



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 21, 2025 – 02:27 PM EST

PDB ID : 9E4W
Title : Structure of Bacillus phage SPO1 anti-CBASS 4 (Acb4) in complex with 3'3'-cGAMP
Authors : Chang, R.B.; Toyoda, H.C.; Hobbs, S.J.; Richmond-Buccola, D.; Wein, T.; Burger, N.; Chouchani, E.T.; Sorek, R.; Kranzusch, P.J.
Deposited on : 2024-10-25
Resolution : 2.08 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

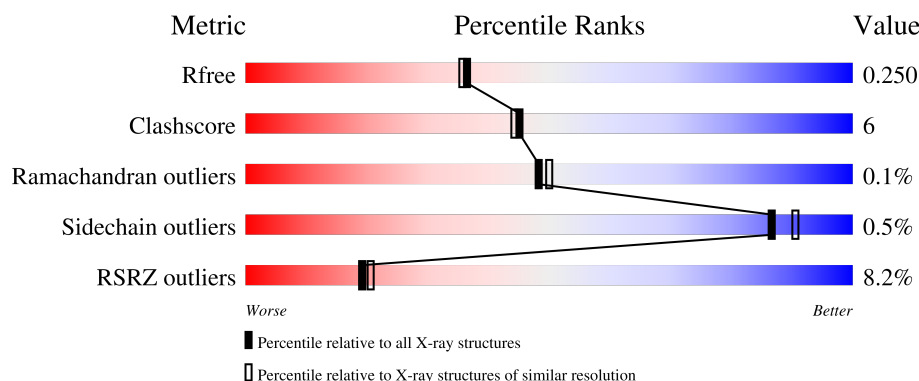
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.08 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7574 (2.10-2.06)
Clashscore	180529	8325 (2.10-2.06)
Ramachandran outliers	177936	8271 (2.10-2.06)
Sidechain outliers	177891	8272 (2.10-2.06)
RSRZ outliers	164620	7574 (2.10-2.06)

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

Mol	Chain	Length	Quality of chain
1	A	97	
1	B	97	
1	C	97	
1	D	97	

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Mol	Chain	Length	Quality of chain
1	E	97	
1	F	97	
1	G	97	
1	H	97	
1	I	97	
1	J	97	
1	K	97	
1	L	97	
1	M	97	
1	N	97	
1	O	97	
1	P	97	
1	Q	97	
1	R	97	
1	S	97	
1	T	97	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16539 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 anti-CBASS 4 (Acb4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	95	Total	C	N	O	S	0	0	0
			756	477	124	153	2			
1	B	94	Total	C	N	O	S	0	0	0
			747	471	122	152	2			
1	C	93	Total	C	N	O	S	0	0	0
			738	465	121	150	2			
1	D	93	Total	C	N	O	S	0	0	0
			738	465	121	150	2			
1	E	93	Total	C	N	O	S	0	0	0
			738	465	121	150	2			
1	F	93	Total	C	N	O	S	0	0	0
			738	465	121	150	2			
1	G	93	Total	C	N	O	S	0	0	0
			738	467	121	147	3			
1	H	93	Total	C	N	O	S	0	0	0
			738	465	121	150	2			
1	I	95	Total	C	N	O	S	0	0	0
			755	477	124	152	2			
1	J	88	Total	C	N	O	S	0	0	0
			698	439	115	142	2			
1	K	94	Total	C	N	O	S	0	0	0
			747	471	123	151	2			
1	L	94	Total	C	N	O	S	0	0	0
			747	471	123	151	2			
1	M	87	Total	C	N	O	S	0	0	0
			691	437	113	139	2			
1	N	86	Total	C	N	O	S	0	0	0
			682	431	112	137	2			
1	O	83	Total	C	N	O	S	0	0	0
			648	407	106	133	2			
1	P	90	Total	C	N	O	S	0	0	0
			713	450	117	144	2			

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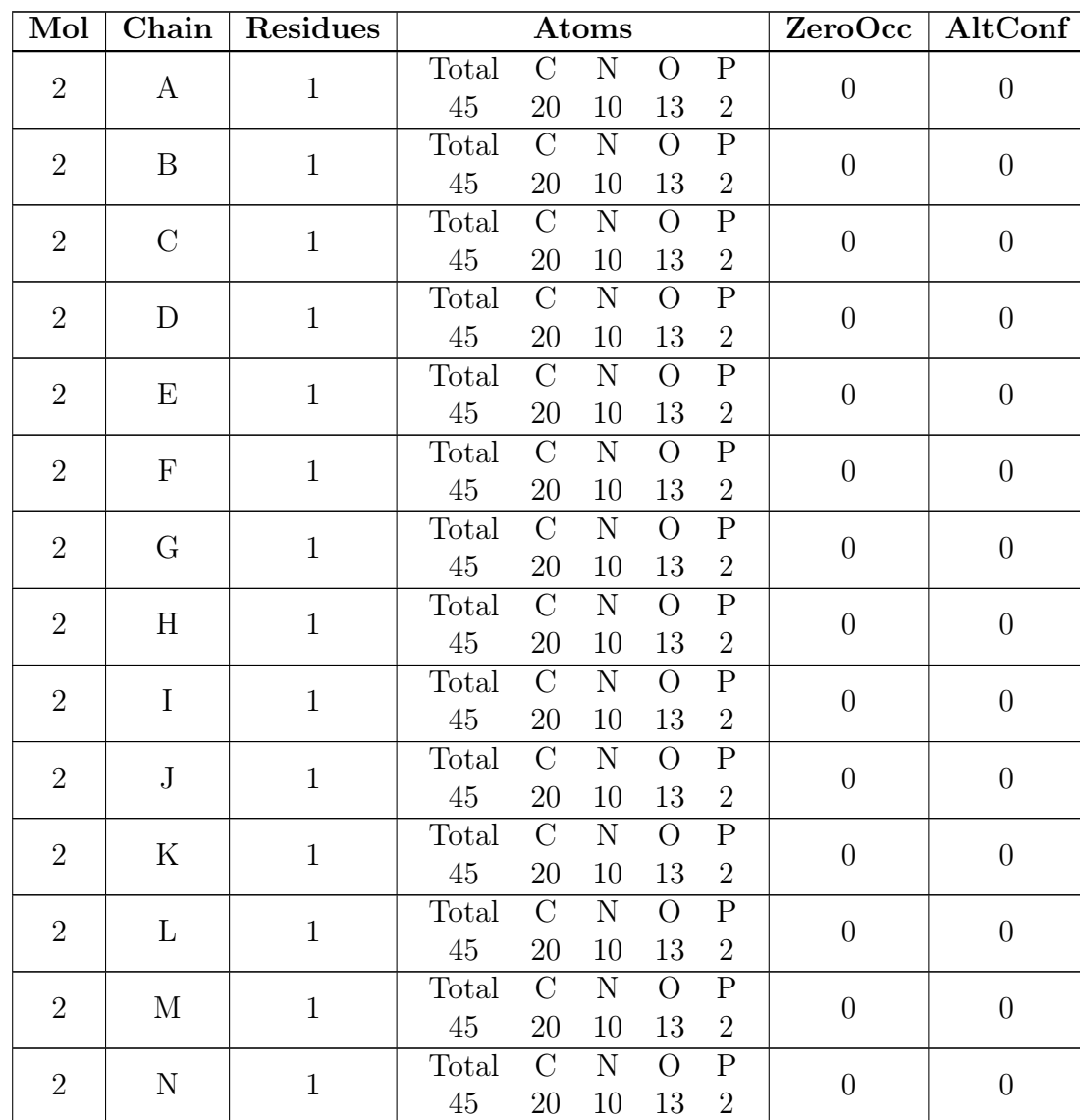
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	90	Total	C	N	O	S	0	0	0
			713	450	117	144	2			
1	R	94	Total	C	N	O	S	0	0	0
			747	471	123	151	2			
1	S	90	Total	C	N	O	S	0	0	0
			715	451	118	144	2			
1	T	92	Total	C	N	O	S	0	0	0
			730	459	120	149	2			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP B6V2Y3
B	0	SER	-	expression tag	UNP B6V2Y3
C	0	SER	-	expression tag	UNP B6V2Y3
D	0	SER	-	expression tag	UNP B6V2Y3
E	0	SER	-	expression tag	UNP B6V2Y3
F	0	SER	-	expression tag	UNP B6V2Y3
G	0	SER	-	expression tag	UNP B6V2Y3
H	0	SER	-	expression tag	UNP B6V2Y3
I	0	SER	-	expression tag	UNP B6V2Y3
J	0	SER	-	expression tag	UNP B6V2Y3
K	0	SER	-	expression tag	UNP B6V2Y3
L	0	SER	-	expression tag	UNP B6V2Y3
M	0	SER	-	expression tag	UNP B6V2Y3
N	0	SER	-	expression tag	UNP B6V2Y3
O	0	SER	-	expression tag	UNP B6V2Y3
P	0	SER	-	expression tag	UNP B6V2Y3
Q	0	SER	-	expression tag	UNP B6V2Y3
R	0	SER	-	expression tag	UNP B6V2Y3
S	0	SER	-	expression tag	UNP B6V2Y3
T	0	SER	-	expression tag	UNP B6V2Y3

- Molecule 2 is 2-amino-9-[(2R,3R,3aS,5R,7aR,9R,10R,10aS,12R,14aR)-9-(6-amino-9H-purin-9-yl)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecin-2-yl]-1,9-dihydro-6H-purin-6-one (three-letter code: 4BW) (formula: C₂₀H₂₄N₁₀O₁₃P₂) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total 45	C 20	N 10	O 13	P 2	0	0
2	P	1	Total 45	C 20	N 10	O 13	P 2	0	0
2	Q	1	Total 45	C 20	N 10	O 13	P 2	0	0
2	R	1	Total 45	C 20	N 10	O 13	P 2	0	0
2	S	1	Total 45	C 20	N 10	O 13	P 2	0	0
2	T	1	Total 45	C 20	N 10	O 13	P 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	98	Total 98	O 98	0	0
3	B	88	Total 88	O 88	0	0
3	C	82	Total 82	O 82	0	0
3	D	81	Total 81	O 81	0	0
3	E	83	Total 83	O 83	0	0
3	F	88	Total 88	O 88	0	0
3	G	63	Total 63	O 63	0	0
3	H	72	Total 72	O 72	0	0
3	I	65	Total 65	O 65	0	0
3	J	56	Total 56	O 56	0	0
3	K	44	Total 44	O 44	0	0
3	L	45	Total 45	O 45	0	0
3	M	38	Total 38	O 38	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	N	30	Total 30	O 30	0	0
3	O	20	Total 20	O 20	0	0
3	P	27	Total 27	O 27	0	0
3	Q	41	Total 41	O 41	0	0
3	R	41	Total 41	O 41	0	0
3	S	26	Total 26	O 26	0	0
3	T	34	Total 34	O 34	0	0

- Molecule 1: anti-CBASS 4 (Acb4)



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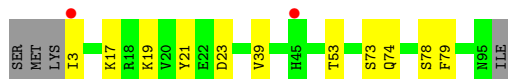
- Molecule 1: anti-CBASS 4 (Acb4)




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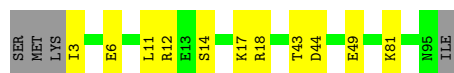


- Molecule 1: anti-CBASS 4 (Acb4)

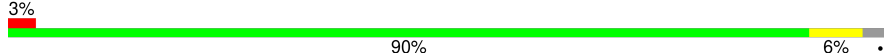


- Molecule 1: anti-CBASS 4 (Acb4)

Chain F:  85% 11% .




- Molecule 1: anti-CBASS 4 (Acb4)

Chain G:  3% 90% 6% .



- Molecule 1: anti-CBASS 4 (Acb4)

Chain H:  0% 87% 9% .




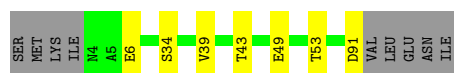
- Molecule 1: anti-CBASS 4 (Acb4)

Chain I:  94% . .




- Molecule 1: anti-CBASS 4 (Acb4)

Chain J:  84% 7% 9%




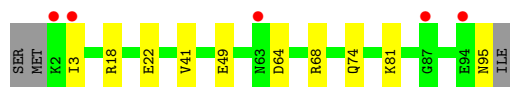
- Molecule 1: anti-CBASS 4 (Acb4)

Chain K:  5% 82% 14% .

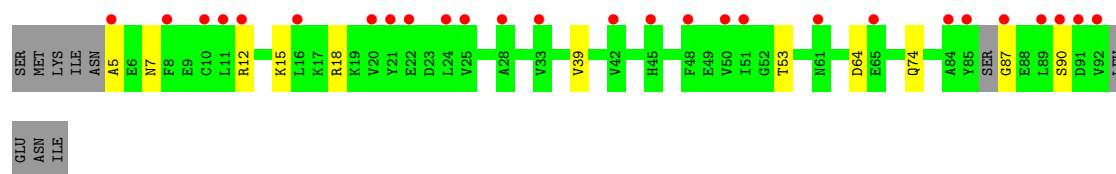
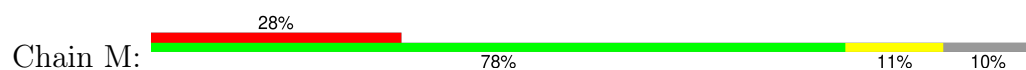


- Molecule 1: anti-CBASS 4 (Acb4)

Chain L:  5% 87% 10% .



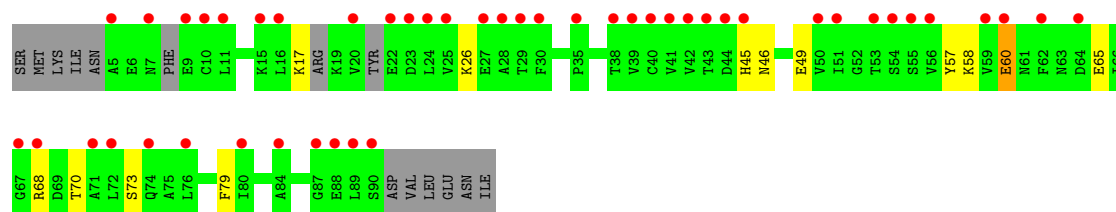
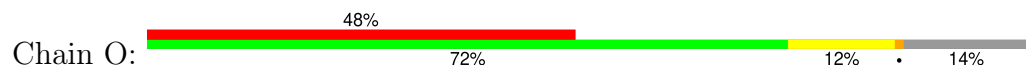
- Molecule 1: anti-CBASS 4 (Acb4)



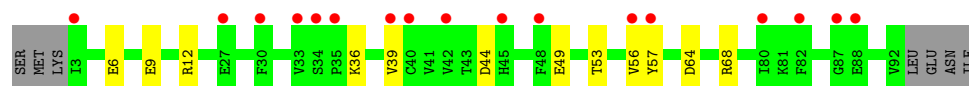
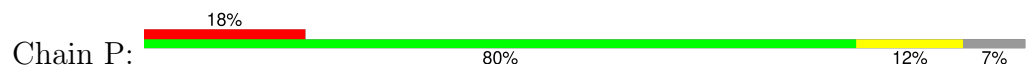
- Molecule 1: anti-CBASS 4 (Acb4)



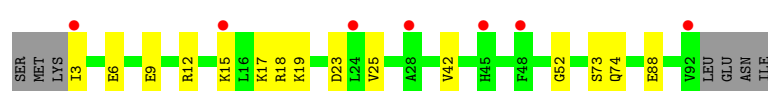
- Molecule 1: anti-CBASS 4 (Acb4)



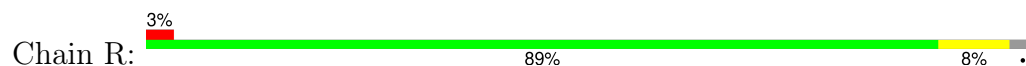
- Molecule 1: anti-CBASS 4 (Acb4)

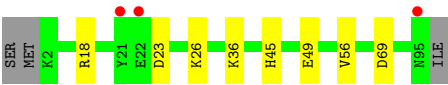


- Molecule 1: anti-CBASS 4 (Acb4)

