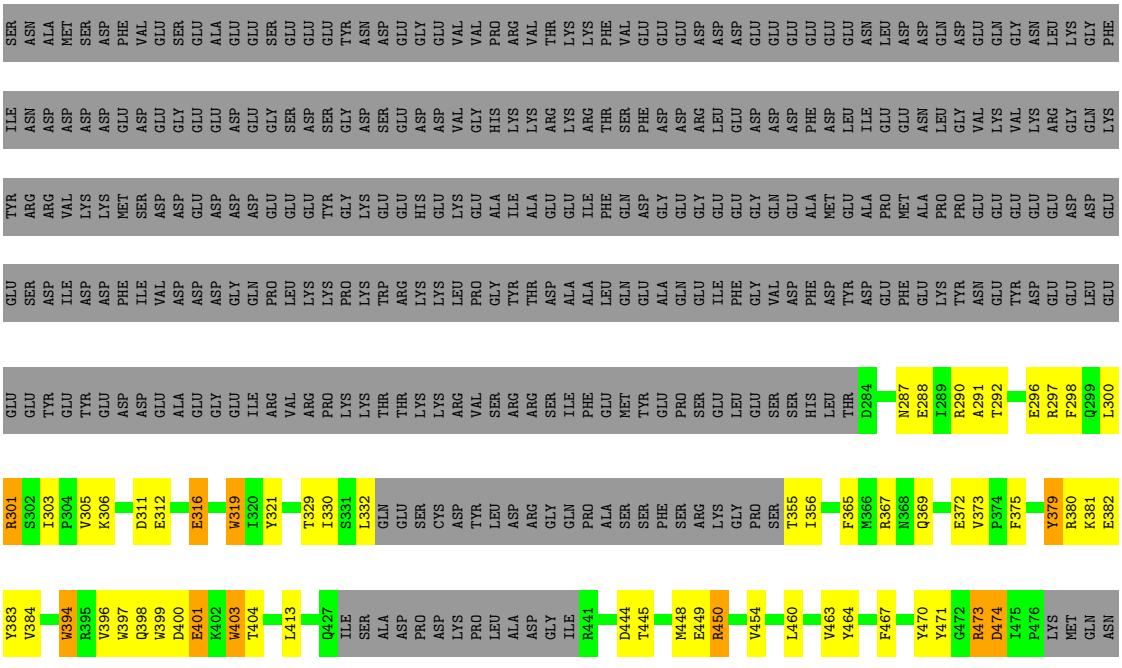
• Molecule 12: RNA polymerase II subunit K

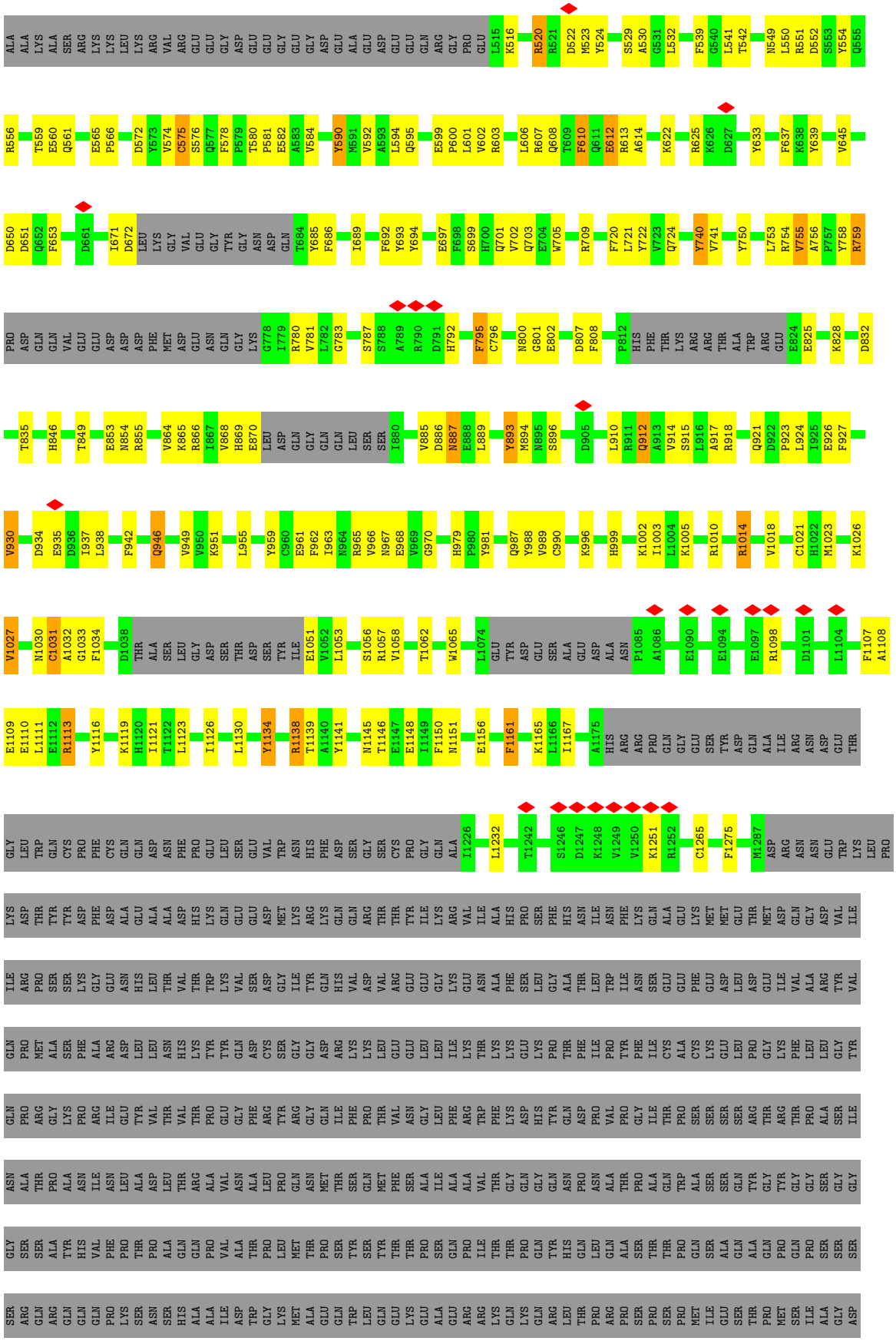




• Molecule 13: Transcription elongation factor SPT6





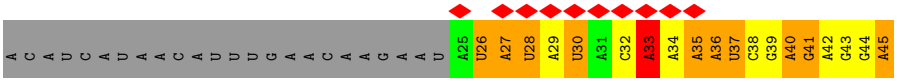


• Molecule 14: NTS

Chain N:

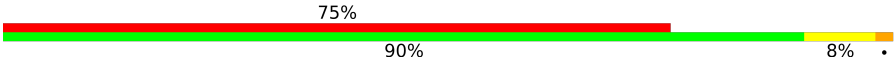
• Molecule 15: RNA

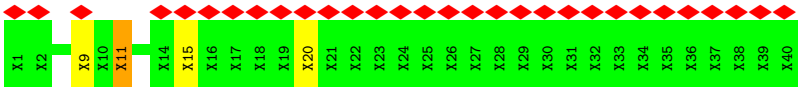
Chain P:



• Molecule 16: LEO1 helix

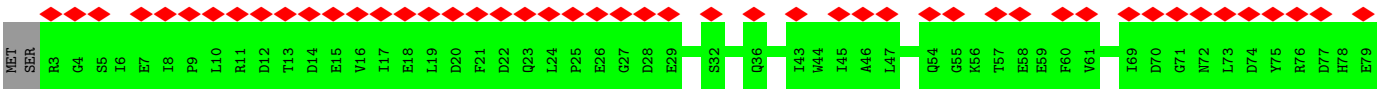
Chain R:

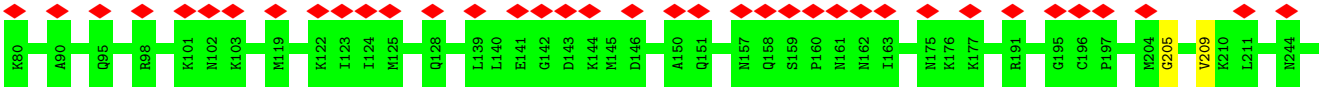


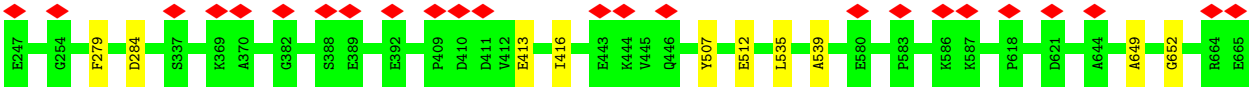


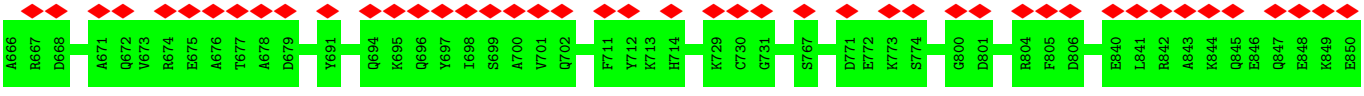
• Molecule 17: RNA polymerase-associated protein CTR9 homolog

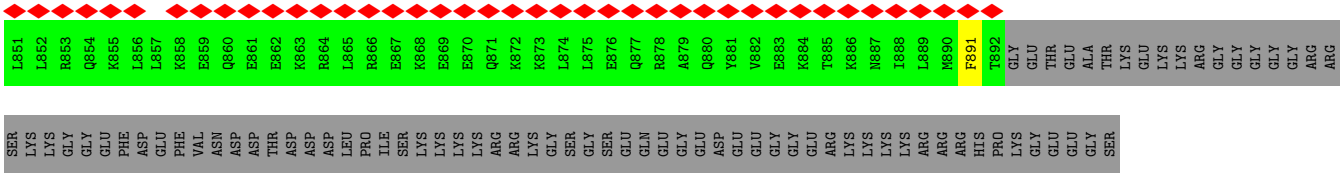
Chain S:

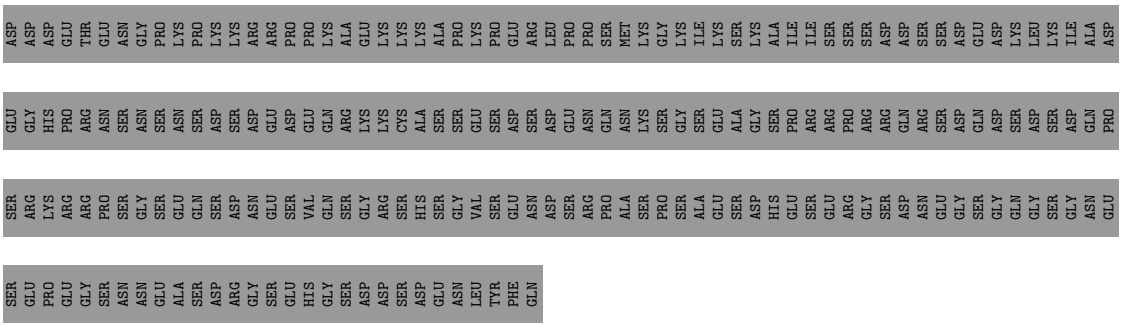




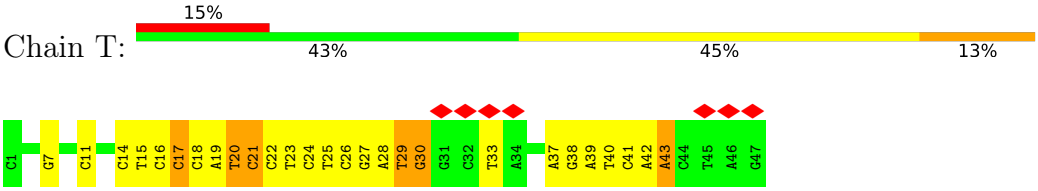




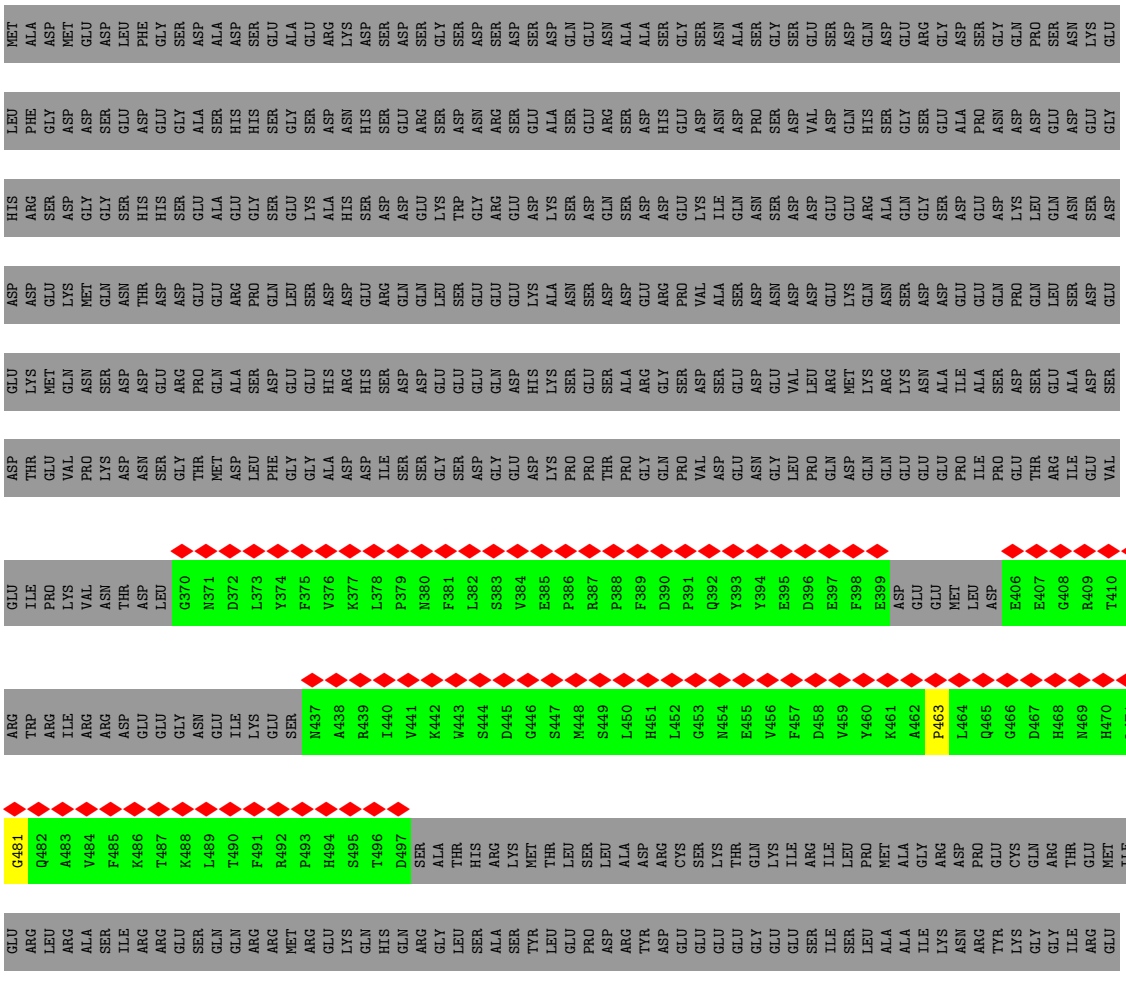


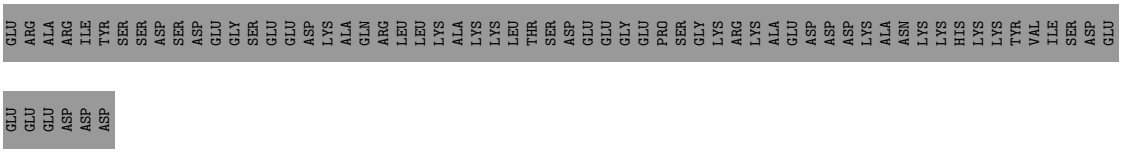


• Molecule 18: TS



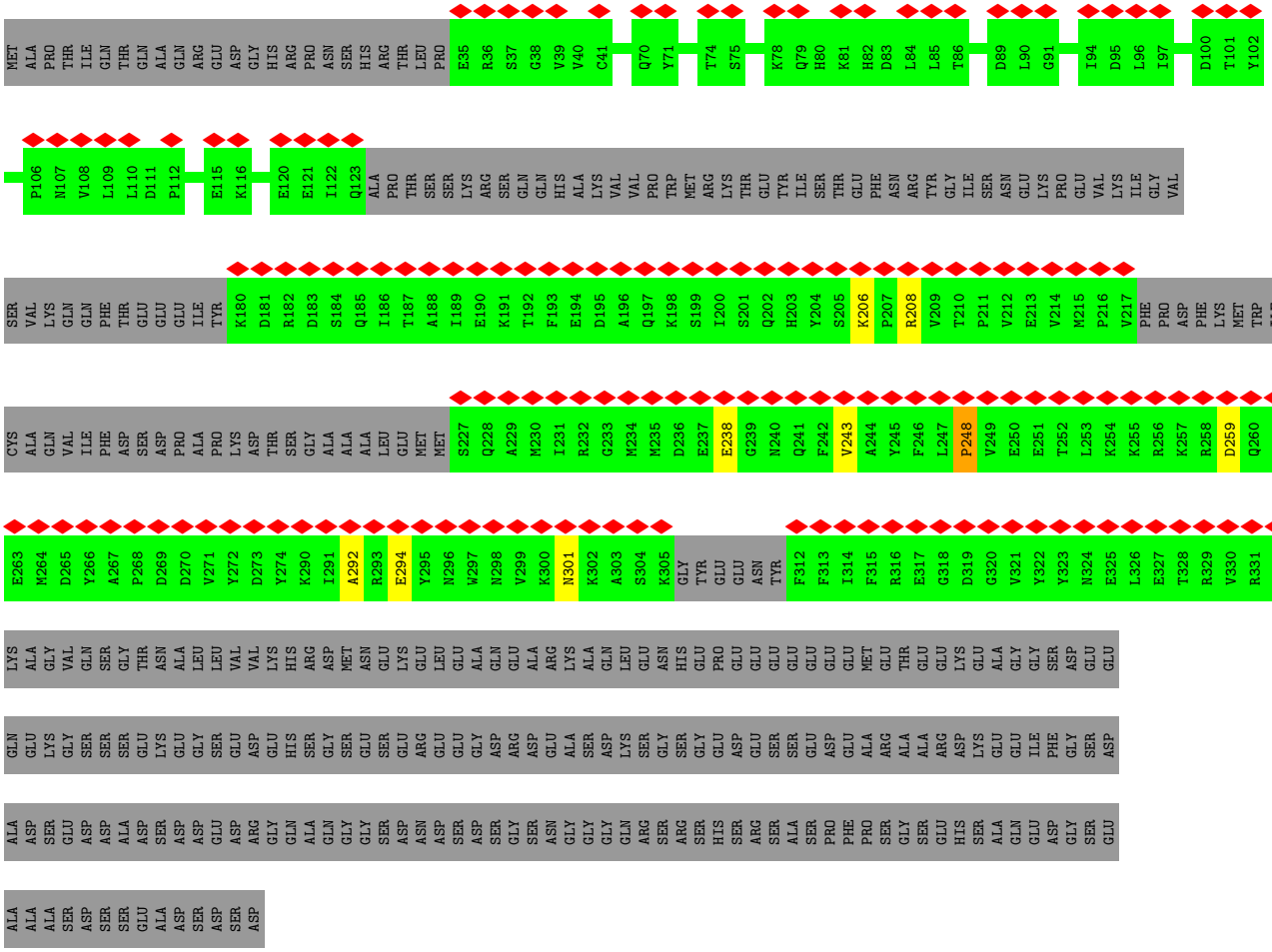
• Molecule 19: RNA polymerase-associated protein LEO1





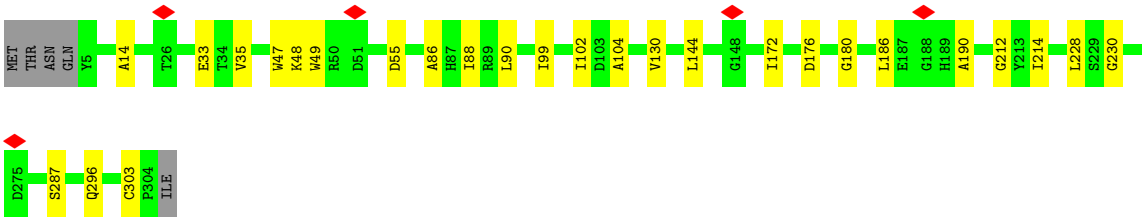
• Molecule 20: RNA polymerase II-associated factor 1 homolog

