wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 02:11 am GMT

PDB ID	:	6GEN
EMDB ID	:	EMD-4396
Title	:	Chromatin remodeller-nucleosome complex at 4.5 A resolution.
Authors	:	Willhoft, O.; Chua, E.Y.D.; Wilkinson, M.; Wigley, D.B.
Deposited on	:	2018-04-27
Resolution	:	3.60 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

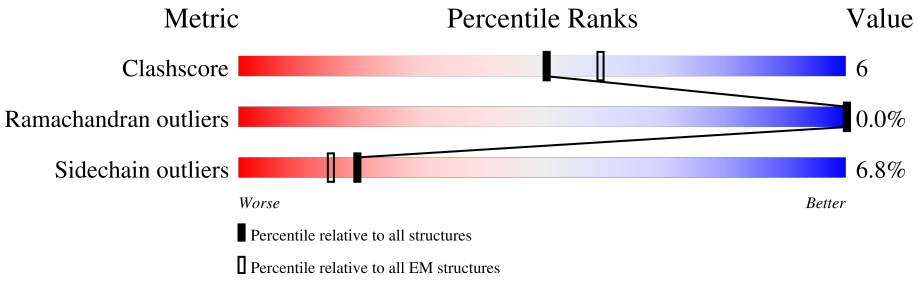
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

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



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

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	Z	131	8% 100%
2	A	136	59% 12% 29%
2	B	136	60% 12% 29%
3	C	103	65% 14% 20%
3	D	103	66% 11% 22%
4	E	132	69% 8% 22%
4	F	132	70% 6% 23%
5	G	131	61% 11% 27%

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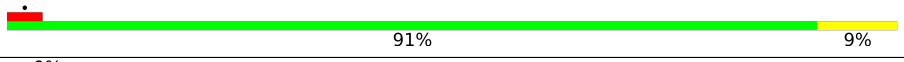
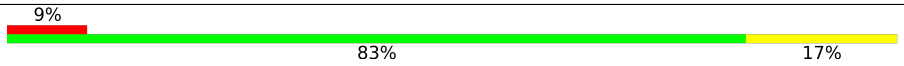
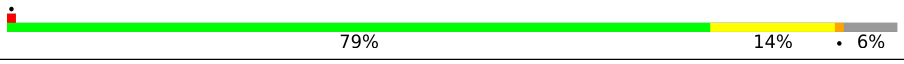
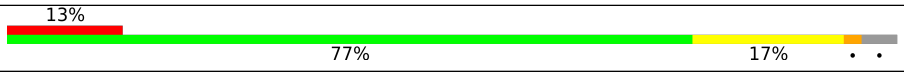
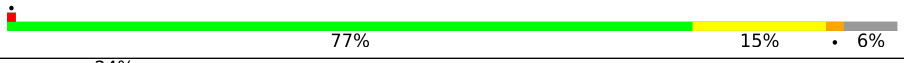
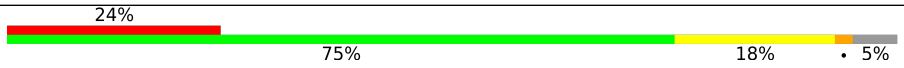
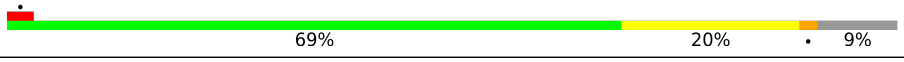
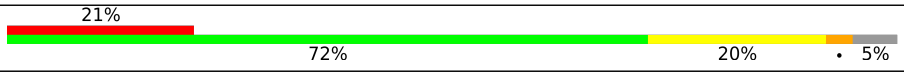
Mol	Chain	Length	Quality of chain
5	H	131	
6	I	173	
7	J	173	
8	M	1514	
9	R	438	
10	S	280	
11	T	463	
11	V	463	
11	X	463	
12	U	471	
12	W	471	
12	Y	471	

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 44481 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 Vacuolar protein sorting-associated protein 72.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	Z	131	Total 655	C 393	N 131	O 131	0	0

- Molecule 2 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	A	97	Total 796	C 506	N 152	O 138	0	0
2	B	97	Total 796	C 506	N 152	O 138	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	GLU	ASP	conflict	UNP P61830
B	123	GLU	ASP	conflict	UNP P61830

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	82	Total 651	C 410	N 126	O 115	0	0
3	D	80	Total 638	C 401	N 124	O 113	0	0

- Molecule 4 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	103	Total 795	C 499	N 156	O 140	0	0
4	F	101	Total 779	C 489	N 153	O 137	0	0

- Molecule 5 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	96	Total	C	N	O	S	0	0
			746	468	131	146	1		
5	H	91	Total	C	N	O	S	0	0
			712	449	125	137	1		

- Molecule 6 is a DNA chain called DNA (173-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	173	Total	C	N	O	P	0	0
			3525	1673	640	1039	173		

- Molecule 7 is a DNA chain called DNA (173-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	173	Total	C	N	O	P	0	0
			3568	1687	671	1037	173		

- Molecule 8 is a protein called Helicase SWR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	688	Total	C	N	O	S	0	0
			5398	3438	960	974	26		

- Molecule 9 is a protein called Actin-like protein ARP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	411	Total	C	N	O	S	0	0
			3335	2156	544	619	16		

- Molecule 10 is a protein called Vacuolar protein sorting-associated protein 71.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	208	Total	C	N	O	S	0	0
			1695	1071	302	312	10		

- Molecule 11 is a protein called RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	443	Total	C	N	O	S	0	0
			3391	2140	584	657	10		

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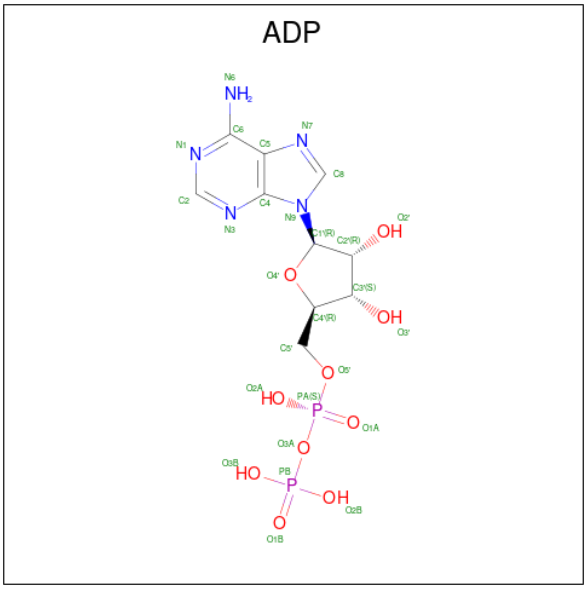
Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	434	Total	C	N	O	S	0	0
			3336	2107	574	645	10		
11	X	442	Total	C	N	O	S	0	0
			3397	2144	584	659	10		

- Molecule 12 is a protein called RuvB-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	430	Total	C	N	O	S	0	0
			3299	2063	570	655	11		
12	W	433	Total	C	N	O	S	0	0
			3325	2085	572	657	11		
12	Y	447	Total	C	N	O	S	0	0
			3410	2133	590	675	12		

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
13	M	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	R	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	T	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	U	1	Total	C	N	O	P	0
			27	10	5	10	2	

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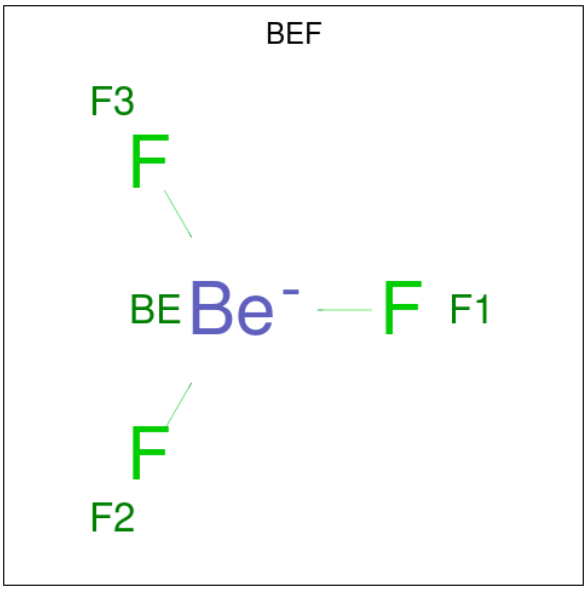
Mol	Chain	Residues	Atoms					AltConf
13	V	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	W	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 14 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			AltConf
14	M	1	Total	Be	F	0
			4	1	3	
14	R	1	Total	Be	F	0
			4	1	3	

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
15	M	1	Total	Mg	0
			1	1	
15	R	1	Total	Mg	0
			1	1	
15	U	2	Total	Mg	0
			2	2	

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Mol	Chain	Residues	Atoms	AltConf
15	V	1	Total Mg 1 1	0
15	W	1	Total Mg 1 1	0
15	Y	2	Total Mg 2 2	0

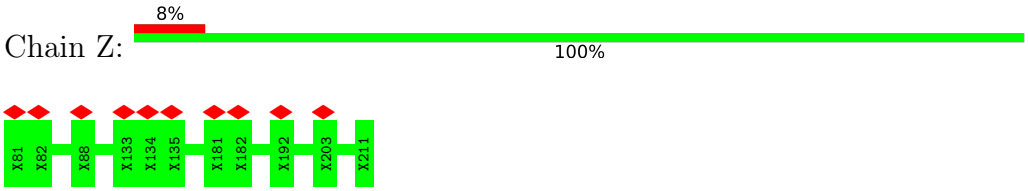
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
16	S	2	Total Zn 2 2	0

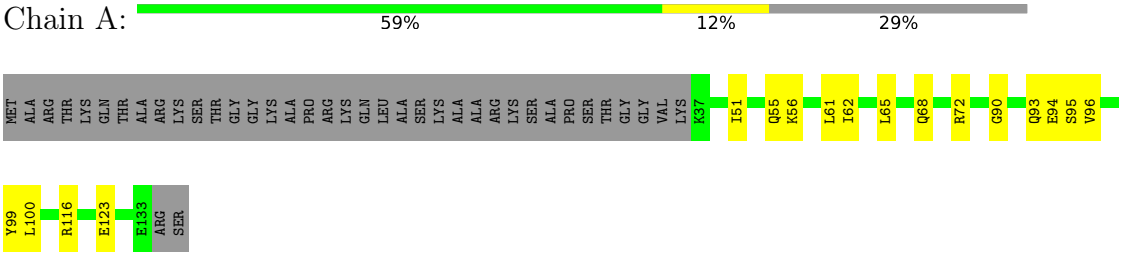
3 Residue-property plots (i)

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.

