Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/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:

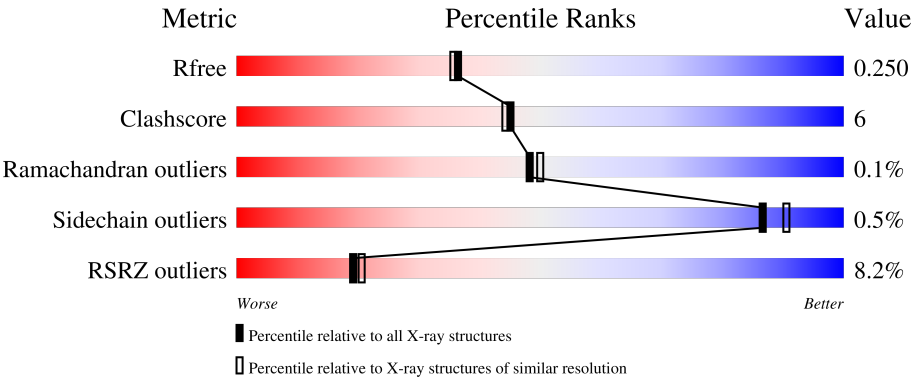
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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 <=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	82% 15%
1	B	97	90% 7%
1	C	97	88% 7%
1	D	97	2% 87% 9%

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Mol	Chain	Length	Quality of chain
1	E	97	2% 85% 11%
1	F	97	85% 11%
1	G	97	3% 90% 6%
1	H	97	% 87% 9%
1	I	97	94%
1	J	97	84% 7% 9%
1	K	97	5% 82% 14%
1	L	97	5% 87% 10%
1	M	97	28% 78% 11% 10%
1	N	97	21% 71% 18% 11%
1	O	97	48% 72% 12% 14%
1	P	97	18% 80% 12% 7%
1	Q	97	7% 77% 15% 7%
1	R	97	3% 89% 8%
1	S	97	5% 79% 12% 7%
1	T	97	6% 91% 5%

2 Entry composition (i)

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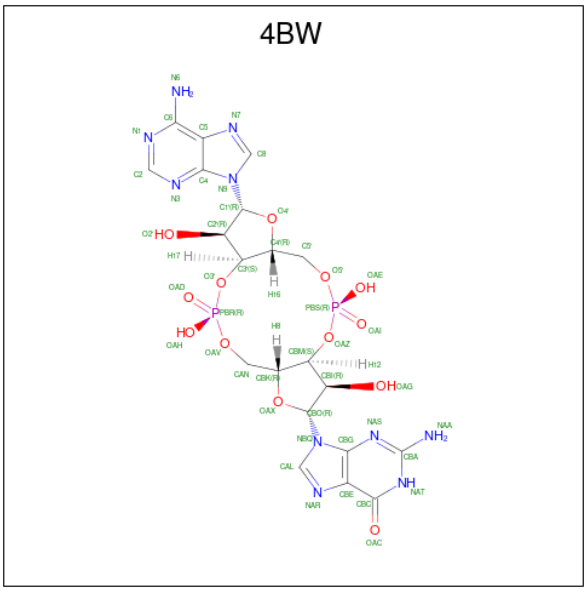
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	90	Total	C	N	O	S	0	0	0
			713	450	117	144	2			
1	R	94	Total	C	N	O	S	0	0	0
			747	471	123	151	2			
1	S	90	Total	C	N	O	S	0	0	0
			715	451	118	144	2			
1	T	92	Total	C	N	O	S	0	0	0
			730	459	120	149	2			

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-dioxidooctahydro-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: $C_{20}H_{24}N_{10}O_{13}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			45	20	10	13	2		
2	B	1	Total	C	N	O	P	0	0
			45	20	10	13	2		
2	C	1	Total	C	N	O	P	0	0
			45	20	10	13	2		
2	D	1	Total	C	N	O	P	0	0
			45	20	10	13	2		
2	E	1	Total	C	N	O	P	0	0
			45	20	10	13	2		
2	F	1	Total	C	N	O	P	0	0
			45	20	10	13	2		
2	G	1	Total	C	N	O	P	0	0
			45	20	10	13	2		
2	H	1	Total	C	N	O	P	0	0
			45	20	10	13	2		
2	I	1	Total	C	N	O	P	0	0
			45	20	10	13	2		
2	J	1	Total	C	N	O	P	0	0
			45	20	10	13	2		
2	K	1	Total	C	N	O	P	0	0
			45	20	10	13	2		
2	L	1	Total	C	N	O	P	0	0
			45	20	10	13	2		
2	M	1	Total	C	N	O	P	0	0
			45	20	10	13	2		
2	N	1	Total	C	N	O	P	0	0
			45	20	10	13	2		