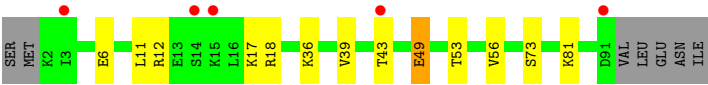
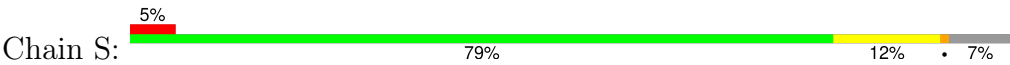


- Molecule 1: anti-CBASS 4 (Acb4)

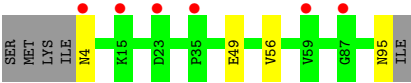




• Molecule 1: anti-CBASS 4 (Acb4)



• Molecule 1: anti-CBASS 4 (Acb4)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.28Å 56.50Å 167.58Å 87.53° 89.02° 81.58°	Depositor
Resolution (Å)	45.60 – 2.08 45.60 – 2.08	Depositor EDS
% Data completeness (in resolution range)	69.4 (45.60-2.08) 69.8 (45.60-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.219 , 0.252 0.218 , 0.250	Depositor DCC
R_{free} test set	113016 reflections (1.71%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16539	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4BW

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	0.24	0/766	0.44	0/1031
1	B	0.24	0/757	0.44	0/1020
1	C	0.25	0/748	0.44	0/1009
1	D	0.24	0/748	0.44	0/1009
1	E	0.24	0/748	0.44	0/1009
1	F	0.24	0/748	0.44	0/1009
1	G	0.24	0/748	0.44	0/1007
1	H	0.23	0/748	0.44	0/1009
1	I	0.24	0/765	0.44	0/1031
1	J	0.24	0/708	0.45	0/954
1	K	0.24	0/757	0.44	0/1020
1	L	0.28	0/757	0.45	0/1020
1	M	0.24	0/700	0.44	0/942
1	N	0.24	0/692	0.44	0/932
1	O	0.24	0/653	0.44	0/875
1	P	0.24	0/723	0.44	0/975
1	Q	0.24	0/723	0.44	0/975
1	R	0.24	0/757	0.44	0/1020
1	S	0.24	0/725	0.46	0/976
1	T	0.24	0/740	0.44	0/998
All	All	0.24	0/14711	0.44	0/19821

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	756	0	749	10	0
1	B	747	0	736	7	0
1	C	738	0	725	9	0
1	D	738	0	725	8	0
1	E	738	0	725	6	0
1	F	738	0	725	8	0
1	G	738	0	738	4	0
1	H	738	0	725	4	0
1	I	755	0	749	3	0
1	J	698	0	682	6	0
1	K	747	0	738	11	0
1	L	747	0	738	7	0
1	M	691	0	679	10	0
1	N	682	0	672	12	0
1	O	648	0	638	9	0
1	P	713	0	702	8	0
1	Q	713	0	702	10	0
1	R	747	0	738	6	0
1	S	715	0	706	8	0
1	T	730	0	714	5	0
2	A	45	0	22	1	0
2	B	45	0	22	1	0
2	C	45	0	22	4	0
2	D	45	0	22	2	0
2	E	45	0	22	3	0
2	F	45	0	22	2	0
2	G	45	0	22	1	0
2	H	45	0	22	1	0
2	I	45	0	22	4	0
2	J	45	0	22	2	0
2	K	45	0	22	3	0
2	L	45	0	22	1	0
2	M	45	0	22	1	0
2	N	45	0	22	2	0
2	O	45	0	22	4	0
2	P	45	0	22	2	0
2	Q	45	0	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	45	0	22	2	0
2	S	45	0	22	3	0
2	T	45	0	22	3	0
3	A	98	0	0	4	0
3	B	88	0	0	6	3
3	C	82	0	0	4	1
3	D	81	0	0	3	1
3	E	83	0	0	2	0
3	F	88	0	0	4	4
3	G	63	0	0	1	4
3	H	72	0	0	1	2
3	I	65	0	0	2	2
3	J	56	0	0	2	0
3	K	44	0	0	5	0
3	L	45	0	0	2	0
3	M	38	0	0	7	1
3	N	30	0	0	3	0
3	O	20	0	0	3	0
3	P	27	0	0	2	0
3	Q	41	0	0	2	1
3	R	41	0	0	3	4
3	S	26	0	0	2	0
3	T	34	0	0	3	1
All	All	16539	0	14746	175	12

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 175 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:101:4BW:OAX	2:G:101:4BW:CBO	1.67	1.22
2:F:101:4BW:OAX	2:F:101:4BW:CBO	1.67	1.20
2:S:4201:4BW:OAX	2:S:4201:4BW:CBO	1.68	1.19
2:N:101:4BW:OAX	2:N:101:4BW:CBO	1.68	1.19
2:I:101:4BW:OAX	2:I:101:4BW:CBO	1.67	1.17

The worst 5 of 12 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:251:HOH:O	3:I:238:HOH:O[1_645]	1.61	0.59
3:H:207:HOH:O	3:R:232:HOH:O[1_556]	1.89	0.31
3:M:228:HOH:O	3:T:221:HOH:O[1_645]	1.92	0.28
3:G:237:HOH:O	3:R:227:HOH:O[1_546]	1.98	0.22
3:G:256:HOH:O	3:R:239:HOH:O[1_556]	1.98	0.22

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 X-ray entries followed by that with respect to entries of similar resolution.

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	93/97 (96%)	92 (99%)	1 (1%)	0	100	100
1	B	92/97 (95%)	92 (100%)	0	0	100	100
1	C	91/97 (94%)	91 (100%)	0	0	100	100
1	D	91/97 (94%)	90 (99%)	1 (1%)	0	100	100
1	E	91/97 (94%)	91 (100%)	0	0	100	100
1	F	91/97 (94%)	91 (100%)	0	0	100	100
1	G	91/97 (94%)	90 (99%)	1 (1%)	0	100	100
1	H	91/97 (94%)	91 (100%)	0	0	100	100
1	I	93/97 (96%)	93 (100%)	0	0	100	100
1	J	86/97 (89%)	86 (100%)	0	0	100	100
1	K	92/97 (95%)	90 (98%)	2 (2%)	0	100	100
1	L	92/97 (95%)	90 (98%)	2 (2%)	0	100	100
1	M	83/97 (86%)	82 (99%)	1 (1%)	0	100	100
1	N	84/97 (87%)	84 (100%)	0	0	100	100
1	O	75/97 (77%)	73 (97%)	2 (3%)	0	100	100
1	P	88/97 (91%)	88 (100%)	0	0	100	100
1	Q	88/97 (91%)	88 (100%)	0	0	100	100
1	R	92/97 (95%)	92 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	88/97 (91%)	87 (99%)	0	1 (1%)	12	7
1	T	90/97 (93%)	90 (100%)	0	0	100	100
All	All	1782/1940 (92%)	1771 (99%)	10 (1%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	49	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	87/89 (98%)	86 (99%)	1 (1%)	70	76
1	B	86/89 (97%)	86 (100%)	0	100	100
1	C	85/89 (96%)	84 (99%)	1 (1%)	67	73
1	D	85/89 (96%)	85 (100%)	0	100	100
1	E	85/89 (96%)	84 (99%)	1 (1%)	67	73
1	F	85/89 (96%)	85 (100%)	0	100	100
1	G	85/89 (96%)	85 (100%)	0	100	100
1	H	85/89 (96%)	83 (98%)	2 (2%)	44	47
1	I	87/89 (98%)	87 (100%)	0	100	100
1	J	80/89 (90%)	80 (100%)	0	100	100
1	K	86/89 (97%)	86 (100%)	0	100	100
1	L	86/89 (97%)	85 (99%)	1 (1%)	67	73
1	M	79/89 (89%)	79 (100%)	0	100	100
1	N	78/89 (88%)	78 (100%)	0	100	100
1	O	75/89 (84%)	73 (97%)	2 (3%)	40	43
1	P	82/89 (92%)	82 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	82/89 (92%)	82 (100%)	0	100	100
1	R	86/89 (97%)	86 (100%)	0	100	100
1	S	82/89 (92%)	82 (100%)	0	100	100
1	T	84/89 (94%)	84 (100%)	0	100	100
All	All	1670/1780 (94%)	1662 (100%)	8 (0%)	86	90

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	79	PHE
1	O	60	GLU
1	H	79	PHE
1	H	4	ASN
1	L	3	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

20 ligands are modelled in this entry.

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
2	4BW	S	4201	-	43,51,51	4.77	18 (41%)	49,80,80	1.78	10 (20%)
2	4BW	O	101	-	43,51,51	4.76	19 (44%)	49,80,80	1.82	10 (20%)
2	4BW	D	301	-	43,51,51	4.75	18 (41%)	49,80,80	1.80	9 (18%)
2	4BW	I	101	-	43,51,51	4.76	18 (41%)	49,80,80	1.79	9 (18%)
2	4BW	C	101	-	43,51,51	4.75	18 (41%)	49,80,80	1.73	9 (18%)
2	4BW	H	101	-	43,51,51	4.76	18 (41%)	49,80,80	1.78	9 (18%)
2	4BW	M	101	-	43,51,51	4.78	19 (44%)	49,80,80	1.81	10 (20%)
2	4BW	Q	101	-	43,51,51	4.78	18 (41%)	49,80,80	1.78	9 (18%)
2	4BW	B	201	-	43,51,51	4.77	19 (44%)	49,80,80	1.81	9 (18%)
2	4BW	L	101	-	43,51,51	4.77	18 (41%)	49,80,80	1.81	9 (18%)
2	4BW	K	101	-	43,51,51	4.79	18 (41%)	49,80,80	1.82	9 (18%)
2	4BW	E	101	-	43,51,51	4.75	17 (39%)	49,80,80	1.72	10 (20%)
2	4BW	R	101	-	43,51,51	4.78	19 (44%)	49,80,80	1.85	10 (20%)
2	4BW	T	101	-	43,51,51	4.79	19 (44%)	49,80,80	1.79	9 (18%)
2	4BW	F	101	-	43,51,51	4.76	18 (41%)	49,80,80	1.79	9 (18%)
2	4BW	G	101	-	43,51,51	4.76	19 (44%)	49,80,80	1.80	9 (18%)
2	4BW	A	201	-	43,51,51	4.75	18 (41%)	49,80,80	1.82	8 (16%)
2	4BW	J	101	-	43,51,51	4.77	18 (41%)	49,80,80	1.79	9 (18%)
2	4BW	P	101	-	43,51,51	4.77	19 (44%)	49,80,80	1.85	10 (20%)
2	4BW	N	101	-	43,51,51	4.77	19 (44%)	49,80,80	1.78	9 (18%)

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
2	4BW	S	4201	-	-	1/22/62/62	0/6/7/7
2	4BW	O	101	-	-	6/22/62/62	0/6/7/7
2	4BW	D	301	-	-	1/22/62/62	0/6/7/7
2	4BW	I	101	-	-	6/22/62/62	0/6/7/7
2	4BW	C	101	-	-	3/22/62/62	0/6/7/7
2	4BW	H	101	-	-	2/22/62/62	0/6/7/7

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4BW	M	101	-	-	1/22/62/62	0/6/7/7
2	4BW	Q	101	-	-	1/22/62/62	0/6/7/7
2	4BW	B	201	-	-	3/22/62/62	0/6/7/7
2	4BW	L	101	-	-	3/22/62/62	0/6/7/7
2	4BW	K	101	-	-	0/22/62/62	0/6/7/7
2	4BW	E	101	-	-	3/22/62/62	0/6/7/7
2	4BW	R	101	-	-	2/22/62/62	0/6/7/7
2	4BW	T	101	-	-	2/22/62/62	0/6/7/7
2	4BW	F	101	-	-	1/22/62/62	0/6/7/7
2	4BW	G	101	-	-	1/22/62/62	0/6/7/7
2	4BW	A	201	-	-	2/22/62/62	0/6/7/7
2	4BW	J	101	-	-	4/22/62/62	0/6/7/7
2	4BW	P	101	-	-	6/22/62/62	0/6/7/7
2	4BW	N	101	-	-	6/22/62/62	0/6/7/7

The worst 5 of 367 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	101	4BW	OAX-CBO	20.70	1.68	1.40
2	M	101	4BW	OAX-CBO	20.66	1.68	1.40
2	Q	101	4BW	OAX-CBO	20.66	1.68	1.40
2	R	101	4BW	OAX-CBO	20.66	1.68	1.40
2	S	4201	4BW	OAX-CBO	20.64	1.68	1.40

The worst 5 of 185 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	101	4BW	C4'-O4'-C1'	-5.63	104.77	109.92
2	F	101	4BW	N3-C2-N1	-5.42	121.31	128.67
2	A	201	4BW	N3-C2-N1	-5.41	121.33	128.67
2	P	101	4BW	N3-C2-N1	-5.37	121.38	128.67
2	H	101	4BW	N3-C2-N1	-5.37	121.38	128.67

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	4BW	CAN-OAV-PBR-OAD
2	B	201	4BW	CAN-OAV-PBR-OAD

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Mol	Chain	Res	Type	Atoms
2	B	201	4BW	C5'-O5'-PBS-OAI
2	F	101	4BW	CAN-OAV-PBR-OAD
2	I	101	4BW	CAN-OAV-PBR-O3'

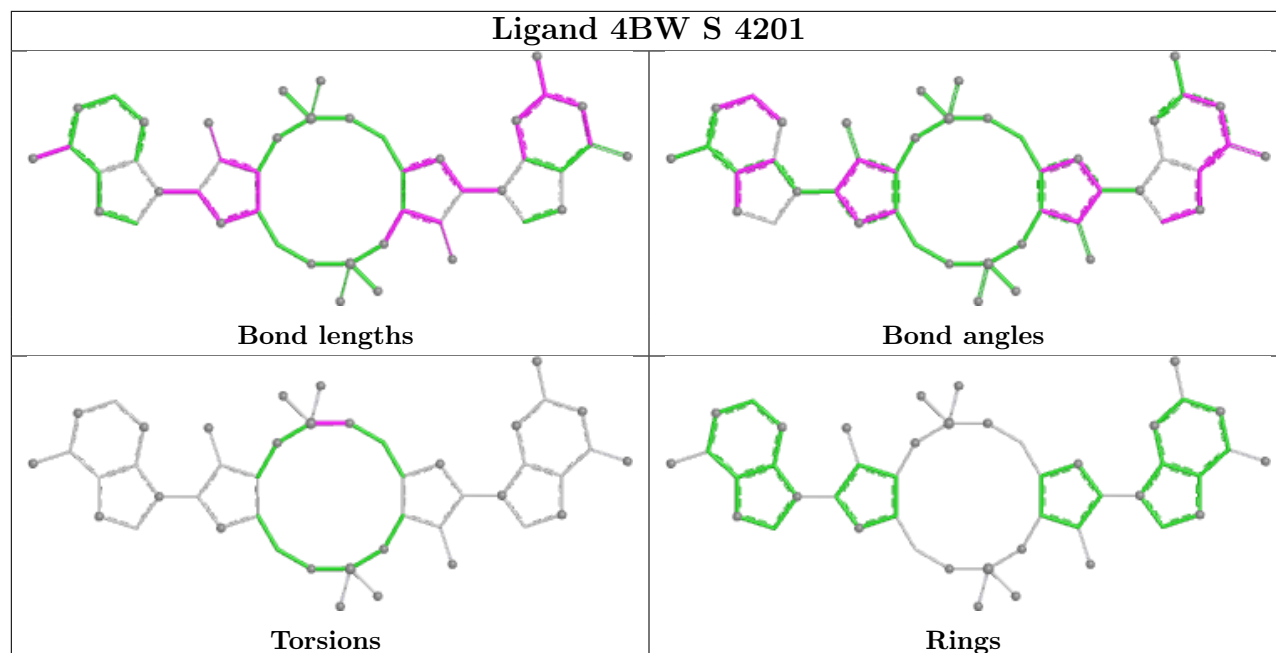
There are no ring outliers.