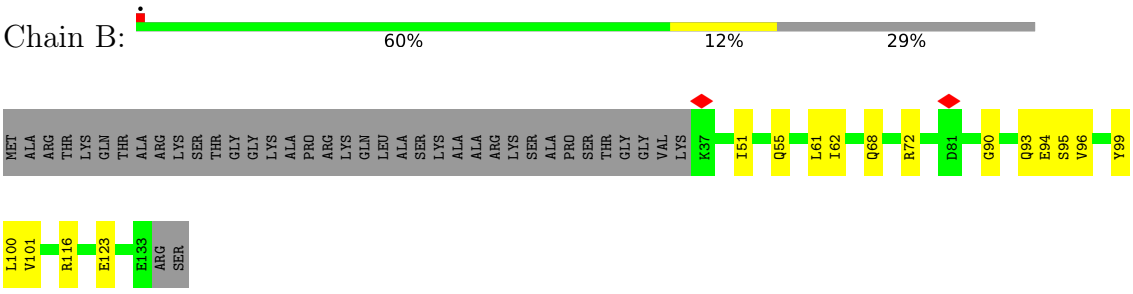
• Molecule 1: Vacuolar protein sorting-associated protein 72



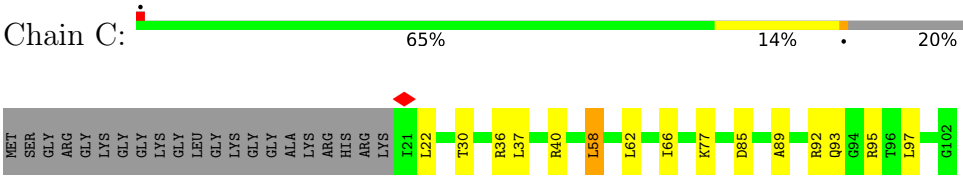
• Molecule 2: Histone H3



• Molecule 2: Histone H3

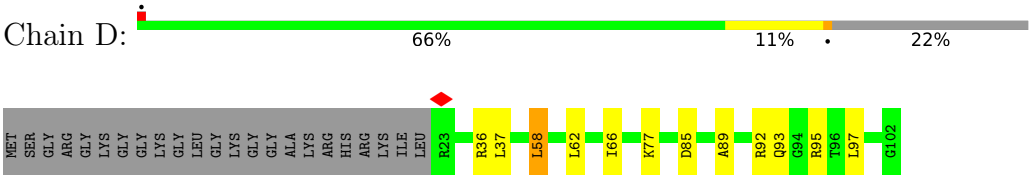


• Molecule 3: Histone H4



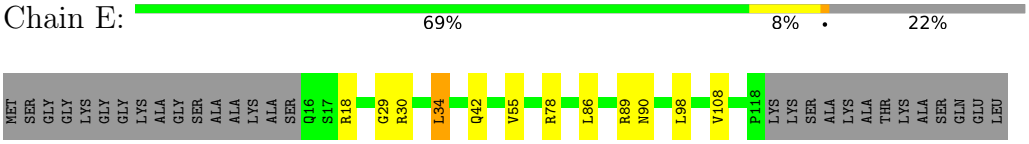
• Molecule 3: Histone H4

Chain D:



• Molecule 4: Histone H2A.1

Chain E:

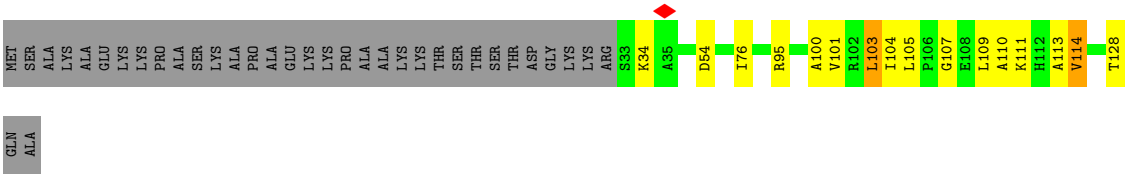


• Molecule 4: Histone H2A.1

Chain F:

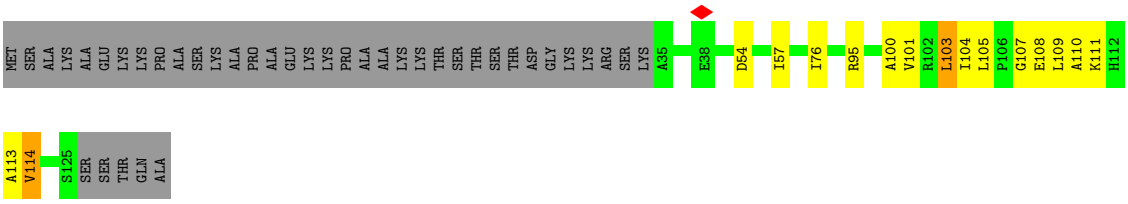
• Molecule 5: Histone H2B.1

Chain G:



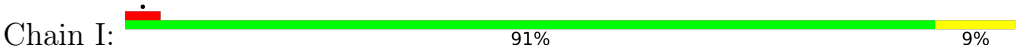
• Molecule 5: Histone H2B.1

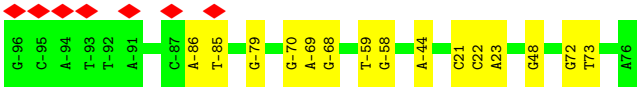
Chain H:



• Molecule 6: DNA (173-MER)

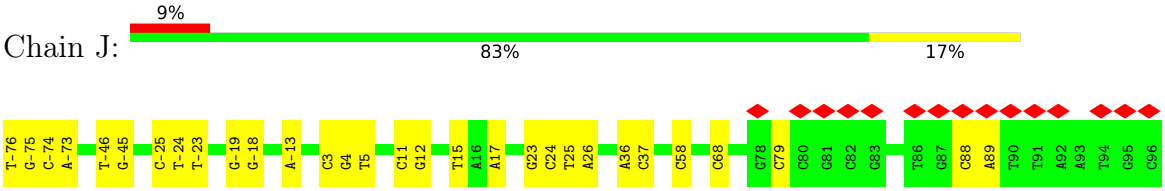
Chain I:





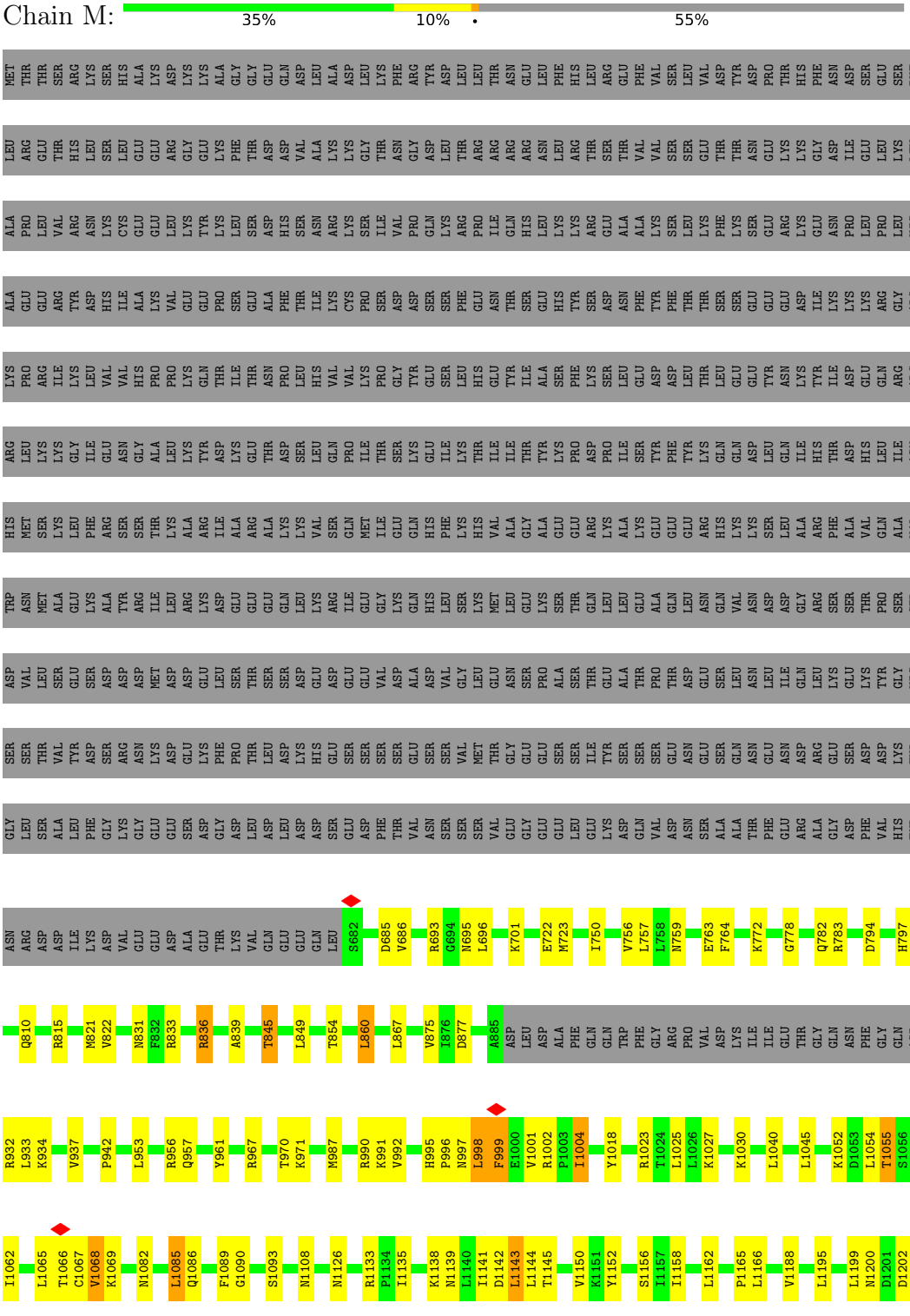
• Molecule 7: DNA (173-MER)

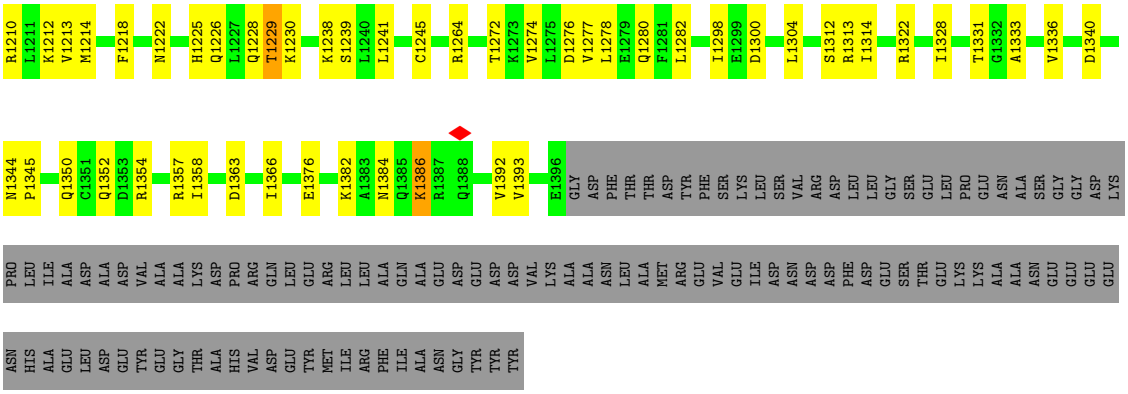
Chain J:



• Molecule 8: Helicase SWR1

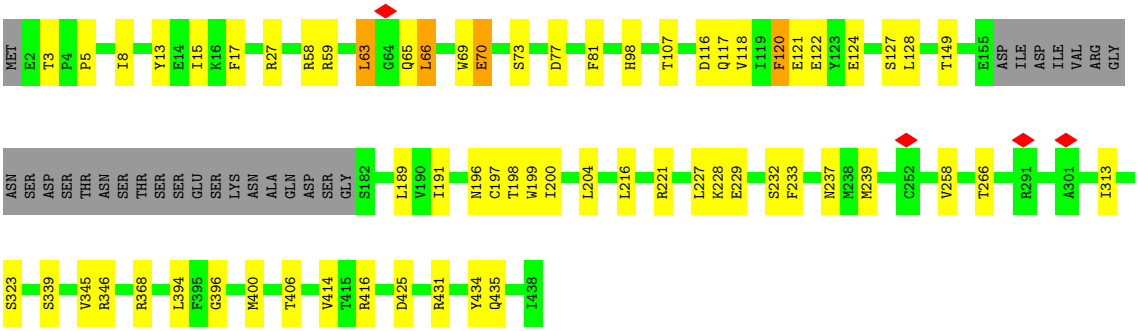
Chain M:





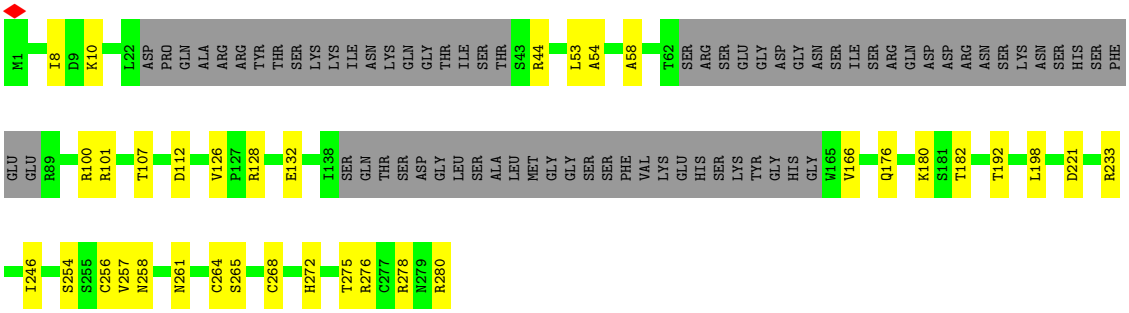
• Molecule 9: Actin-like protein ARP6

Chain R:



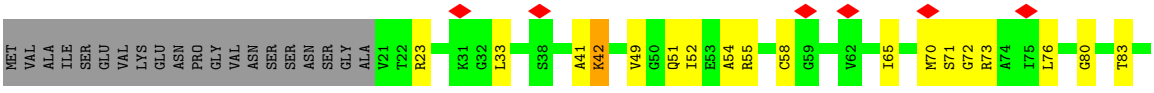
• Molecule 10: Vacuolar protein sorting-associated protein 71

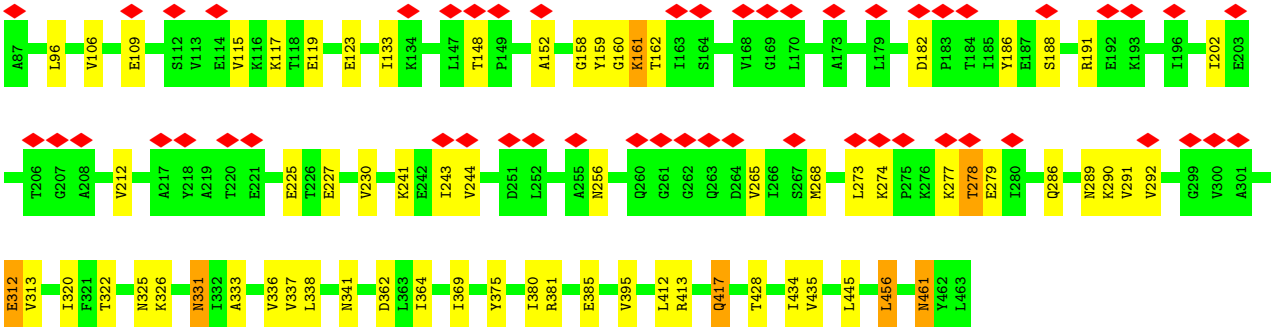
Chain S:



• Molecule 11: RuvB-like protein 1

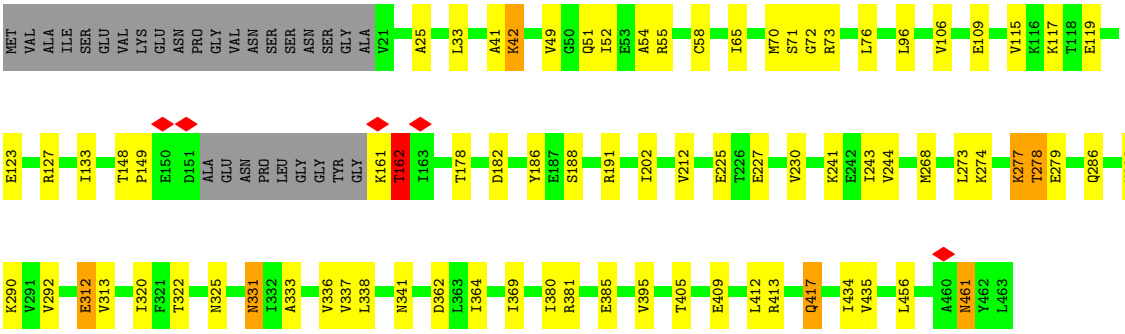
Chain T:





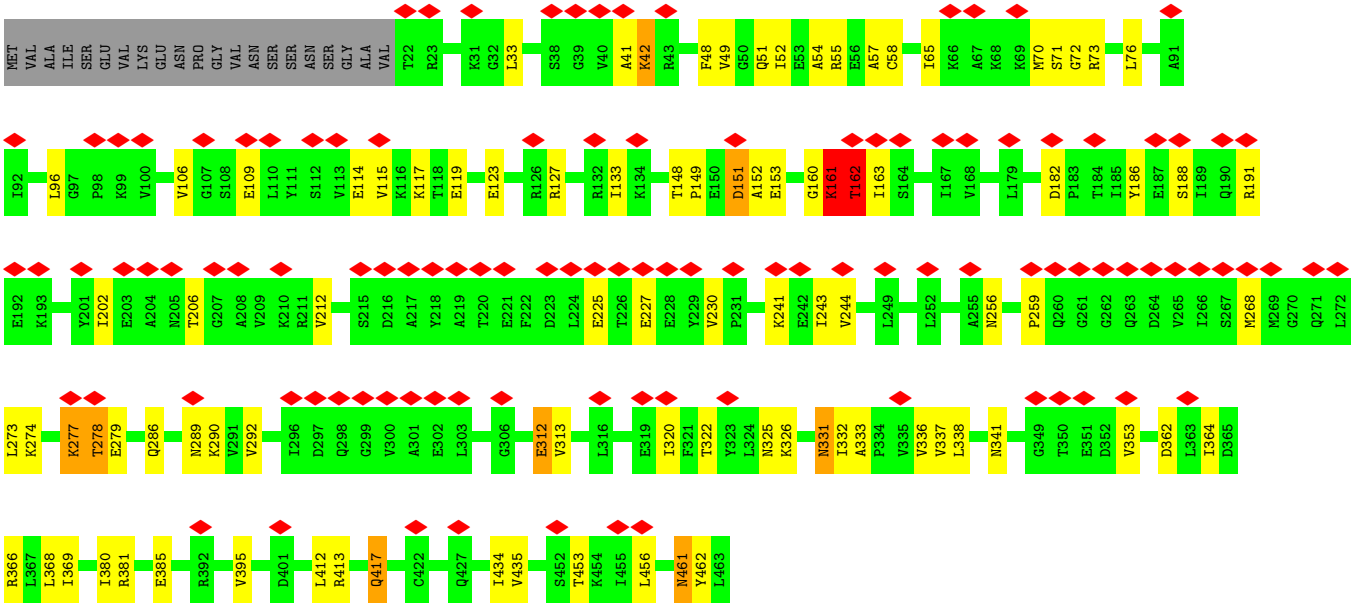
• Molecule 11: RuvB-like protein 1

Chain V:



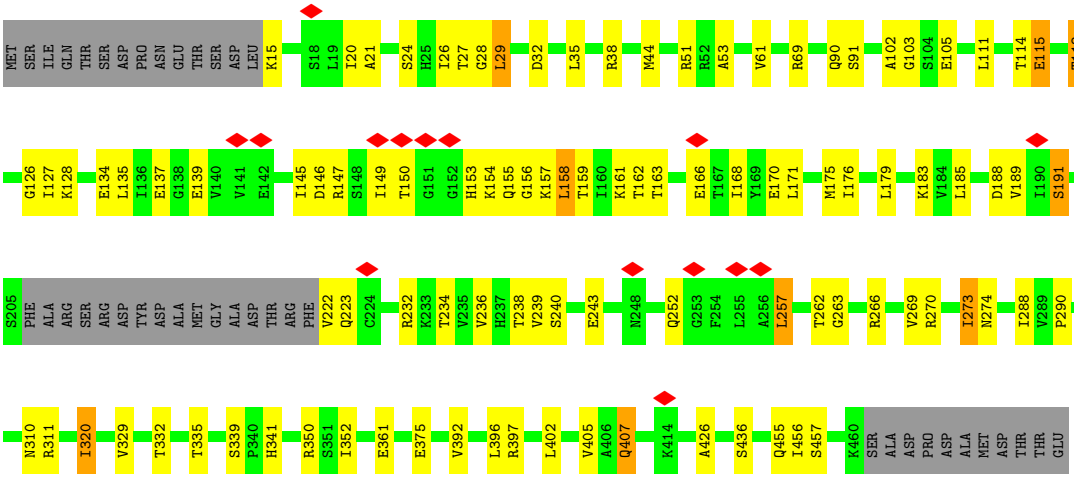
• Molecule 11: RuvB-like protein 1

Chain X:



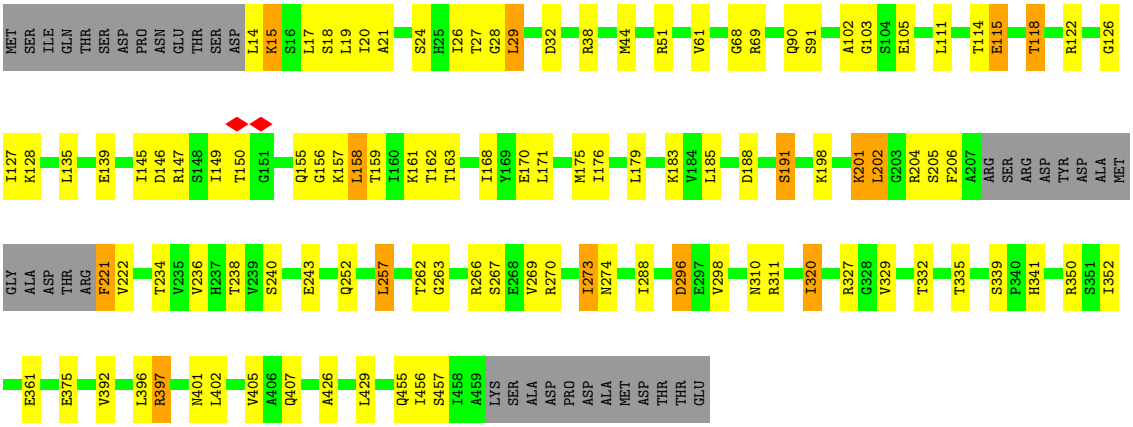
• Molecule 12: RuvB-like protein 2

Chain U:



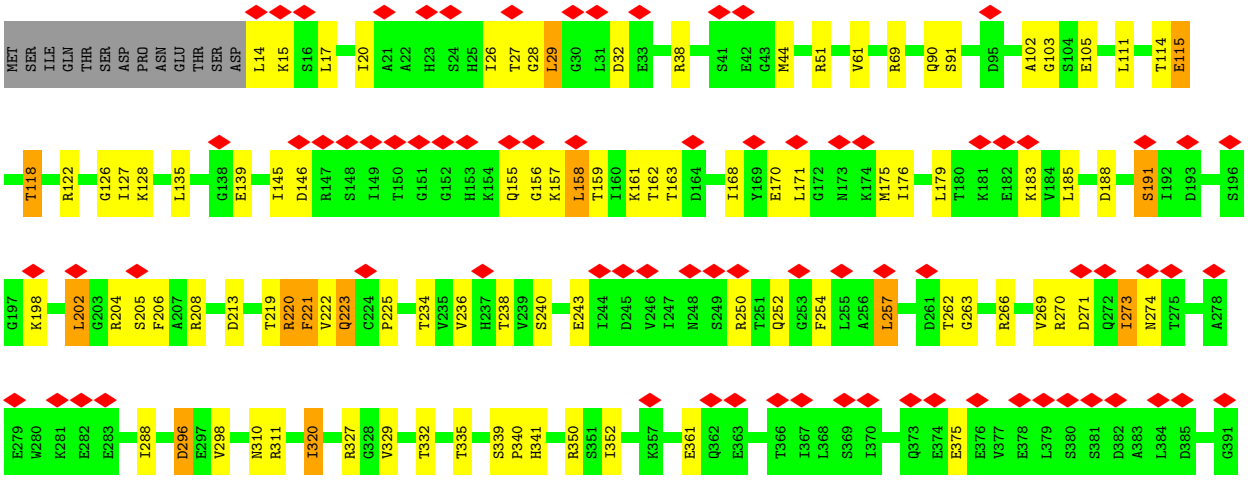
• Molecule 12: RuvB-like protein 2

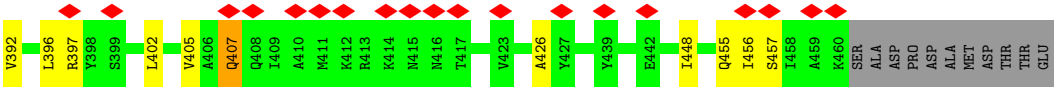
Chain W:



• Molecule 12: RuvB-like protein 2

Chain Y:




V392
L396
R397
Y398
S399
L402
V405
A406
Q407
Q408
I409
A410
M411
K412
R413
K414
N415
N416
T417
V423
A426
Y427
Y439
E442
I448
Q455
I456
S457
I458
A459
K460
SER
ALA
ASP
PRO
ASP
ALA
MET
ASP
THR
THR
GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98529	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 ($e^-/Å^2$)	1.71794871794872	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.207	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0359	Depositor
Map size (Å)	426.24, 426.24, 426.24	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ZN, BEF, 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
2	A	0.24	0/807	0.42	0/1081
2	B	0.25	0/807	0.42	0/1081
3	C	0.24	0/658	0.45	0/880
3	D	0.24	0/645	0.45	0/862
4	E	0.24	0/806	0.42	0/1091
4	F	0.24	0/789	0.42	0/1067
5	G	0.25	0/756	0.41	0/1017
5	H	0.24	0/722	0.41	0/972
6	I	0.58	0/3949	0.97	1/6087 (0.0%)
7	J	0.56	0/4007	0.94	0/6188
8	M	0.26	0/5495	0.48	3/7442 (0.0%)
9	R	0.25	0/3429	0.43	2/4650 (0.0%)
10	S	0.25	0/1722	0.42	0/2320
11	T	0.25	0/3433	0.47	0/4646
11	V	0.25	0/3375	0.46	0/4565
11	X	0.25	0/3439	0.47	0/4652
12	U	0.24	0/3333	0.45	0/4492
12	W	0.25	0/3361	0.45	0/4530
12	Y	0.25	0/3447	0.46	0/4649
All	All	0.33	0/44980	0.59	6/62272 (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
8	M	0	2
11	T	0	4
11	V	0	2
11	X	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	U	0	1
12	W	0	3
12	Y	0	3
All	All	0	20

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	999	PHE	CB-CG-CD2	7.75	126.22	120.80
9	R	66	LEU	CA-CB-CG	6.60	130.49	115.30
9	R	63	LEU	CA-CB-CG	6.30	129.80	115.30
8	M	998	LEU	C-N-CA	5.59	135.68	121.70
6	I	48	DG	O4'-C4'-C3'	-5.39	102.34	104.50

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	M	1067	CYS	Peptide
8	M	1344	ASN	Peptide
11	T	152	ALA	Peptide
11	T	160	GLY	Peptide
11	T	161	LYS	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	Z	655	0	147	0	0
2	A	796	0	841	11	0
2	B	796	0	841	10	0
3	C	651	0	690	9	0
3	D	638	0	677	8	0
4	E	795	0	834	9	0
4	F	779	0	819	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	746	0	771	12	0
5	H	712	0	736	11	0
6	I	3525	0	1941	11	0
7	J	3568	0	1940	21	0
8	M	5398	0	5352	85	0
9	R	3335	0	3256	37	0
10	S	1695	0	1746	27	0
11	T	3391	0	3513	47	0
11	V	3336	0	3475	38	0
11	X	3397	0	3533	55	0
12	U	3299	0	3387	51	0
12	W	3325	0	3413	55	0
12	Y	3410	0	3466	57	0
13	M	27	0	12	3	0
13	R	27	0	12	0	0
13	T	27	0	12	0	0
13	U	27	0	12	0	0
13	V	27	0	12	0	0
13	W	27	0	12	0	0
13	X	27	0	12	2	0
13	Y	27	0	12	0	0
14	M	4	0	0	0	0
14	R	4	0	0	0	0
15	M	1	0	0	0	0
15	R	1	0	0	0	0
15	U	2	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	2	0	0	0	0
16	S	2	0	0	0	0
All	All	44481	0	41474	479	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 6.

The worst 5 of 479 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)
12:W:269:VAL:O	12:W:273:ILE:HB	1.65	0.97
12:U:269:VAL:O	12:U:273:ILE:HB	1.65	0.95
12:Y:269:VAL:O	12:Y:273:ILE:HB	1.65	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:62:LEU:O	3:C:66:ILE:HB	1.70	0.92
3:D:62:LEU:O	3:D:66:ILE:HB	1.70	0.92

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	
2	A	95/136 (70%)	93 (98%)	2 (2%)	0	100	100
2	B	95/136 (70%)	93 (98%)	2 (2%)	0	100	100
3	C	80/103 (78%)	78 (98%)	2 (2%)	0	100	100
3	D	78/103 (76%)	76 (97%)	2 (3%)	0	100	100
4	E	101/132 (76%)	101 (100%)	0	0	100	100
4	F	99/132 (75%)	99 (100%)	0	0	100	100
5	G	94/131 (72%)	90 (96%)	4 (4%)	0	100	100
5	H	89/131 (68%)	87 (98%)	2 (2%)	0	100	100
8	M	684/1514 (45%)	627 (92%)	56 (8%)	1 (0%)	51	83
9	R	407/438 (93%)	401 (98%)	6 (2%)	0	100	100
10	S	200/280 (71%)	199 (100%)	1 (0%)	0	100	100
11	T	441/463 (95%)	417 (95%)	23 (5%)	1 (0%)	47	79
11	V	430/463 (93%)	411 (96%)	19 (4%)	0	100	100
11	X	440/463 (95%)	420 (96%)	20 (4%)	0	100	100
12	U	426/471 (90%)	414 (97%)	12 (3%)	0	100	100
12	W	429/471 (91%)	415 (97%)	14 (3%)	0	100	100
12	Y	445/471 (94%)	427 (96%)	18 (4%)	0	100	100
All	All	4633/6038 (77%)	4448 (96%)	183 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	M	1345	PRO
11	T	161	LYS

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	
2	A	84/113 (74%)	84 (100%)	0	100	100
2	B	84/113 (74%)	84 (100%)	0	100	100
3	C	68/81 (84%)	64 (94%)	4 (6%)	19	55
3	D	67/81 (83%)	64 (96%)	3 (4%)	27	62
4	E	82/99 (83%)	80 (98%)	2 (2%)	49	75
4	F	80/99 (81%)	78 (98%)	2 (2%)	47	75
5	G	83/109 (76%)	80 (96%)	3 (4%)	35	67
5	H	78/109 (72%)	76 (97%)	2 (3%)	46	74
8	M	574/1376 (42%)	518 (90%)	56 (10%)	8	36
9	R	372/396 (94%)	359 (96%)	13 (4%)	36	68
10	S	199/261 (76%)	193 (97%)	6 (3%)	41	71
11	T	371/391 (95%)	343 (92%)	28 (8%)	13	45
11	V	368/391 (94%)	340 (92%)	28 (8%)	13	45
11	X	374/391 (96%)	343 (92%)	31 (8%)	11	42
12	U	367/403 (91%)	335 (91%)	32 (9%)	10	41
12	W	369/403 (92%)	339 (92%)	30 (8%)	11	43
12	Y	372/403 (92%)	339 (91%)	33 (9%)	9	40
All	All	3992/5219 (76%)	3719 (93%)	273 (7%)	19	50

5 of 273 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	X	322	THR

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Mol	Chain	Res	Type
11	X	456	LEU
12	Y	252	GLN
11	T	159	TYR
11	T	115	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
12	W	63	ASN
11	X	271	GLN
12	W	401	ASN
11	X	124	ASN
12	Y	63	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	ADP	M	1601	14	24,29,29	0.96	1 (4%)	29,45,45	1.36	3 (10%)
13	ADP	Y	502	15	24,29,29	0.94	1 (4%)	29,45,45	1.39	4 (13%)
14	BEF	R	502	-	0,3,3	-	-	-		
14	BEF	M	1602	13	0,3,3	-	-	-		
13	ADP	U	502	15	24,29,29	0.98	1 (4%)	29,45,45	1.53	4 (13%)
13	ADP	X	501	15	24,29,29	0.96	1 (4%)	29,45,45	1.47	4 (13%)
13	ADP	W	501	15	24,29,29	0.99	1 (4%)	29,45,45	1.46	4 (13%)
13	ADP	T	501	15	24,29,29	0.96	1 (4%)	29,45,45	1.44	4 (13%)
13	ADP	V	501	15	24,29,29	0.96	1 (4%)	29,45,45	1.44	4 (13%)
13	ADP	R	501	15	24,29,29	0.96	1 (4%)	29,45,45	1.37	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ADP	M	1601	14	-	6/12/32/32	0/3/3/3
13	ADP	Y	502	15	-	1/12/32/32	0/3/3/3
13	ADP	U	502	15	-	2/12/32/32	0/3/3/3
13	ADP	X	501	15	-	2/12/32/32	0/3/3/3
13	ADP	W	501	15	-	0/12/32/32	0/3/3/3
13	ADP	T	501	15	-	3/12/32/32	0/3/3/3
13	ADP	V	501	15	-	3/12/32/32	0/3/3/3
13	ADP	R	501	15	-	4/12/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	W	501	ADP	C5-C4	2.59	1.47	1.40
13	U	502	ADP	C5-C4	2.56	1.47	1.40
13	R	501	ADP	C5-C4	2.50	1.47	1.40
13	X	501	ADP	C5-C4	2.50	1.47	1.40
13	M	1601	ADP	C5-C4	2.49	1.47	1.40

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	U	502	ADP	PA-O3A-PB	-3.78	119.84	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Y	502	ADP	PA-O3A-PB	-3.73	120.02	132.83
13	W	501	ADP	PA-O3A-PB	-3.64	120.33	132.83
13	Y	502	ADP	N3-C2-N1	-3.39	123.38	128.68
13	X	501	ADP	PA-O3A-PB	-3.37	121.25	132.83