Chain V:



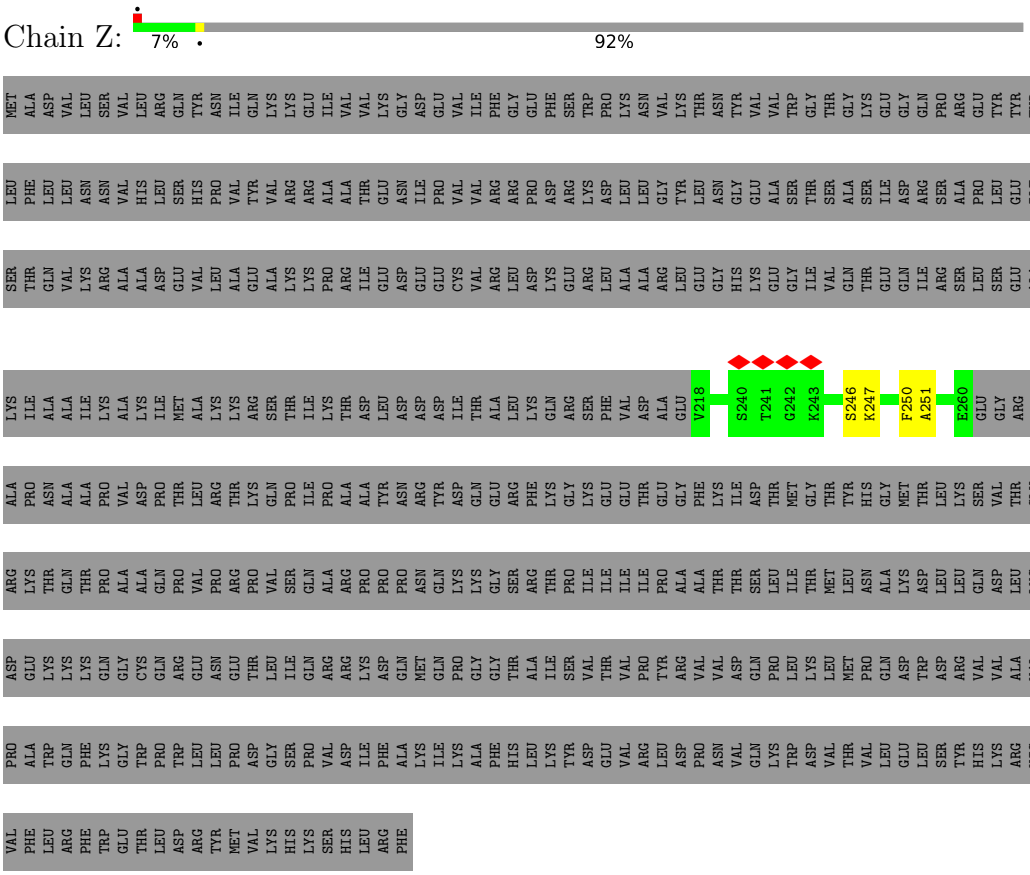
• Molecule 21: WD repeat-containing protein 61

Chain Y:



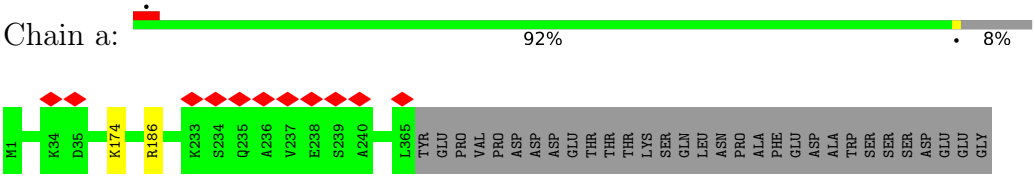
• Molecule 22: Parafibromin

Chain Z:



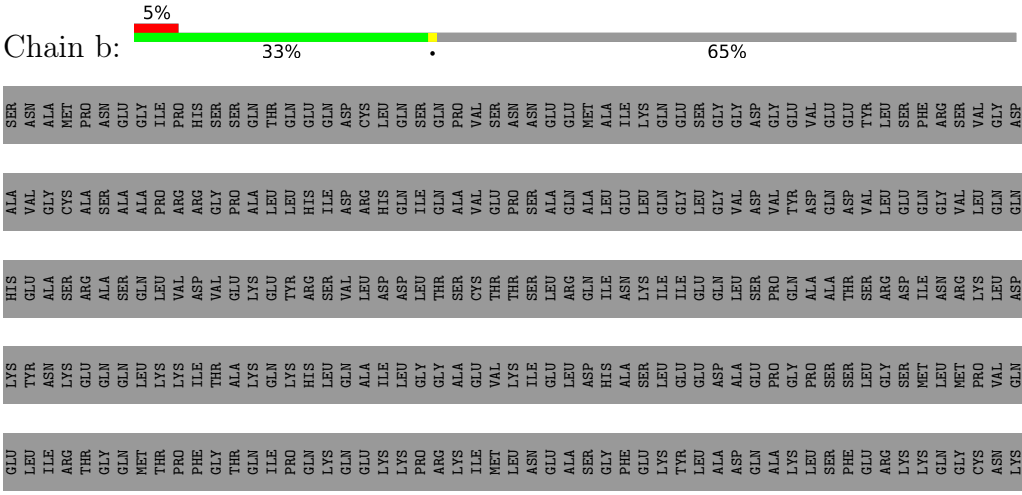
• Molecule 23: DNA excision repair protein ERCC-8

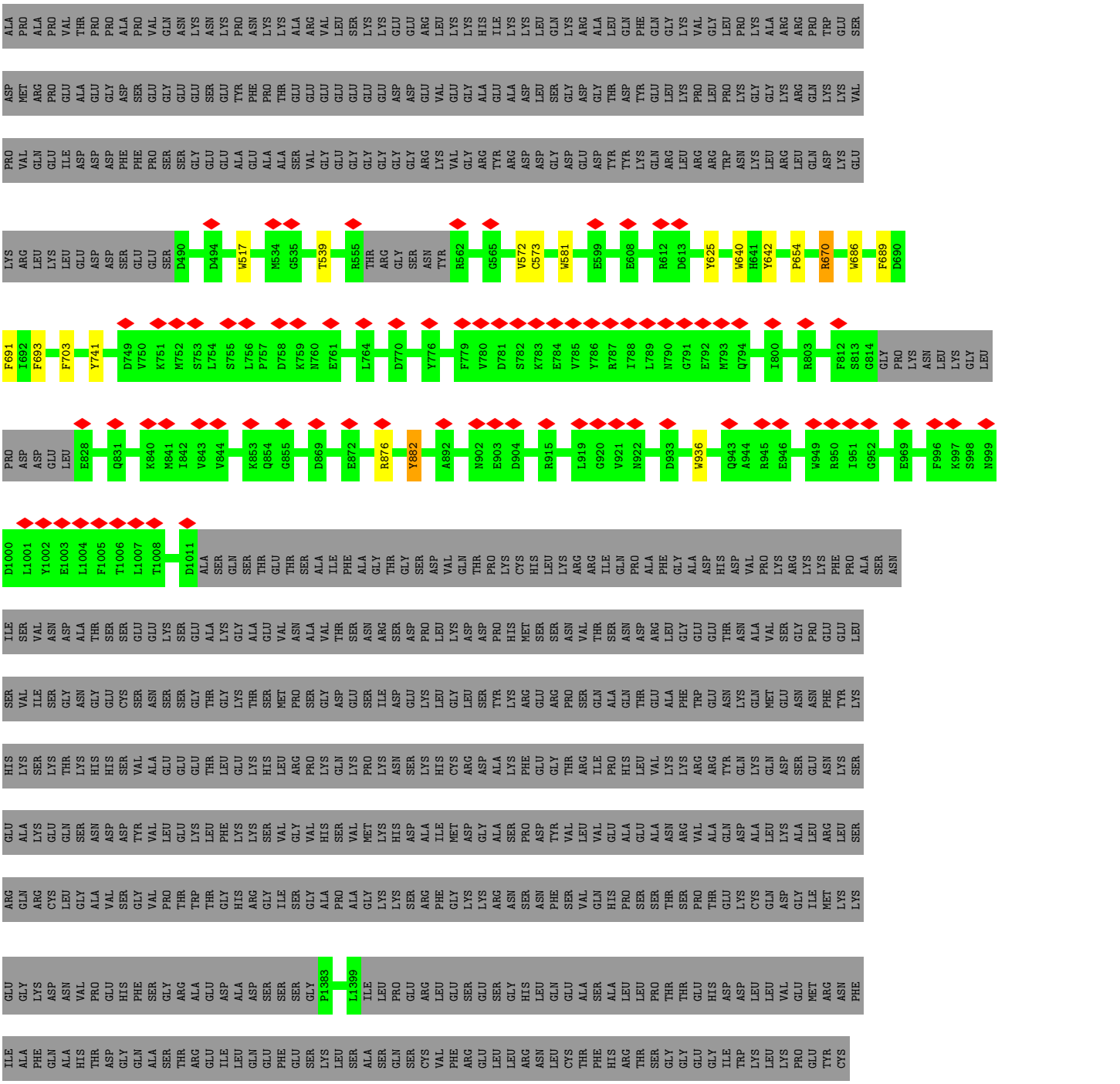
Chain a:



• Molecule 24: DNA excision repair protein ERCC-6

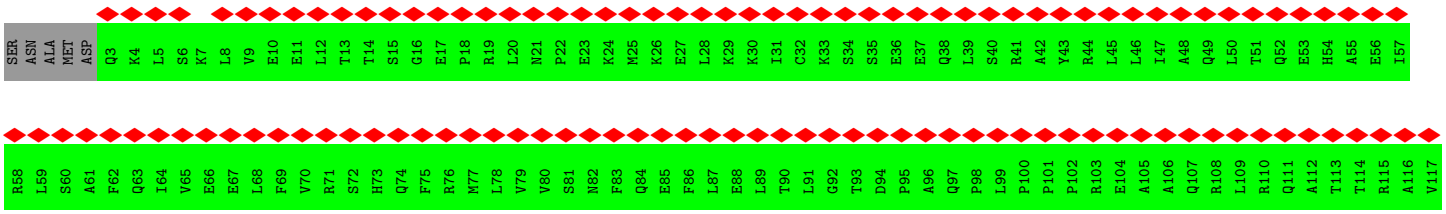
Chain b:

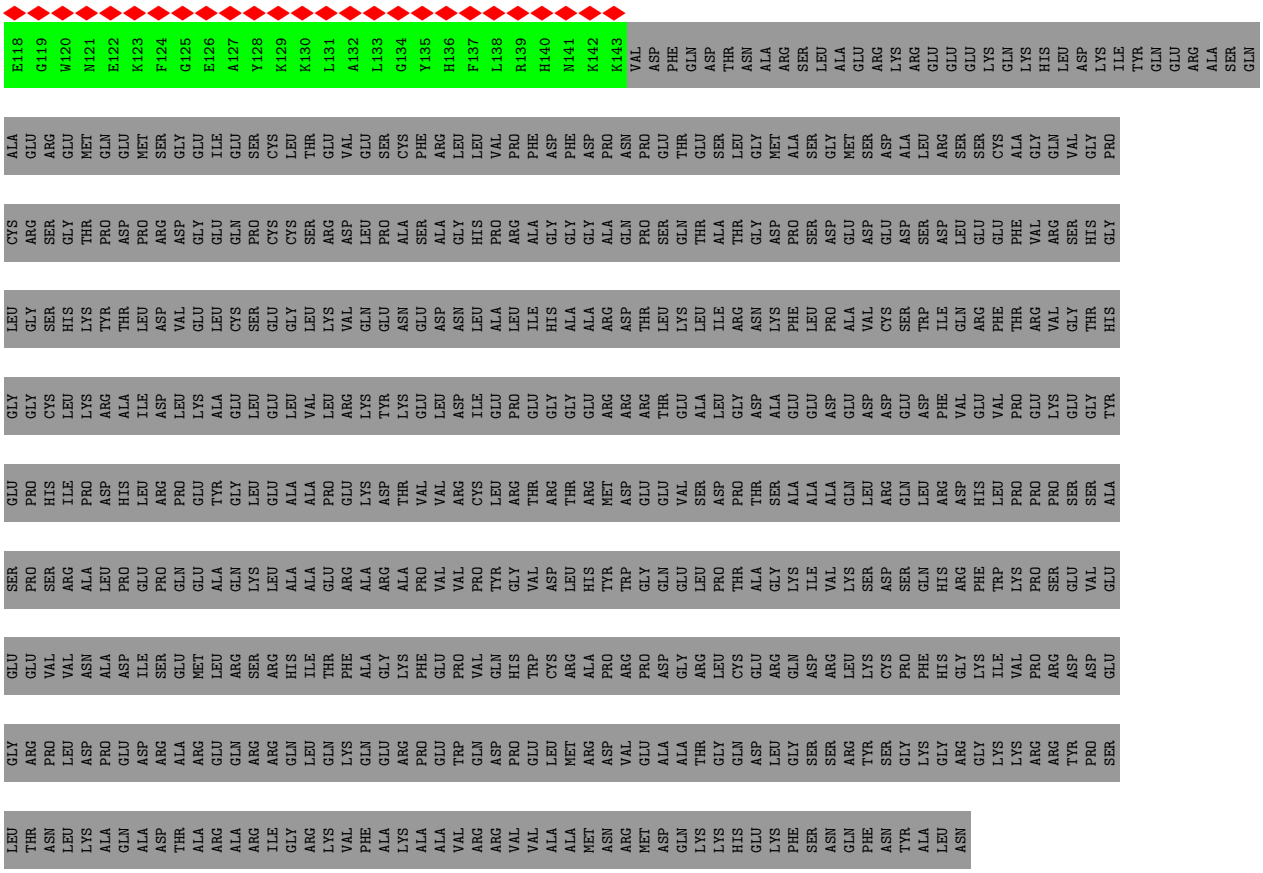




• Molecule 25: UV-stimulated scaffold protein A

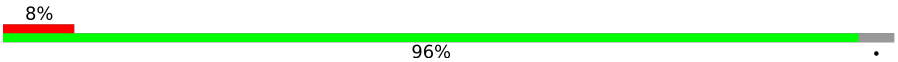
Chain c:

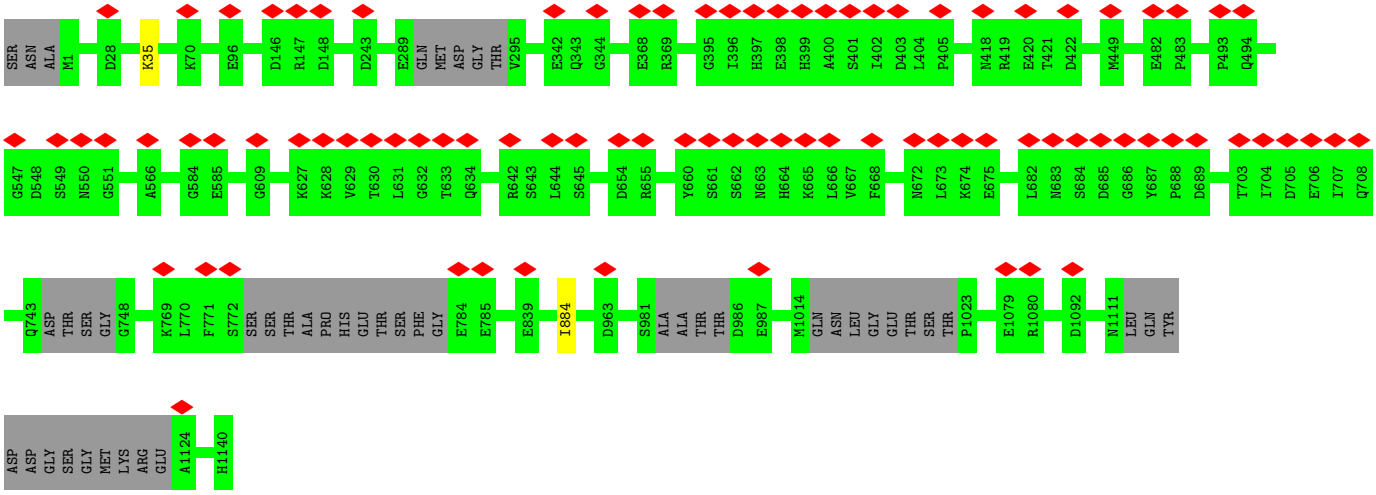




• Molecule 26: DNA damage-binding protein 1

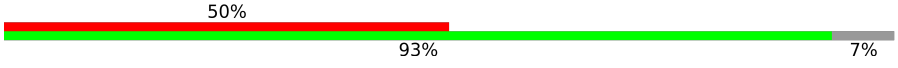
Chain d:

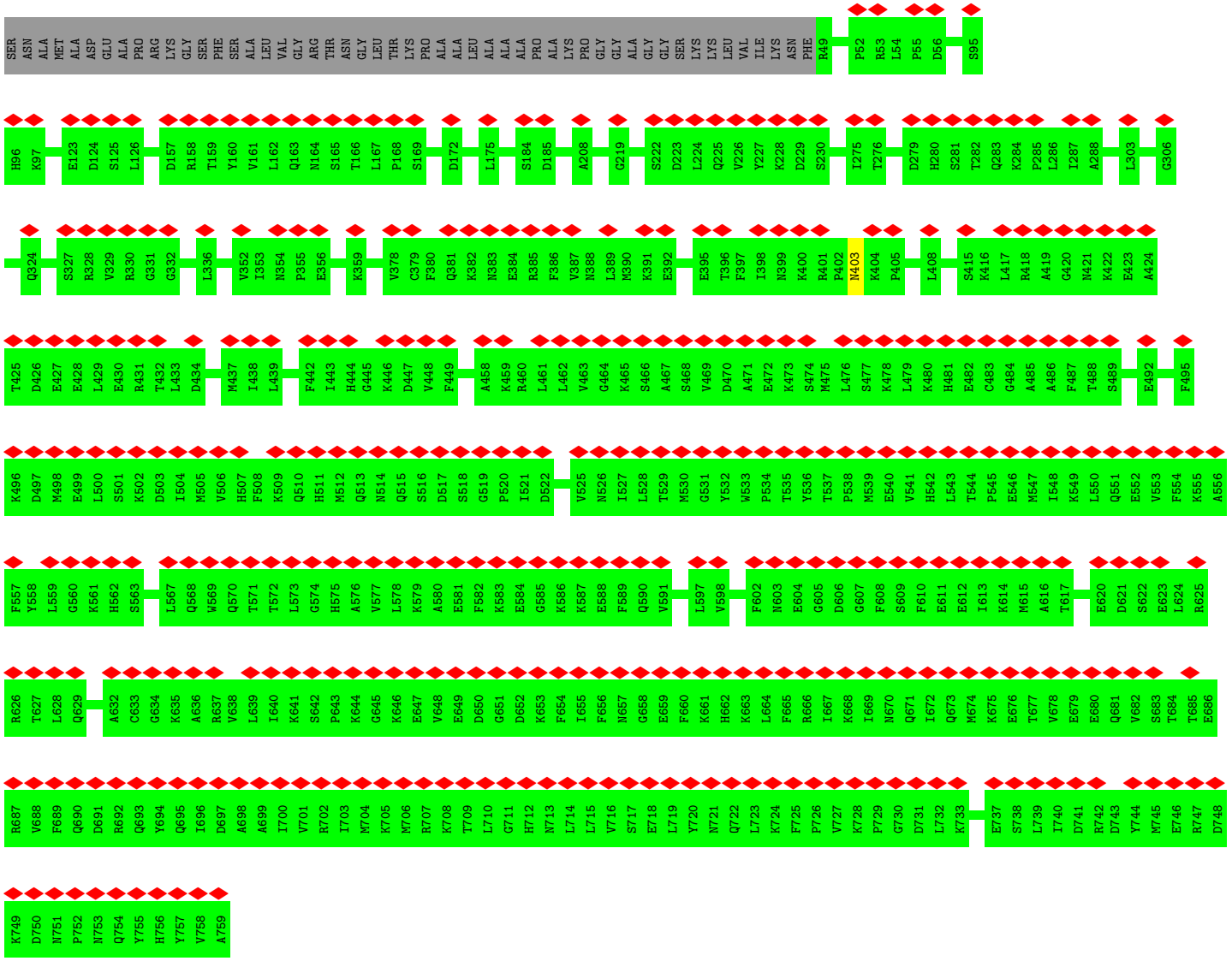




• Molecule 27: Cullin-4A

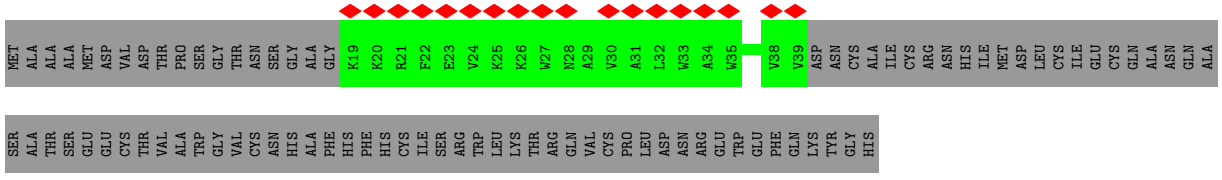
Chain e:





• Molecule 28: E3 ubiquitin-protein ligase RBX1

Chain f:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.112	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	440.99997, 440.99997, 440.99997	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.30	0/11382	0.54	1/15368 (0.0%)
2	B	0.32	0/9233	0.54	0/12463
3	C	0.35	0/2132	0.57	1/2896 (0.0%)
4	D	0.85	1/1027 (0.1%)	0.77	1/1384 (0.1%)
5	E	0.30	0/1751	0.54	0/2366
6	F	0.32	0/667	0.50	0/901
7	G	1.28	12/1365 (0.9%)	0.86	5/1853 (0.3%)
8	H	0.35	0/1207	0.53	0/1628
9	I	0.31	0/972	0.55	0/1316
10	J	0.32	0/542	0.51	0/730
11	K	0.31	0/939	0.49	0/1271
12	L	0.36	0/394	0.60	0/524
13	M	1.76	177/6770 (2.6%)	0.98	14/9119 (0.2%)
14	N	2.38	41/817 (5.0%)	1.00	0/1258
15	P	4.52	108/510 (21.2%)	2.04	32/793 (4.0%)
17	S	0.28	0/3559	0.52	0/4447
18	T	4.09	207/1056 (19.6%)	1.40	18/1624 (1.1%)
19	U	0.29	0/413	0.47	0/511
20	V	0.28	0/864	0.54	0/1073
21	Y	0.32	0/1199	0.62	1/1497 (0.1%)
22	Z	0.29	0/171	0.53	0/212
23	a	0.60	0/2908	0.67	1/3939 (0.0%)
24	b	1.16	29/4364 (0.7%)	0.73	2/5893 (0.0%)
25	c	0.22	0/563	0.42	0/702
26	d	0.35	0/7547	0.54	0/10071
27	e	0.29	0/2844	0.57	0/3552
28	f	0.23	0/83	0.61	0/102
All	All	1.02	575/65279 (0.9%)	0.69	76/87493 (0.1%)

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
1	A	0	1
13	M	0	1
16	R	0	1
23	a	0	1
26	d	0	2
27	e	0	1
All	All	0	7