20 monomers are involved in 44 short contacts:

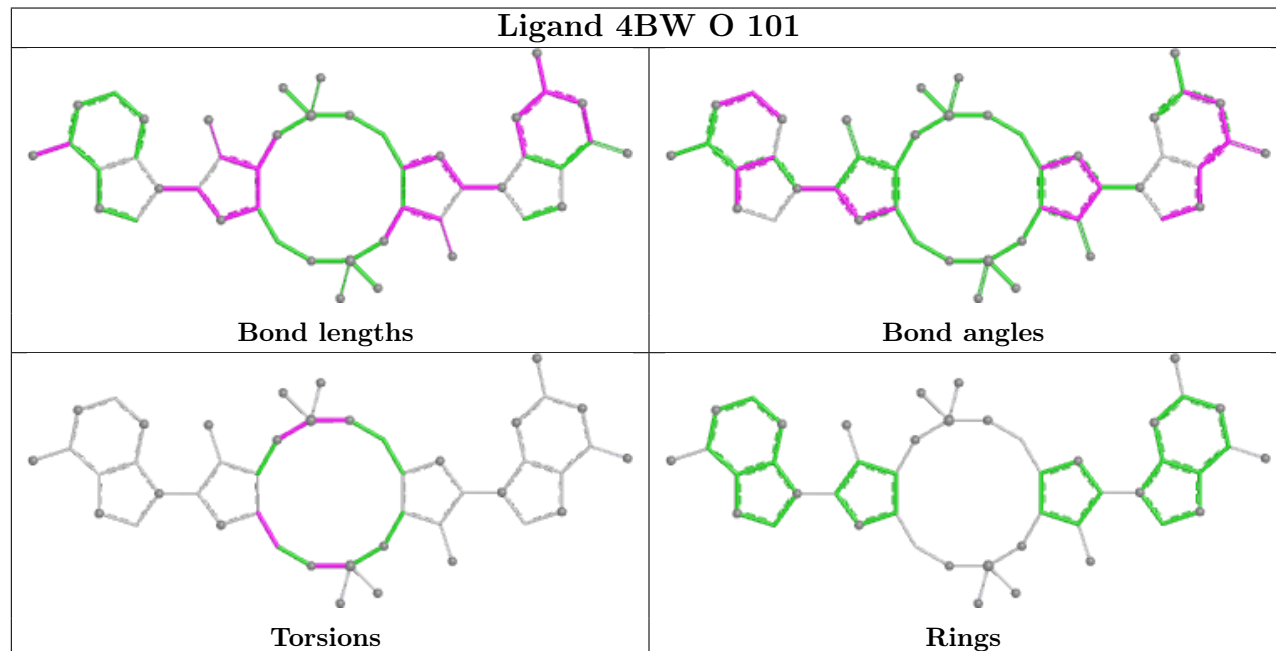
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	S	4201	4BW	3	0
2	O	101	4BW	4	0
2	D	301	4BW	2	0
2	I	101	4BW	4	0
2	C	101	4BW	4	0
2	H	101	4BW	1	0
2	M	101	4BW	1	0
2	Q	101	4BW	2	0
2	B	201	4BW	1	0
2	L	101	4BW	1	0
2	K	101	4BW	3	0
2	E	101	4BW	3	0
2	R	101	4BW	2	0
2	T	101	4BW	3	0
2	F	101	4BW	2	0
2	G	101	4BW	1	0
2	A	201	4BW	1	0
2	J	101	4BW	2	0
2	P	101	4BW	2	0
2	N	101	4BW	2	0

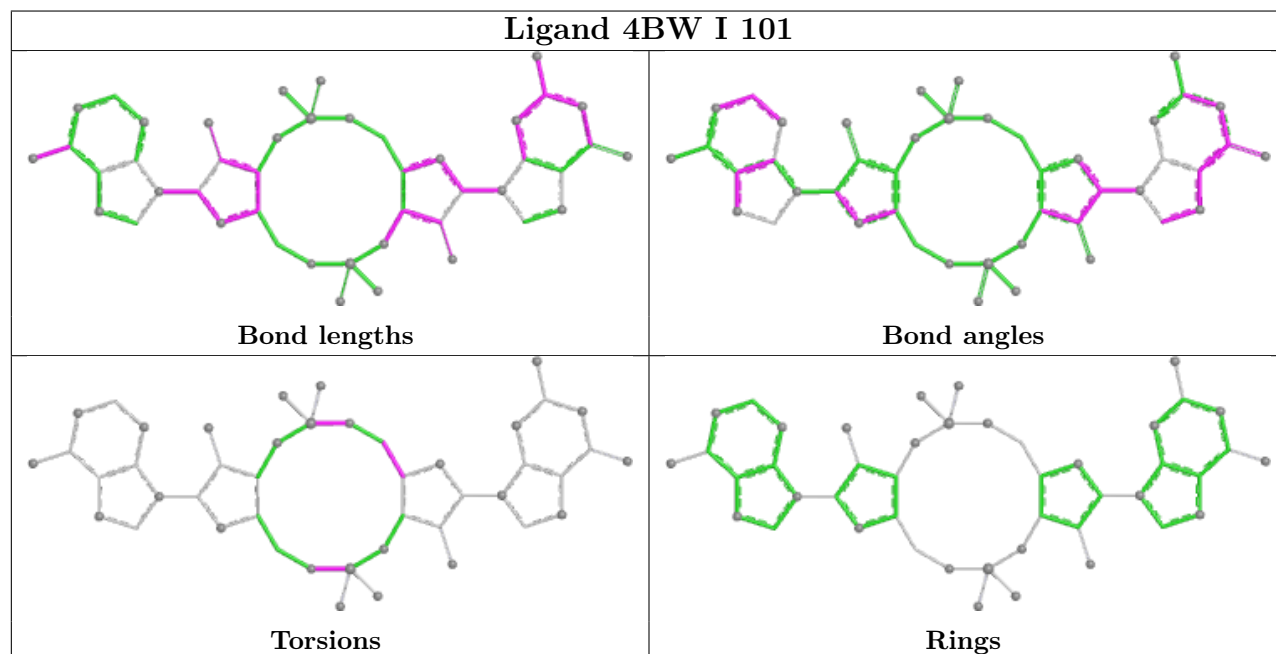
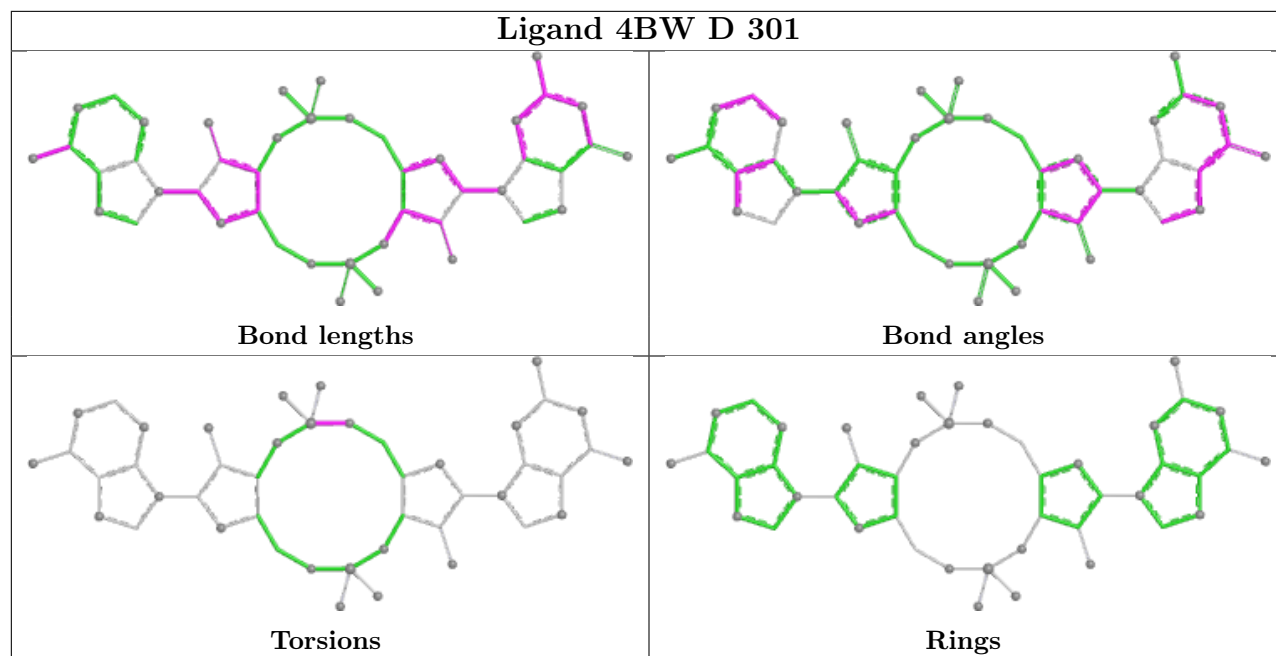
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

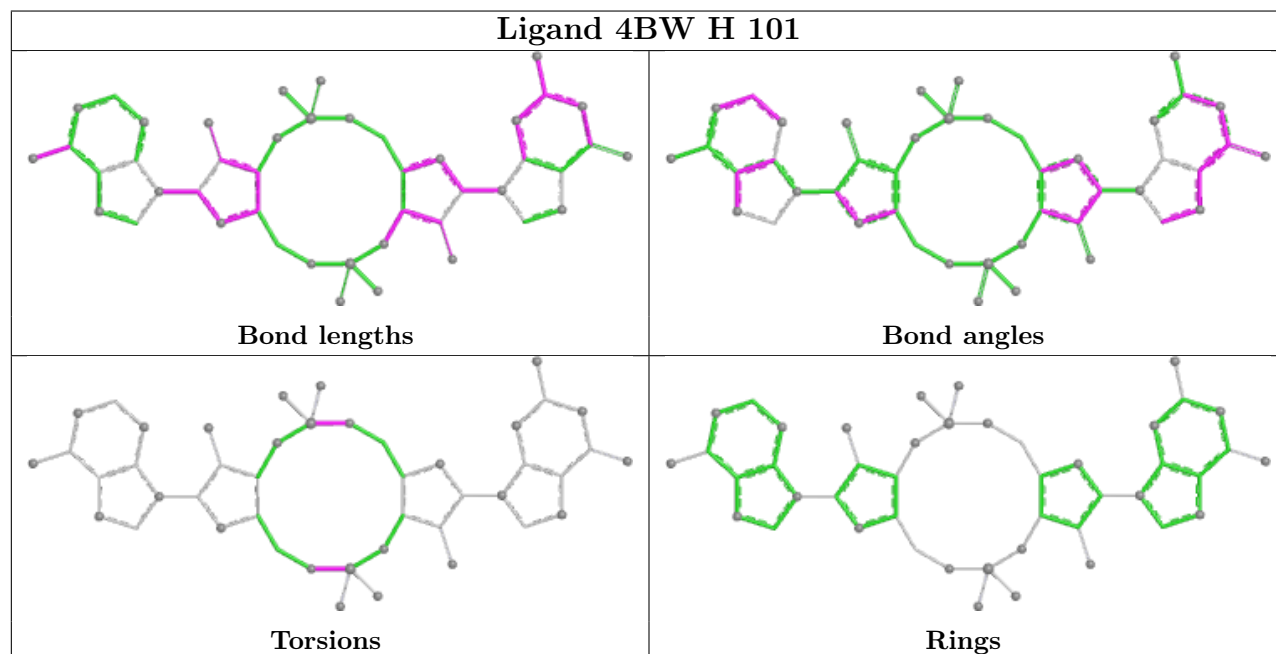
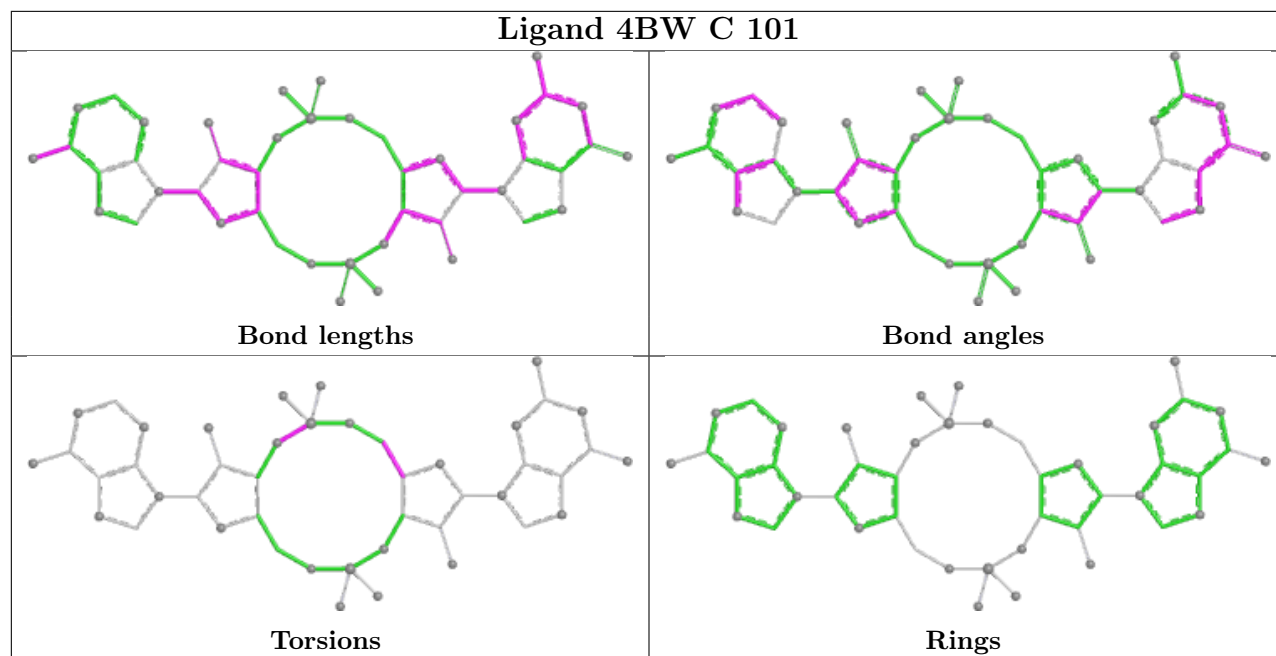
Ligand 4BW S 4201