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

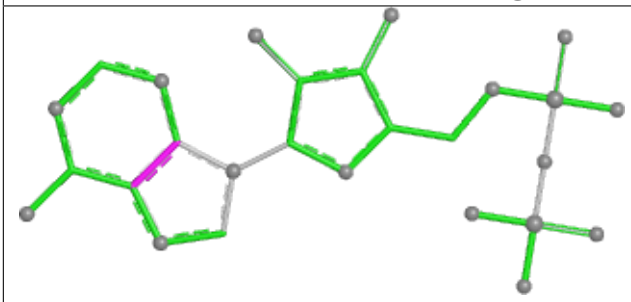
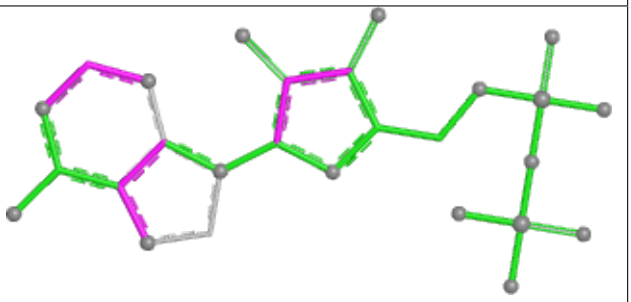
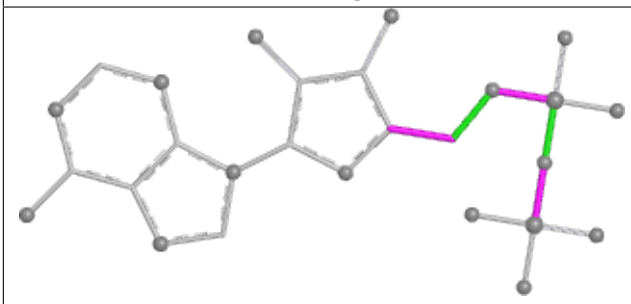
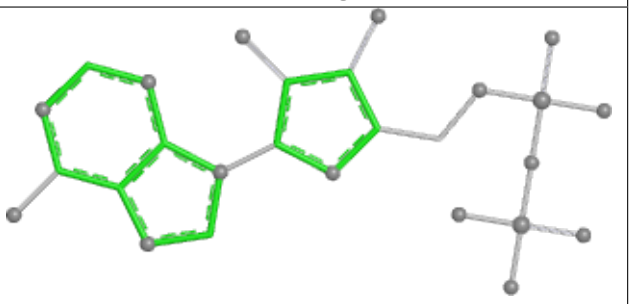
Mol	Chain	Res	Type	Atoms
13	M	1601	ADP	PA-O3A-PB-O2B
13	M	1601	ADP	C5'-O5'-PA-O1A
13	M	1601	ADP	C5'-O5'-PA-O2A
13	R	501	ADP	C5'-O5'-PA-O1A
13	R	501	ADP	C5'-O5'-PA-O2A

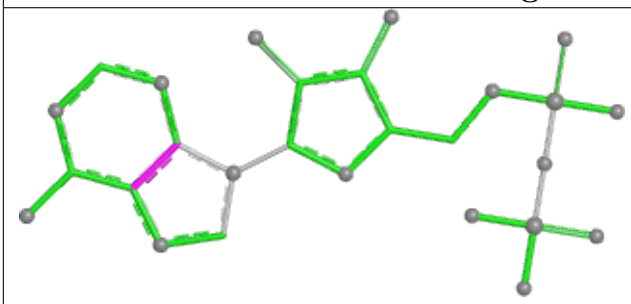
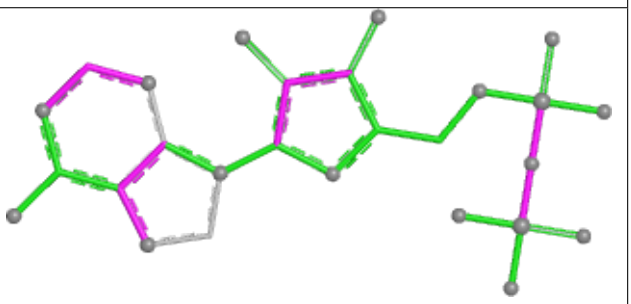
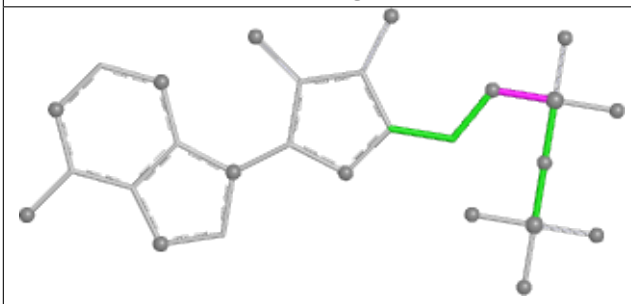
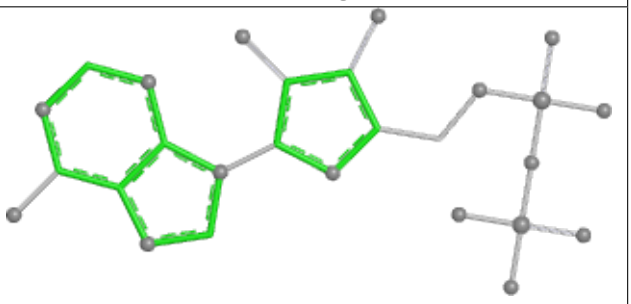
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	1601	ADP	3	0
13	X	501	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP M 1601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP Y 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

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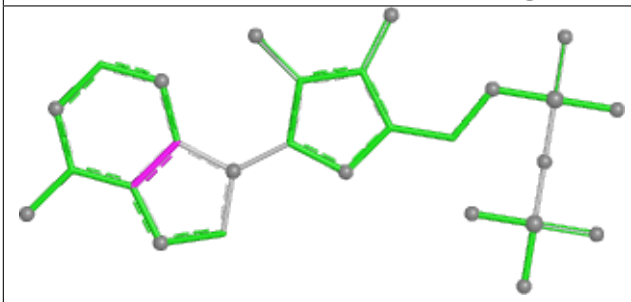
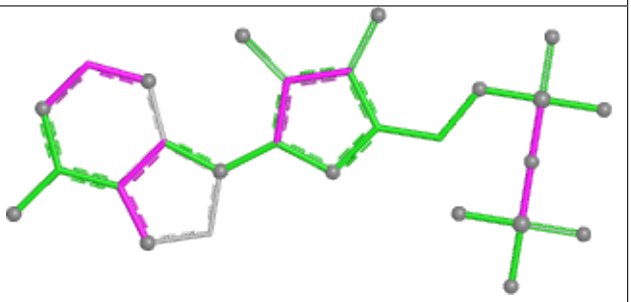
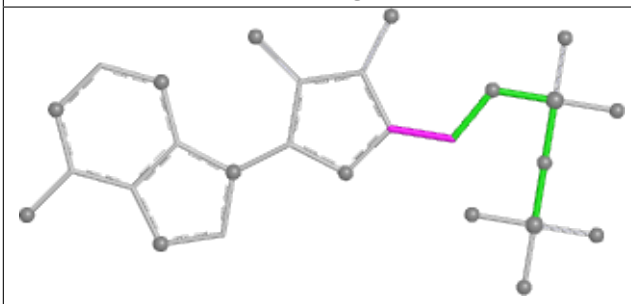
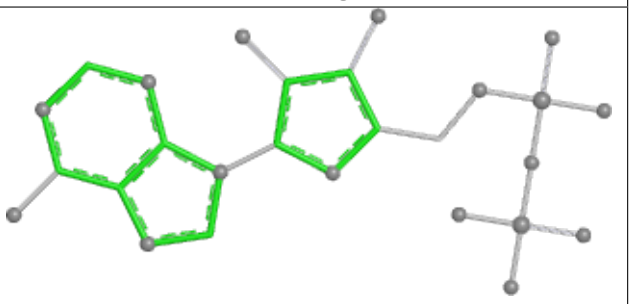
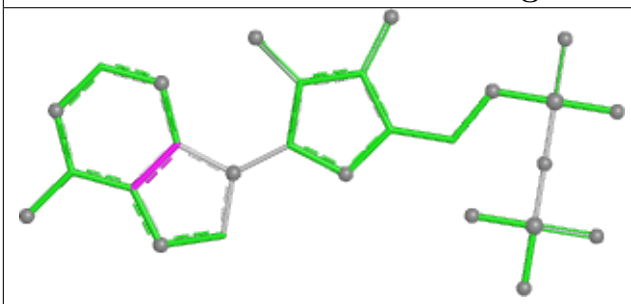
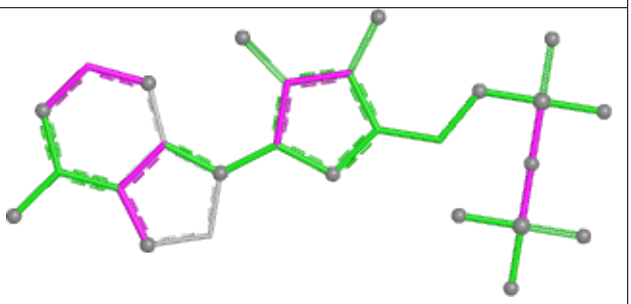
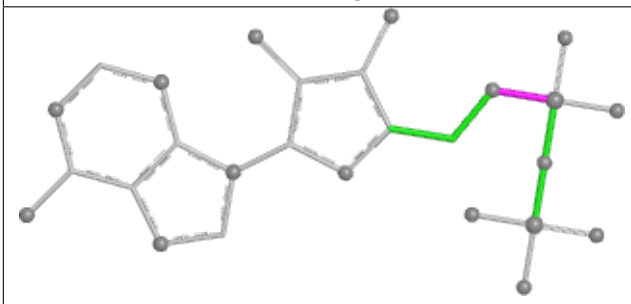
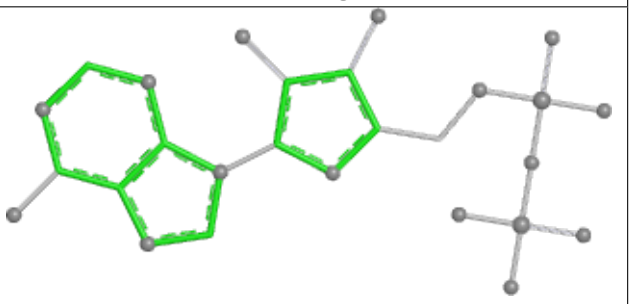
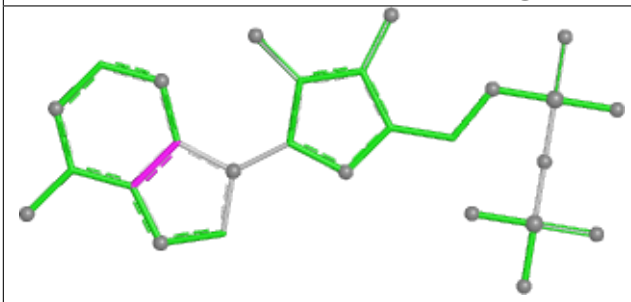
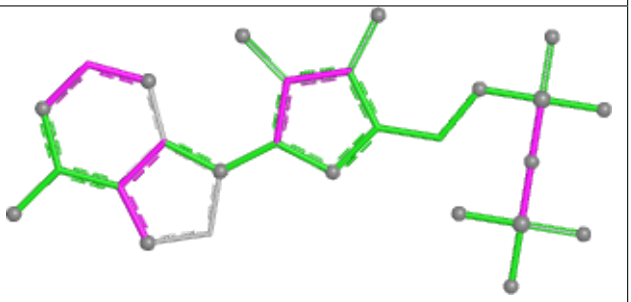
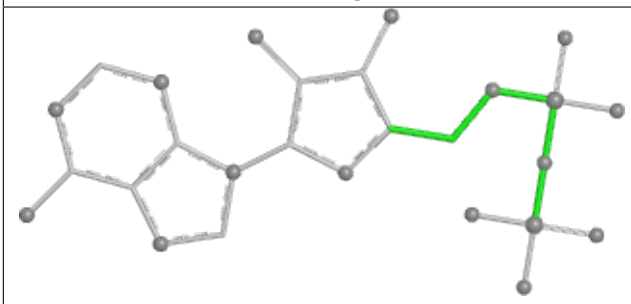
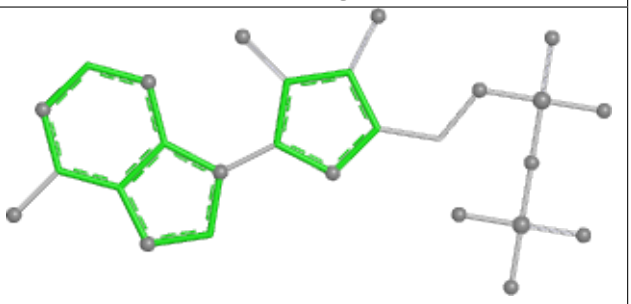
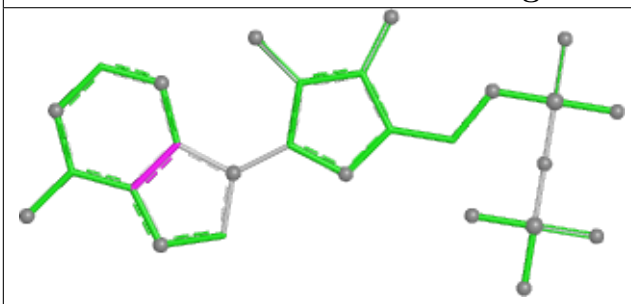
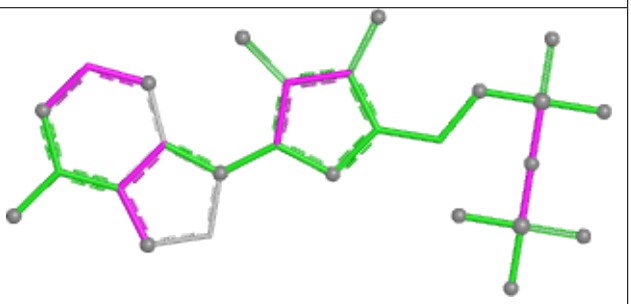
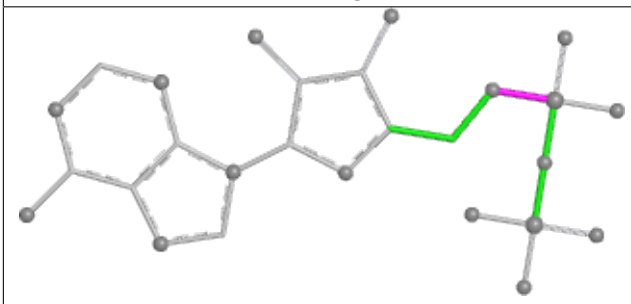
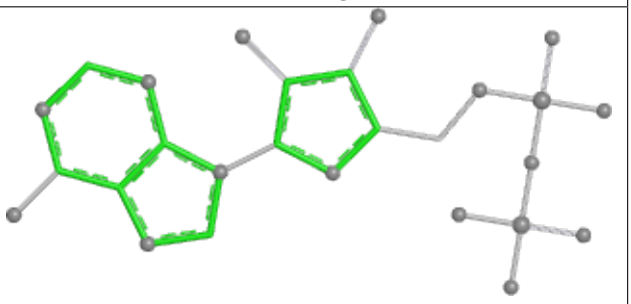
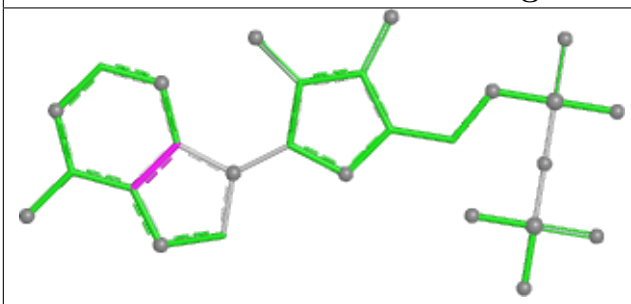
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP X 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