All (575) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	P	43	G	C5-C4	-17.85	1.25	1.38
18	T	25	DT	C5-C6	-16.39	1.22	1.34
18	T	22	DC	N3-C4	-16.37	1.22	1.33
18	T	27	DG	N7-C5	-15.77	1.29	1.39
15	P	41	G	N9-C8	-15.30	1.27	1.37
15	P	41	G	C2-N3	-15.28	1.20	1.32
15	P	41	G	C5-C4	-15.18	1.27	1.38
15	P	41	G	C8-N7	-14.45	1.22	1.30
15	P	41	G	N1-C2	-14.23	1.26	1.37
15	P	44	G	C5-C4	-14.23	1.28	1.38
18	T	28	DA	N9-C4	-14.09	1.29	1.37
18	T	25	DT	N1-C2	-13.90	1.26	1.38
15	P	41	G	N9-C4	-13.88	1.26	1.38
15	P	44	G	N1-C2	-13.88	1.26	1.37
15	P	41	G	N3-C4	-13.82	1.25	1.35
15	P	43	G	C8-N7	-13.79	1.22	1.30
18	T	27	DG	C8-N7	-13.75	1.22	1.30
15	P	41	G	C6-N1	-13.66	1.29	1.39
18	T	22	DC	N1-C6	-13.28	1.29	1.37
15	P	42	A	C5-C4	-13.16	1.29	1.38
15	P	43	G	N9-C8	-13.10	1.28	1.37
15	P	42	A	C8-N7	-13.05	1.22	1.31
15	P	44	G	C8-N7	-12.93	1.23	1.30
18	T	26	DC	N3-C4	-12.78	1.25	1.33
18	T	25	DT	C4-C5	-12.74	1.33	1.45
18	T	25	DT	C2-N3	-12.73	1.27	1.37
15	P	43	G	N7-C5	-12.45	1.31	1.39
15	P	39	G	C2-N3	-12.34	1.22	1.32
15	P	44	G	C6-N1	-12.34	1.30	1.39
18	T	28	DA	C5-C4	-12.20	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	23	DT	C3'-O3'	-12.09	1.28	1.44
15	P	40	A	C5-C4	-12.02	1.30	1.38
18	T	27	DG	N9-C4	-11.93	1.28	1.38
15	P	43	G	C2-N3	-11.92	1.23	1.32
18	T	19	DA	N7-C5	-11.92	1.32	1.39
18	T	25	DT	N1-C6	-11.86	1.29	1.38
18	T	23	DT	C2-N3	-11.76	1.28	1.37
15	P	42	A	C6-N1	-11.70	1.27	1.35
18	T	21	DC	N1-C6	-11.70	1.30	1.37
18	T	23	DT	C2-O2	-11.55	1.13	1.22
18	T	24	DC	C2-O2	-11.48	1.14	1.24
18	T	25	DT	C5-C7	-11.41	1.43	1.50
15	P	39	G	C5-C4	-11.40	1.30	1.38
18	T	27	DG	C5-C4	-11.37	1.30	1.38
18	T	25	DT	N3-C4	-11.33	1.29	1.38
15	P	40	A	C5-C6	-11.23	1.30	1.41
18	T	27	DG	C5-C6	-11.18	1.31	1.42
18	T	24	DC	N3-C4	-11.17	1.26	1.33
15	P	40	A	C8-N7	-11.10	1.23	1.31
15	P	45	A	N9-C8	-11.08	1.28	1.37
18	T	21	DC	C3'-O3'	-11.06	1.29	1.44
18	T	23	DT	C5-C6	-10.92	1.26	1.34
15	P	44	G	N9-C8	-10.89	1.30	1.37
18	T	19	DA	C3'-O3'	-10.85	1.29	1.44
18	T	22	DC	C3'-O3'	-10.79	1.29	1.44
18	T	28	DA	N7-C5	-10.77	1.32	1.39
18	T	20	DT	C5-C6	-10.71	1.26	1.34
15	P	40	A	N7-C5	-10.70	1.32	1.39
15	P	44	G	C2-N3	-10.70	1.24	1.32
15	P	45	A	C5-C4	-10.59	1.31	1.38
18	T	23	DT	N1-C2	-10.52	1.29	1.38
18	T	21	DC	N3-C4	-10.50	1.26	1.33
15	P	43	G	N1-C2	-10.49	1.29	1.37
18	T	19	DA	C5-C4	-10.42	1.31	1.38
18	T	25	DT	C3'-O3'	-10.38	1.30	1.44
18	T	23	DT	N3-C4	-10.33	1.30	1.38
18	T	21	DC	C4-C5	-10.27	1.34	1.43
15	P	45	A	N9-C4	-10.26	1.31	1.37
15	P	40	A	N9-C8	-10.21	1.29	1.37
15	P	43	G	C6-N1	-10.17	1.32	1.39
18	T	24	DC	N1-C2	-10.12	1.30	1.40
18	T	24	DC	C2-N3	-10.12	1.27	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	P	42	A	N7-C5	-10.04	1.33	1.39
13	M	722	TYR	CD1-CE1	-9.94	1.24	1.39
13	M	693	TYR	CD1-CE1	-9.91	1.24	1.39
15	P	39	G	C5-C6	-9.91	1.32	1.42
15	P	42	A	N1-C2	-9.90	1.25	1.34
18	T	25	DT	C2-O2	-9.87	1.14	1.22
15	P	45	A	C8-N7	-9.84	1.24	1.31
18	T	20	DT	C3'-O3'	-9.82	1.31	1.44
14	N	13	DA	N9-C4	-9.80	1.31	1.37
18	T	27	DG	N9-C8	-9.77	1.31	1.37
18	T	26	DC	C3'-O3'	-9.74	1.31	1.44
15	P	40	A	C2-N3	-9.70	1.24	1.33
18	T	19	DA	C8-N7	-9.65	1.24	1.31
18	T	24	DC	C3'-O3'	-9.62	1.31	1.44
15	P	40	A	C6-N1	-9.51	1.28	1.35
18	T	24	DC	N1-C6	-9.50	1.31	1.37
18	T	28	DA	N3-C4	-9.46	1.29	1.34
18	T	26	DC	C2-O2	-9.42	1.16	1.24
18	T	23	DT	C1'-N1	-9.36	1.34	1.47
18	T	22	DC	C4-C5	-9.34	1.35	1.43
7	G	68	TYR	CD1-CE1	-9.32	1.25	1.39
15	P	40	A	N9-C4	-9.25	1.32	1.37
18	T	23	DT	C4'-C3'	-9.21	1.43	1.52
13	M	990	CYS	CB-SG	-9.18	1.66	1.82
18	T	28	DA	N9-C8	-9.17	1.30	1.37
18	T	22	DC	C4-N4	-9.08	1.25	1.33
18	T	22	DC	C2-N3	-9.06	1.28	1.35
15	P	41	G	N7-C5	-8.98	1.33	1.39
18	T	24	DC	C4-C5	-8.93	1.35	1.43
18	T	26	DC	C4-C5	-8.93	1.35	1.43
13	M	397	TRP	CB-CG	-8.92	1.34	1.50
13	M	755	VAL	CB-CG2	-8.91	1.34	1.52
18	T	19	DA	N9-C4	-8.91	1.32	1.37
18	T	26	DC	N1-C2	-8.88	1.31	1.40
15	P	39	G	N9-C8	-8.85	1.31	1.37
13	M	988	TYR	CD2-CE2	-8.84	1.26	1.39
13	M	912	GLN	CB-CG	-8.81	1.28	1.52
18	T	23	DT	C5-C7	-8.78	1.44	1.50
18	T	21	DC	C4-N4	-8.76	1.26	1.33
18	T	22	DC	C4'-C3'	-8.74	1.43	1.52
15	P	45	A	P-OP1	-8.73	1.34	1.49
18	T	21	DC	C2-N3	-8.73	1.28	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	34	DG	C3'-O3'	-8.72	1.32	1.44
13	M	471	TYR	CD1-CE1	-8.71	1.26	1.39
13	M	633	TYR	CD1-CE1	-8.68	1.26	1.39
13	M	693	TYR	CD2-CE2	-8.62	1.26	1.39
13	M	319	TRP	CB-CG	-8.60	1.34	1.50
7	G	66	VAL	CB-CG1	-8.55	1.34	1.52
13	M	316	GLU	CB-CG	-8.51	1.35	1.52
13	M	988	TYR	CD1-CE1	-8.51	1.26	1.39
18	T	25	DT	P-O5'	-8.47	1.51	1.59
15	P	39	G	C8-N7	-8.46	1.25	1.30
18	T	21	DC	P-O5'	-8.46	1.51	1.59
14	N	10	DC	N1-C6	-8.43	1.32	1.37
15	P	43	G	N3-C4	-8.41	1.29	1.35
24	b	741	TYR	CD1-CE1	-8.40	1.26	1.39
13	M	1034	PHE	CD2-CE2	-8.37	1.22	1.39
18	T	23	DT	C2'-C1'	-8.34	1.44	1.52
15	P	39	G	N1-C2	-8.31	1.31	1.37
15	P	41	G	C2-N2	-8.27	1.26	1.34
18	T	28	DA	C3'-O3'	-8.27	1.33	1.44
18	T	39	DA	C3'-O3'	-8.24	1.33	1.44
24	b	936	TRP	CB-CG	-8.24	1.35	1.50
18	T	20	DT	C4-C5	-8.22	1.37	1.45
15	P	39	G	N3-C4	-8.18	1.29	1.35
18	T	20	DT	N3-C4	-8.18	1.32	1.38
18	T	24	DC	C4'-C3'	-8.17	1.44	1.52
24	b	741	TYR	CD2-CE2	-8.16	1.27	1.39
18	T	16	DC	N1-C6	-8.14	1.32	1.37
18	T	22	DC	P-O5'	-8.14	1.51	1.59
18	T	38	DG	C3'-O3'	-8.14	1.33	1.44
15	P	44	G	N3-C4	-8.12	1.29	1.35
15	P	45	A	P-O5'	-8.12	1.51	1.59
13	M	741	VAL	CB-CG2	-8.09	1.35	1.52
13	M	893	TYR	CB-CG	-8.08	1.39	1.51
13	M	653	PHE	CB-CG	-8.07	1.37	1.51
18	T	26	DC	O4'-C1'	-8.07	1.32	1.42
14	N	43	DG	C3'-O3'	-8.06	1.33	1.44
18	T	28	DA	C6-N1	-8.05	1.29	1.35
15	P	42	A	C6-N6	-8.05	1.27	1.33
18	T	26	DC	N1-C6	-8.04	1.32	1.37
18	T	19	DA	N9-C8	-8.04	1.31	1.37
15	P	42	A	C5-C6	-8.00	1.33	1.41
14	N	13	DA	N7-C5	-8.00	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	P	44	G	P-OP1	-8.00	1.35	1.49
14	N	12	DC	C3'-O3'	-7.97	1.33	1.44
14	N	12	DC	N1-C6	-7.97	1.32	1.37
18	T	25	DT	C4-O4	-7.95	1.16	1.23
18	T	28	DA	C8-N7	-7.95	1.25	1.31
24	b	882	TYR	CD1-CE1	-7.95	1.27	1.39
18	T	27	DG	P-O5'	-7.95	1.51	1.59
18	T	23	DT	C4-C5	-7.94	1.37	1.45
15	P	44	G	N7-C5	-7.93	1.34	1.39
18	T	29	DT	C5-C6	-7.93	1.28	1.34
13	M	720	PHE	CB-CG	-7.92	1.37	1.51
13	M	394	TRP	CG-CD1	-7.91	1.25	1.36
15	P	45	A	C6-N1	-7.91	1.30	1.35
13	M	401	GLU	CB-CG	-7.88	1.37	1.52
13	M	722	TYR	CD2-CE2	-7.87	1.27	1.39
18	T	28	DA	C5-C6	-7.84	1.33	1.41
13	M	321	TYR	CD1-CE1	-7.83	1.27	1.39
18	T	20	DT	N1-C2	-7.80	1.31	1.38
15	P	45	A	N1-C2	-7.78	1.27	1.34
15	P	38	C	N1-C6	-7.77	1.32	1.37
18	T	23	DT	C4-O4	-7.75	1.16	1.23
18	T	25	DT	C2'-C1'	-7.75	1.44	1.52
13	M	319	TRP	CE3-CZ3	-7.71	1.25	1.38
13	M	524	TYR	CD2-CE2	-7.70	1.27	1.39
18	T	25	DT	C4'-O4'	-7.70	1.37	1.45
13	M	403	TRP	CE3-CZ3	-7.69	1.25	1.38
18	T	19	DA	C5-C6	-7.67	1.34	1.41
13	M	379	TYR	CB-CG	-7.66	1.40	1.51
18	T	23	DT	P-OP1	-7.66	1.35	1.49
18	T	19	DA	C6-N6	-7.65	1.27	1.33
13	M	693	TYR	CB-CG	-7.64	1.40	1.51
18	T	21	DC	C4'-C3'	-7.63	1.45	1.52
15	P	45	A	C6-N6	-7.60	1.27	1.33
15	P	40	A	N1-C2	-7.58	1.27	1.34
13	M	946	GLN	CB-CG	-7.57	1.32	1.52
15	P	44	G	C2-N2	-7.55	1.26	1.34
18	T	20	DT	N1-C6	-7.54	1.32	1.38
18	T	24	DC	C4-N4	-7.53	1.27	1.33
13	M	592	VAL	CB-CG2	-7.52	1.37	1.52
18	T	24	DC	C5-C6	-7.51	1.28	1.34
13	M	653	PHE	CD2-CE2	-7.50	1.24	1.39
15	P	42	A	N9-C4	-7.49	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	640	TRP	CB-CG	-7.49	1.36	1.50
24	b	882	TYR	CD2-CE2	-7.49	1.28	1.39
13	M	750	TYR	CE2-CZ	-7.48	1.28	1.38
14	N	44	DA	C3'-O3'	-7.48	1.34	1.44
18	T	28	DA	P-O5'	-7.47	1.52	1.59
18	T	26	DC	C2-N3	-7.44	1.29	1.35
15	P	41	G	C5-C6	-7.44	1.34	1.42
15	P	43	G	C6-O6	-7.43	1.17	1.24
7	G	18	PHE	CD1-CE1	-7.41	1.24	1.39
15	P	45	A	N7-C5	-7.41	1.34	1.39
13	M	319	TRP	CD2-CE2	-7.40	1.32	1.41
15	P	42	A	N9-C8	-7.39	1.31	1.37
18	T	22	DC	C1'-N1	-7.38	1.36	1.47
14	N	13	DA	C5-C4	-7.38	1.33	1.38
18	T	17	DC	N1-C6	-7.38	1.32	1.37
15	P	39	G	N7-C5	-7.36	1.34	1.39
13	M	989	VAL	CB-CG2	-7.29	1.37	1.52
15	P	44	G	C6-O6	-7.27	1.17	1.24
15	P	44	G	P-OP2	-7.27	1.36	1.49
13	M	590	TYR	CD1-CE1	-7.25	1.28	1.39
18	T	21	DC	N1-C2	-7.25	1.32	1.40
13	M	394	TRP	CB-CG	-7.24	1.37	1.50
13	M	383	TYR	CB-CG	-7.24	1.40	1.51
18	T	16	DC	C3'-O3'	-7.24	1.34	1.44
18	T	27	DG	N1-C2	-7.21	1.31	1.37
15	P	44	G	N9-C4	-7.20	1.32	1.38
18	T	18	DC	N1-C6	-7.20	1.32	1.37
13	M	375	PHE	CD1-CE1	-7.19	1.24	1.39
18	T	22	DC	C2-O2	-7.17	1.18	1.24
18	T	26	DC	C4-N4	-7.17	1.27	1.33
15	P	43	G	O3'-P	-7.14	1.52	1.61
18	T	17	DC	C3'-O3'	-7.14	1.34	1.44
13	M	321	TYR	CD2-CE2	-7.13	1.28	1.39
13	M	705	TRP	CB-CG	-7.11	1.37	1.50
13	M	373	VAL	CB-CG2	-7.09	1.38	1.52
15	P	44	G	C5-C6	-7.08	1.35	1.42
18	T	18	DC	C3'-O3'	-7.08	1.34	1.44
13	M	1141	TYR	CD1-CE1	-7.07	1.28	1.39
13	M	1034	PHE	CB-CG	-7.05	1.39	1.51
15	P	42	A	C2-N3	-7.03	1.27	1.33
14	N	14	DT	C1'-N1	-7.02	1.37	1.47
13	M	1034	PHE	CG-CD2	-7.01	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	24	DC	C4'-O4'	-6.99	1.38	1.45
13	M	603	ARG	CG-CD	-6.99	1.34	1.51
13	M	893	TYR	CD1-CE1	-6.98	1.28	1.39
15	P	39	G	C6-O6	-6.98	1.17	1.24
13	M	988	TYR	CE1-CZ	-6.98	1.29	1.38
18	T	19	DA	P-O5'	-6.96	1.52	1.59
18	T	20	DT	C2'-C1'	-6.93	1.45	1.52
18	T	22	DC	N1-C2	-6.93	1.33	1.40
18	T	19	DA	C6-N1	-6.91	1.30	1.35
13	M	539	PHE	CD1-CE1	-6.88	1.25	1.39
15	P	40	A	C6-N6	-6.86	1.28	1.33
13	M	893	TYR	CD2-CE2	-6.84	1.29	1.39
18	T	27	DG	C3'-O3'	-6.83	1.35	1.44
18	T	22	DC	O4'-C1'	-6.82	1.34	1.42
14	N	13	DA	C3'-O3'	-6.79	1.35	1.44
18	T	23	DT	C4'-O4'	-6.77	1.38	1.45
15	P	38	C	C4-C5	-6.77	1.37	1.43
13	M	1031	CYS	CB-SG	-6.76	1.70	1.82
7	G	17	TYR	CD1-CE1	-6.76	1.29	1.39
13	M	396	VAL	CB-CG2	-6.75	1.38	1.52
14	N	13	DA	N3-C4	-6.75	1.30	1.34
15	P	44	G	P-O5'	-6.75	1.53	1.59
18	T	24	DC	O4'-C1'	-6.73	1.34	1.42
18	T	38	DG	N9-C8	-6.73	1.33	1.37
18	T	29	DT	N3-C4	-6.65	1.33	1.38
24	b	882	TYR	CG-CD1	-6.64	1.30	1.39
15	P	45	A	P-OP2	-6.64	1.37	1.49
13	M	1034	PHE	CG-CD1	-6.63	1.28	1.38
7	G	68	TYR	CD2-CE2	-6.62	1.29	1.39
13	M	471	TYR	CB-CG	-6.62	1.41	1.51
18	T	20	DT	P-O5'	-6.62	1.53	1.59
15	P	39	G	C2-N2	-6.62	1.27	1.34
14	N	14	DT	N1-C6	-6.61	1.33	1.38
15	P	43	G	N9-C4	-6.61	1.32	1.38
18	T	21	DC	C5-C6	-6.60	1.29	1.34
15	P	45	A	N3-C4	-6.60	1.30	1.34
13	M	1014	ARG	CZ-NH1	-6.59	1.24	1.33
13	M	578	PHE	C-N	-6.58	1.21	1.34
15	P	42	A	P-O5'	-6.58	1.53	1.59
14	N	11	DT	C3'-O3'	-6.58	1.35	1.44
13	M	781	VAL	CB-CG2	-6.58	1.39	1.52
18	T	17	DC	C4-C5	-6.57	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	740	TYR	CB-CG	-6.56	1.41	1.51
18	T	20	DT	C5-C7	-6.55	1.46	1.50
18	T	20	DT	C2-N3	-6.54	1.32	1.37
18	T	21	DC	C1'-N1	-6.54	1.38	1.47
18	T	26	DC	C5-C6	-6.54	1.29	1.34
13	M	693	TYR	CE1-CZ	-6.54	1.30	1.38
18	T	28	DA	O4'-C1'	-6.54	1.34	1.42
13	M	633	TYR	CD2-CE2	-6.54	1.29	1.39
13	M	987	GLN	CB-CG	-6.54	1.34	1.52
18	T	20	DT	C4'-C3'	-6.52	1.46	1.52
13	M	399	TRP	CB-CG	-6.51	1.38	1.50
14	N	12	DC	N3-C4	-6.51	1.29	1.33
18	T	28	DA	N1-C2	-6.51	1.28	1.34
18	T	20	DT	C2-O2	-6.50	1.17	1.22
24	b	691	PHE	CD2-CE2	-6.49	1.26	1.39
18	T	25	DT	C1'-N1	-6.49	1.38	1.47
13	M	464	TYR	CD1-CE1	-6.48	1.29	1.39
15	P	39	G	C6-N1	-6.46	1.35	1.39
13	M	301	ARG	CG-CD	-6.44	1.35	1.51
13	M	397	TRP	CE3-CZ3	-6.43	1.27	1.38
18	T	23	DT	N1-C6	-6.43	1.33	1.38
14	N	9	DT	C5-C6	-6.41	1.29	1.34
15	P	43	G	C5-C6	-6.39	1.35	1.42
13	M	379	TYR	CE1-CZ	-6.38	1.30	1.38
15	P	43	G	P-O5'	-6.38	1.53	1.59
13	M	637	PHE	CB-CG	-6.37	1.40	1.51
15	P	38	C	N3-C4	-6.36	1.29	1.33
24	b	693	PHE	CD1-CE1	-6.36	1.26	1.39
14	N	8	DA	N9-C4	-6.35	1.34	1.37
24	b	689	PHE	CB-CG	-6.34	1.40	1.51
7	G	17	TYR	CD2-CE2	-6.32	1.29	1.39
18	T	25	DT	P-OP2	-6.30	1.38	1.49
15	P	37	U	N1-C6	-6.29	1.32	1.38
24	b	670	ARG	CG-CD	-6.28	1.36	1.51
14	N	11	DT	C2-N3	-6.28	1.32	1.37
15	P	42	A	N3-C4	-6.28	1.31	1.34
13	M	463	VAL	CB-CG1	-6.28	1.39	1.52
13	M	653	PHE	CG-CD2	-6.27	1.29	1.38
18	T	27	DG	C6-N1	-6.26	1.35	1.39
18	T	28	DA	C2'-C1'	-6.26	1.46	1.52
13	M	379	TYR	CD1-CE1	-6.25	1.29	1.39
18	T	37	DA	C3'-O3'	-6.25	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	691	PHE	CB-CG	-6.24	1.40	1.51
18	T	22	DC	P-OP1	-6.24	1.38	1.49
13	M	396	VAL	CB-CG1	-6.22	1.39	1.52
18	T	19	DA	N3-C4	-6.21	1.31	1.34
13	M	383	TYR	CD2-CE2	-6.21	1.30	1.39
14	N	10	DC	N3-C4	-6.21	1.29	1.33
13	M	633	TYR	CG-CD2	-6.19	1.31	1.39
18	T	21	DC	C4'-O4'	-6.17	1.38	1.45
24	b	741	TYR	CE1-CZ	-6.15	1.30	1.38
24	b	642	TYR	CD2-CE2	-6.12	1.30	1.39
13	M	471	TYR	CG-CD1	-6.10	1.31	1.39
13	M	653	PHE	CD1-CE1	-6.10	1.27	1.39
13	M	403	TRP	CD2-CE2	-6.09	1.34	1.41
18	T	23	DT	P-O5'	-6.08	1.53	1.59
13	M	750	TYR	CD2-CE2	-6.08	1.30	1.39
13	M	397	TRP	CG-CD2	-6.08	1.33	1.43
13	M	1134	TYR	CE2-CZ	-6.08	1.30	1.38
18	T	24	DC	P-O5'	-6.08	1.53	1.59
13	M	1030	ASN	CB-CG	-6.07	1.37	1.51
14	N	10	DC	C1'-N1	-6.07	1.38	1.47
13	M	750	TYR	CD1-CE1	-6.06	1.30	1.39
13	M	373	VAL	CB-CG1	-6.05	1.40	1.52
18	T	27	DG	O4'-C1'	-6.05	1.34	1.42
13	M	470	TYR	CE1-CZ	-6.05	1.30	1.38
13	M	961	GLU	CB-CG	-6.05	1.40	1.52
18	T	16	DC	N3-C4	-6.05	1.29	1.33
13	M	599	GLU	CB-CG	-6.05	1.40	1.52
14	N	14	DT	C3'-O3'	-6.04	1.36	1.44
18	T	22	DC	C5'-C4'	-6.04	1.44	1.51
18	T	20	DT	C4-O4	-6.03	1.17	1.23
14	N	13	DA	C5-C6	-6.03	1.35	1.41
13	M	942	PHE	CD2-CE2	-6.02	1.27	1.39
15	P	39	G	N9-C4	-6.02	1.33	1.38
18	T	15	DT	N1-C6	-6.02	1.34	1.38
13	M	795	PHE	CD2-CE2	-6.01	1.27	1.39
18	T	26	DC	O5'-C5'	-6.00	1.27	1.42
18	T	17	DC	C5-C6	-6.00	1.29	1.34
18	T	39	DA	N9-C4	-6.00	1.34	1.37
13	M	693	TYR	CG-CD2	-6.00	1.31	1.39
18	T	23	DT	P-OP2	-6.00	1.38	1.49
14	N	14	DT	N3-C4	-5.98	1.33	1.38
7	G	66	VAL	CB-CG2	-5.97	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	96	GLU	CD-OE1	-5.97	1.19	1.25
13	M	539	PHE	CD2-CE2	-5.97	1.27	1.39
13	M	1034	PHE	CE1-CZ	-5.97	1.26	1.37
13	M	1014	ARG	CD-NE	-5.97	1.36	1.46
13	M	949	VAL	CB-CG1	-5.96	1.40	1.52
18	T	37	DA	C5-C4	-5.95	1.34	1.38
18	T	21	DC	O4'-C1'	-5.94	1.35	1.42
18	T	14	DC	C3'-O3'	-5.94	1.36	1.44
13	M	686	PHE	CB-CG	-5.93	1.41	1.51
13	M	375	PHE	CE2-CZ	-5.93	1.26	1.37
24	b	642	TYR	CD1-CE1	-5.92	1.30	1.39
13	M	962	PHE	CD1-CE1	-5.91	1.27	1.39
13	M	365	PHE	CB-CG	-5.91	1.41	1.51
18	T	14	DC	N1-C6	-5.91	1.33	1.37
14	N	11	DT	C4-C5	-5.90	1.39	1.45
18	T	37	DA	N7-C5	-5.90	1.35	1.39
13	M	1065	TRP	CB-CG	-5.89	1.39	1.50
13	M	959	TYR	CD1-CE1	-5.89	1.30	1.39
15	P	37	U	C2-N3	-5.89	1.33	1.37
18	T	24	DC	C2'-C1'	-5.88	1.46	1.52
13	M	592	VAL	CB-CG1	-5.88	1.40	1.52
18	T	37	DA	N9-C8	-5.88	1.33	1.37
24	b	573	CYS	CB-SG	-5.88	1.72	1.81
15	P	32	C	C1'-N1	5.88	1.57	1.48
18	T	27	DG	P-OP1	-5.87	1.39	1.49
18	T	25	DT	P-OP1	-5.87	1.39	1.49
24	b	581	TRP	CB-CG	-5.87	1.39	1.50
13	M	394	TRP	CD2-CE2	-5.86	1.34	1.41
15	P	26	U	C1'-N1	5.86	1.57	1.48
13	M	962	PHE	CB-CG	-5.85	1.41	1.51
13	M	403	TRP	CB-CG	-5.84	1.39	1.50
13	M	600	PRO	CB-CG	-5.84	1.20	1.50
13	M	740	TYR	CD1-CE1	-5.84	1.30	1.39
18	T	41	DC	N1-C6	-5.84	1.33	1.37
13	M	400	ASP	CB-CG	-5.82	1.39	1.51
13	M	720	PHE	CD2-CE2	-5.82	1.27	1.39
18	T	17	DC	C2-N3	-5.82	1.31	1.35
15	P	44	G	O3'-P	-5.81	1.54	1.61
18	T	27	DG	C6-O6	-5.81	1.19	1.24
18	T	20	DT	P-OP1	-5.81	1.39	1.49
13	M	1034	PHE	CE2-CZ	-5.80	1.26	1.37
18	T	15	DT	C2-N3	-5.78	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	639	TYR	CD1-CE1	-5.76	1.30	1.39
18	T	29	DT	C2-N3	-5.75	1.33	1.37
18	T	40	DT	C3'-O3'	-5.74	1.36	1.44
24	b	686	TRP	CB-CG	-5.74	1.40	1.50
13	M	375	PHE	CD2-CE2	-5.73	1.27	1.39
15	P	41	G	C6-O6	-5.72	1.19	1.24
13	M	467	PHE	CD1-CE1	-5.71	1.27	1.39
13	M	927	PHE	CD1-CE1	-5.71	1.27	1.39
13	M	893	TYR	CG-CD2	-5.71	1.31	1.39
18	T	39	DA	C5-C4	-5.71	1.34	1.38
15	P	44	G	C2'-C1'	-5.71	1.47	1.53
13	M	942	PHE	CD1-CE1	-5.70	1.27	1.39
18	T	37	DA	C5-C6	-5.69	1.35	1.41
18	T	28	DA	C1'-N9	-5.68	1.39	1.47
18	T	21	DC	P-OP1	-5.67	1.39	1.49
13	M	612	GLU	CD-OE1	-5.66	1.19	1.25
18	T	27	DG	C2'-C1'	-5.65	1.46	1.52
13	M	795	PHE	CB-CG	-5.64	1.41	1.51
13	M	962	PHE	CD2-CE2	-5.64	1.27	1.39
15	P	45	A	C5-C6	-5.64	1.35	1.41
13	M	298	PHE	CB-CG	-5.64	1.41	1.51
13	M	524	TYR	CD1-CE1	-5.64	1.30	1.39
18	T	38	DG	P-O5'	-5.64	1.54	1.59
13	M	637	PHE	CD2-CE2	-5.63	1.27	1.39
18	T	19	DA	C2'-C1'	-5.63	1.46	1.52
13	M	722	TYR	CE1-CZ	-5.63	1.31	1.38
18	T	24	DC	P-OP1	-5.63	1.39	1.49
13	M	637	PHE	CG-CD1	-5.62	1.30	1.38
13	M	590	TYR	CD2-CE2	-5.62	1.30	1.39
18	T	29	DT	P-O5'	-5.62	1.54	1.59
13	M	633	TYR	CE1-CZ	-5.61	1.31	1.38
24	b	691	PHE	CG-CD1	-5.61	1.30	1.38
18	T	27	DG	C3'-C2'	-5.60	1.45	1.52
14	N	9	DT	C2-N3	-5.59	1.33	1.37
13	M	1027	VAL	CB-CG2	-5.59	1.41	1.52
13	M	927	PHE	CD2-CE2	-5.59	1.28	1.39
13	M	645	VAL	CB-CG1	-5.58	1.41	1.52
18	T	22	DC	C5-C6	-5.58	1.29	1.34
18	T	16	DC	C5-C6	-5.58	1.29	1.34
13	M	590	TYR	CE1-CZ	-5.58	1.31	1.38
13	M	549	ASN	CB-CG	-5.57	1.38	1.51
24	b	517	TRP	CB-CG	-5.55	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	15	DT	N3-C4	-5.55	1.34	1.38
7	G	68	TYR	CE1-CZ	-5.54	1.31	1.38
13	M	463	VAL	CB-CG2	-5.53	1.41	1.52
15	P	30	U	C1'-N1	5.53	1.57	1.48
18	T	11	DC	N1-C6	-5.53	1.33	1.37
13	M	686	PHE	CD1-CE1	-5.52	1.28	1.39
15	P	38	C	C5-C6	-5.52	1.29	1.34
13	M	403	TRP	CE2-CZ2	-5.51	1.30	1.39
15	P	42	A	C2'-C1'	-5.51	1.47	1.53
18	T	19	DA	C4'-O4'	-5.50	1.39	1.45
14	N	14	DT	C2-N3	-5.50	1.33	1.37
13	M	471	TYR	CG-CD2	-5.49	1.32	1.39
7	G	18	PHE	CD2-CE2	-5.48	1.28	1.39
14	N	13	DA	N9-C8	-5.48	1.33	1.37
15	P	43	G	C2-N2	-5.47	1.29	1.34
18	T	28	DA	C2-N3	-5.46	1.28	1.33
13	M	454	VAL	CB-CG1	-5.45	1.41	1.52
18	T	26	DC	C4'-C3'	-5.43	1.47	1.52
13	M	653	PHE	CG-CD1	-5.43	1.30	1.38
14	N	9	DT	C4-C5	-5.42	1.40	1.45
15	P	42	A	P-OP2	-5.42	1.39	1.49
15	P	37	U	N1-C2	-5.42	1.33	1.38
18	T	15	DT	N1-C2	-5.41	1.33	1.38
14	N	14	DT	C4-C5	-5.40	1.40	1.45
13	M	471	TYR	CD2-CE2	-5.40	1.31	1.39
18	T	26	DC	C2'-C1'	-5.39	1.46	1.52
7	G	58	VAL	CB-CG2	-5.38	1.41	1.52
13	M	795	PHE	CG-CD2	-5.38	1.30	1.38
15	P	42	A	C4'-C3'	-5.38	1.47	1.52
24	b	572	VAL	CB-CG1	-5.38	1.41	1.52
15	P	41	G	C2'-C1'	-5.37	1.47	1.53
13	M	602	VAL	CB-CG1	-5.37	1.41	1.52
13	M	1134	TYR	CD2-CE2	-5.37	1.31	1.39
13	M	1138	ARG	CG-CD	-5.36	1.38	1.51
15	P	45	A	C2-N3	-5.35	1.28	1.33
13	M	1141	TYR	CE1-CZ	-5.35	1.31	1.38
13	M	1161	PHE	CB-CG	-5.34	1.42	1.51
18	T	29	DT	C2-O2	-5.34	1.18	1.22
13	M	379	TYR	CE2-CZ	-5.34	1.31	1.38
13	M	1027	VAL	CB-CG1	-5.34	1.41	1.52
14	N	8	DA	N7-C5	-5.33	1.36	1.39
15	P	42	A	P-OP1	-5.33	1.39	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	722	TYR	CB-CG	-5.33	1.43	1.51
13	M	693	TYR	CE2-CZ	-5.32	1.31	1.38
18	T	24	DC	P-OP2	-5.32	1.40	1.49
14	N	10	DC	C5-C6	-5.31	1.30	1.34
14	N	33	DA	N7-C5	-5.31	1.36	1.39
18	T	37	DA	N9-C4	-5.31	1.34	1.37
13	M	566	PRO	CB-CG	-5.30	1.23	1.50
13	M	590	TYR	CE2-CZ	-5.30	1.31	1.38
7	G	58	VAL	CB-CG1	-5.30	1.41	1.52
13	M	988	TYR	CG-CD2	-5.29	1.32	1.39
15	P	40	A	N3-C4	-5.29	1.31	1.34
18	T	18	DC	C4'-O4'	-5.29	1.39	1.45
13	M	301	ARG	CB-CG	-5.28	1.38	1.52
13	M	693	TYR	CG-CD1	-5.28	1.32	1.39
13	M	471	TYR	CE1-CZ	-5.27	1.31	1.38
14	N	11	DT	N1-C6	-5.27	1.34	1.38
13	M	946	GLN	CG-CD	-5.26	1.39	1.51
18	T	25	DT	O4'-C1'	-5.26	1.35	1.42
15	P	41	G	C4'-C3'	-5.25	1.47	1.52
13	M	590	TYR	CB-CG	-5.24	1.43	1.51
14	N	12	DC	C5-C6	-5.24	1.30	1.34
13	M	524	TYR	CE2-CZ	-5.23	1.31	1.38
13	M	539	PHE	CB-CG	-5.22	1.42	1.51
13	M	1265	CYS	CB-SG	-5.21	1.73	1.81
14	N	34	DG	C5'-C4'	-5.21	1.45	1.51
13	M	893	TYR	CE2-CZ	-5.21	1.31	1.38
13	M	914	VAL	CB-CG2	-5.21	1.42	1.52
13	M	379	TYR	CA-CB	-5.20	1.42	1.53
13	M	379	TYR	CG-CD2	-5.20	1.32	1.39
18	T	41	DC	C5-C6	-5.19	1.30	1.34
18	T	16	DC	C4-C5	-5.19	1.38	1.43
18	T	28	DA	P-OP1	-5.18	1.40	1.49
13	M	930	VAL	CB-CG1	-5.18	1.42	1.52
18	T	27	DG	C4'-C3'	-5.17	1.47	1.52
24	b	703	PHE	CD1-CE1	-5.17	1.28	1.39
13	M	383	TYR	CD1-CE1	-5.17	1.31	1.39
24	b	654	PRO	CB-CG	-5.17	1.24	1.50
13	M	464	TYR	CB-CG	-5.17	1.44	1.51
13	M	962	PHE	CG-CD2	-5.17	1.30	1.38
24	b	691	PHE	CE2-CZ	-5.17	1.27	1.37
13	M	962	PHE	CG-CD1	-5.16	1.31	1.38
18	T	27	DG	C1'-N9	-5.16	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	722	TYR	CG-CD2	-5.16	1.32	1.39
18	T	38	DG	N7-C5	-5.15	1.36	1.39
14	N	15	DA	C3'-O3'	-5.15	1.37	1.44
18	T	29	DT	C4-C5	-5.14	1.40	1.45
13	M	464	TYR	CE1-CZ	-5.14	1.31	1.38
14	N	34	DG	C4'-C3'	-5.14	1.47	1.52
18	T	43	DA	N9-C4	-5.14	1.34	1.37
13	M	610	PHE	CB-CG	-5.13	1.42	1.51
13	M	602	VAL	CB-CG2	-5.13	1.42	1.52
18	T	41	DC	N3-C4	-5.11	1.30	1.33
18	T	37	DA	C8-N7	-5.11	1.27	1.31
13	M	653	PHE	CE2-CZ	-5.10	1.27	1.37
7	G	65	PHE	CB-CG	-5.10	1.42	1.51
18	T	22	DC	P-OP2	-5.10	1.40	1.49
18	T	38	DG	N9-C4	-5.10	1.33	1.38
13	M	893	TYR	CG-CD1	-5.09	1.32	1.39
18	T	15	DT	C4-C5	-5.09	1.40	1.45
13	M	397	TRP	CE2-CZ2	-5.08	1.31	1.39
24	b	625	TYR	CB-CG	-5.07	1.44	1.51
13	M	633	TYR	CB-CG	-5.07	1.44	1.51
18	T	22	DC	C3'-C2'	-5.07	1.46	1.52
18	T	26	DC	P-O5'	-5.06	1.54	1.59
18	T	27	DG	P-OP2	-5.06	1.40	1.49
24	b	689	PHE	CD1-CE1	-5.05	1.29	1.39
13	M	319	TRP	CZ3-CH2	-5.05	1.31	1.40
14	N	7	DG	C3'-O3'	-5.05	1.37	1.44
14	N	13	DA	C8-N7	-5.04	1.28	1.31
13	M	685	TYR	CD1-CE1	-5.03	1.31	1.39
14	N	9	DT	N3-C4	-5.03	1.34	1.38
13	M	720	PHE	CD1-CE1	-5.03	1.29	1.39
24	b	642	TYR	CE1-CZ	-5.02	1.32	1.38
24	b	689	PHE	CD2-CE2	-5.02	1.29	1.39
18	T	40	DT	C2-N3	-5.02	1.33	1.37
13	M	590	TYR	CG-CD2	-5.02	1.32	1.39
18	T	23	DT	O4'-C1'	-5.02	1.36	1.42
18	T	28	DA	C4'-O4'	-5.02	1.40	1.45
13	M	887	ASN	CA-CB	-5.01	1.40	1.53
14	N	12	DC	C4-C5	-5.01	1.39	1.43
18	T	28	DA	C4'-C3'	-5.01	1.47	1.52
13	M	595	GLN	CG-CD	-5.01	1.39	1.51
24	b	693	PHE	CG-CD1	-5.00	1.31	1.38