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

- Molecule 3 is water.

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

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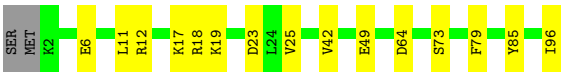
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	N	30	Total O 30 30	0	0
3	O	20	Total O 20 20	0	0
3	P	27	Total O 27 27	0	0
3	Q	41	Total O 41 41	0	0
3	R	41	Total O 41 41	0	0
3	S	26	Total O 26 26	0	0
3	T	34	Total O 34 34	0	0

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: anti-CBASS 4 (Acb4)

Chain A:



• Molecule 1: anti-CBASS 4 (Acb4)

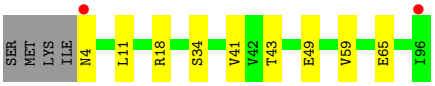
Chain B:

• Molecule 1: anti-CBASS 4 (Acb4)

Chain C:

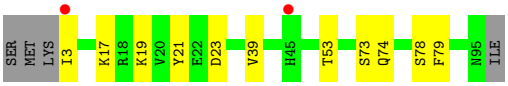
• Molecule 1: anti-CBASS 4 (Acb4)

Chain D:



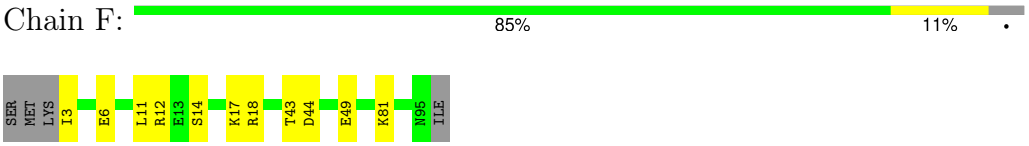
• Molecule 1: anti-CBASS 4 (Acb4)

Chain E:



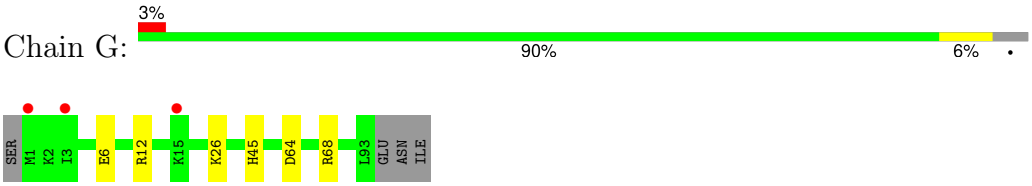
• Molecule 1: anti-CBASS 4 (Acb4)

Chain F:



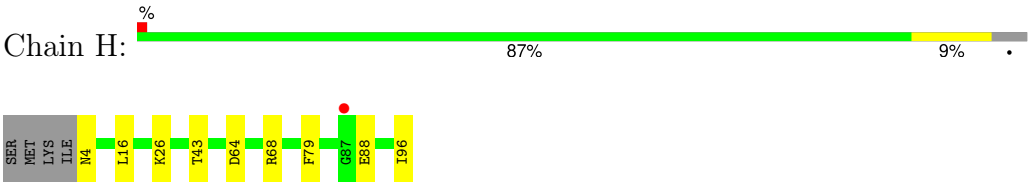
• Molecule 1: anti-CBASS 4 (Acb4)

Chain G:



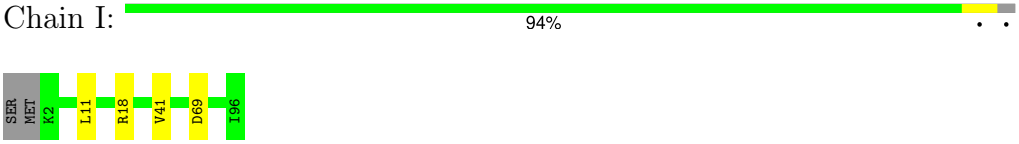
• Molecule 1: anti-CBASS 4 (Acb4)

Chain H:



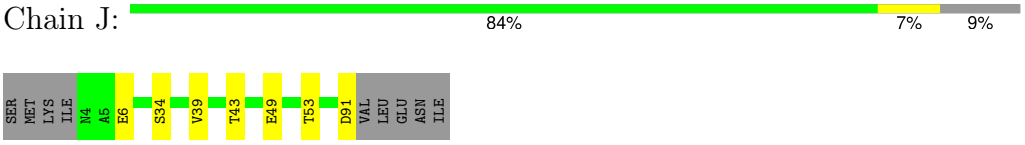
• Molecule 1: anti-CBASS 4 (Acb4)

Chain I:



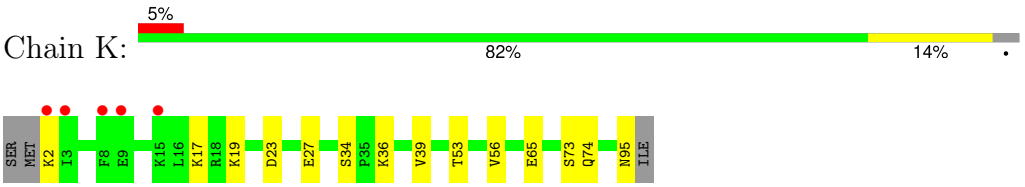
• Molecule 1: anti-CBASS 4 (Acb4)

Chain J:



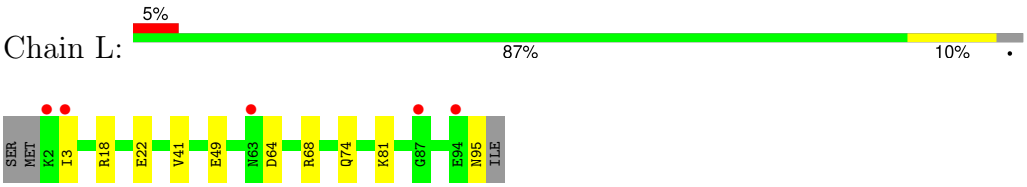
• Molecule 1: anti-CBASS 4 (Acb4)

Chain K:



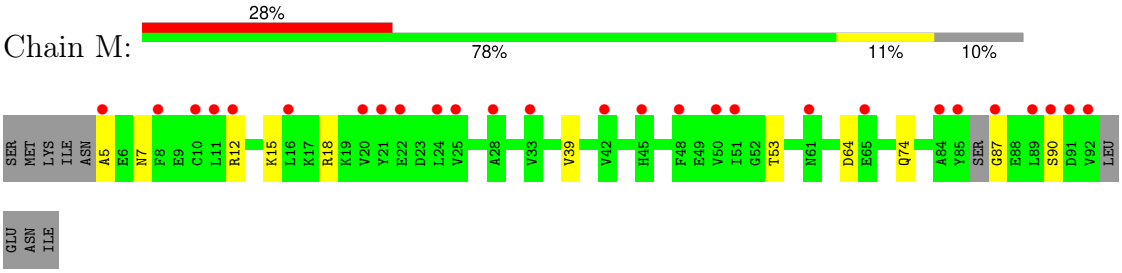
• Molecule 1: anti-CBASS 4 (Acb4)

Chain L:



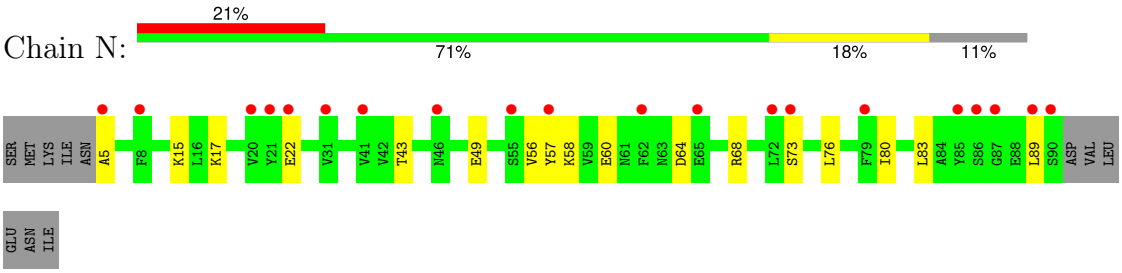
• Molecule 1: anti-CBASS 4 (Acb4)

Chain M:



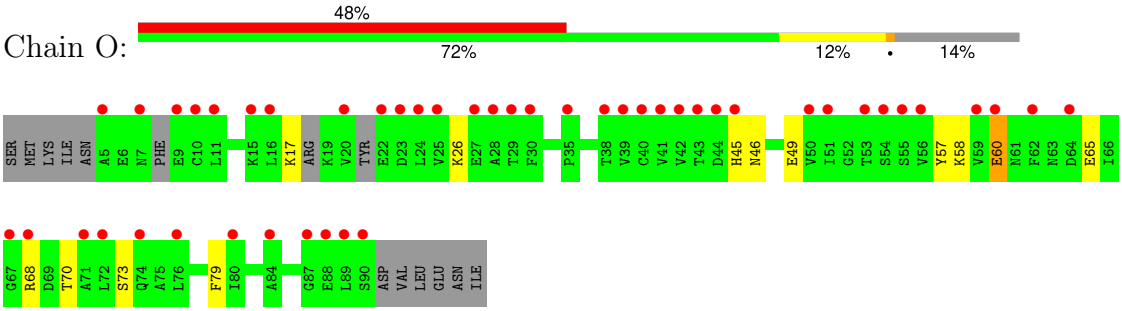
• Molecule 1: anti-CBASS 4 (Acb4)

Chain N:



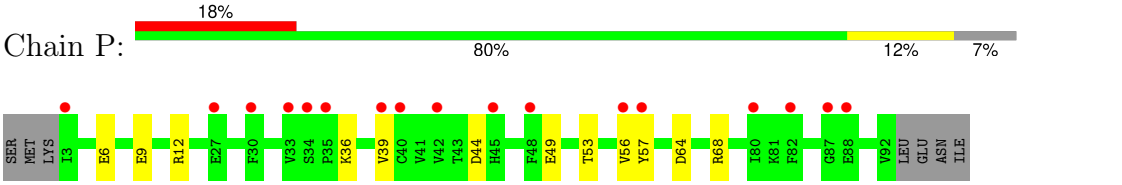
• Molecule 1: anti-CBASS 4 (Acb4)

Chain O:



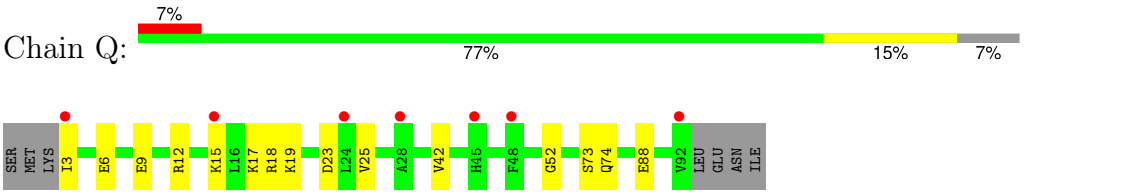
• Molecule 1: anti-CBASS 4 (Acb4)

Chain P:



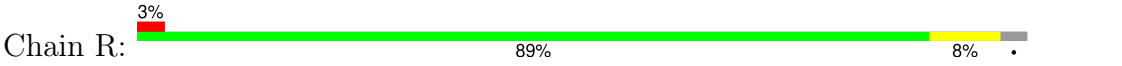
• Molecule 1: anti-CBASS 4 (Acb4)

Chain Q:



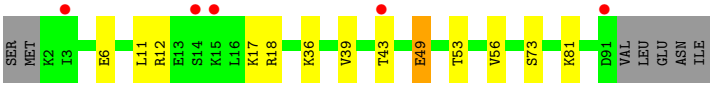
• Molecule 1: anti-CBASS 4 (Acb4)

Chain R:



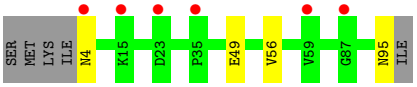
• Molecule 1: anti-CBASS 4 (Acb4)

Chain S:



• Molecule 1: anti-CBASS 4 (Acb4)

Chain T:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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.