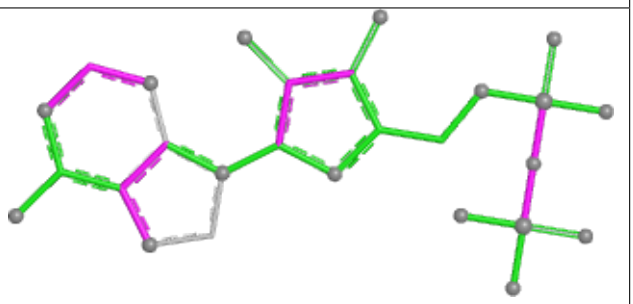
Ligand ADP W 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP T 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

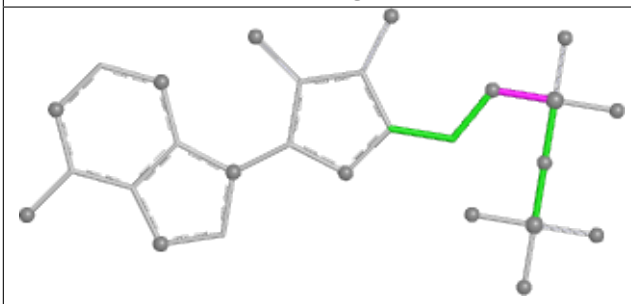
Ligand ADP V 501



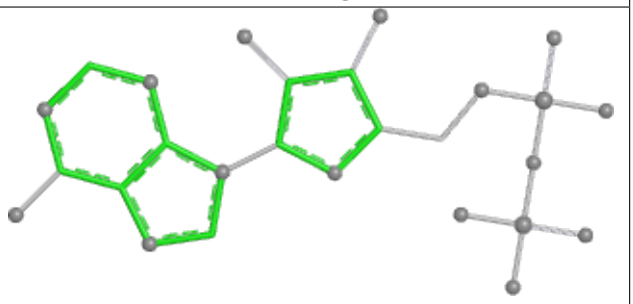
Bond lengths



Bond angles

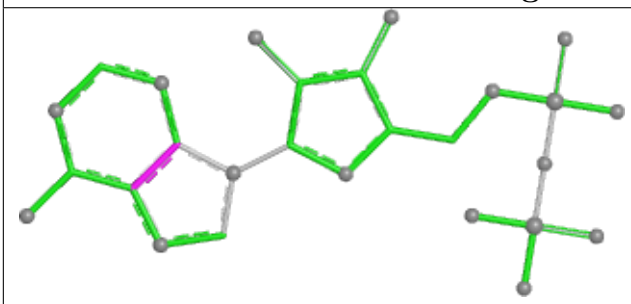


Torsions

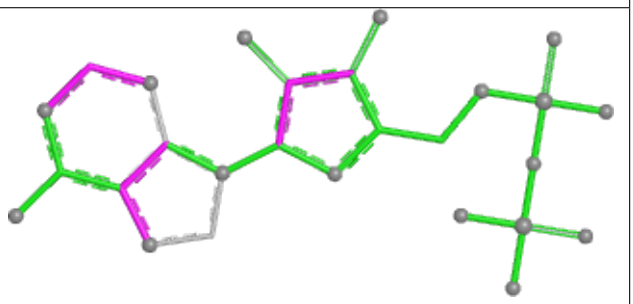


Rings

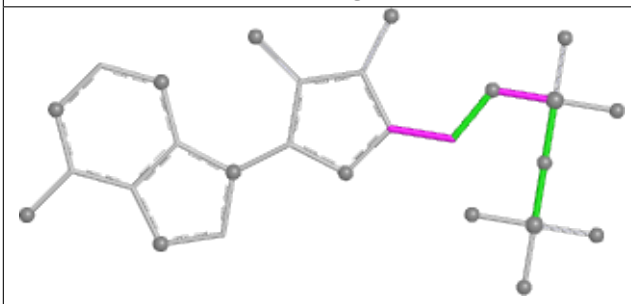
Ligand ADP R 501



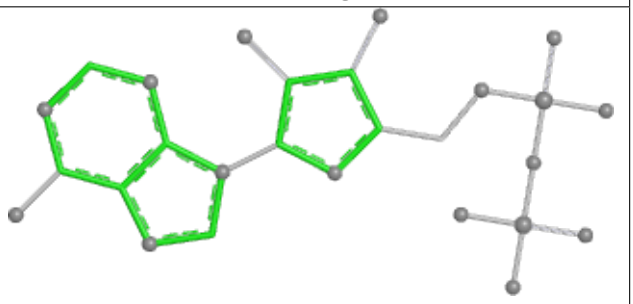
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

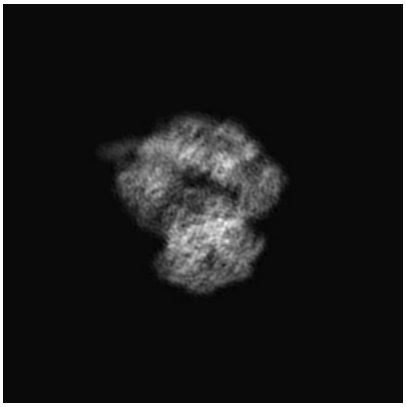
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4396. These allow visual inspection of the internal detail of the map and identification of artifacts.

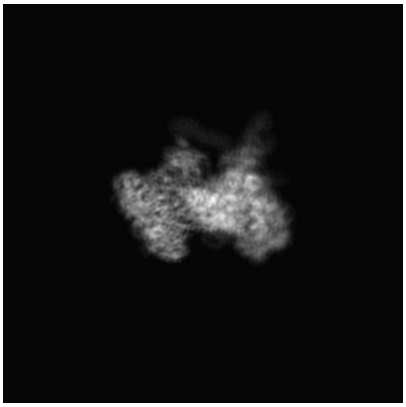
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

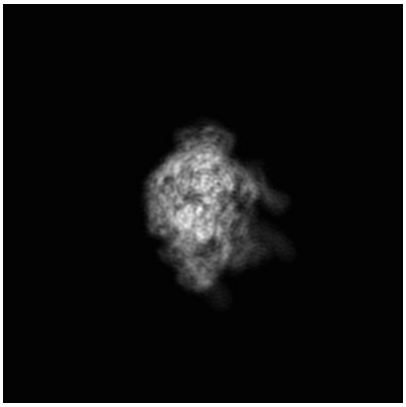
6.1.1 Primary map



X



Y

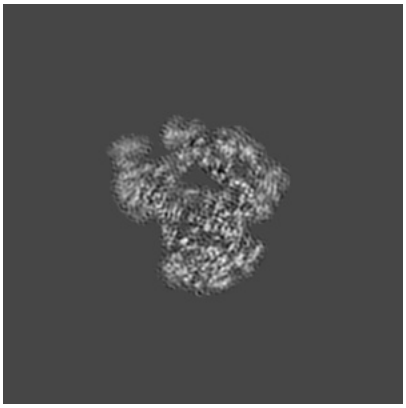


Z

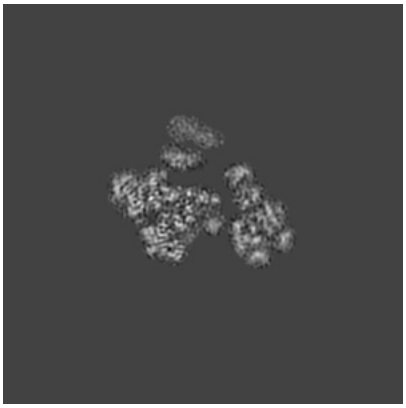
The images above show the map projected in three orthogonal directions.