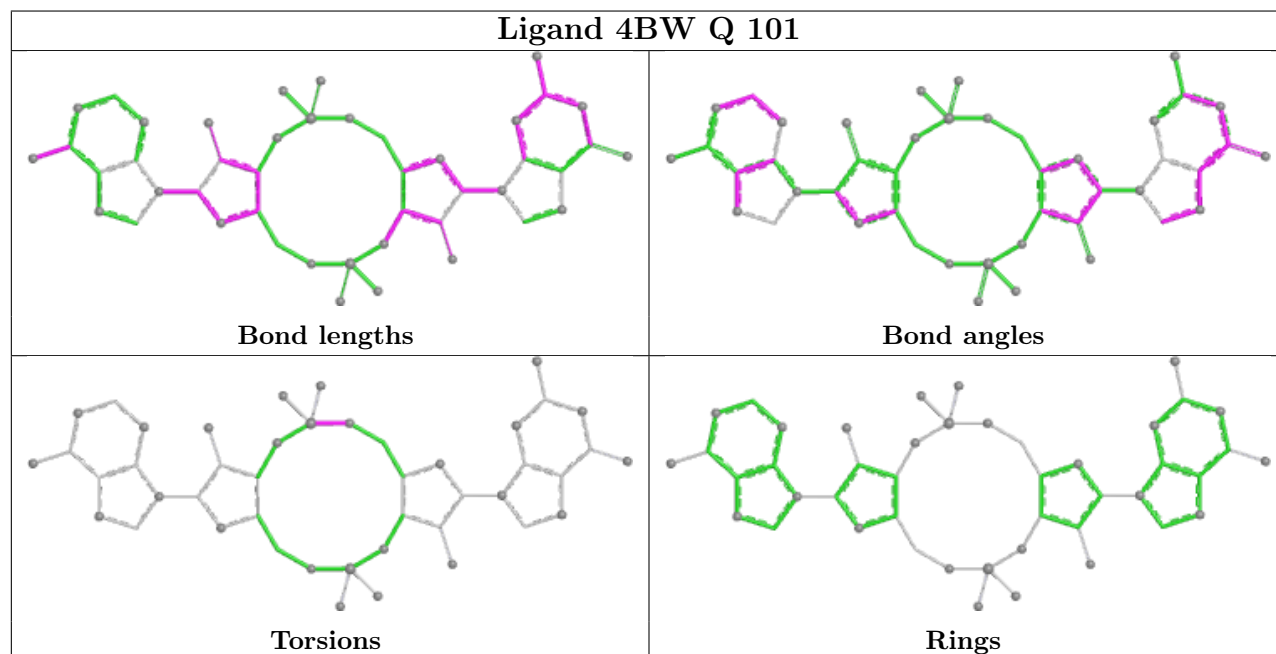
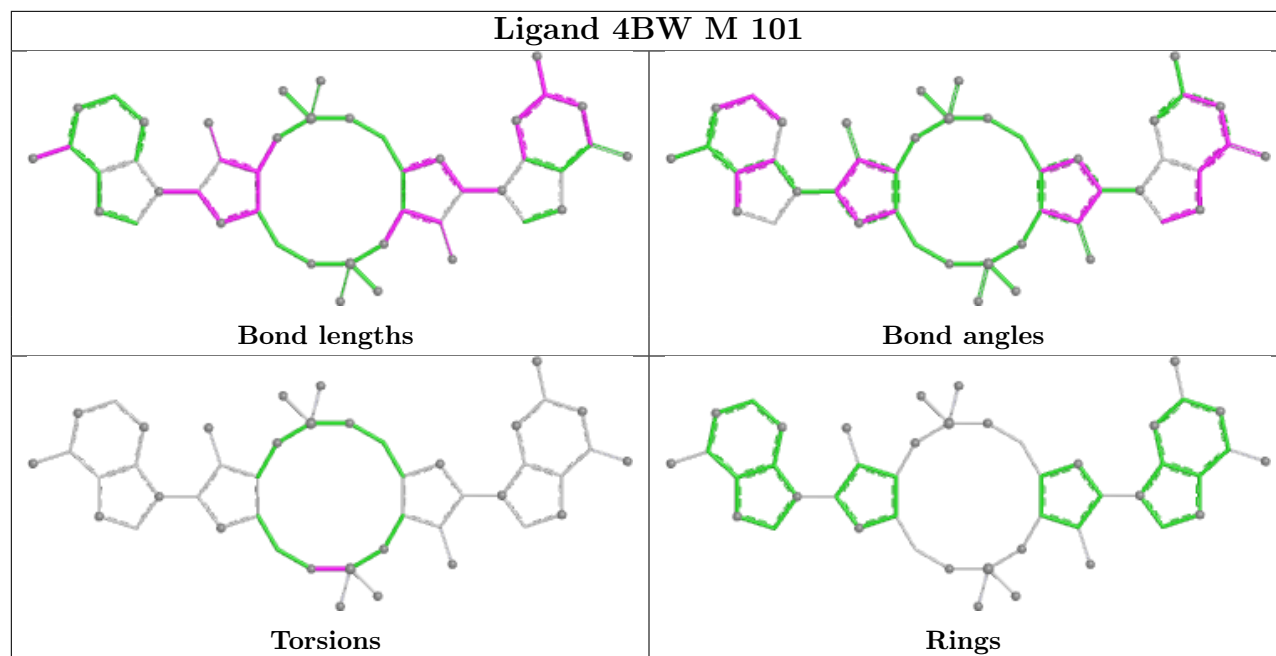


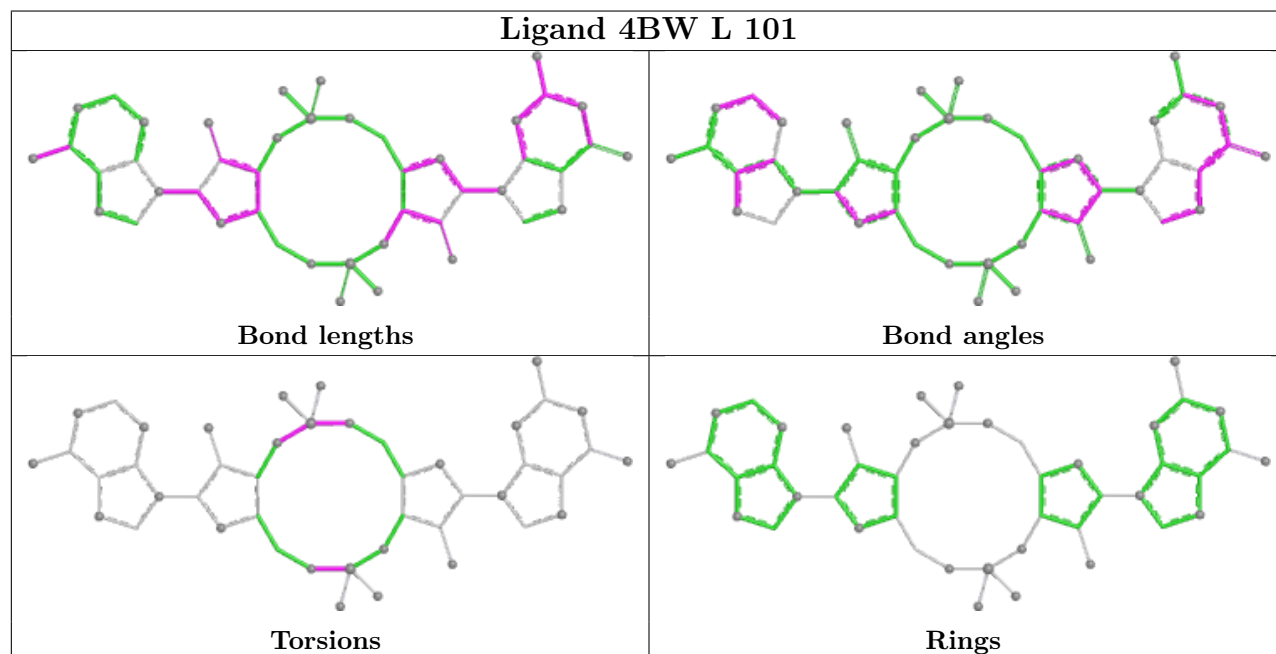
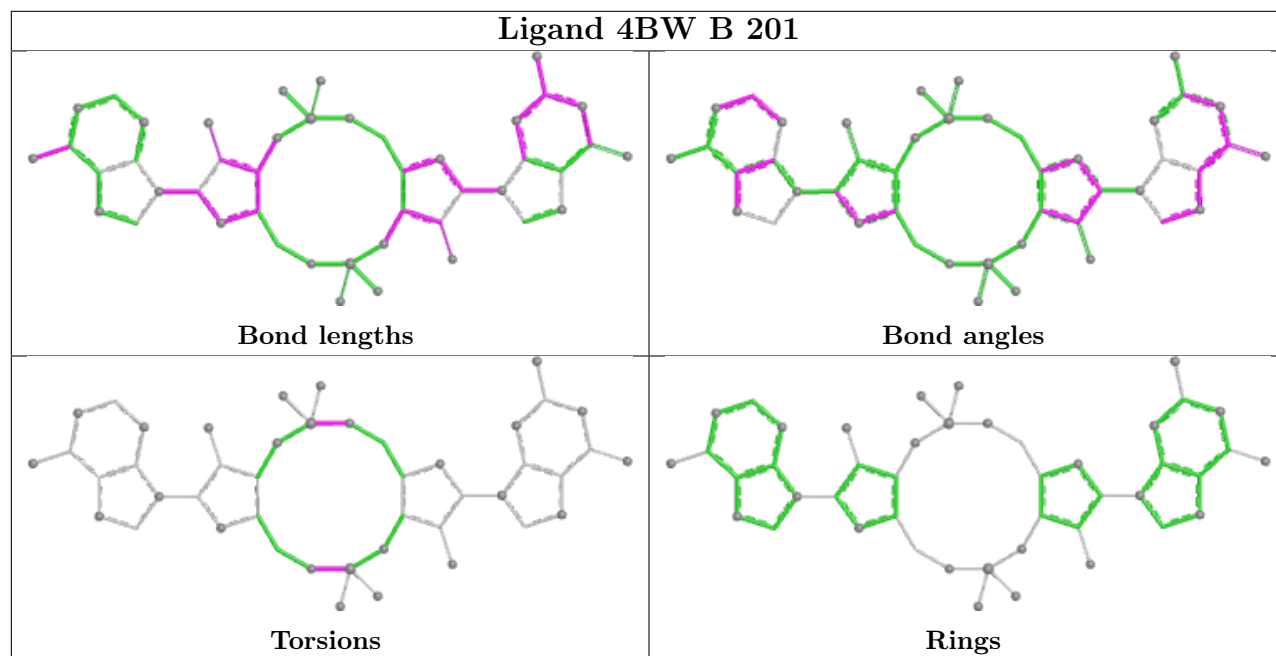
Ligand 4BW O 101

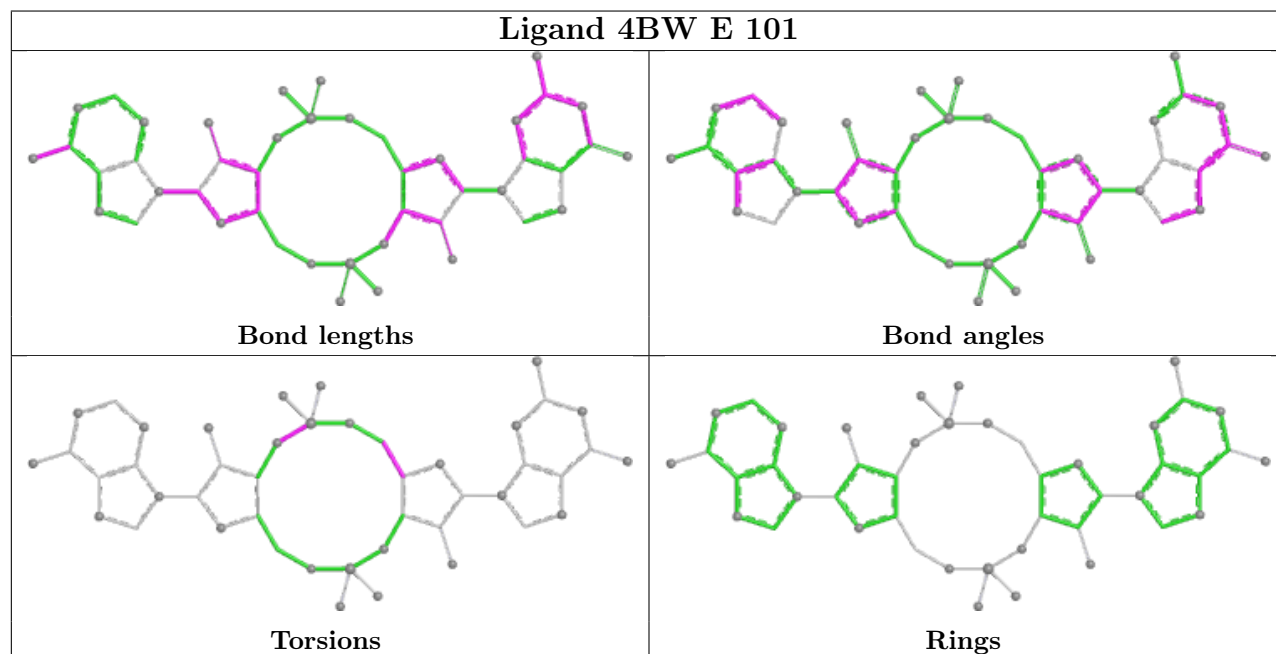
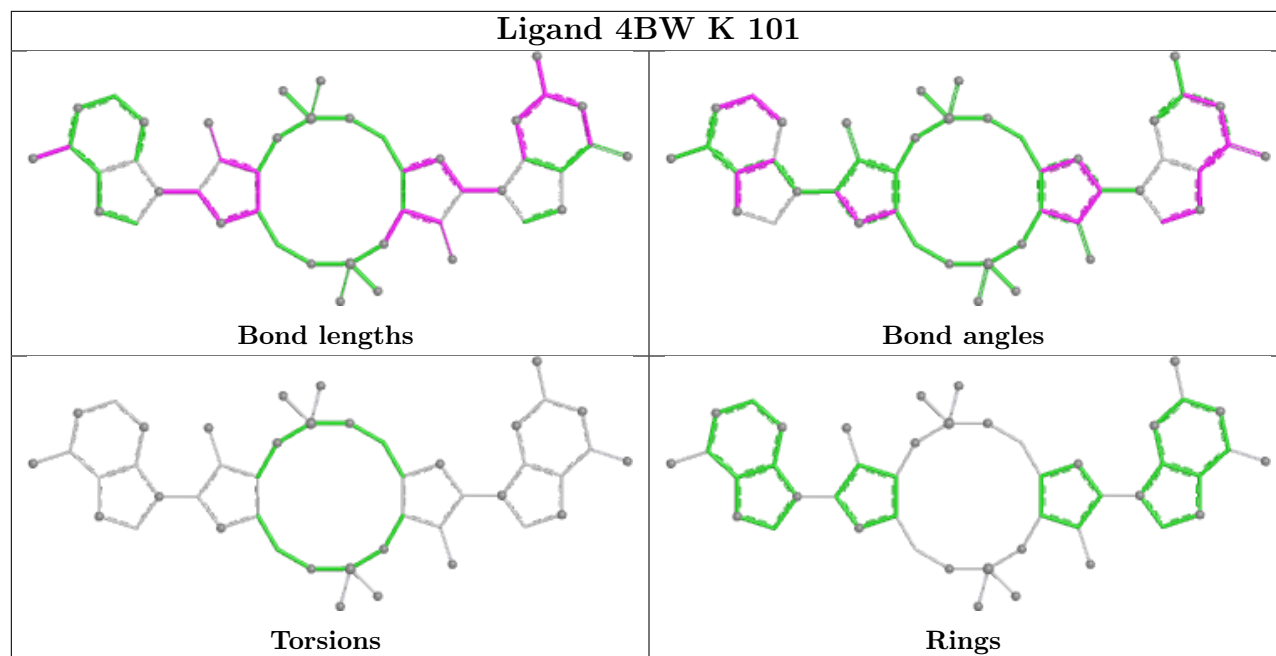