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	P	45	A	O5'-P-OP1	-15.91	91.38	105.70
13	M	1014	ARG	NE-CZ-NH1	-13.18	113.71	120.30
18	T	19	DA	O5'-P-OP2	-11.54	95.32	105.70
13	M	1014	ARG	NE-CZ-NH2	10.53	125.57	120.30
15	P	40	A	N1-C6-N6	-10.48	112.31	118.60
15	P	43	G	N1-C6-O6	-10.19	113.79	119.90
18	T	21	DC	O4'-C4'-C3'	-10.00	100.00	106.00
18	T	29	DT	O4'-C1'-N1	9.03	114.32	108.00
18	T	30	DG	O4'-C1'-C2'	-8.76	98.89	105.90
13	M	520	ARG	NE-CZ-NH2	-8.67	115.97	120.30
13	M	474	ASP	CB-CG-OD1	-8.41	110.73	118.30
15	P	43	G	C6-C5-N7	8.00	135.20	130.40
15	P	40	A	C4-C5-C6	-7.98	113.01	117.00
13	M	450	ARG	NE-CZ-NH2	7.91	124.25	120.30
15	P	45	A	N1-C6-N6	-7.77	113.94	118.60
15	P	41	G	O5'-P-OP1	-7.72	98.76	105.70
15	P	40	A	O5'-P-OP1	-7.47	98.98	105.70
18	T	30	DG	C4'-C3'-C2'	-7.43	96.41	103.10
15	P	43	G	C4-C5-N7	-7.32	107.87	110.80
13	M	473	ARG	NE-CZ-NH2	-7.28	116.66	120.30
13	M	603	ARG	NE-CZ-NH2	-7.11	116.74	120.30
18	T	30	DG	C8-N9-C4	-7.06	103.58	106.40
15	P	43	G	N9-C4-C5	6.96	108.19	105.40
23	a	186	ARG	NE-CZ-NH1	6.75	123.67	120.30
13	M	603	ARG	NE-CZ-NH1	6.70	123.65	120.30
15	P	44	G	C6-C5-N7	6.69	134.41	130.40
15	P	44	G	N9-C4-C5	6.67	108.07	105.40
15	P	42	A	C5-C6-N1	6.62	121.01	117.70
24	b	876	ARG	NE-CZ-NH2	-6.58	117.01	120.30
15	P	40	A	N9-C4-C5	-6.44	103.22	105.80
15	P	43	G	C5-C6-O6	6.43	132.46	128.60
18	T	22	DC	O4'-C4'-C3'	-6.37	101.95	104.50
4	D	138	ARG	NE-CZ-NH2	-6.36	117.12	120.30
24	b	670	ARG	NE-CZ-NH2	-6.33	117.14	120.30
15	P	43	G	C5-N7-C8	6.30	107.45	104.30
7	G	144	ARG	NE-CZ-NH1	6.25	123.42	120.30
18	T	30	DG	OP1-P-OP2	6.20	128.90	119.60
15	P	44	G	C4-C5-N7	-6.09	108.36	110.80
18	T	23	DT	O4'-C4'-C3'	-6.08	102.07	104.50
7	G	22	LEU	CA-CB-CG	6.04	129.19	115.30
13	M	1010	ARG	NE-CZ-NH1	5.93	123.26	120.30
18	T	29	DT	O4'-C1'-C2'	-5.88	101.20	105.90
15	P	44	G	OP2-P-O3'	5.86	118.10	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	P	39	G	N3-C4-C5	5.81	131.50	128.60
15	P	39	G	C4-C5-C6	-5.78	115.33	118.80
13	M	474	ASP	CB-CG-OD2	5.72	123.45	118.30
3	C	67	ARG	NE-CZ-NH2	-5.66	117.47	120.30
18	T	19	DA	O4'-C4'-C3'	-5.61	102.25	104.50
18	T	29	DT	C5-C4-O4	-5.60	120.98	124.90
15	P	33	A	O4'-C1'-N9	-5.59	103.72	108.20
15	P	45	A	C8-N9-C4	5.59	108.04	105.80
15	P	40	A	C4-C5-N7	5.57	113.49	110.70
15	P	42	A	OP2-P-O3'	5.53	117.37	105.20
15	P	41	G	C5-N7-C8	-5.50	101.55	104.30
13	M	1021	CYS	CA-CB-SG	-5.49	104.12	114.00
7	G	63	ARG	NE-CZ-NH1	5.43	123.02	120.30
15	P	40	A	C5-C6-N1	5.41	120.40	117.70
15	P	40	A	N1-C2-N3	-5.38	126.61	129.30
15	P	41	G	N3-C4-C5	5.35	131.28	128.60
18	T	26	DC	O5'-P-OP2	-5.33	100.91	105.70
18	T	25	DT	C4-C5-C7	5.31	122.19	119.00
18	T	24	DC	OP2-P-O3'	5.31	116.88	105.20
15	P	37	U	C5-C6-N1	5.30	125.35	122.70
13	M	709	ARG	NE-CZ-NH1	5.28	122.94	120.30
13	M	724	GLN	N-CA-CB	5.25	120.06	110.60
1	A	483	ARG	CG-CD-NE	5.25	122.83	111.80
18	T	23	DT	C4-C5-C7	5.21	122.12	119.00
18	T	29	DT	N3-C4-O4	5.19	123.01	119.90
15	P	41	G	C4-C5-C6	-5.17	115.70	118.80
7	G	16	ARG	NE-CZ-NH1	5.14	122.87	120.30
7	G	144	ARG	NE-CZ-NH2	-5.13	117.73	120.30
18	T	33	DT	C5-C4-O4	-5.13	121.31	124.90
15	P	37	U	C5-C4-O4	-5.06	122.86	125.90
15	P	45	A	C6-C5-N7	5.05	135.84	132.30
13	M	607	ARG	NE-CZ-NH2	-5.03	117.78	120.30
21	Y	190	ALA	C-N-CA	5.01	134.23	121.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	538	VAL	Peptide
13	M	575	CYS	Peptide
16	R	11	UNK	Peptide
23	a	174	LYS	Peptide