All (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
2:A:201:4BW:CBO	2:A:201:4BW:OAX	1.67	1.17
2:O:101:4BW:CBO	2:O:101:4BW:OAX	1.68	1.17
2:Q:101:4BW:OAX	2:Q:101:4BW:CBO	1.67	1.17
2:H:101:4BW:CBO	2:H:101:4BW:OAX	1.67	1.16
2:D:301:4BW:CBO	2:D:301:4BW:OAX	1.67	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:101:4BW:OAX	2:M:101:4BW:CBO	1.68	1.15
2:T:101:4BW:CBO	2:T:101:4BW:OAX	1.68	1.15
2:B:201:4BW:OAX	2:B:201:4BW:CBO	1.67	1.14
2:P:101:4BW:CBO	2:P:101:4BW:OAX	1.67	1.14
2:E:101:4BW:OAX	2:E:101:4BW:CBO	1.67	1.14
2:C:101:4BW:OAX	2:C:101:4BW:CBO	1.67	1.12
2:K:101:4BW:CBO	2:K:101:4BW:OAX	1.68	1.12
2:L:101:4BW:CBO	2:L:101:4BW:OAX	1.67	1.11
2:J:101:4BW:OAX	2:J:101:4BW:CBO	1.67	1.11
2:C:101:4BW:OAI	3:C:201:HOH:O	1.71	1.05
2:R:101:4BW:OAX	2:R:101:4BW:CBO	1.68	1.04
1:N:56:VAL:O	3:N:201:HOH:O	1.77	1.03
1:R:23:ASP:OD1	3:R:201:HOH:O	1.88	0.91
1:L:95:ASN:O	3:L:201:HOH:O	1.93	0.86
1:A:64:ASP:OD2	3:A:301:HOH:O	1.92	0.86
2:F:101:4BW:OAI	3:F:201:HOH:O	1.96	0.84
1:F:3:ILE:N	3:F:202:HOH:O	2.13	0.82
1:B:88:GLU:OE2	3:B:302:HOH:O	2.03	0.76
1:Q:88:GLU:OE1	3:Q:201:HOH:O	2.03	0.76
1:M:15:LYS:NZ	3:M:202:HOH:O	2.19	0.76
1:M:74:GLN:NE2	3:M:201:HOH:O	2.03	0.74
1:T:4:ASN:N	3:T:202:HOH:O	2.22	0.72
1:B:22:GLU:OE2	3:B:303:HOH:O	2.08	0.72
1:L:18:ARG:NE	1:L:22:GLU:OE2	2.19	0.72
1:A:96:ILE:O	3:A:303:HOH:O	2.07	0.71
1:H:88:GLU:OE2	3:H:201:HOH:O	2.07	0.71
2:I:101:4BW:H4	2:I:101:4BW:H10	1.71	0.71
1:B:74:GLN:NE2	3:B:306:HOH:O	2.22	0.71
1:Q:3:ILE:N	3:Q:202:HOH:O	2.24	0.71
1:P:44:ASP:OD2	3:P:201:HOH:O	2.08	0.71
1:M:5:ALA:N	3:M:204:HOH:O	2.23	0.70
1:P:9:GLU:OE2	3:P:202:HOH:O	2.10	0.69
1:A:6:GLU:O	1:A:12:ARG:NH1	2.24	0.69
2:C:101:4BW:H4	2:C:101:4BW:H9	1.75	0.68
1:Q:6:GLU:O	1:Q:12:ARG:NH1	2.27	0.68
1:C:77:ASP:OD2	3:C:202:HOH:O	2.12	0.68
1:O:68:ARG:NH1	3:O:201:HOH:O	2.26	0.67
1:R:69:ASP:OD1	3:R:202:HOH:O	2.12	0.67
1:D:11:LEU:O	1:D:18:ARG:NH1	2.28	0.67
1:S:17:LYS:NZ	1:S:73:SER:OG	2.29	0.66