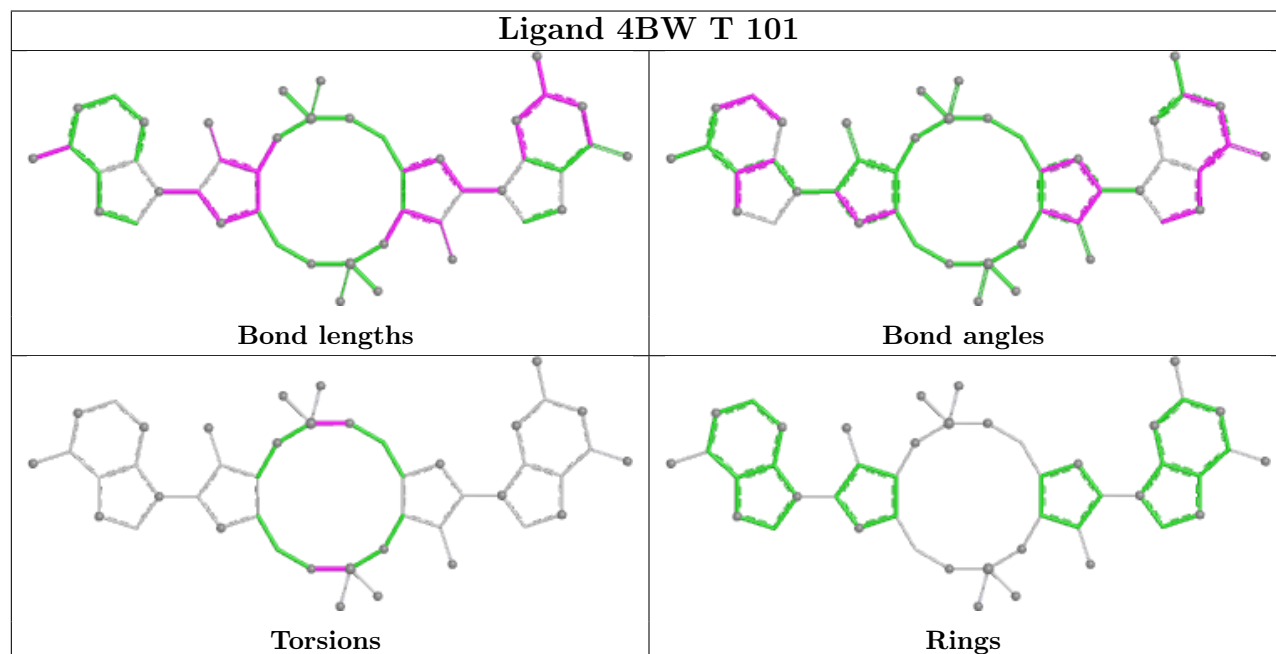
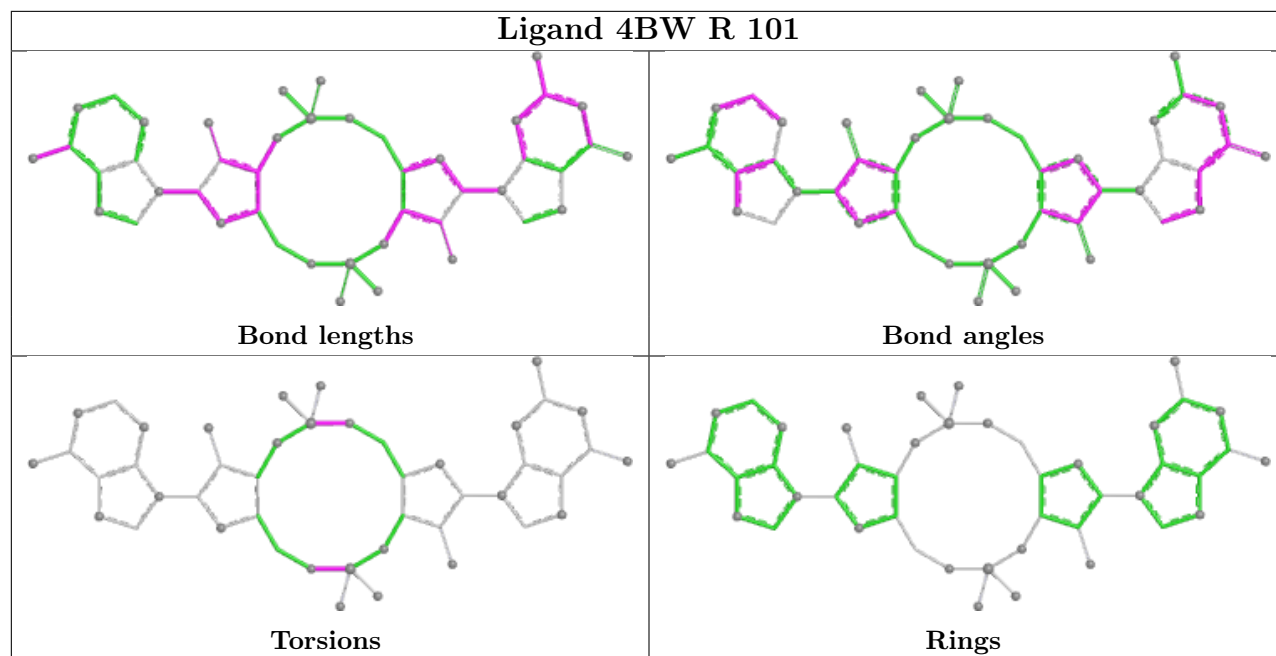




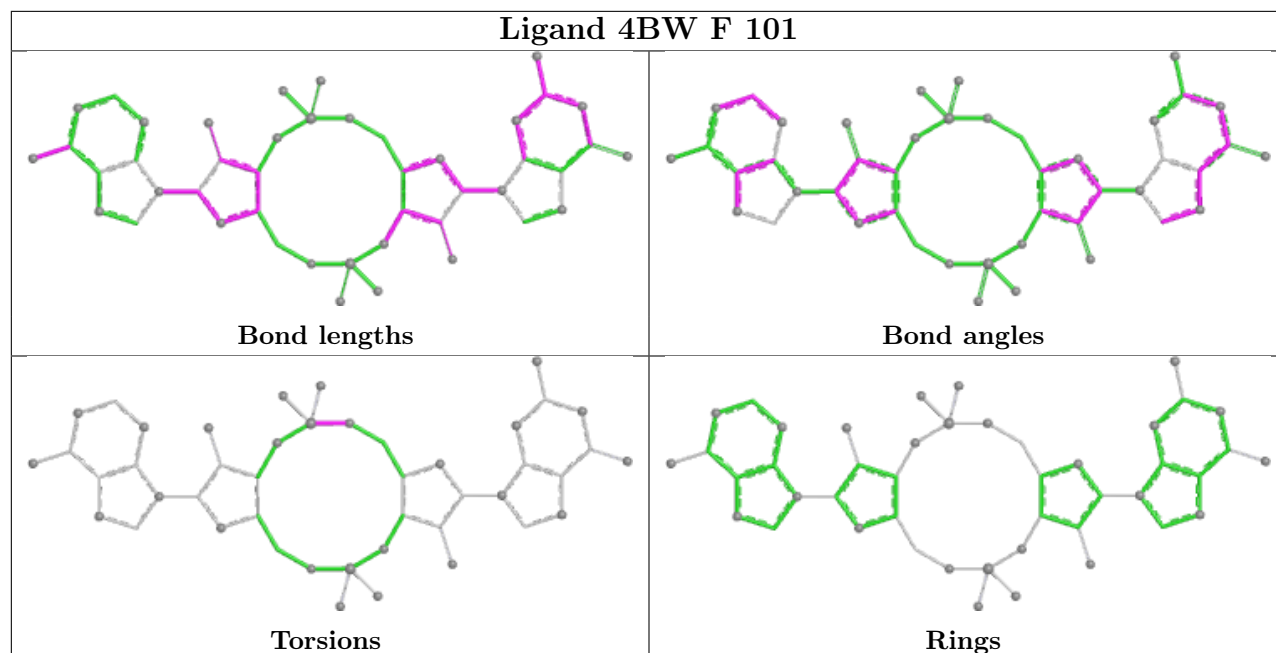




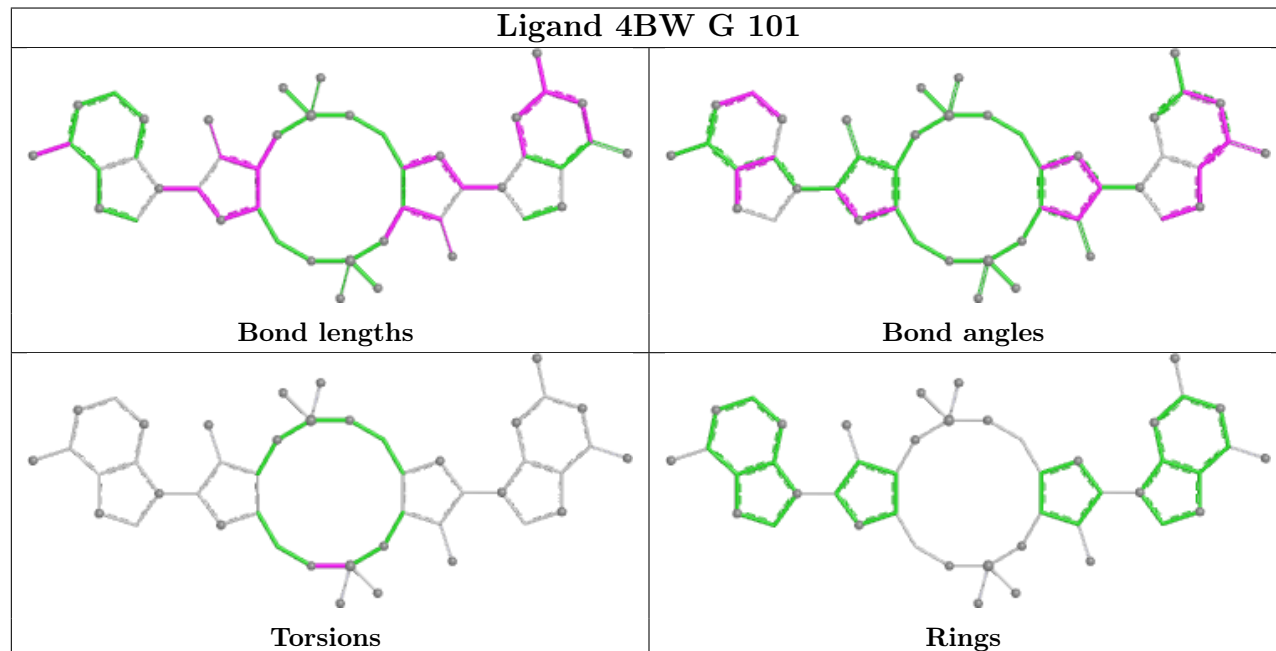


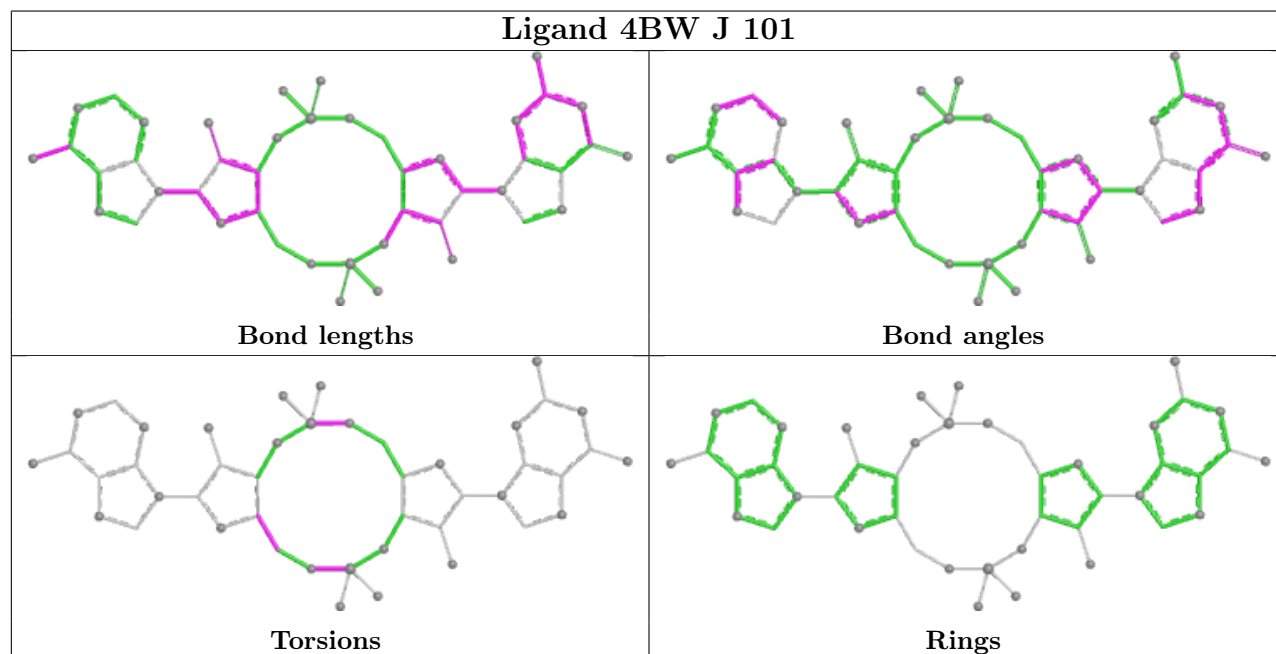
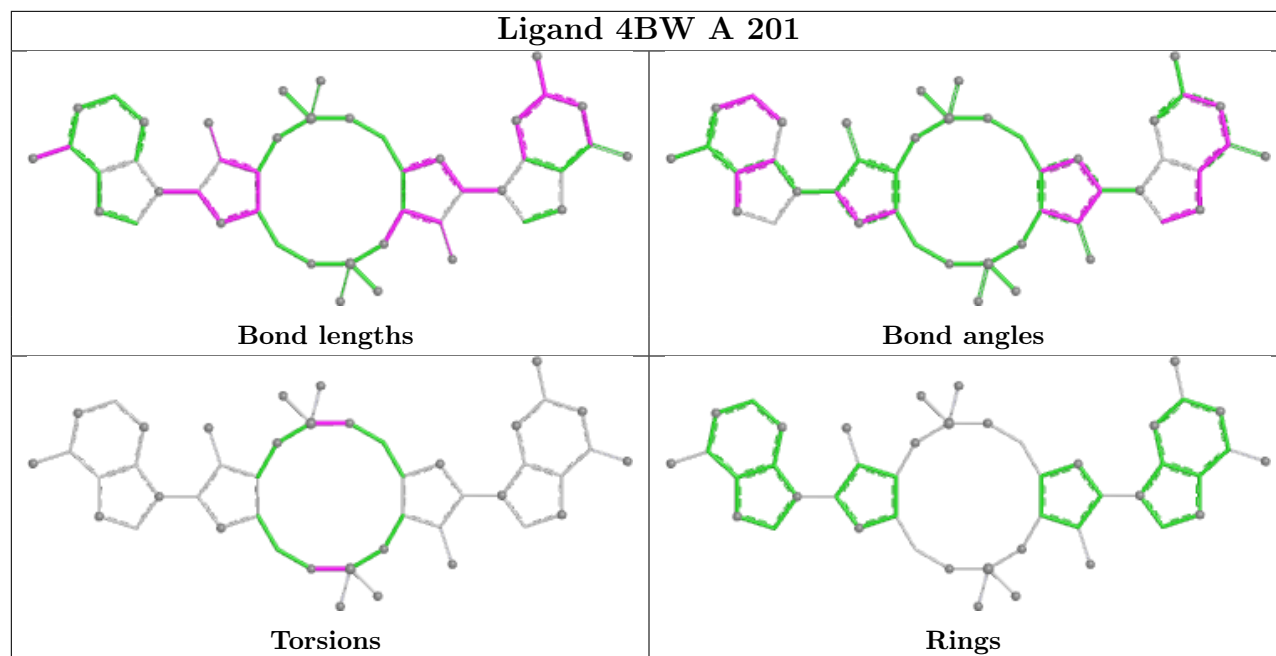