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Mol	Chain	Res	Type	Group
26	d	35	LYS	Peptide
26	d	884	ILE	Peptide
27	e	403	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11179	0	11313	104	0
2	B	9052	0	9087	56	0
3	C	2089	0	2031	14	0
4	D	1013	0	972	18	0
5	E	1720	0	1737	14	0
6	F	657	0	684	4	0
7	G	1334	0	1333	26	0
8	H	1186	0	1147	5	0
9	I	949	0	879	9	0
10	J	533	0	553	5	0
11	K	920	0	942	6	0
12	L	388	0	393	2	0
13	M	6648	0	6644	138	0
14	N	727	0	393	1	0
15	P	454	0	210	12	0
16	R	160	0	2	3	0
17	S	3560	0	940	8	0
18	T	947	0	519	13	0
19	U	416	0	111	0	0
20	V	868	0	212	3	0
21	Y	1200	0	341	15	0
22	Z	172	0	44	2	0
23	a	2849	0	2778	0	0
24	b	4261	0	4302	0	0
25	c	564	0	143	0	0
26	d	7439	0	6530	0	0
27	e	2845	0	753	0	0
28	f	84	0	20	0	0
29	A	2	0	0	0	0
29	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	C	1	0	0	0	0
29	I	2	0	0	0	0
29	J	1	0	0	0	0
29	L	1	0	0	0	0
30	A	1	0	0	0	0
All	All	64223	0	55013	407	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 (407) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:CYS:SG	1:A:184:CYS:HB3	1.83	1.18
13:M:926:GLU:OE1	13:M:981:TYR:OH	1.90	0.88
1:A:338:SER:OG	1:A:341:GLN:OE1	1.92	0.88
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.57	0.87
13:M:1014:ARG:NH1	13:M:1032:ALA:O	2.08	0.87
2:B:565:THR:OG1	2:B:610:ARG:O	1.95	0.85
13:M:886:ASP:OD1	13:M:887:ASN:N	2.12	0.83
13:M:1167:ILE:HD12	13:M:1232:LEU:HD11	1.60	0.81
1:A:266:MET:HE3	1:A:270:ALA:HB3	1.63	0.80
1:A:114:CYS:SG	1:A:184:CYS:CB	2.68	0.79
9:I:68:ILE:O	9:I:122:ARG:NH1	2.16	0.79
13:M:561:GLN:NE2	13:M:697:GLU:OE2	2.15	0.79
1:A:1190:GLN:O	1:A:1194:ASN:ND2	2.16	0.78
13:M:825:GLU:O	13:M:828:LYS:N	2.15	0.78
13:M:893:TYR:O	13:M:896:SER:OG	2.01	0.77
4:D:93:HIS:HB3	4:D:96:GLU:OE1	1.85	0.76
2:B:357:CYS:SG	2:B:361:LYS:NZ	2.58	0.76
4:D:90:LYS:HE2	4:D:130:ILE:HD12	1.66	0.75
2:B:924:ARG:NH1	3:C:62:GLU:OE1	2.21	0.74
13:M:445:THR:O	13:M:448:MET:N	2.20	0.74
2:B:352:GLY:O	2:B:361:LYS:NZ	2.20	0.74
1:A:374:SER:OG	1:A:376:ASP:OD1	2.06	0.73
2:B:430:ASN:ND2	16:R:20:UNK:O	2.22	0.72
1:A:70:ARG:NH2	1:A:75:ALA:O	2.21	0.72
1:A:576:GLN:O	1:A:590:GLN:NE2	2.23	0.72
1:A:538:VAL:HG12	1:A:539:GLN:H	1.53	0.72
13:M:445:THR:O	13:M:449:GLU:N	2.21	0.71
3:C:180:ALA:O	10:J:42:ARG:NH2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:TYR:OH	1:A:450:MET:O	2.08	0.71
1:A:549:THR:O	1:A:589:LYS:NZ	2.24	0.71
1:A:233:CYS:SG	1:A:244:ARG:NH1	2.64	0.70
1:A:67:ARG:NH2	15:P:33:A:OP1	2.24	0.70
2:B:198:GLU:OE2	2:B:388:TYR:OH	2.09	0.70
1:A:461:GLN:NE2	2:B:1090:GLU:OE2	2.24	0.70
13:M:692:PHE:O	13:M:694:TYR:N	2.25	0.70
2:B:957:THR:OG1	2:B:959:GLU:O	2.11	0.69
1:A:321:GLU:OE1	1:A:341:GLN:NE2	2.26	0.69
13:M:1145:ASN:O	13:M:1148:GLU:N	2.26	0.69
13:M:1148:GLU:N	13:M:1148:GLU:OE1	2.26	0.68
13:M:580:THR:O	13:M:582:GLU:N	2.26	0.68
1:A:266:MET:SD	18:T:30:DG:N3	2.67	0.68
1:A:457:ILE:HD11	1:A:515:ILE:HD12	1.76	0.68
1:A:431:PHE:HE2	15:P:33:A:H61	1.42	0.67
2:B:551:GLU:OE2	2:B:578:LYS:NZ	2.27	0.67
7:G:100:GLU:N	7:G:100:GLU:OE1	2.28	0.67
1:A:1182:GLN:O	1:A:1190:GLN:NE2	2.29	0.66
13:M:1145:ASN:OD1	13:M:1146:THR:N	2.28	0.66
2:B:329:GLY:O	2:B:335:ARG:NE	2.29	0.65
1:A:1198:GLU:OE1	1:A:1198:GLU:N	2.29	0.65
7:G:91:GLN:NE2	7:G:93:ASN:OD1	2.28	0.65
13:M:529:SER:OG	13:M:530:ALA:N	2.30	0.65
7:G:49:THR:OG1	7:G:50:THR:N	2.31	0.64
13:M:582:GLU:N	13:M:582:GLU:OE1	2.30	0.64
1:A:373:LEU:O	1:A:485:ASN:ND2	2.30	0.64
1:A:413:TYR:O	1:A:415:GLY:N	2.30	0.64
13:M:979:HIS:O	13:M:981:TYR:N	2.30	0.64
2:B:1104:ARG:NH1	2:B:1109:GLU:OE2	2.31	0.63
13:M:934:ASP:OD1	13:M:935:GLU:N	2.32	0.63
13:M:1031:CYS:SG	13:M:1032:ALA:N	2.72	0.62
3:C:190:ASN:O	3:C:193:ARG:NH1	2.33	0.62
7:G:149:GLY:O	7:G:160:ILE:N	2.33	0.62
1:A:668:PHE:CE1	1:A:672:ILE:HD11	2.35	0.62
2:B:841:ARG:NH2	15:P:35:A:N7	2.48	0.62
1:A:507:GLN:N	2:B:1105:GLU:OE2	2.33	0.62
13:M:551:ARG:NH1	13:M:552:ASP:OD1	2.32	0.62
13:M:1123:LEU:O	13:M:1126:ILE:N	2.33	0.62
1:A:1311:LEU:HD12	1:A:1332:GLN:HG3	1.82	0.61
11:K:63:VAL:HG22	11:K:71:ILE:HG22	1.82	0.61
2:B:210:LYS:NZ	2:B:212:ASP:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:50:ASN:O	9:I:51:SER:OG	2.16	0.61
13:M:474:ASP:OD1	13:M:474:ASP:N	2.22	0.61
13:M:572:ASP:OD1	13:M:572:ASP:N	2.33	0.61
2:B:927:ARG:NH1	2:B:1057:ASP:OD2	2.33	0.61
1:A:760:LEU:HD22	1:A:764:ASN:ND2	2.14	0.61
1:A:808:PRO:HG2	2:B:675:LEU:HD12	1.83	0.61
4:D:33:LEU:HD22	4:D:101:ALA:HB3	1.81	0.61
13:M:444:ASP:OD1	13:M:444:ASP:N	2.33	0.61
7:G:95:VAL:O	7:G:110:ARG:N	2.34	0.60
16:R:11:UNK:O	16:R:15:UNK:N	2.34	0.60
13:M:369:GLN:O	13:M:1026:LYS:NZ	2.30	0.60
1:A:659:GLU:OE2	1:A:985:ARG:NH1	2.34	0.60
8:H:71:ASP:OD2	8:H:142:TYR:OH	2.19	0.60
5:E:93:ARG:CZ	17:S:891:PHE:CA	2.79	0.60
1:A:41:ILE:HD12	1:A:255:VAL:HG11	1.83	0.60
2:B:794:VAL:HG12	2:B:967:ILE:HG22	1.83	0.60
1:A:862:ARG:NH2	1:A:1432:PHE:O	2.34	0.60
13:M:853:GLU:OE1	13:M:854:ASN:ND2	2.35	0.60
20:V:243:VAL:O	20:V:248:PRO:N	2.35	0.60
13:M:1108:ALA:HA	13:M:1111:LEU:HD12	1.84	0.59
5:E:134:GLU:OE2	5:E:181:ARG:NH2	2.36	0.58
13:M:800:ASN:OD1	13:M:801:GLY:N	2.36	0.58
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.86	0.58
13:M:699:SER:OG	13:M:701:GLN:N	2.36	0.58
1:A:266:MET:CE	18:T:30:DG:H2'	2.34	0.58
8:H:102:ASP:OD2	8:H:110:THR:OG1	2.21	0.58
21:Y:212:GLY:O	21:Y:230:GLY:N	2.37	0.58
13:M:870:GLU:OE1	13:M:870:GLU:N	2.36	0.58
13:M:1062:THR:HG21	13:M:1126:ILE:HD11	1.86	0.58
2:B:501:LEU:HD12	2:B:505:LEU:CD1	2.32	0.58
21:Y:48:LYS:N	21:Y:55:ASP:O	2.37	0.58
2:B:565:THR:HG21	2:B:580:PRO:HB3	1.86	0.58
5:E:56:THR:OG1	5:E:78:GLU:OE2	2.18	0.57
13:M:473:ARG:NE	13:M:473:ARG:HA	2.18	0.57
7:G:109:SER:O	7:G:112:SER:OG	2.22	0.56
2:B:413:LYS:O	2:B:417:ILE:HD12	2.03	0.56
4:D:36:GLU:OE2	4:D:84:ARG:NH1	2.39	0.56
13:M:787:SER:HG	13:M:792:HIS:CE1	2.21	0.56
1:A:421:ARG:NH1	1:A:444:TYR:OH	2.39	0.56
1:A:904:GLN:NE2	1:A:981:CYS:O	2.37	0.56
21:Y:172:ILE:O	21:Y:186:LEU:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:297:ARG:NE	13:M:372:GLU:OE2	2.39	0.56
1:A:1180:ASN:ND2	1:A:1183:SER:OG	2.38	0.56
13:M:565:GLU:N	13:M:565:GLU:OE1	2.39	0.56
13:M:1002:LYS:O	13:M:1005:LYS:N	2.38	0.56
5:E:120:ASP:OD1	5:E:121:MET:N	2.38	0.56
2:B:847:LYS:NZ	2:B:864:ASP:OD2	2.22	0.56
13:M:650:ASP:OD1	13:M:651:ASP:N	2.37	0.56
4:D:33:LEU:O	4:D:36:GLU:N	2.39	0.55
13:M:807:ASP:OD1	13:M:807:ASP:N	2.37	0.55
13:M:1151:ASN:ND2	13:M:1156:GLU:O	2.38	0.55
13:M:965:ARG:NH1	13:M:968:GLU:OE2	2.40	0.55
1:A:54:LEU:O	1:A:61:ARG:NH2	2.40	0.55
2:B:1090:GLU:OE1	2:B:1090:GLU:N	2.39	0.55
13:M:610:PHE:O	13:M:614:ALA:HB2	2.07	0.55
13:M:316:GLU:O	13:M:319:TRP:N	2.39	0.55
3:C:59:LEU:HD13	3:C:63:PHE:CD1	2.42	0.55
2:B:602:SER:OG	2:B:620:ARG:NH1	2.41	0.54
7:G:138:GLN:N	7:G:141:ASP:OD2	2.36	0.54
2:B:274:ARG:NH2	2:B:281:ASP:OD1	2.41	0.54
2:B:625:LEU:HD13	2:B:675:LEU:HD21	1.90	0.54
13:M:951:LYS:O	13:M:955:LEU:HD23	2.07	0.54
5:E:78:GLU:OE1	5:E:78:GLU:N	2.41	0.54
6:F:84:GLU:OE2	6:F:84:GLU:N	2.40	0.54
13:M:306:LYS:O	13:M:367:ARG:NH2	2.41	0.54
1:A:108:ARG:NH2	1:A:191:ILE:O	2.41	0.54
13:M:301:ARG:NH2	13:M:305:VAL:HG22	2.23	0.54
1:A:499:ASP:OD1	15:P:45:A:H4'	2.09	0.53
2:B:959:GLU:O	2:B:961:ILE:N	2.40	0.53
4:D:103:LEU:O	7:G:144:ARG:NH2	2.41	0.53
13:M:552:ASP:OD2	13:M:556:ARG:NE	2.41	0.53
13:M:1031:CYS:O	13:M:1033:GLY:N	2.42	0.53
1:A:413:TYR:O	1:A:449:HIS:ND1	2.41	0.53
17:S:279:PHE:O	17:S:284:ASP:N	2.40	0.53
13:M:613:ARG:O	13:M:613:ARG:HG3	2.09	0.52
1:A:461:GLN:OE1	1:A:502:ASN:ND2	2.42	0.52
13:M:287:ASN:O	13:M:290:ARG:HG2	2.10	0.52
1:A:862:ARG:NH1	2:B:1088:GLU:OE2	2.42	0.52
13:M:288:GLU:O	13:M:292:THR:N	2.41	0.52
1:A:889:LEU:O	1:A:890:ARG:NH1	2.42	0.52
13:M:802:GLU:N	13:M:802:GLU:OE2	2.42	0.52
3:C:7:PRO:O	11:K:104:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:622:LYS:HA	13:M:625:ARG:HE	1.75	0.52
1:A:865:ILE:HD13	1:A:1092:ALA:HB3	1.91	0.51
13:M:1056:SER:OG	13:M:1058:VAL:HG22	2.09	0.51
7:G:39:THR:O	7:G:43:GLY:N	2.40	0.51
13:M:551:ARG:HD3	13:M:601:LEU:HD11	1.92	0.51
21:Y:86:ALA:O	21:Y:104:ALA:N	2.43	0.51
3:C:86:ARG:HD3	11:K:11:LEU:HD11	1.93	0.51
13:M:1051:GLU:OE1	13:M:1051:GLU:N	2.44	0.51
13:M:329:THR:HG22	13:M:329:THR:O	2.11	0.51
13:M:1113:ARG:HA	13:M:1116:TYR:HE1	1.76	0.51
1:A:951:GLU:OE2	1:A:954:ARG:NH2	2.44	0.51
4:D:90:LYS:CE	4:D:130:ILE:HD12	2.36	0.51
13:M:532:LEU:HD11	13:M:584:VAL:HG23	1.93	0.51
13:M:1165:LYS:HE3	13:M:1167:ILE:CG2	2.41	0.51
13:M:574:VAL:O	13:M:574:VAL:HG13	2.10	0.50
7:G:90:THR:O	7:G:139:GLN:NE2	2.43	0.50
1:A:601:ASN:ND2	1:A:989:ASN:OD1	2.43	0.50
13:M:316:GLU:HG2	13:M:403:TRP:CE2	2.46	0.50
5:E:114:ALA:O	5:E:117:SER:OG	2.26	0.50
7:G:100:GLU:O	7:G:100:GLU:HG2	2.11	0.50
5:E:141:GLU:N	5:E:141:GLU:OE1	2.45	0.50
13:M:288:GLU:O	13:M:291:ALA:N	2.44	0.50
7:G:11:ILE:HD11	7:G:26:VAL:HG13	1.94	0.50
13:M:963:ILE:O	13:M:967:ASN:ND2	2.45	0.50
4:D:90:LYS:HD2	4:D:92:LEU:HD12	1.93	0.49
13:M:1156:GLU:OE1	13:M:1156:GLU:N	2.46	0.49
13:M:606:LEU:HD23	13:M:721:LEU:HD22	1.93	0.49
13:M:999:HIS:O	13:M:1003:ILE:HD12	2.12	0.49
1:A:481:THR:O	1:A:483:ARG:NE	2.46	0.49
2:B:312:GLN:NE2	9:I:22:ASN:OD1	2.46	0.49
13:M:550:LEU:HD22	13:M:689:ILE:CD1	2.43	0.49
13:M:575:CYS:SG	13:M:576:SER:N	2.85	0.49
13:M:1109:GLU:OE2	13:M:1113:ARG:NH1	2.46	0.49
21:Y:35:VAL:N	21:Y:47:TRP:O	2.44	0.49
21:Y:176:ASP:O	21:Y:180:GLY:N	2.38	0.49
1:A:1477:ALA:HB1	7:G:23:LEU:HD21	1.95	0.49
9:I:72:VAL:HG22	9:I:78:LEU:HD11	1.95	0.49
2:B:812:ARG:NH2	2:B:900:GLU:OE2	2.45	0.48
5:E:209:VAL:O	5:E:210:GLN:NE2	2.44	0.48
3:C:70:LEU:O	10:J:6:ARG:NE	2.40	0.48
21:Y:130:VAL:O	21:Y:144:LEU:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:THR:H	1:A:736:THR:HG21	1.79	0.48
2:B:777:ASN:O	10:J:47:ARG:NH1	2.40	0.48
2:B:975:ARG:NE	2:B:975:ARG:HA	4.43	0.48
13:M:450:ARG:HH21	13:M:450:ARG:HG3	1.77	0.48
13:M:1062:THR:O	13:M:1062:THR:HG22	2.14	0.48
13:M:394:TRP:O	13:M:398:GLN:HG3	2.12	0.48
1:A:523:ARG:NH1	6:F:127:ASP:OD2	2.47	0.48
7:G:21:ASN:OD1	7:G:24:ASN:HB2	2.14	0.48
9:I:50:ASN:ND2	9:I:52:CYS:O	2.46	0.48
1:A:1005:HIS:ND1	1:A:1007:ILE:HG22	2.29	0.48
2:B:15:ASP:OD1	2:B:15:ASP:N	2.47	0.48
13:M:865:LYS:O	13:M:869:HIS:ND1	2.41	0.48
1:A:1229:GLU:OE1	1:A:1229:GLU:N	2.45	0.48
13:M:780:ARG:O	13:M:846:HIS:N	2.47	0.48
21:Y:14:ALA:N	21:Y:296:GLN:O	2.47	0.48
13:M:311:ASP:N	13:M:311:ASP:OD1	2.38	0.48
13:M:795:PHE:CD2	13:M:910:LEU:HG	2.49	0.48
2:B:1035:ARG:NH1	2:B:1036:LYS:O	2.47	0.47
4:D:96:GLU:OE2	4:D:117:SER:HB3	2.14	0.47
18:T:20:DT:H2'	18:T:21:DC:O4'	2.13	0.47
21:Y:33:GLU:O	21:Y:49:TRP:N	2.48	0.47
4:D:34:ASN:OD1	4:D:102:ASN:ND2	2.48	0.47
7:G:20:PRO:O	7:G:21:ASN:HB3	2.14	0.47
21:Y:90:LEU:O	21:Y:99:ILE:N	2.41	0.47
1:A:455:ILE:HG23	1:A:520:MET:HE1	1.97	0.47
2:B:105:PRO:HG2	16:R:9:UNK:C	2.44	0.47
3:C:144:GLU:OE1	3:C:144:GLU:N	2.48	0.47
13:M:808:PHE:HB2	13:M:910:LEU:HD21	1.96	0.47
17:S:205:GLY:O	17:S:209:VAL:N	2.48	0.47
1:A:114:CYS:HG	1:A:184:CYS:CB	2.22	0.47
4:D:125:GLU:OE2	4:D:125:GLU:N	2.42	0.47
13:M:1111:LEU:O	13:M:1116:TYR:N	2.45	0.47
1:A:1297:THR:HG23	1:A:1297:THR:O	2.15	0.46
1:A:1357:THR:O	5:E:142:HIS:NE2	2.45	0.46
1:A:823:VAL:CG1	1:A:831:LEU:HD22	2.46	0.46
2:B:905:ASP:N	2:B:922:ARG:O	2.47	0.46
4:D:140:PHE:CZ	13:M:523:MET:HE1	2.50	0.46
1:A:1478:GLU:N	1:A:1478:GLU:OE1	2.49	0.46
2:B:808:SER:OG	2:B:1050:ARG:NH1	2.48	0.46
1:A:760:LEU:HD22	1:A:764:ASN:HD22	1.79	0.46
3:C:189:ASP:O	3:C:191:ALA:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:438:ARG:NH2	2:B:442:ASP:OD1	2.48	0.46
13:M:311:ASP:OD1	13:M:312:GLU:N	2.49	0.46
1:A:78:MET:O	2:B:1072:ARG:NH2	2.49	0.46
4:D:84:ARG:O	4:D:87:LEU:N	2.48	0.46
7:G:117:MET:HE2	7:G:135:ILE:HG13	1.98	0.46
1:A:67:ARG:NH2	15:P:33:A:H5'	2.31	0.45
1:A:321:GLU:OE1	1:A:321:GLU:N	2.50	0.45
1:A:844:ARG:NH2	2:B:501:LEU:HD13	2.31	0.45
7:G:117:MET:CE	7:G:135:ILE:HG13	2.46	0.45
9:I:109:ARG:HE	9:I:124:THR:HG21	1.81	0.45
13:M:296:GLU:HB2	13:M:996:LYS:HD2	1.98	0.45
13:M:754:ARG:HD2	13:M:754:ARG:O	2.16	0.45
13:M:755:VAL:HG23	13:M:923:PRO:HG2	1.98	0.45
13:M:1150:PHE:CZ	13:M:1161:PHE:CE2	3.04	0.45
13:M:296:GLU:OE2	13:M:300:LEU:HD21	2.16	0.45
13:M:542:THR:O	13:M:542:THR:HG23	2.15	0.45
13:M:915:SER:O	13:M:918:ARG:N	2.50	0.45
7:G:27:LYS:HE3	7:G:51:ILE:HD11	1.97	0.45
1:A:332:SER:HB3	18:T:29:DT:H5"	1.97	0.45
1:A:668:PHE:CZ	1:A:672:ILE:HD11	2.52	0.45
13:M:379:TYR:O	13:M:380:ARG:NH1	2.46	0.45
13:M:590:TYR:CZ	13:M:594:LEU:HD21	2.52	0.45
13:M:1023:MET:HE2	13:M:1027:VAL:HG23	1.99	0.45
21:Y:35:VAL:O	21:Y:47:TRP:N	2.40	0.45
5:E:112:PRO:HB3	18:T:7:DG:H5'	1.98	0.45
7:G:62:GLY:O	7:G:63:ARG:HG2	2.17	0.45
9:I:109:ARG:NE	9:I:124:THR:HG21	2.32	0.45
13:M:783:GLY:O	13:M:796:CYS:HA	2.17	0.45
13:M:1126:ILE:O	13:M:1130:LEU:HD23	2.16	0.45
1:A:823:VAL:HG11	1:A:831:LEU:HD22	1.98	0.45
13:M:554:TYR:O	13:M:556:ARG:N	2.49	0.45
4:D:76:ASN:O	4:D:79:THR:OG1	2.24	0.44
13:M:413:LEU:HD12	13:M:460:LEU:HD11	1.99	0.44
13:M:753:LEU:HD13	13:M:924:LEU:HD13	1.98	0.44
1:A:1378:LEU:HD21	1:A:1405:MET:HE3	2.00	0.44
13:M:1113:ARG:HA	13:M:1116:TYR:CE1	2.51	0.44
18:T:29:DT:O3'	18:T:30:DG:O4'	2.35	0.44
22:Z:247:LYS:O	22:Z:251:ALA:N	2.44	0.44
1:A:332:SER:HB3	18:T:29:DT:C5'	2.47	0.44
2:B:294:ASP:OD1	2:B:379:ARG:NH2	2.48	0.44
13:M:849:THR:HB	13:M:885:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:LEU:O	1:A:1396:ARG:NH1	2.50	0.44
13:M:613:ARG:HG3	13:M:671:ILE:HG23	1.99	0.44
18:T:29:DT:C4	18:T:30:DG:C2	3.05	0.44
21:Y:88:ILE:N	21:Y:102:ILE:O	2.39	0.44
1:A:883:ILE:HD11	1:A:1424:THR:HA	1.99	0.44
3:C:5:ASN:OD1	11:K:52:LYS:NZ	2.51	0.44
3:C:175:LYS:NZ	12:L:57:ALA:O	2.44	0.44
8:H:88:PHE:CD1	8:H:144:LEU:HD12	2.52	0.44
21:Y:214:ILE:O	21:Y:228:LEU:N	2.40	0.44
4:D:108:ALA:O	4:D:111:SER:OG	2.20	0.44
13:M:355:THR:HG23	13:M:356:ILE:N	2.33	0.44
1:A:272:ASN:ND2	18:T:30:DG:H2"	2.32	0.44
1:A:1189:ASP:OD2	1:A:1258:ARG:NE	2.51	0.44
8:H:71:ASP:OD1	8:H:72:ASP:N	2.51	0.44
11:K:7:PHE:CD1	11:K:11:LEU:HD12	2.53	0.44
13:M:522:ASP:C	13:M:523:MET:HG3	2.38	0.44
13:M:756:ALA:N	13:M:1139:THR:O	2.48	0.44
17:S:413:GLU:O	17:S:416:ILE:N	2.51	0.44
1:A:114:CYS:SG	1:A:184:CYS:SG	3.16	0.43
1:A:266:MET:CE	1:A:270:ALA:HB3	2.40	0.43
1:A:863:ARG:HB3	1:A:1414:ILE:HG22	2.00	0.43
4:D:138:ARG:HH12	13:M:523:MET:HG2	1.83	0.43
2:B:84:TYR:HE2	2:B:132:VAL:HG22	1.83	0.43
1:A:467:MET:SD	1:A:524:MET:HB3	2.58	0.43
11:K:81:TYR:OH	11:K:89:ASN:OD1	2.33	0.43
13:M:699:SER:OG	13:M:702:VAL:N	2.51	0.43
15:P:40:A:H2'	15:P:41:G:O4'	2.17	0.43
2:B:256:ILE:HD11	2:B:373:LEU:HD21	2.00	0.43
2:B:887:TYR:O	2:B:888:THR:HG22	2.17	0.43
5:E:93:ARG:NH2	17:S:891:PHE:CA	2.81	0.43
13:M:608:GLN:O	13:M:612:GLU:OE1	2.36	0.43
1:A:937:ASP:OD1	1:A:938:LEU:N	2.51	0.43
13:M:1119:LYS:O	13:M:1123:LEU:HD23	2.18	0.43
21:Y:287:SER:O	21:Y:303:CYS:N	2.46	0.43
2:B:628:VAL:HG12	2:B:629:GLU:O	2.18	0.43
3:C:123:ASN:OD1	3:C:124:SER:N	2.51	0.43
13:M:330:ILE:HG13	13:M:332:LEU:HD23	2.01	0.43
13:M:966:VAL:O	13:M:970:GLY:N	2.46	0.43
13:M:1002:LYS:O	13:M:1003:ILE:C	2.57	0.43
20:V:206:LYS:O	20:V:208:ARG:N	2.49	0.43
2:B:850:ASP:OD1	2:B:850:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:1145:ASN:HB3	13:M:1148:GLU:OE1	2.19	0.43
1:A:1471:PHE:O	6:F:64:ARG:NH1	2.47	0.43
13:M:473:ARG:NH2	13:M:520:ARG:HE	2.16	0.43
1:A:1475:LEU:HB2	7:G:66:VAL:HG21	2.00	0.43
13:M:755:VAL:HG23	13:M:755:VAL:O	2.17	0.43
22:Z:246:SER:O	22:Z:250:PHE:N	2.42	0.42
2:B:347:MET:HE1	2:B:365:LEU:HD22	2.00	0.42
13:M:303:ILE:HG21	13:M:404:THR:HG21	2.01	0.42
13:M:1018:VAL:HG12	13:M:1023:MET:O	2.19	0.42
1:A:255:VAL:HG23	1:A:280:LEU:HD22	2.01	0.42
4:D:108:ALA:HB1	4:D:112:LYS:HZ3	1.84	0.42
7:G:27:LYS:O	7:G:30:LEU:N	2.51	0.42
1:A:94:VAL:HG21	1:A:311:GLN:HA	2.01	0.42
1:A:381:PRO:HG2	1:A:384:ILE:HD12	2.01	0.42
1:A:413:TYR:HB3	1:A:414:PRO:HD3	2.01	0.42
17:S:535:LEU:O	17:S:539:ALA:N	2.47	0.42
6:F:100:ARG:NH2	6:F:121:ASP:O	2.52	0.42
7:G:1:MET:O	7:G:77:PHE:HA	2.19	0.42
13:M:559:THR:HG22	13:M:560:GLU:N	2.35	0.42
13:M:671:ILE:HG22	13:M:671:ILE:O	2.18	0.42
2:B:1091:ARG:NH2	2:B:1092:ASP:OD1	2.53	0.42
13:M:864:VAL:O	13:M:868:VAL:HG13	2.20	0.42
13:M:866:ARG:O	13:M:870:GLU:OE1	2.38	0.42
15:P:36:A:H2'	15:P:37:U:C6	2.54	0.42
1:A:410:ASN:OD1	1:A:449:HIS:NE2	2.46	0.42
1:A:967:ARG:NH2	1:A:1326:GLY:O	2.52	0.42
1:A:266:MET:SD	18:T:30:DG:H2'	2.60	0.42
1:A:595:ILE:HD11	1:A:675:VAL:HG11	2.02	0.42
1:A:695:ASP:OD1	1:A:695:ASP:N	2.52	0.42
2:B:967:ILE:HG21	2:B:1048:TYR:OH	2.18	0.42
17:S:649:ALA:O	17:S:652:GLY:N	2.53	0.42
1:A:431:PHE:HE2	15:P:33:A:N6	2.12	0.42
2:B:629:GLU:N	2:B:632:LYS:O	2.41	0.42
13:M:702:VAL:HG23	13:M:703:GLN:OE1	2.20	0.42
1:A:1433:GLU:OE1	18:T:17:DC:H4'	2.19	0.41
7:G:79:PRO:HB3	7:G:147:ILE:HD13	2.02	0.41
13:M:381:LYS:O	13:M:384:VAL:N	2.46	0.41
13:M:855:ARG:NE	13:M:1275:PHE:HD2	2.18	0.41
13:M:889:LEU:HG	13:M:930:VAL:HG11	2.00	0.41
13:M:1057:ARG:NH1	13:M:1134:TYR:CE1	2.88	0.41
5:E:110:MET:HG2	5:E:114:ALA:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:382:GLU:HB3	13:M:1121:ILE:HG22	2.01	0.41
13:M:672:ASP:OD1	13:M:672:ASP:N	2.52	0.41
5:E:84:ILE:HG22	14:N:45:DG:P	2.60	0.41
13:M:937:ILE:HG23	13:M:938:LEU:N	2.36	0.41
1:A:431:PHE:CE2	15:P:33:A:N6	2.84	0.41
1:A:883:ILE:O	1:A:883:ILE:HG22	2.20	0.41
1:A:875:TYR:HE2	1:A:1470:CYS:HG	1.68	0.41
5:E:127:LEU:HD23	5:E:127:LEU:H	1.86	0.41
1:A:962:ASP:HB3	1:A:1043:ILE:HG23	2.02	0.41
7:G:60:GLN:O	7:G:62:GLY:O	2.39	0.41
13:M:758:TYR:CD1	13:M:759:ARG:N	2.89	0.41
4:D:126:GLU:O	4:D:130:ILE:HG12	2.21	0.41
9:I:49:ASP:OD1	9:I:49:ASP:N	2.49	0.41
12:L:25:GLU:O	12:L:25:GLU:HG2	2.20	0.41
1:A:388:MET:HE2	1:A:505:LEU:HB2	2.03	0.41
13:M:332:LEU:HD11	13:M:740:TYR:HB2	2.02	0.41
13:M:832:ASP:O	13:M:835:THR:HG22	2.21	0.41
1:A:349:ARG:NH2	2:B:1070:LEU:HD21	2.35	0.41
3:C:210:GLU:O	3:C:210:GLU:HG2	2.21	0.41
7:G:18:PHE:N	7:G:18:PHE:CD1	2.87	0.41
7:G:166:ASP:HB3	13:M:516:LYS:HB2	2.03	0.41
13:M:894:MET:SD	13:M:912:GLN:HG3	2.61	0.41
13:M:917:ALA:O	13:M:921:GLN:HG3	2.21	0.41
15:P:27:A:O2'	15:P:28:U:OP1	2.26	0.41
1:A:848:ILE:HG21	2:B:496:ALA:HB1	2.03	0.41
1:A:883:ILE:HD11	1:A:1424:THR:HG22	2.03	0.41
2:B:735:VAL:HG21	10:J:55:LEU:HD13	2.02	0.41
2:B:962:THR:O	10:J:9:THR:HG23	2.21	0.40
13:M:301:ARG:HD2	13:M:401:GLU:HG2	2.03	0.40
13:M:541:LEU:HD23	13:M:541:LEU:O	2.21	0.40
13:M:1053:LEU:O	13:M:1056:SER:OG	2.30	0.40
13:M:1107:PHE:HA	13:M:1110:GLU:HG2	2.02	0.40
1:A:67:ARG:HH21	15:P:33:A:H5'	1.86	0.40
1:A:457:ILE:HD11	1:A:515:ILE:HG23	2.03	0.40
8:H:49:PRO:O	8:H:147:LYS:NZ	2.50	0.40
13:M:1111:LEU:HD13	13:M:1119:LYS:HB2	2.02	0.40
15:P:36:A:H2'	15:P:37:U:H6	1.87	0.40
21:Y:214:ILE:N	21:Y:228:LEU:O	2.38	0.40
1:A:266:MET:SD	18:T:30:DG:C4	3.15	0.40
1:A:630:VAL:HG21	1:A:652:LEU:HD21	2.04	0.40
1:A:811:ILE:HD12	9:I:79:PRO:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:785:TYR:O	2:B:786:THR:OG1	2.37	0.40
13:M:1156:GLU:HG2	13:M:1161:PHE:CE2	2.56	0.40
1:A:286:ILE:HD12	1:A:309:LEU:HD23	2.04	0.40
1:A:1212:LEU:HD11	1:A:1289:GLU:HB2	2.03	0.40
2:B:864:ASP:OD1	2:B:865:VAL:N	2.51	0.40
3:C:105:VAL:HG11	3:C:115:VAL:HG22	2.03	0.40
13:M:1150:PHE:HD1	13:M:1275:PHE:CE1	2.39	0.40
17:S:507:TYR:O	17:S:512:GLU:N	2.45	0.40
18:T:42:DA:H4'	18:T:43:DA:OP1	2.21	0.40
20:V:292:ALA:C	20:V:294:GLU:H	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1402/1970 (71%)	1365 (97%)	37 (3%)	0	100	100
2	B	1123/1174 (96%)	1076 (96%)	47 (4%)	0	100	100
3	C	256/275 (93%)	249 (97%)	7 (3%)	0	100	100
4	D	126/142 (89%)	118 (94%)	8 (6%)	0	100	100
5	E	207/210 (99%)	204 (99%)	3 (1%)	0	100	100
6	F	80/127 (63%)	75 (94%)	5 (6%)	0	100	100
7	G	169/172 (98%)	158 (94%)	11 (6%)	0	100	100
8	H	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
9	I	115/125 (92%)	111 (96%)	4 (4%)	0	100	100
10	J	65/67 (97%)	65 (100%)	0	0	100	100
11	K	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
12	L	44/58 (76%)	40 (91%)	4 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	M	788/1729 (46%)	711 (90%)	75 (10%)	2 (0%)	41 76
17	S	888/1179 (75%)	842 (95%)	46 (5%)	0	100 100
19	U	98/666 (15%)	82 (84%)	14 (14%)	2 (2%)	7 34
20	V	209/531 (39%)	174 (83%)	31 (15%)	4 (2%)	8 36
21	Y	298/305 (98%)	278 (93%)	20 (7%)	0	100 100
22	Z	41/531 (8%)	40 (98%)	1 (2%)	0	100 100
23	a	363/396 (92%)	342 (94%)	21 (6%)	0	100 100
24	b	512/1496 (34%)	470 (92%)	42 (8%)	0	100 100
25	c	139/712 (20%)	136 (98%)	3 (2%)	0	100 100
26	d	1082/1143 (95%)	1004 (93%)	78 (7%)	0	100 100
27	e	709/762 (93%)	652 (92%)	57 (8%)	0	100 100
28	f	19/108 (18%)	18 (95%)	1 (5%)	0	100 100
All	All	8992/14145 (64%)	8463 (94%)	521 (6%)	8 (0%)	54 85