6.2 Central slices

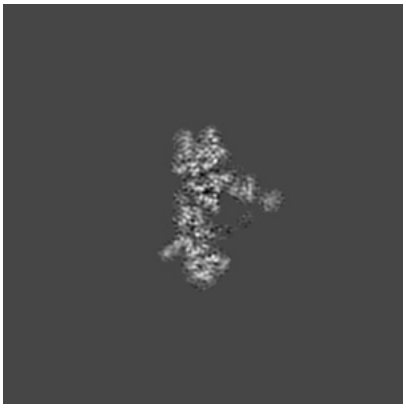
6.2.1 Primary map



X Index: 192



Y Index: 192

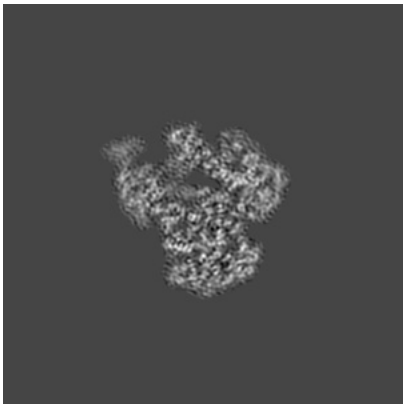


Z Index: 192

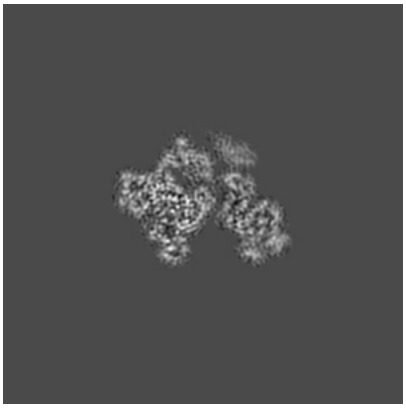
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 197



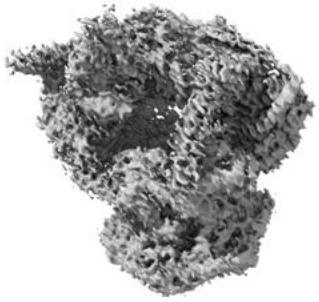
Y Index: 207

Z Index: 154

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 0.0359. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

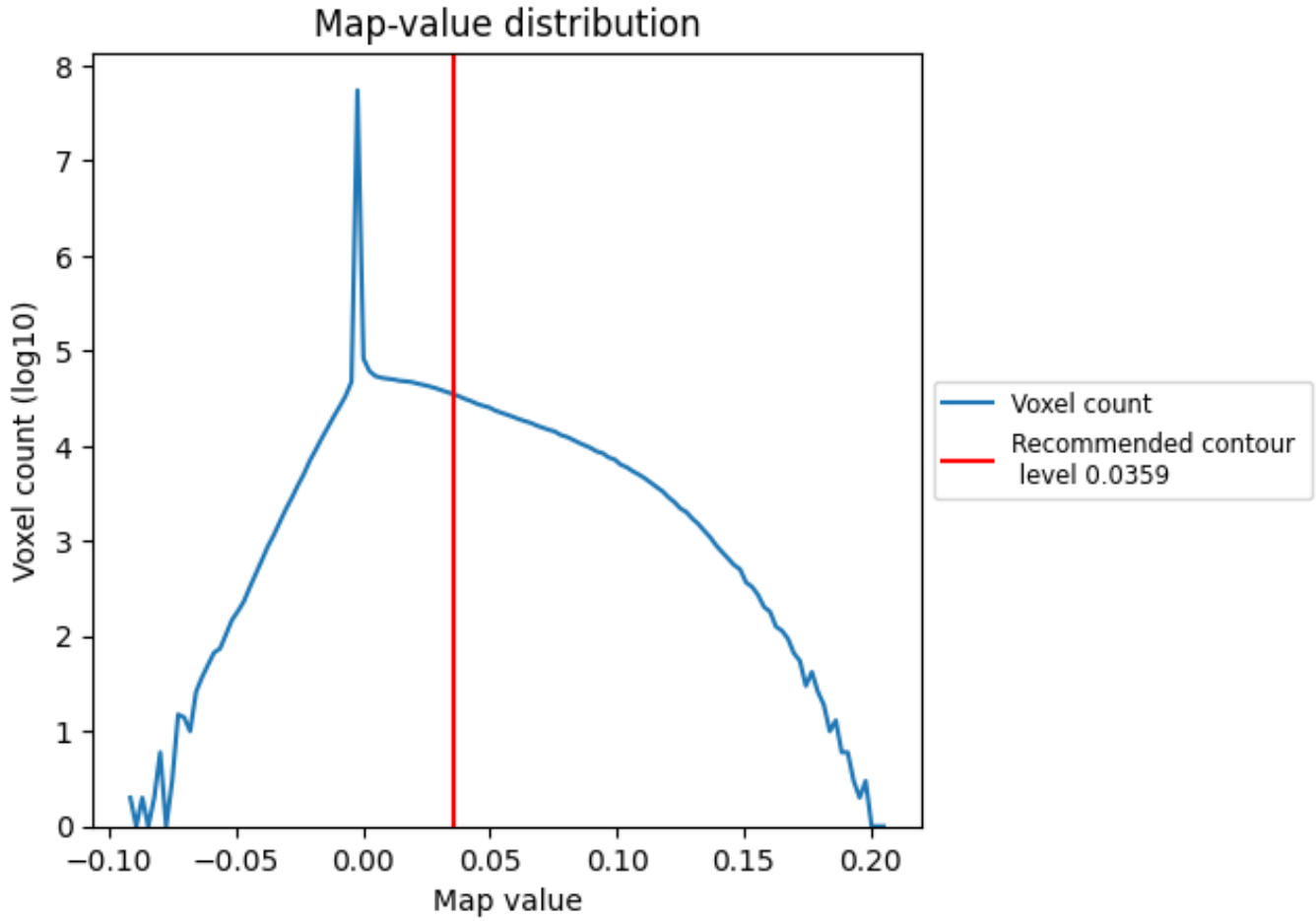
6.5 Mask visualisation (i)

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

7 Map analysis

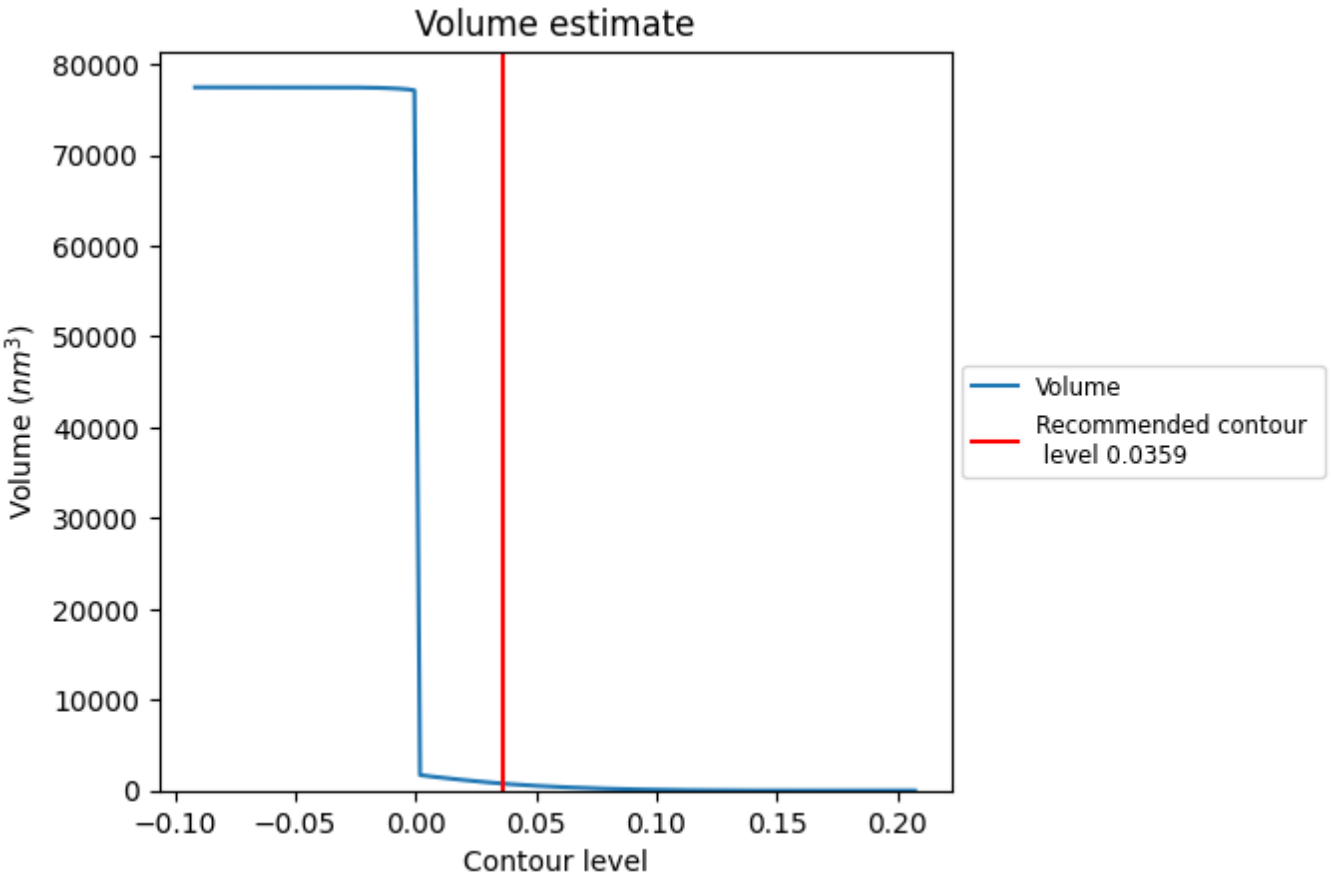
This section contains the results of statistical analysis of the map.

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.