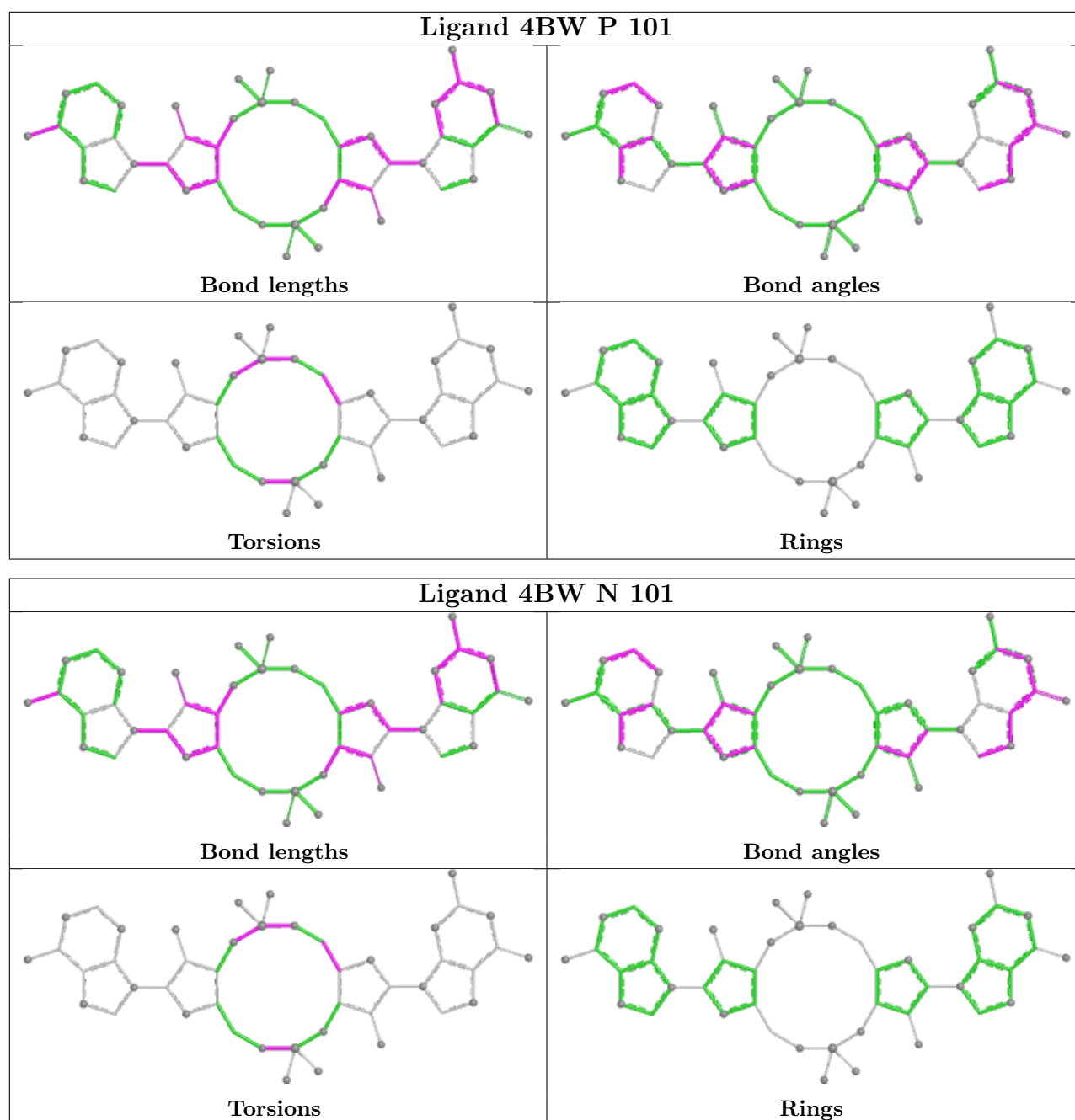
Ligand 4BW F 101



Ligand 4BW G 101







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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	95/97 (97%)	-0.12	0 100 100	10, 16, 30, 35	0
1	B	94/97 (96%)	-0.09	0 100 100	11, 16, 27, 39	0
1	C	93/97 (95%)	-0.01	0 100 100	11, 18, 31, 47	0
1	D	93/97 (95%)	-0.05	2 (2%) 62 63	11, 18, 33, 55	0
1	E	93/97 (95%)	0.08	2 (2%) 62 63	11, 20, 37, 50	0
1	F	93/97 (95%)	-0.15	0 100 100	11, 17, 28, 46	0
1	G	93/97 (95%)	0.21	3 (3%) 50 52	15, 24, 40, 69	0
1	H	93/97 (95%)	0.13	1 (1%) 77 79	15, 23, 34, 39	0
1	I	95/97 (97%)	0.11	0 100 100	18, 24, 36, 43	0
1	J	88/97 (90%)	0.31	0 100 100	18, 29, 41, 51	0
1	K	94/97 (96%)	0.56	5 (5%) 33 35	21, 34, 50, 57	0
1	L	94/97 (96%)	0.51	5 (5%) 33 35	21, 29, 46, 54	0
1	M	87/97 (89%)	1.49	27 (31%) 1 1	30, 42, 70, 76	0
1	N	86/97 (88%)	1.51	20 (23%) 2 2	34, 53, 65, 78	0
1	O	83/97 (85%)	2.26	47 (56%) 0 0	44, 57, 75, 83	0
1	P	90/97 (92%)	1.39	17 (18%) 4 4	37, 47, 63, 71	0
1	Q	90/97 (92%)	0.81	7 (7%) 20 22	27, 36, 53, 64	0
1	R	94/97 (96%)	0.62	3 (3%) 50 52	26, 33, 48, 54	0
1	S	90/97 (92%)	0.82	5 (5%) 31 33	25, 39, 56, 65	0
1	T	92/97 (94%)	0.88	6 (6%) 26 28	26, 39, 54, 59	0
All	All	1830/1940 (94%)	0.54	150 (8%) 19 20	10, 29, 59, 83	0

The worst 5 of 150 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	87	GLY	5.9
1	M	92	VAL	5.6
1	O	25	VAL	5.3
1	H	87	GLY	5.2
1	M	20	VAL	5.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	4BW	O	101	45/45	0.80	0.14	42,52,58,65	0
2	4BW	N	101	45/45	0.85	0.13	40,48,53,61	0
2	4BW	P	101	45/45	0.88	0.12	35,42,47,49	0
2	4BW	T	101	45/45	0.90	0.12	31,41,47,51	0
2	4BW	Q	101	45/45	0.91	0.09	19,28,31,38	0
2	4BW	M	101	45/45	0.92	0.09	30,34,40,41	0
2	4BW	I	101	45/45	0.93	0.08	20,26,29,30	0
2	4BW	R	101	45/45	0.93	0.09	29,34,37,39	0
2	4BW	S	4201	45/45	0.93	0.09	22,29,34,35	0
2	4BW	K	101	45/45	0.93	0.09	26,32,41,45	0
2	4BW	C	101	45/45	0.94	0.08	10,15,20,38	0
2	4BW	E	101	45/45	0.94	0.08	12,15,20,32	0
2	4BW	D	301	45/45	0.95	0.07	10,13,16,18	0
2	4BW	J	101	45/45	0.95	0.07	13,21,26,30	0
2	4BW	F	101	45/45	0.95	0.07	12,15,18,20	0
2	4BW	L	101	45/45	0.95	0.07	16,22,27,32	0
2	4BW	G	101	45/45	0.95	0.07	13,18,20,22	0
2	4BW	H	101	45/45	0.95	0.07	17,21,24,26	0
2	4BW	A	201	45/45	0.96	0.07	10,14,17,20	0

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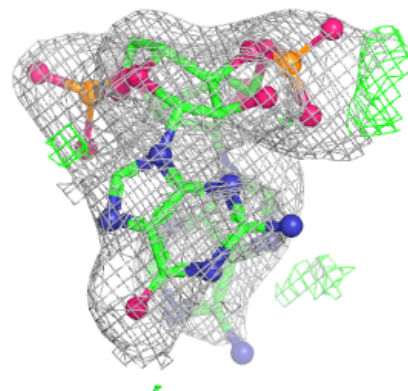
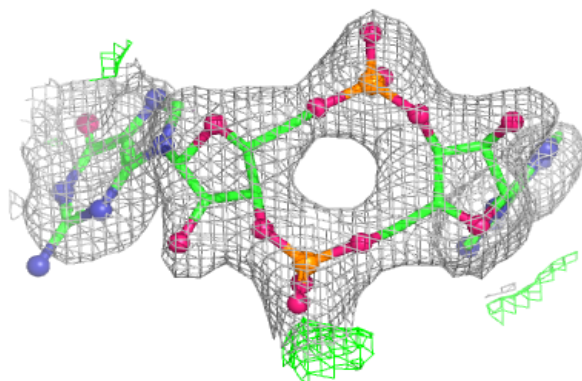
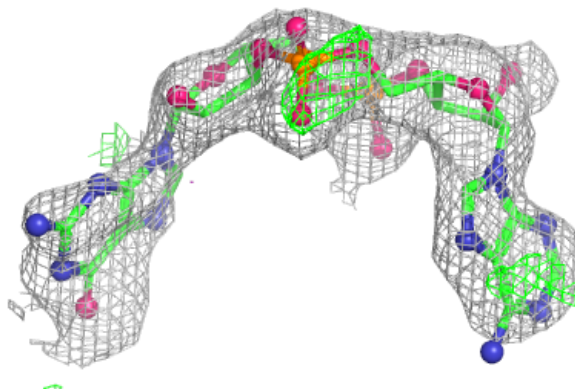
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	4BW	B	201	45/45	0.96	0.06	9,15,18,18	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

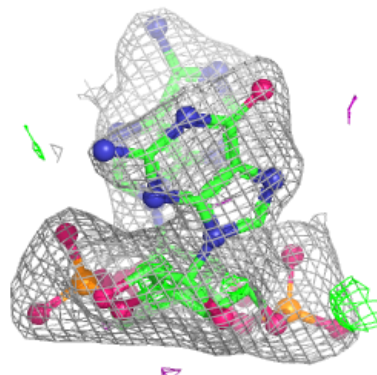
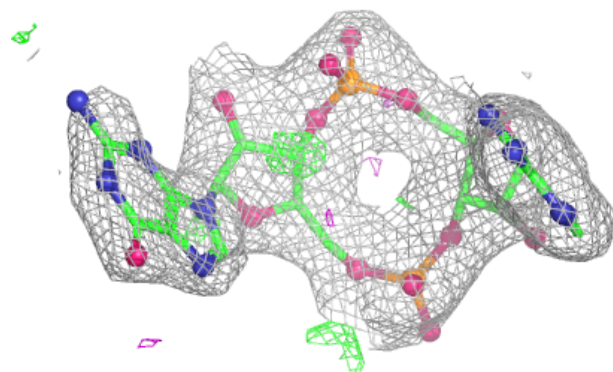
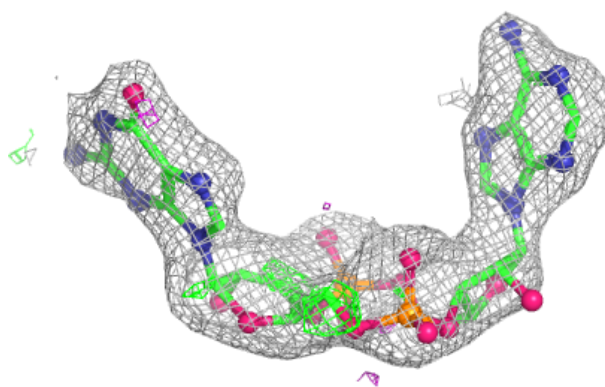
Electron density around 4BW O 101:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

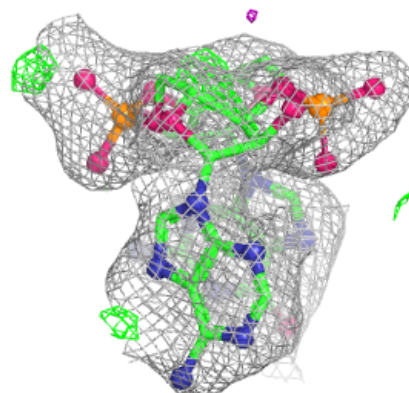
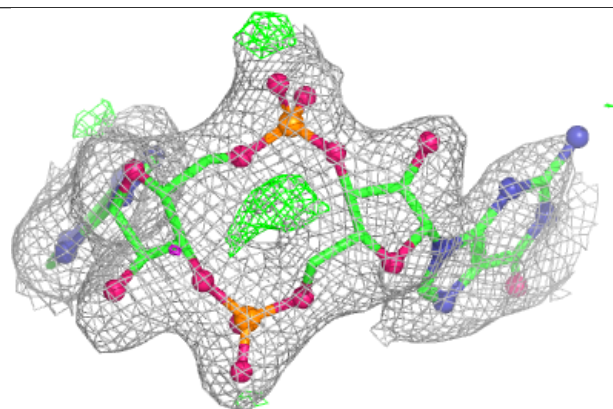
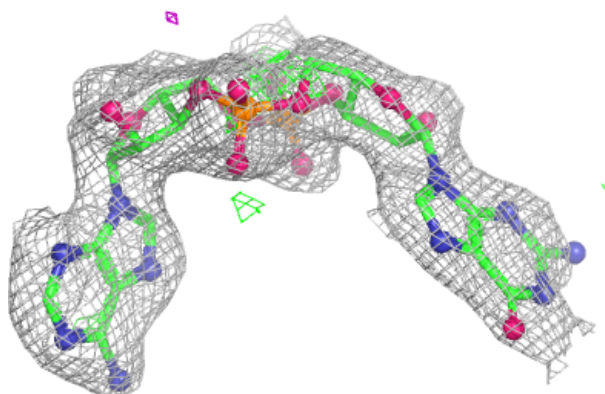


Electron density around 4BW N 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

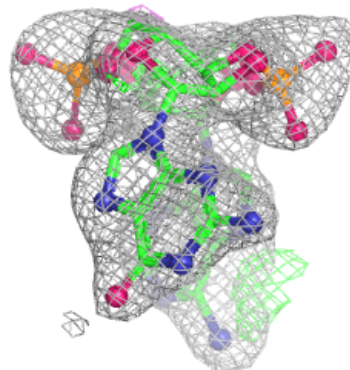
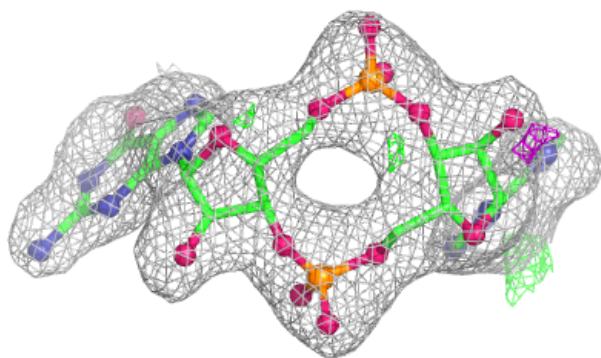
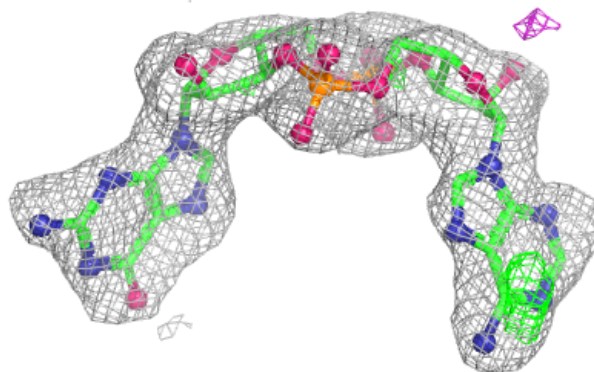
**Electron density around 4BW P 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

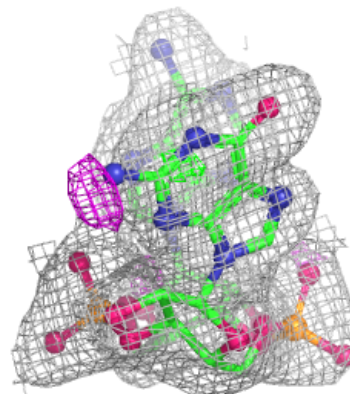
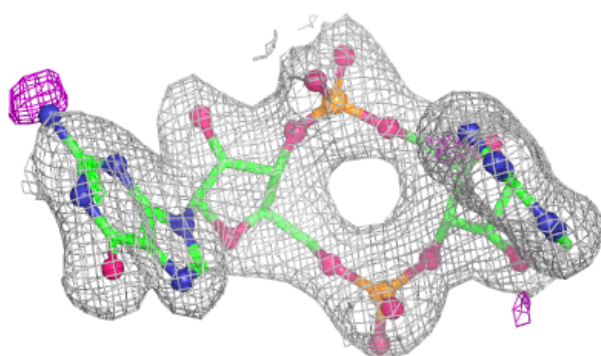
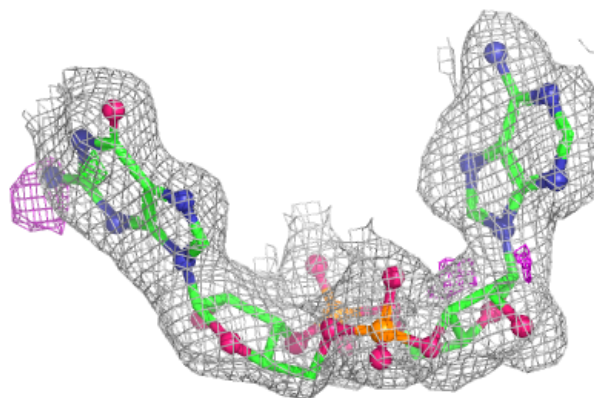


Electron density around 4BW T 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