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	V	248	PRO
19	U	481	GLY
19	U	463	PRO
20	V	238	GLU
20	V	259	ASP
20	V	301	ASN
13	M	946	GLN
13	M	581	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1242/1749 (71%)	1240 (100%)	2 (0%)	93 98

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	992/1027 (97%)	990 (100%)	2 (0%)	93 98
3	C	237/252 (94%)	237 (100%)	0	100 100
4	D	108/126 (86%)	107 (99%)	1 (1%)	78 92
5	E	191/192 (100%)	190 (100%)	1 (0%)	88 96
6	F	71/111 (64%)	71 (100%)	0	100 100
7	G	147/153 (96%)	147 (100%)	0	100 100
8	H	129/131 (98%)	129 (100%)	0	100 100
9	I	105/112 (94%)	105 (100%)	0	100 100
10	J	56/56 (100%)	56 (100%)	0	100 100
11	K	104/106 (98%)	104 (100%)	0	100 100
12	L	43/55 (78%)	43 (100%)	0	100 100
13	M	722/1524 (47%)	717 (99%)	5 (1%)	84 94
23	a	320/348 (92%)	320 (100%)	0	100 100
24	b	466/1299 (36%)	463 (99%)	3 (1%)	86 95
26	d	689/1001 (69%)	689 (100%)	0	100 100
All	All	5622/8242 (68%)	5608 (100%)	14 (0%)	93 98

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	ARG
1	A	1149	ARG
2	B	1072	ARG
2	B	1080	ARG
4	D	48	ASN
5	E	166	ARG
13	M	759	ARG
13	M	1098	ARG
13	M	1113	ARG
13	M	1138	ARG
13	M	1251	LYS
24	b	539	THR
24	b	670	ARG
24	b	882	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	93	HIS
13	M	561	GLN
23	a	183	GLN
26	d	370	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	20/45 (44%)	9 (45%)	1 (5%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	26	U
15	P	27	A
15	P	28	U
15	P	29	A
15	P	30	U
15	P	33	A
15	P	34	A
15	P	35	A
15	P	36	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	27	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

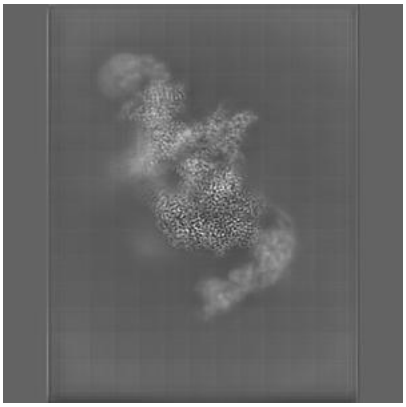
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13015. These allow visual inspection of the internal detail of the map and identification of artifacts.

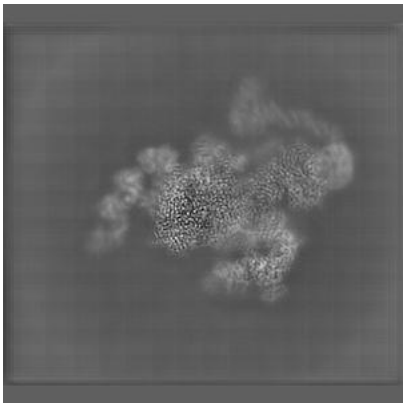
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

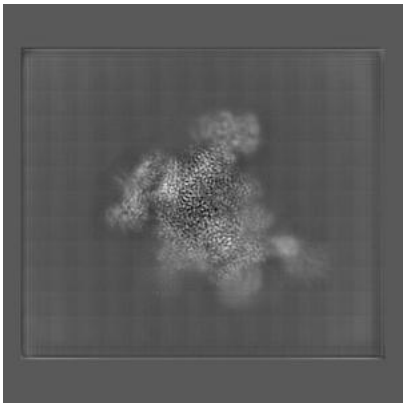
6.1.1 Primary map



X



Y

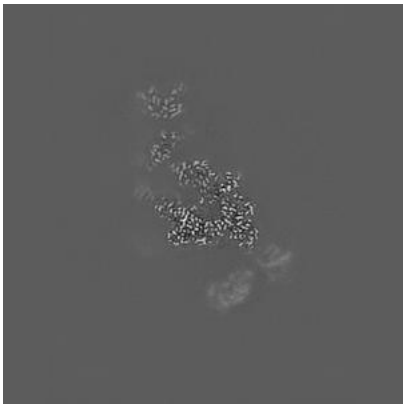


Z

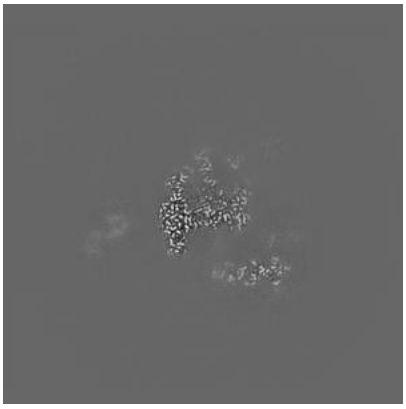
The images above show the map projected in three orthogonal directions.

6.2 Central slices

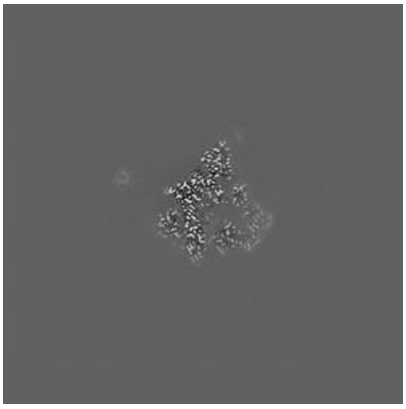
6.2.1 Primary map



X Index: 210



Y Index: 210

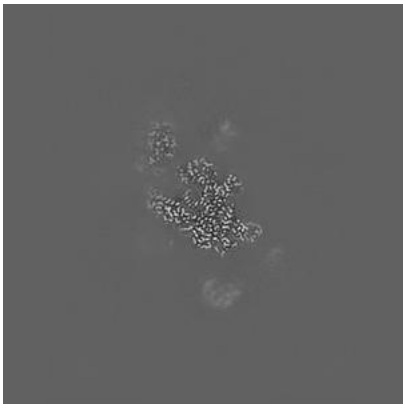


Z Index: 210

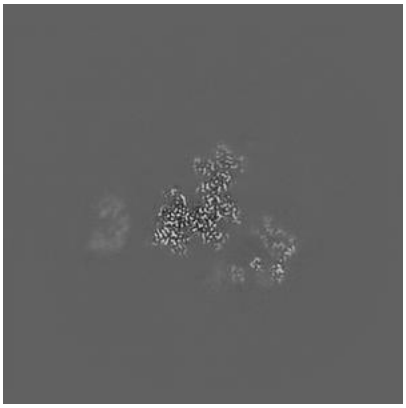
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

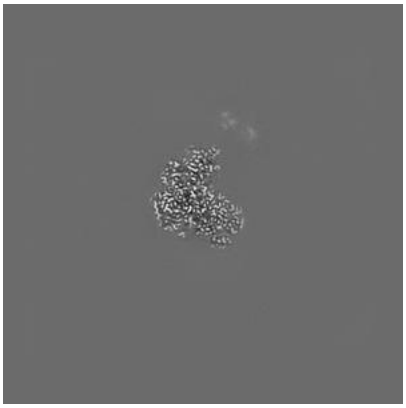
6.3.1 Primary map



X Index: 197



Y Index: 222



Z Index: 183

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

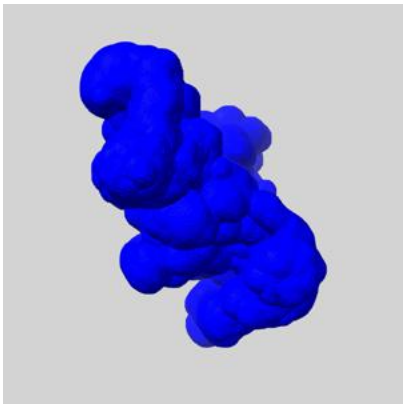
6.5 Mask visualisation (i)

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

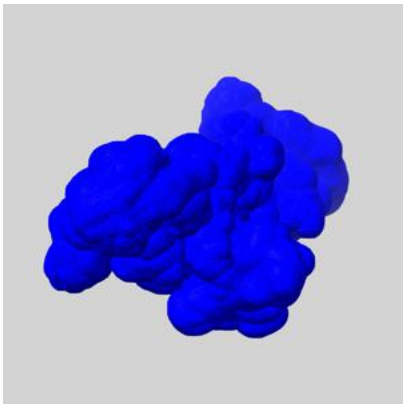
A mask typically either:

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

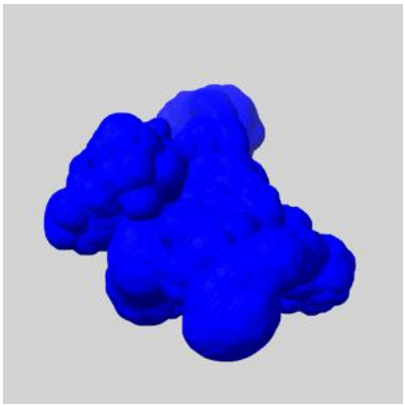
6.5.1 emd_13015_msk_1.map (i)



X

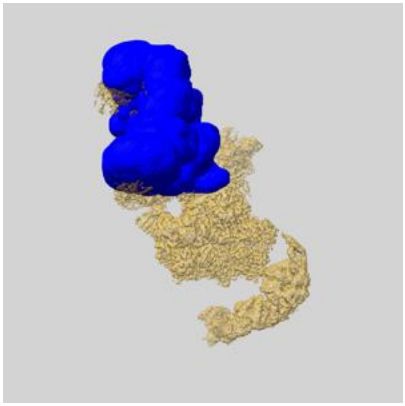


Y

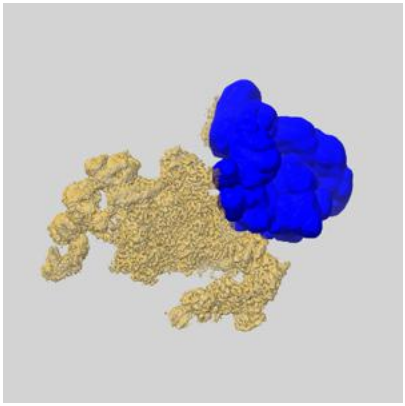


Z

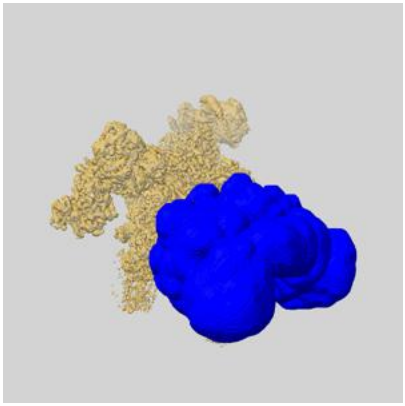
6.5.2 emd_13015_msk_2.map (i)