1:M:87:GLY:N	3:M:205:HOH:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ASN:O	3:B:304:HOH:O	2.13	0.64
1:D:65:GLU:OE2	3:D:401:HOH:O	2.14	0.64
1:N:15:LYS:NZ	3:N:203:HOH:O	2.29	0.64
1:O:65:GLU:OE1	3:O:201:HOH:O	2.15	0.63
2:E:101:4BW:H4	2:E:101:4BW:H9	1.79	0.63
1:K:2:LYS:HE3	1:K:27:GLU:OE2	1.99	0.62
1:M:12:ARG:HA	1:M:18:ARG:HH21	1.64	0.62
2:N:101:4BW:H4	2:N:101:4BW:H9	1.81	0.62
1:K:2:LYS:HB2	3:K:207:HOH:O	1.99	0.61
1:T:95:ASN:ND2	3:T:205:HOH:O	2.32	0.61
1:C:49:GLU:O	2:D:301:4BW:NAT	2.25	0.60
1:Q:52:GLY:HA2	1:Q:74:GLN:HG2	1.85	0.59
1:K:65:GLU:O	3:K:201:HOH:O	2.16	0.59
1:O:49:GLU:O	2:P:101:4BW:NAT	2.31	0.59
1:S:36:LYS:NZ	1:S:56:VAL:O	2.33	0.59
1:M:15:LYS:NZ	3:M:209:HOH:O	2.36	0.58
1:C:3:ILE:N	3:C:207:HOH:O	2.37	0.58
1:B:3:ILE:N	3:B:309:HOH:O	2.36	0.58
1:C:88:GLU:OE2	3:C:203:HOH:O	2.17	0.58
1:K:36:LYS:NZ	1:K:56:VAL:O	2.31	0.58
1:F:44:ASP:HB2	3:F:217:HOH:O	2.03	0.57
2:T:101:4BW:H9	2:T:101:4BW:H15	1.87	0.57
1:K:2:LYS:N	3:K:206:HOH:O	2.37	0.57
1:O:17:LYS:NZ	1:O:73:SER:OG	2.38	0.57
1:J:6:GLU:OE1	3:J:201:HOH:O	2.17	0.56
1:J:43:THR:HG22	1:J:49:GLU:HG2	1.88	0.56
1:G:12:ARG:NH2	3:G:203:HOH:O	2.38	0.55
1:O:46:ASN:ND2	3:O:204:HOH:O	2.38	0.54
1:A:85:TYR:OH	3:A:302:HOH:O	2.03	0.54
1:M:7:ASN:ND2	3:M:204:HOH:O	2.41	0.53
1:L:74:GLN:OE1	3:L:202:HOH:O	2.18	0.53
1:T:56:VAL:HB	2:T:101:4BW:C6	2.39	0.53
1:D:59:VAL:O	3:D:403:HOH:O	2.19	0.53
1:A:17:LYS:NZ	1:A:73:SER:OG	2.42	0.53
1:K:19:LYS:HE2	1:K:23:ASP:OD2	2.09	0.53
2:O:101:4BW:NAT	1:P:49:GLU:O	2.26	0.53
1:P:39:VAL:HG22	1:P:53:THR:HG22	1.91	0.53
1:E:17:LYS:NZ	1:E:73:SER:OG	2.43	0.51
1:C:26:LYS:HB3	1:C:43:THR:HG22	1.92	0.51
1:S:43:THR:HG22	1:S:49:GLU:HG2	1.92	0.51
2:Q:101:4BW:NAT	1:R:49:GLU:O	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6:GLU:O	1:F:12:ARG:NH1	2.43	0.49
2:S:4201:4BW:NAT	1:T:49:GLU:O	2.35	0.49
1:T:4:ASN:ND2	3:T:206:HOH:O	2.35	0.48
2:J:101:4BW:H15	2:J:101:4BW:H9	1.95	0.48
1:K:17:LYS:NZ	1:K:73:SER:OG	2.46	0.48