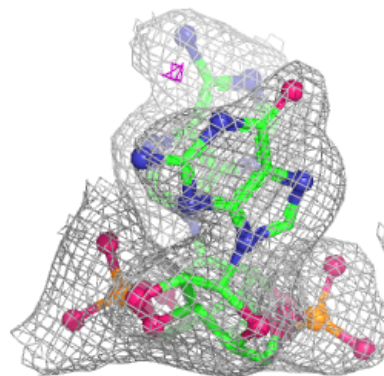
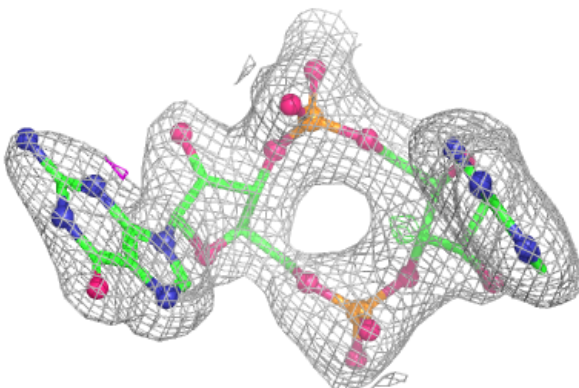
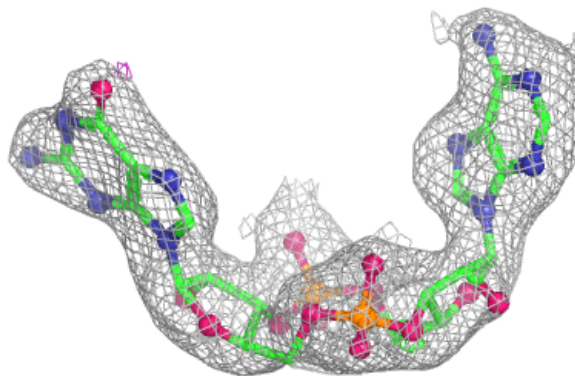
**Electron density around 4BW Q 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



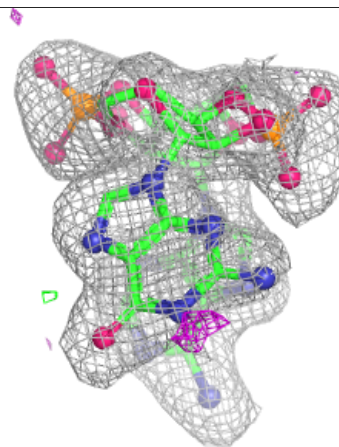
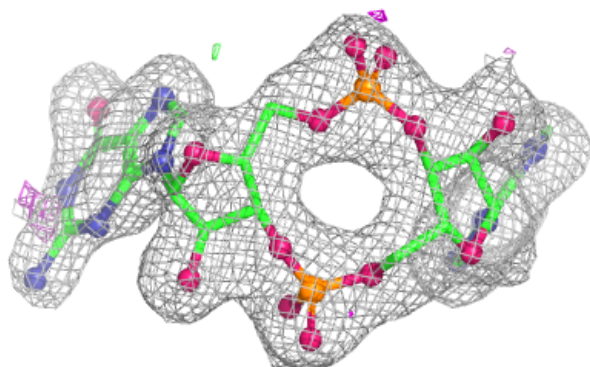
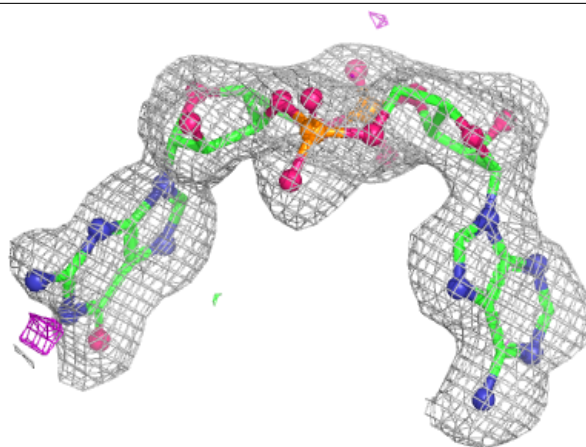
Electron density around 4BW M 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



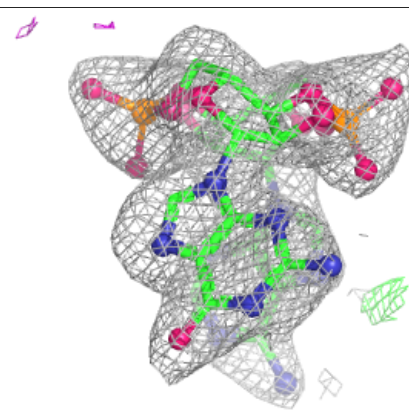
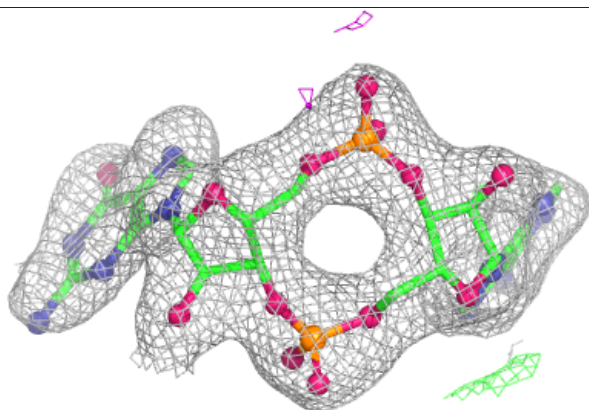
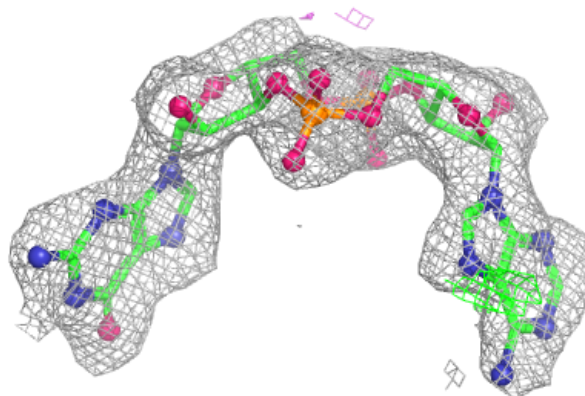
Electron density around 4BW I 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

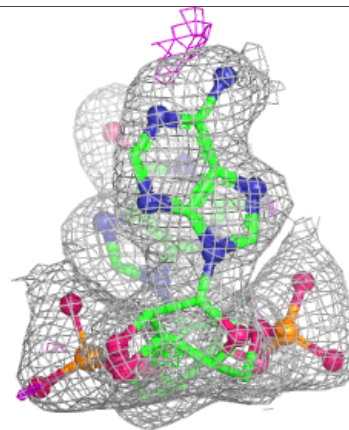
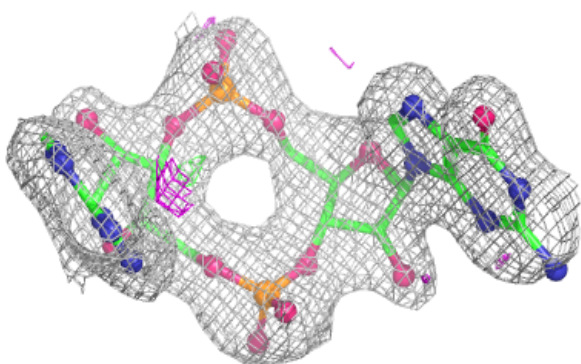
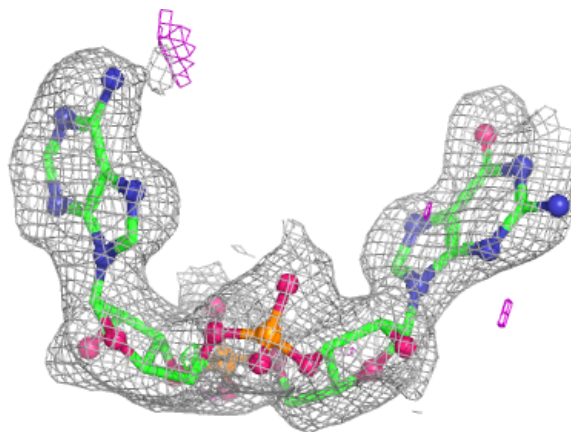


Electron density around 4BW R 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

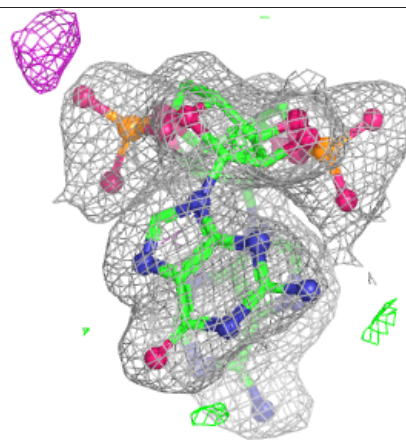
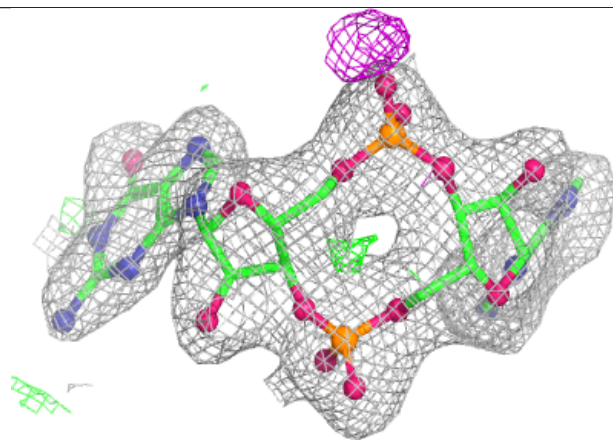
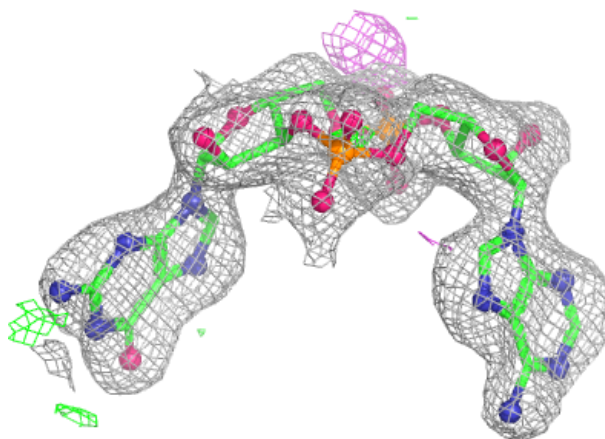
**Electron density around 4BW S 4201:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



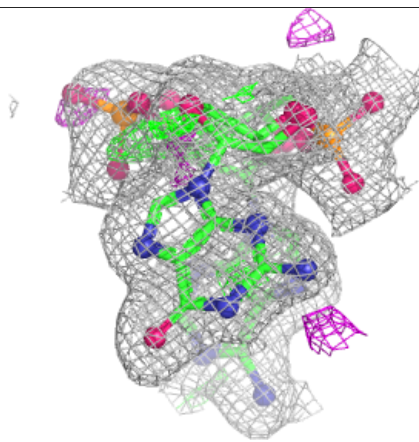
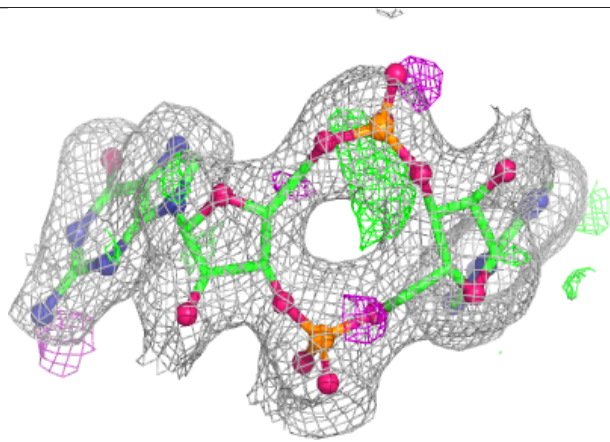
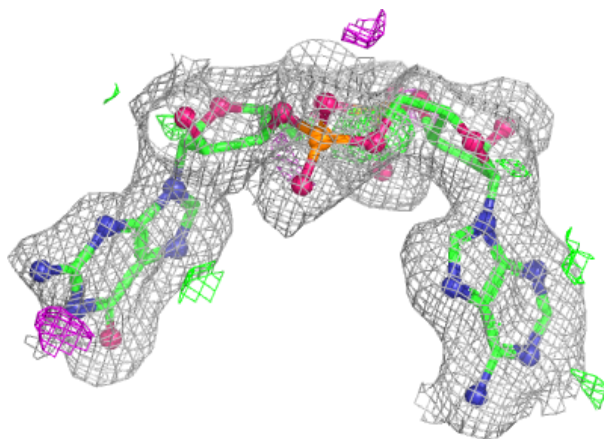
Electron density around 4BW K 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



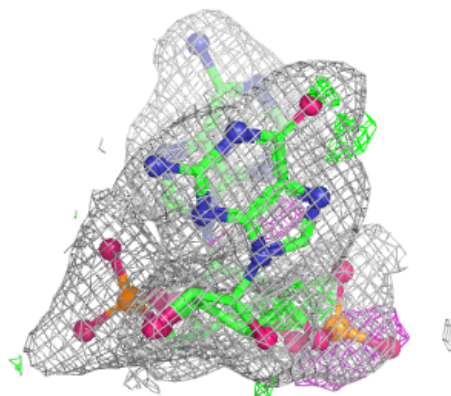
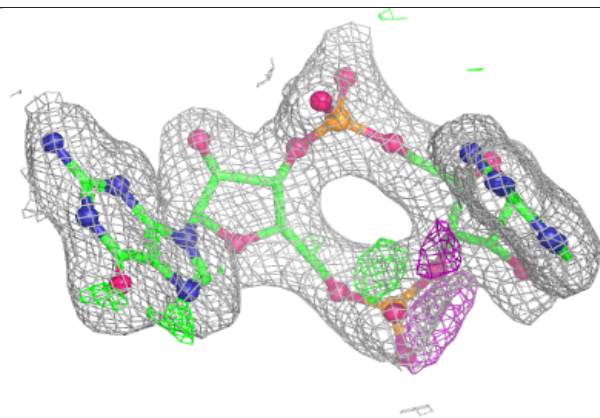
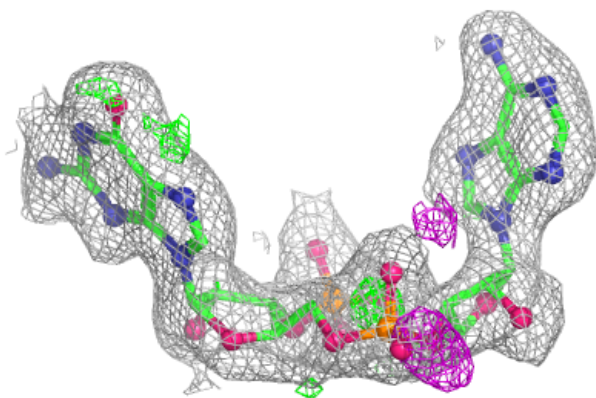
Electron density around 4BW C 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



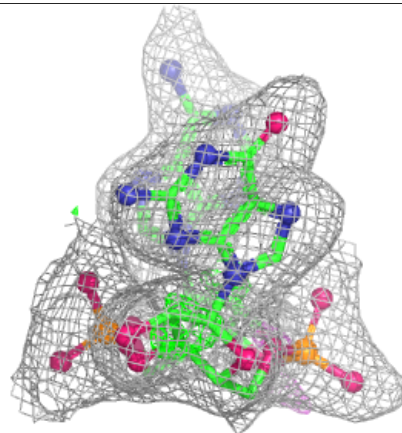
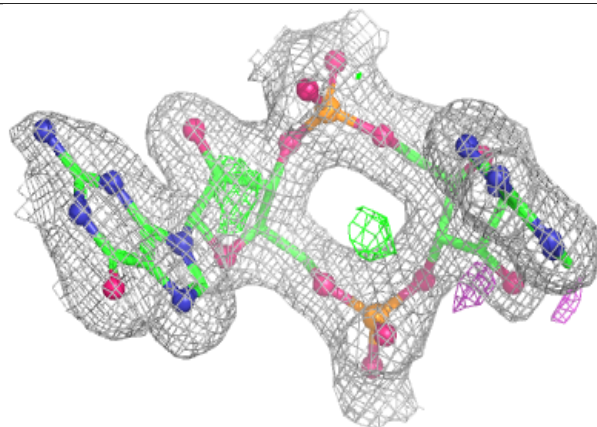
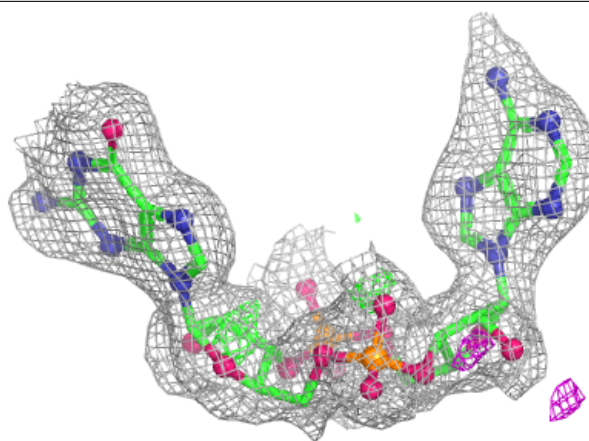
Electron density around 4BW E 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