X

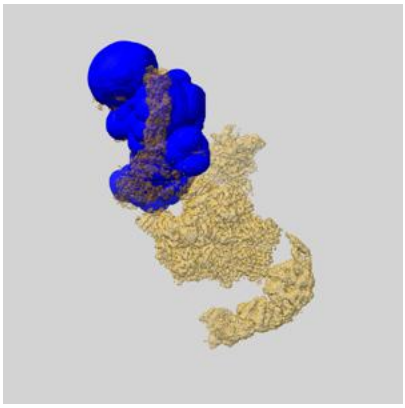


Y

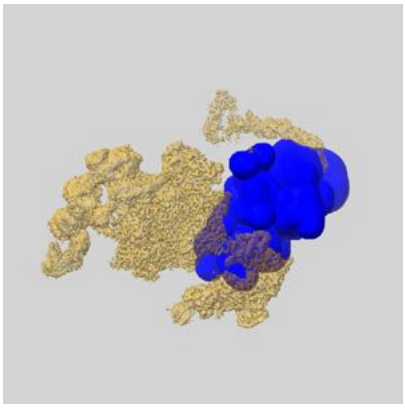


Z

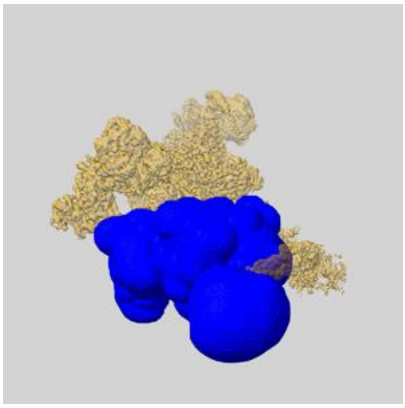
6.5.3 emd_13015_msk_3.map



X

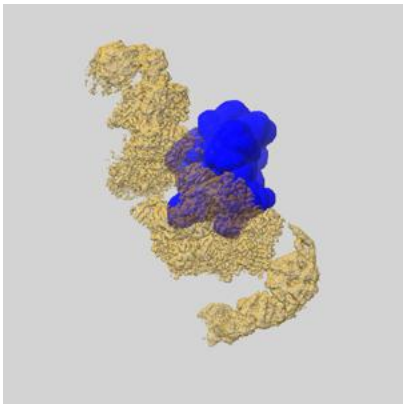


Y

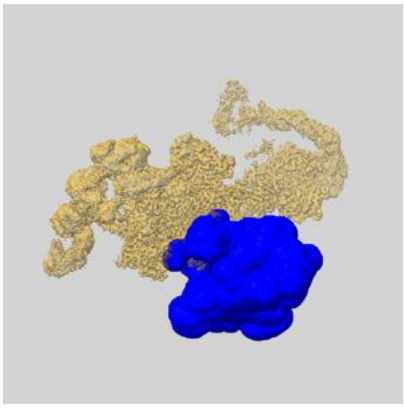


Z

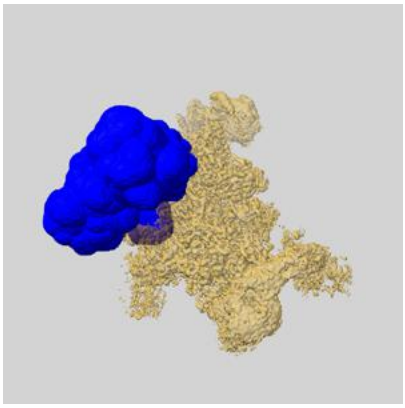
6.5.4 emd_13015_msk_4.map



X

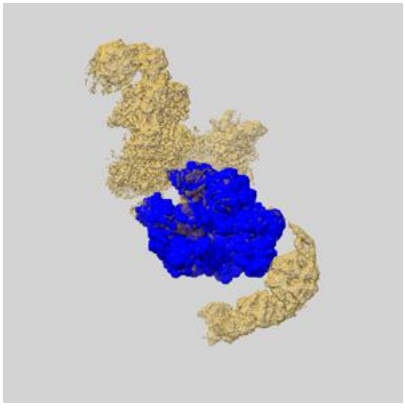


Y

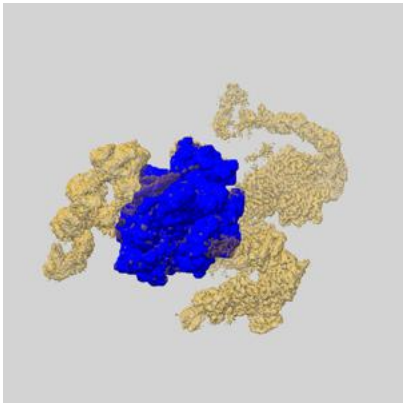


Z

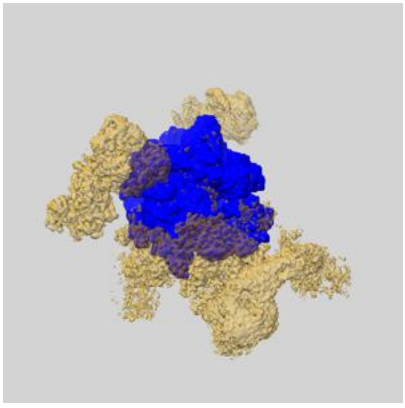
6.5.5 emd_13015_msk_5.map



X



Y

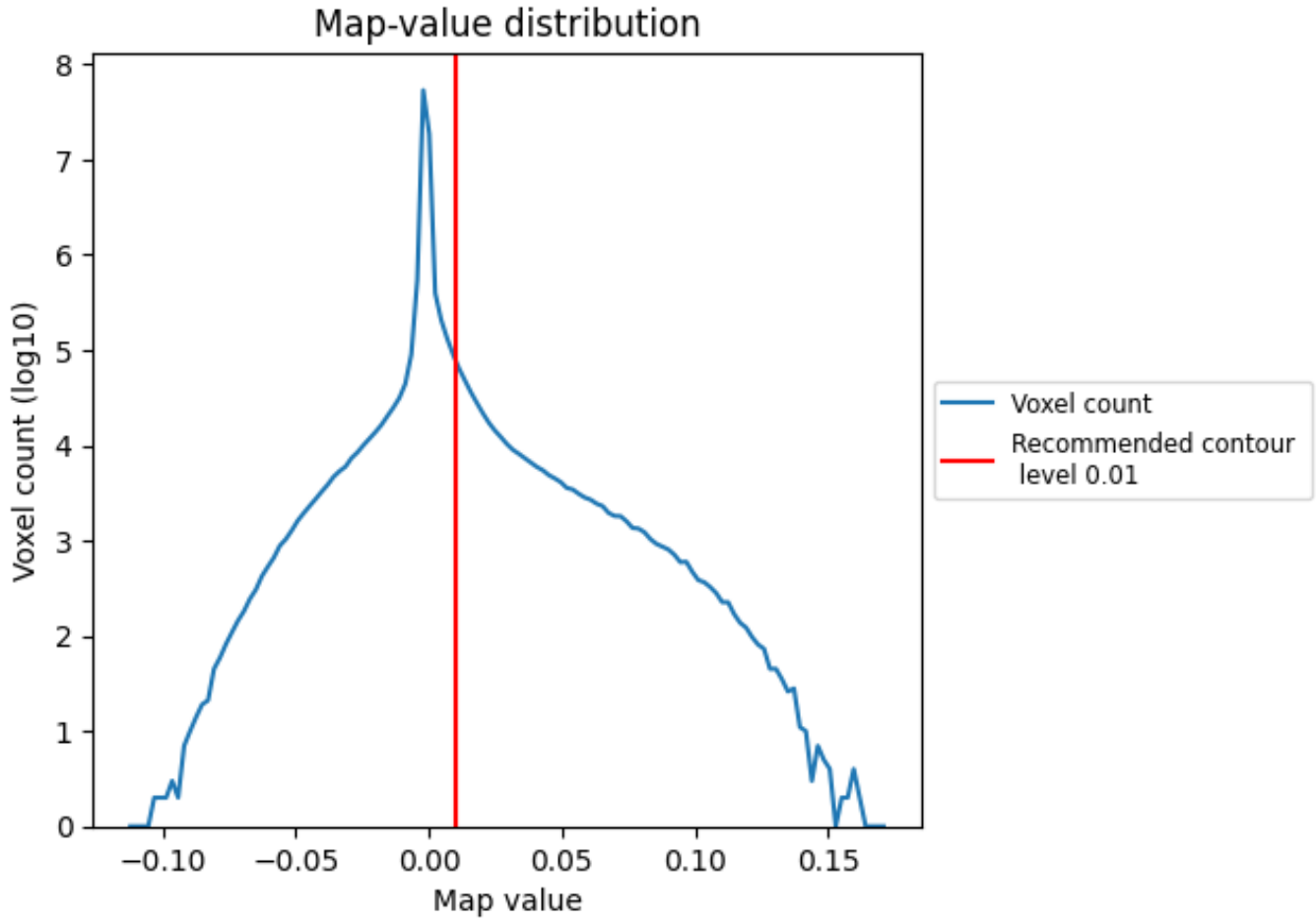


Z

7 Map analysis

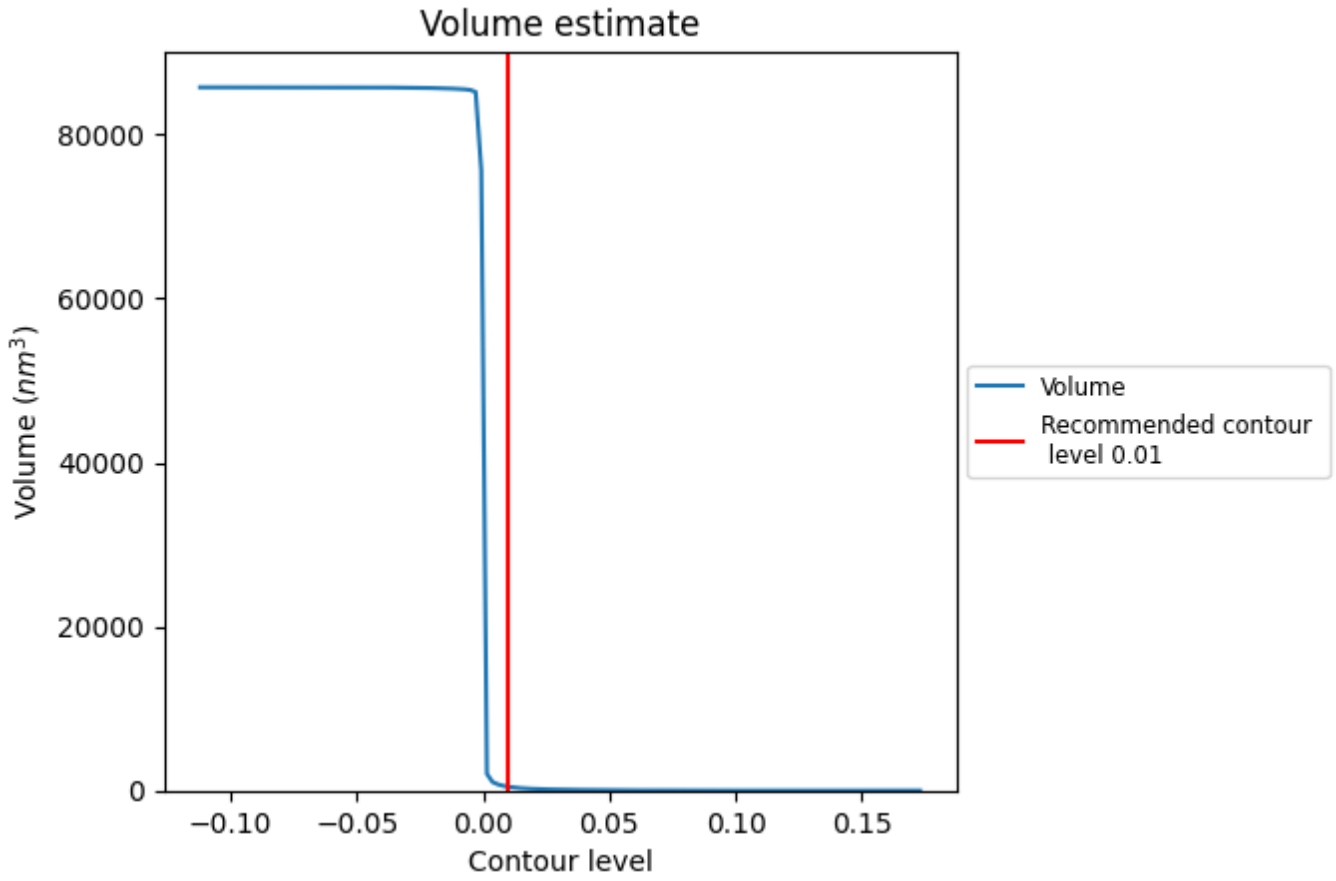
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

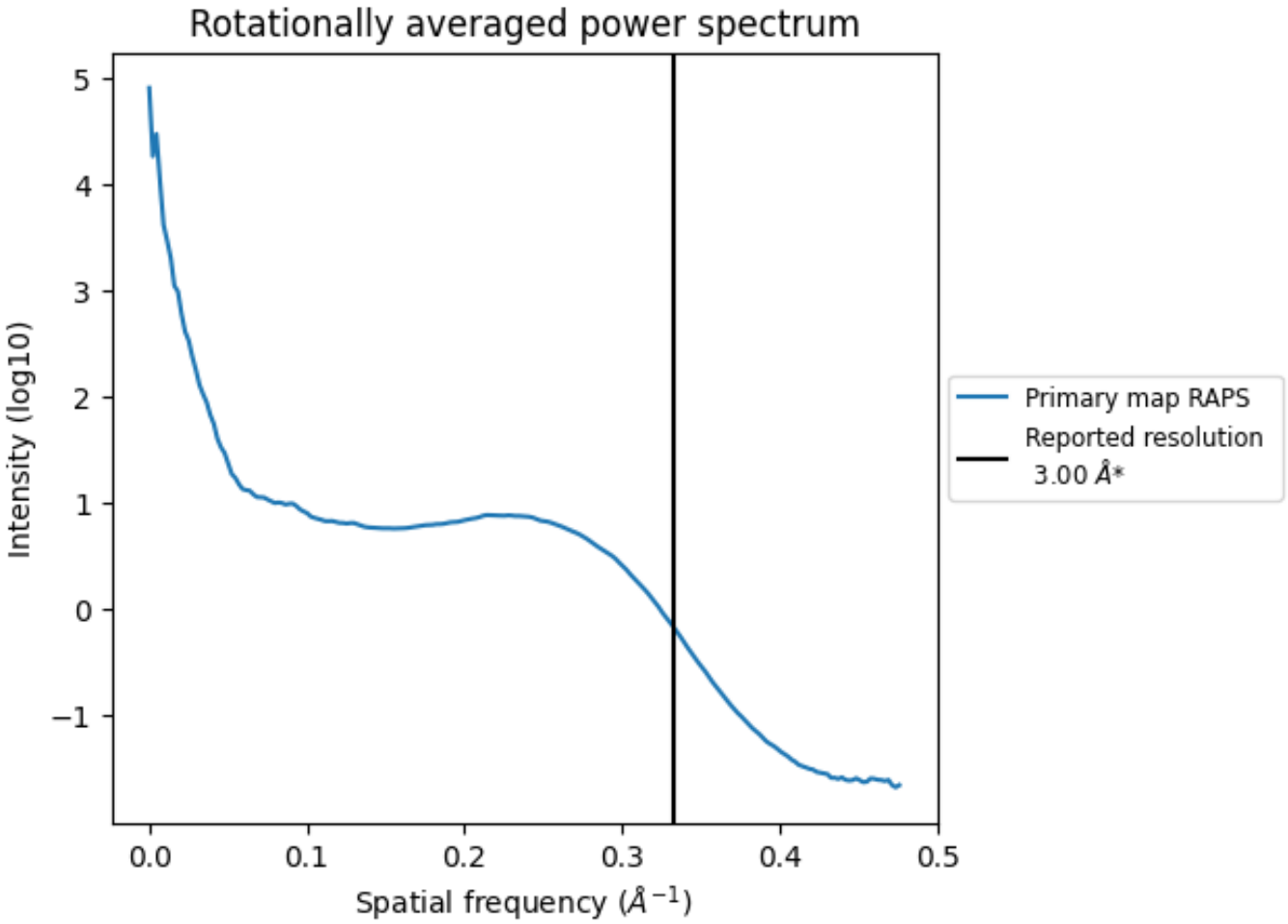
7.2 Volume estimate



The volume at the recommended contour level is 466 nm^3; this corresponds to an approximate mass of 421 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)

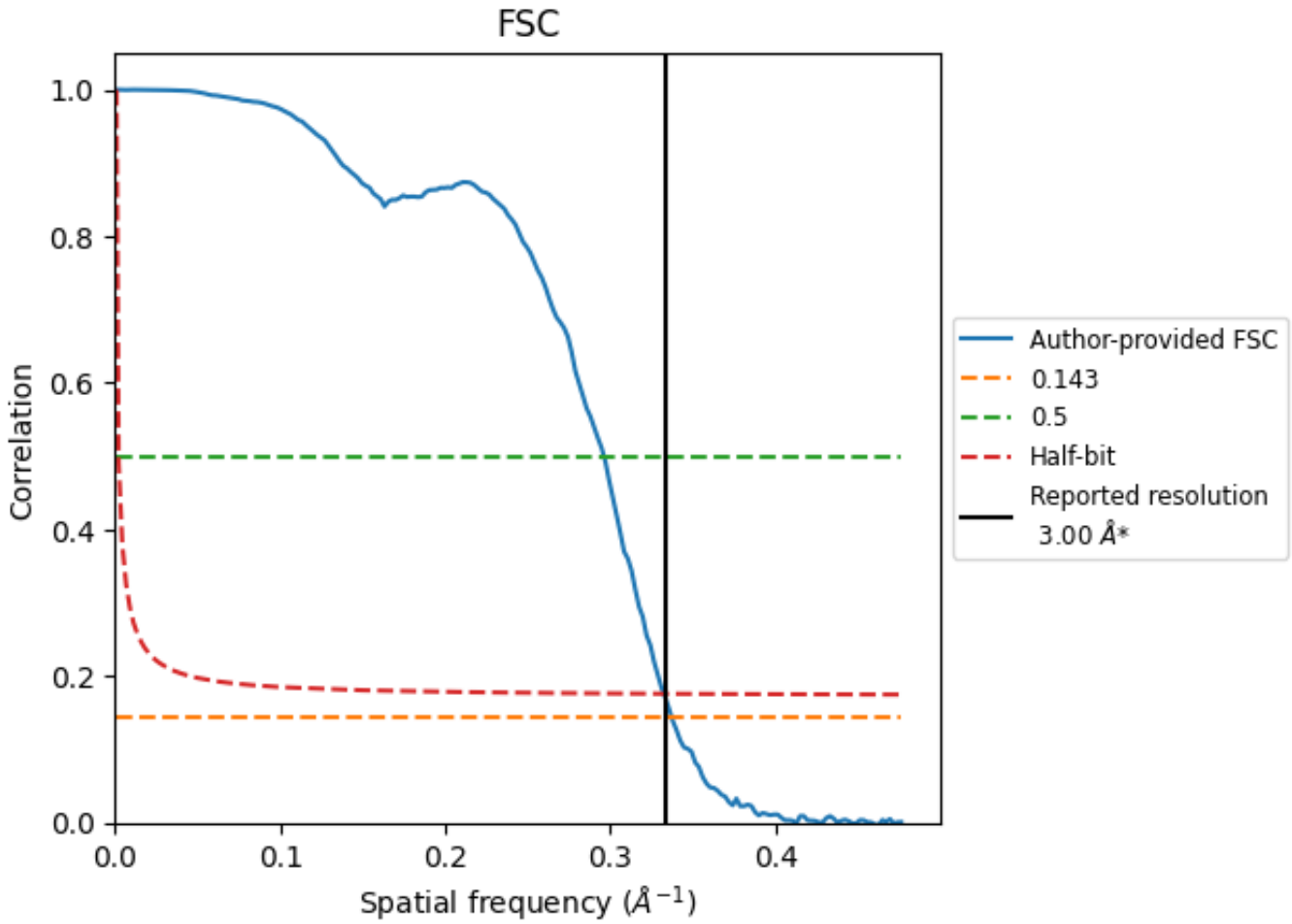


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

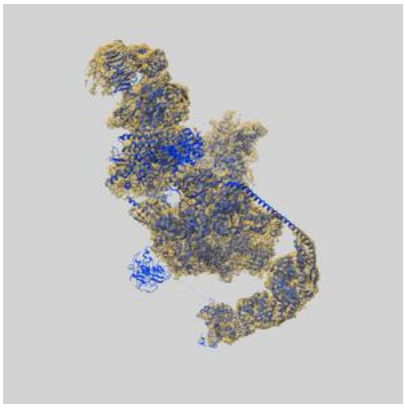
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.97	3.38	3.01
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

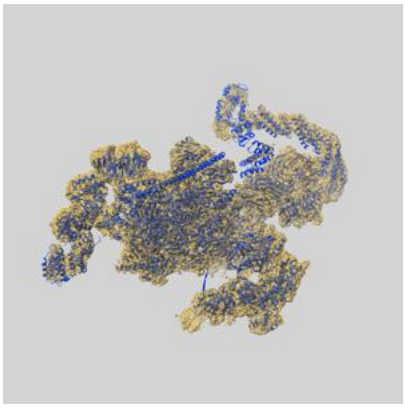
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13015 and PDB model 7OPC. Per-residue inclusion information can be found in section 3 on page 10.

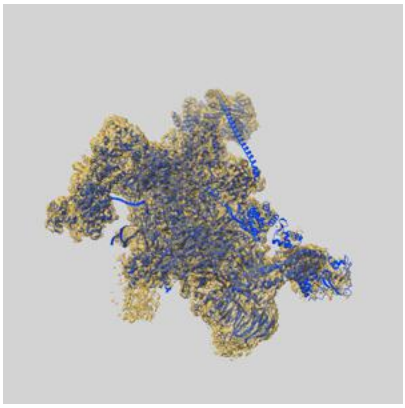
9.1 Map-model overlay



X



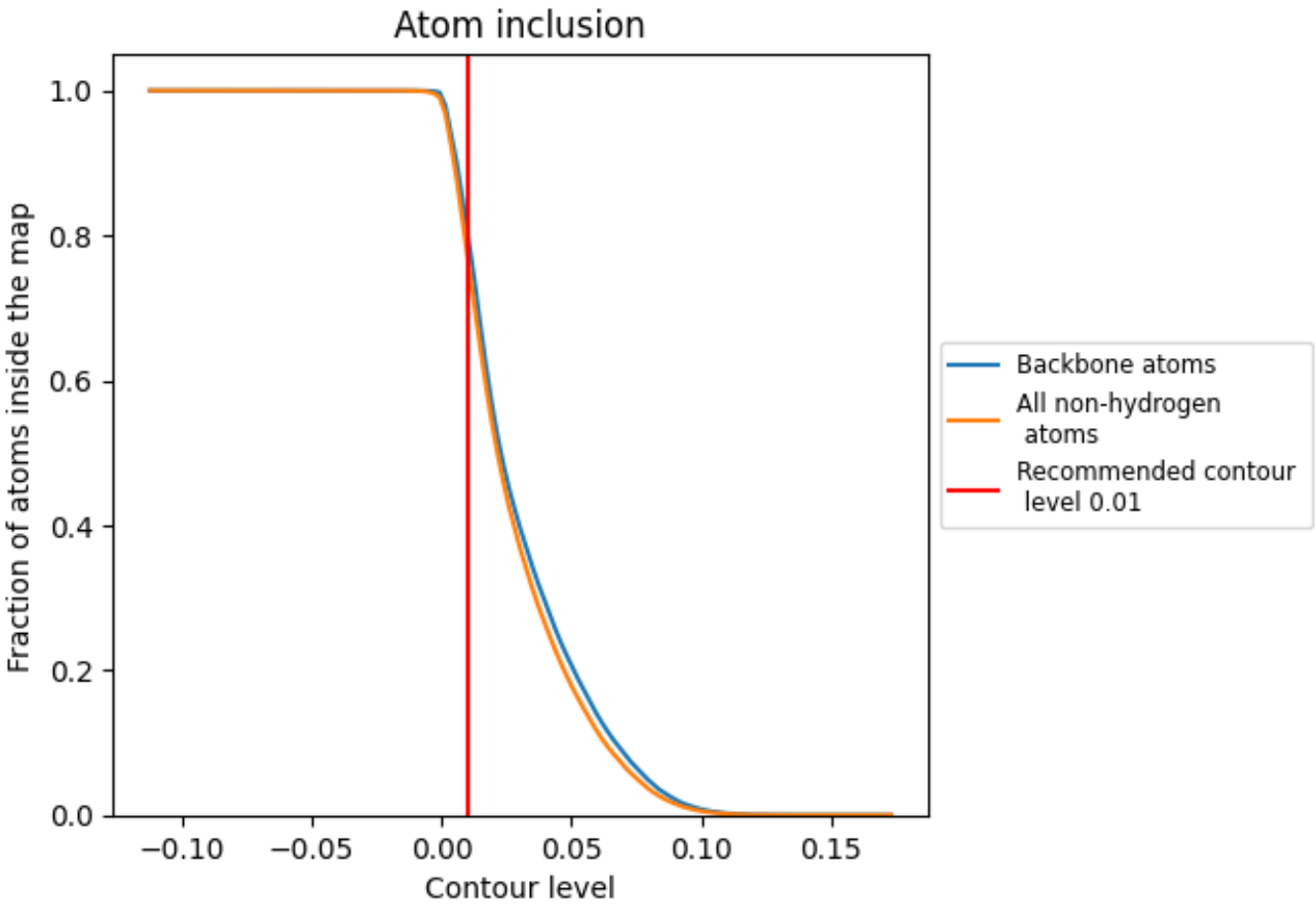
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.