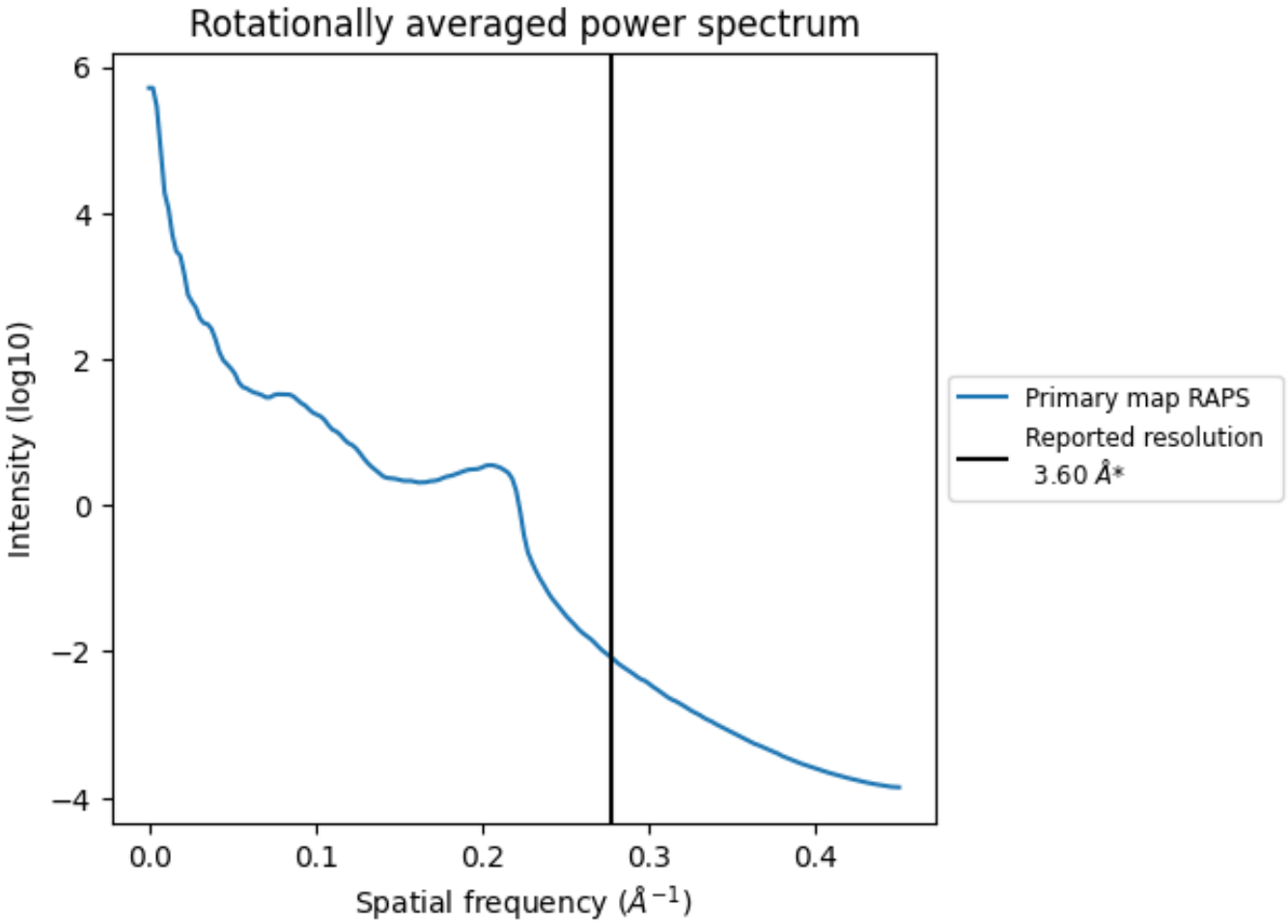
7.2 Volume estimate (i)



The volume at the recommended contour level is 773 nm^3; this corresponds to an approximate mass of 699 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

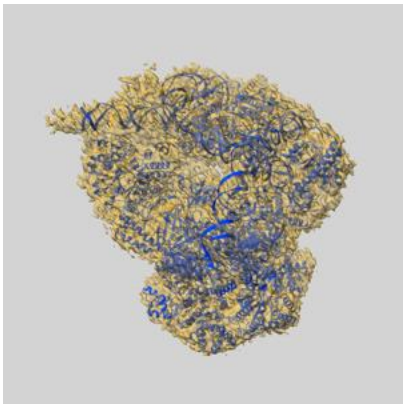
8 Fourier-Shell correlation (i)

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

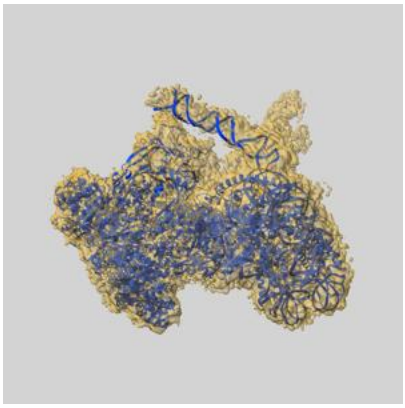
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4396 and PDB model 6GEN. Per-residue inclusion information can be found in section 3 on page 9.

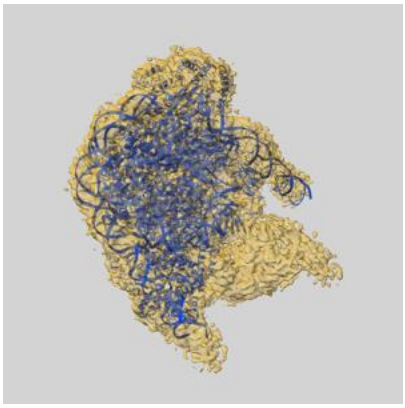
9.1 Map-model overlay



X



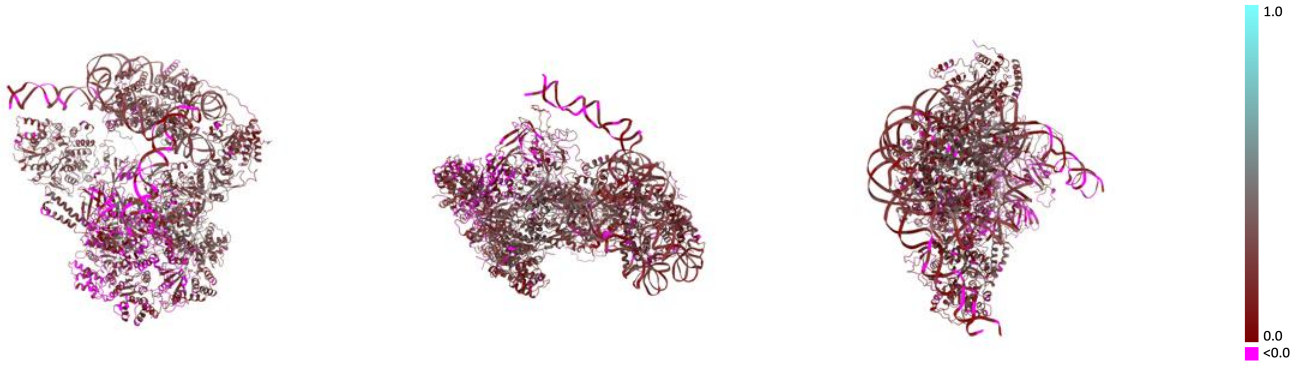
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0359 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.

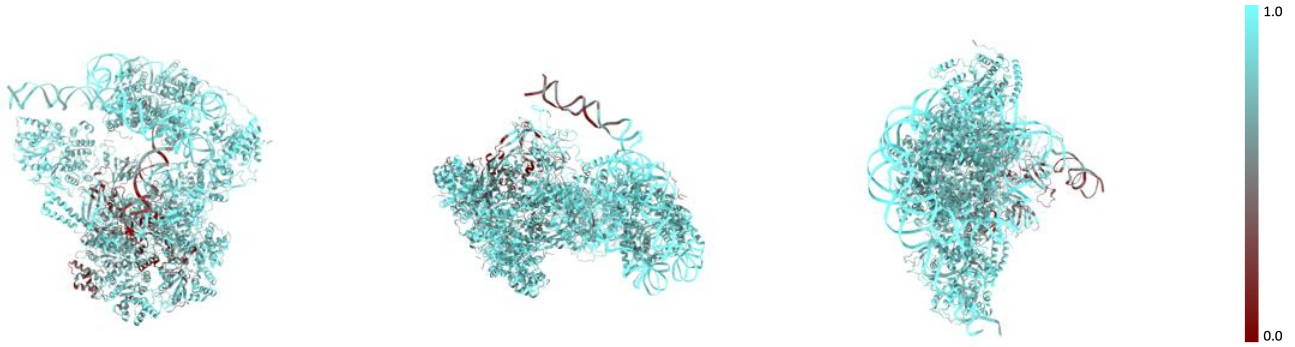
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

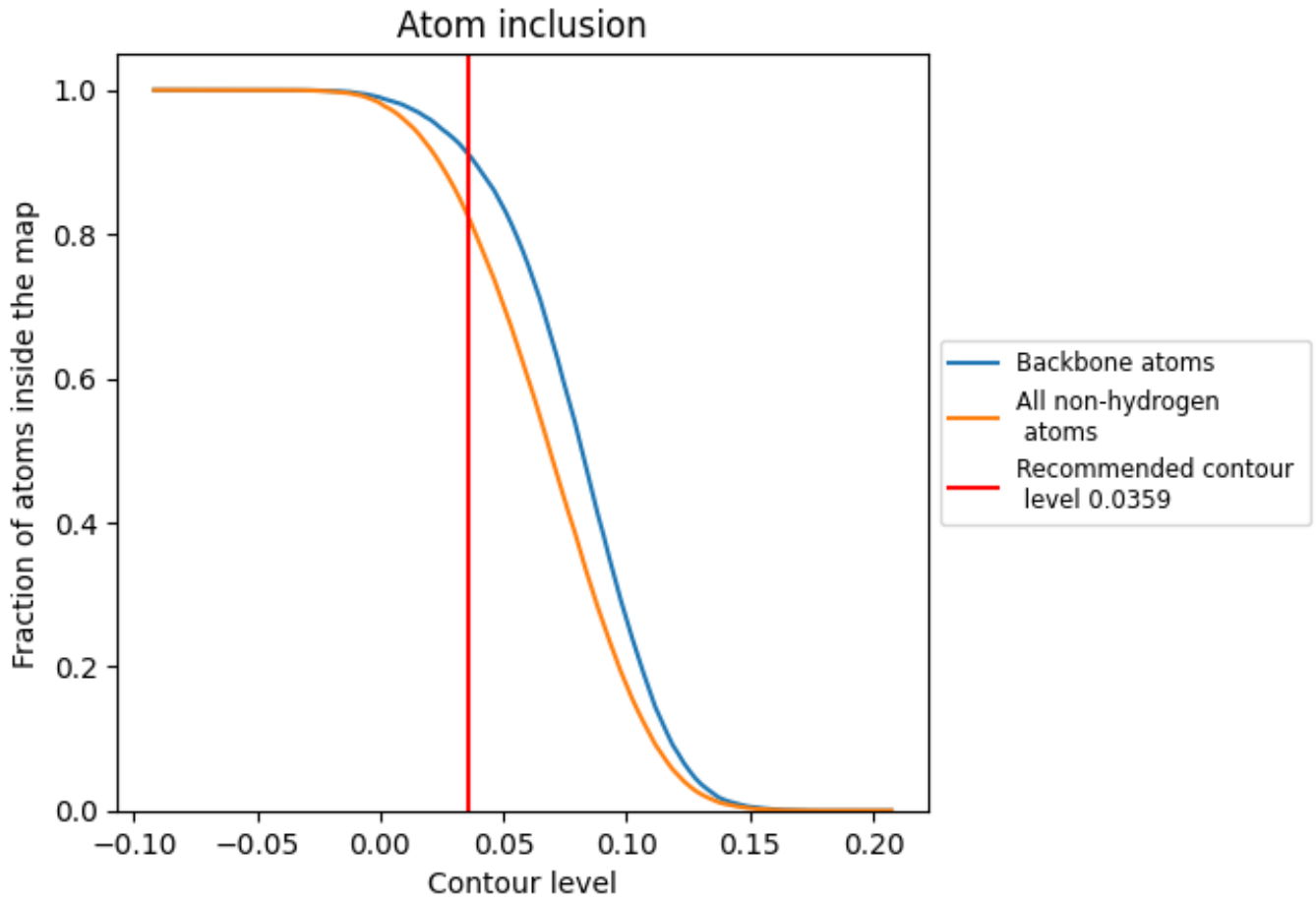
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0359).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 82% 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 (0.0359) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8229	0.1950
A	0.8403	0.2140
B	0.8506	0.2570
C	0.8368	0.2540
D	0.8219	0.2200
E	0.8627	0.2360
F	0.8399	0.2110
G	0.8468	0.2050
H	0.8407	0.2100
I	0.8933	0.1780
J	0.8688	0.1740
M	0.8823	0.2540
R	0.8887	0.2410
S	0.8513	0.2350
T	0.7376	0.1230
U	0.8177	0.2130
V	0.8578	0.2770
W	0.8711	0.2680
X	0.6409	0.0630
Y	0.6728	0.0610
Z	0.8855	0.1990