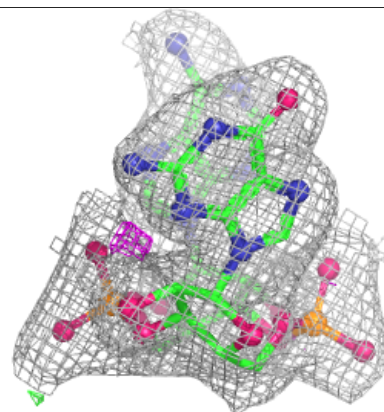
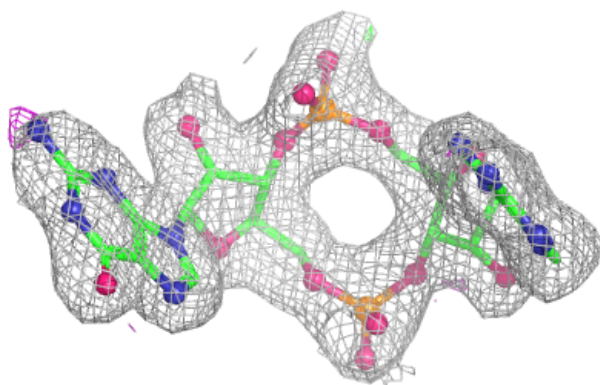
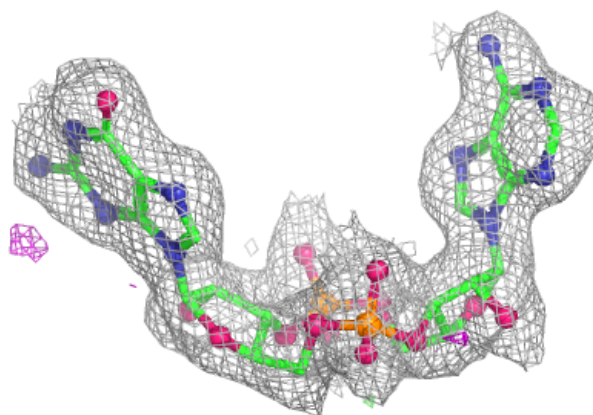
Electron density around 4BW D 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

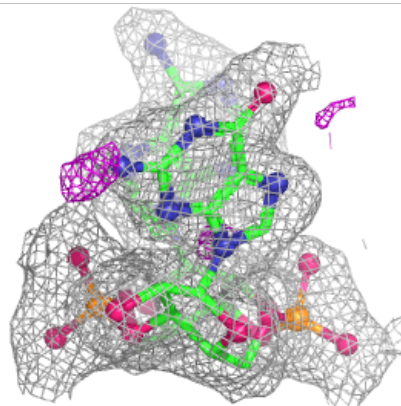
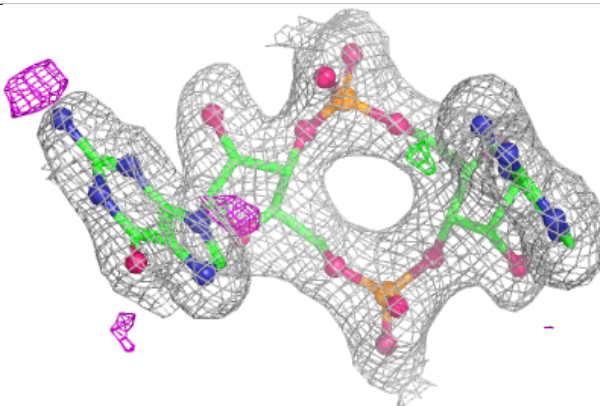
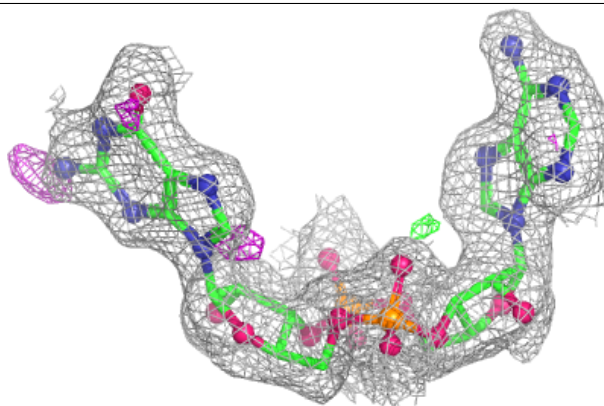


Electron density around 4BW J 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

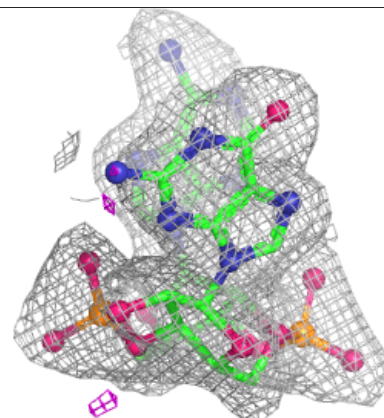
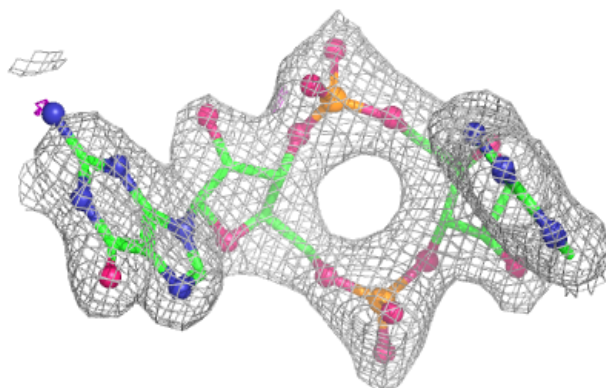
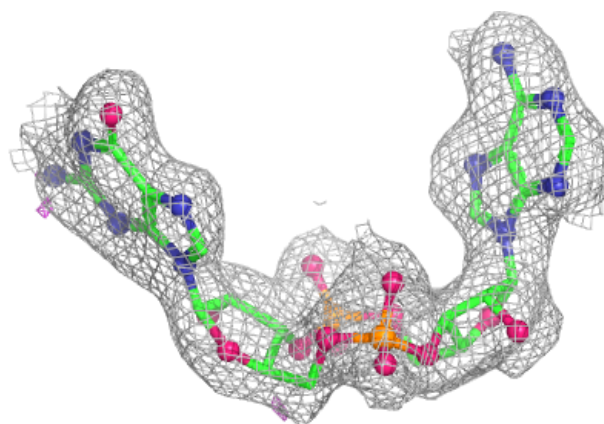
**Electron density around 4BW F 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

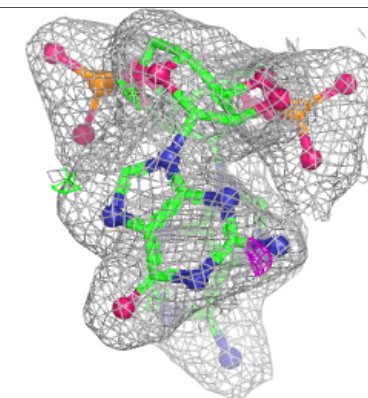
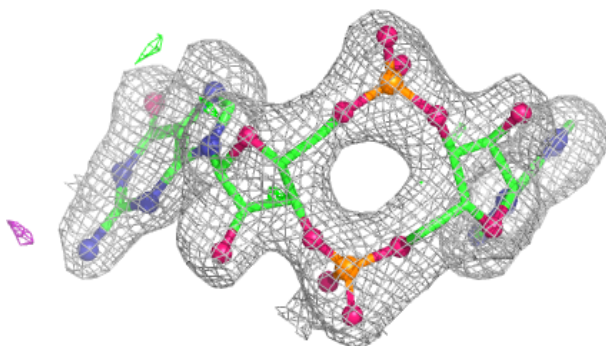
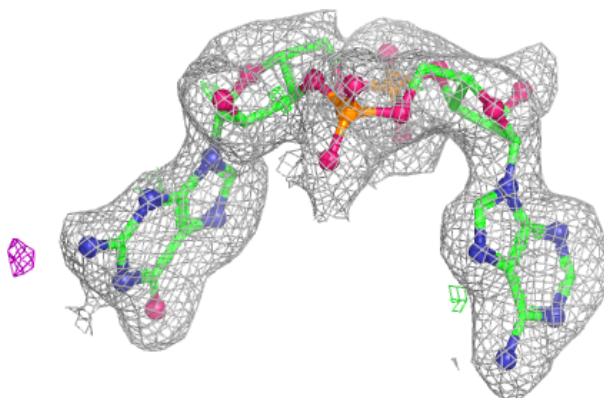


Electron density around 4BW L 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

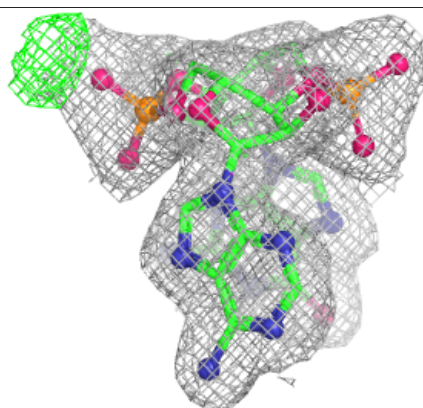
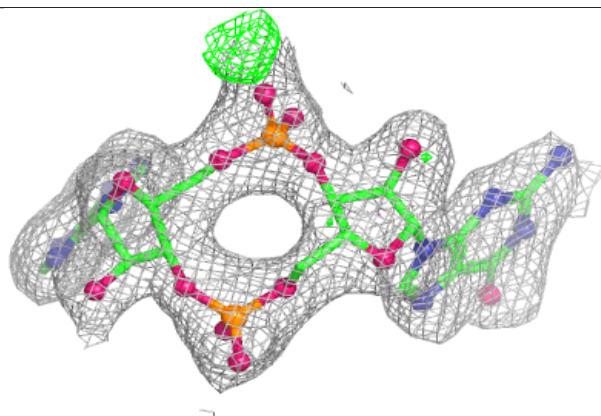
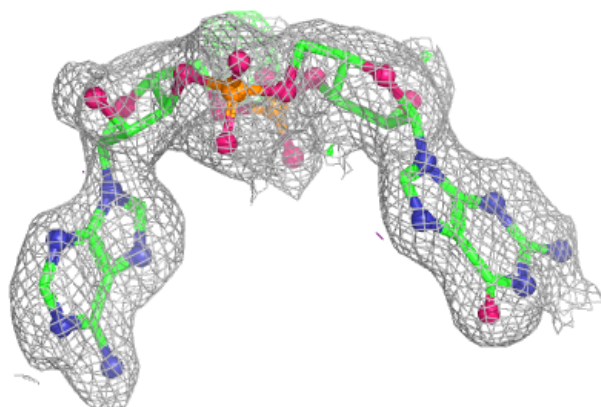
**Electron density around 4BW G 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

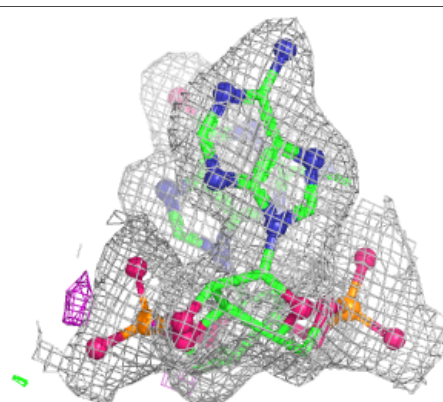
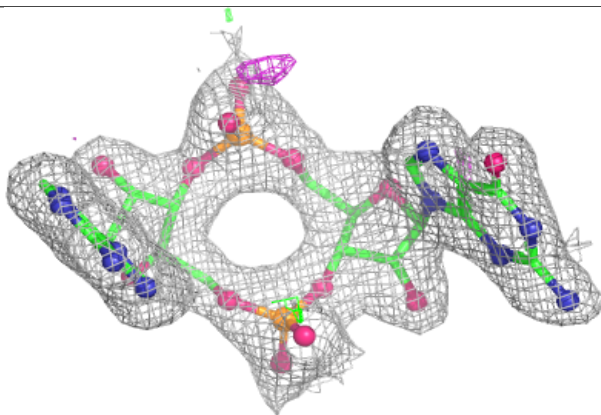
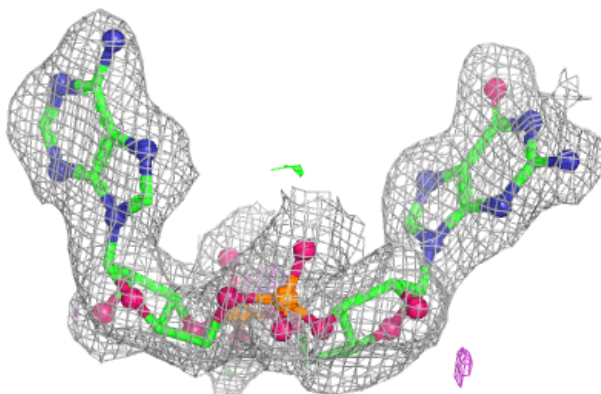


Electron density around 4BW H 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

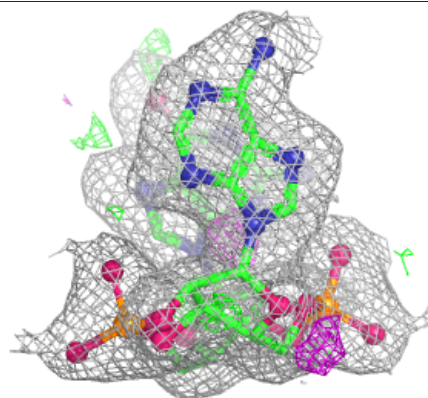
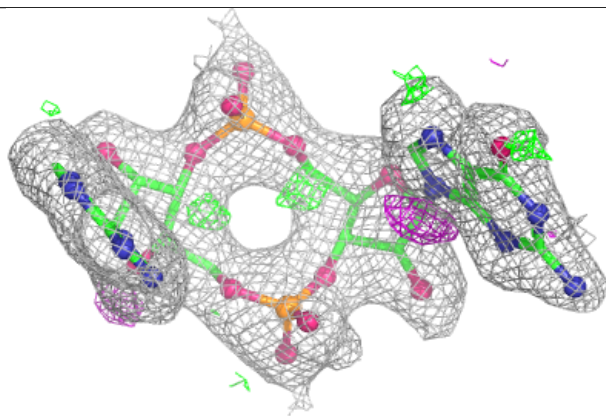
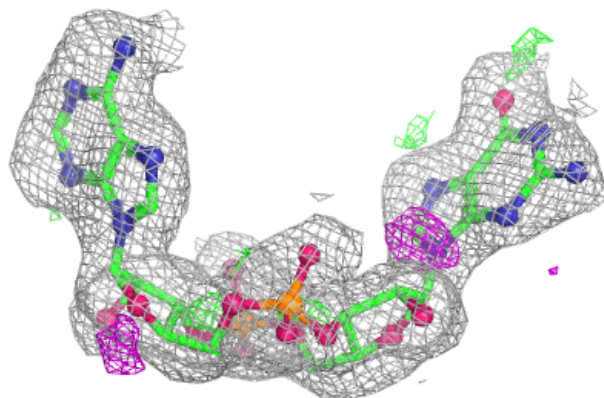
**Electron density around 4BW A 201:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 4BW B 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.