1:S:6:GLU:O	1:S:12:ARG:NH1	2.33	0.48
1:N:17:LYS:NZ	1:N:73:SER:OG	2.47	0.47
1:Q:17:LYS:NZ	1:Q:73:SER:OG	2.47	0.47
1:G:26:LYS:HD2	1:G:45:HIS:HA	1.96	0.47
1:E:39:VAL:HG22	1:E:53:THR:HG22	1.97	0.47
1:F:81:LYS:NZ	3:F:208:HOH:O	2.37	0.47
1:B:85:TYR:OH	3:B:305:HOH:O	2.13	0.46
1:I:69:ASP:OD2	3:I:201:HOH:O	2.20	0.46
1:N:57:TYR:OH	3:N:202:HOH:O	2.20	0.46
2:K:101:4BW:NAT	1:L:49:GLU:O	2.43	0.46
2:O:101:4BW:H21	2:O:101:4BW:H15	1.96	0.46
1:M:90:SER:OG	1:P:57:TYR:OH	2.24	0.46
1:C:26:LYS:N	1:C:43:THR:O	2.37	0.46
1:A:49:GLU:OE1	1:B:34:SER:OG	2.33	0.46
1:E:74:GLN:NE2	3:E:202:HOH:O	2.29	0.45
1:H:64:ASP:HB3	1:H:68:ARG:NH1	2.32	0.45
1:R:26:LYS:HD3	1:R:45:HIS:HA	1.98	0.45
1:G:6:GLU:O	1:G:12:ARG:NH1	2.42	0.45
1:K:95:ASN:O	3:K:202:HOH:O	2.20	0.45
1:E:19:LYS:HE3	1:E:23:ASP:OD2	2.16	0.45
1:O:58:LYS:HB3	1:O:60:GLU:OE2	2.16	0.45
1:D:43:THR:HG22	1:D:49:GLU:HG2	1.98	0.45
2:E:101:4BW:NAT	1:F:49:GLU:O	2.40	0.45
2:I:101:4BW:H5	1:L:81:LYS:HG2	1.99	0.45
1:Q:19:LYS:HE3	1:Q:23:ASP:OD2	2.16	0.45
2:I:101:4BW:NAT	1:J:49:GLU:O	2.39	0.45
1:N:58:LYS:HB3	1:N:60:GLU:OE2	2.17	0.44
1:A:11:LEU:HD22	1:A:18:ARG:HA	2.00	0.44
1:H:16:LEU:HA	1:H:96:ILE:HD11	2.00	0.44
1:J:39:VAL:HG22	1:J:53:THR:HG22	2.00	0.44
1:R:36:LYS:HE3	1:R:56:VAL:O	2.18	0.44
1:E:3:ILE:HB	1:E:21:TYR:OH	2.17	0.44
1:M:39:VAL:HG22	1:M:53:THR:HG22	2.00	0.44
1:P:36:LYS:HE3	1:P:56:VAL:O	2.18	0.44
1:F:11:LEU:HD22	1:F:18:ARG:HA	1.99	0.44
1:K:34:SER:HB3	1:L:41:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:64:ASP:HB3	1:N:68:ARG:NH1	2.33	0.43
1:K:74:GLN:OE1	3:K:203:HOH:O	2.21	0.43
1:D:4:ASN:ND2	3:D:404:HOH:O	2.20	0.43
1:O:26:LYS:HD2	1:O:45:HIS:HA	2.00	0.43
1:A:19:LYS:HE3	1:A:23:ASP:OD2	2.18	0.43
1:S:11:LEU:O	1:S:18:ARG:NH1	2.41	0.43
1:O:70:THR:HG21	2:O:101:4BW:H15	2.01	0.43
1:A:25:VAL:HG13	1:A:42:VAL:HG13	2.01	0.43
1:K:39:VAL:HG22	1:K:53:THR:HG22	2.00	0.42
1:C:34:SER:HB3	1:D:41:VAL:HG11	2.01	0.42
1:N:80:ILE:HD13	1:N:83:LEU:HD12	2.02	0.42
1:A:18:ARG:NH1	3:A:305:HOH:O	2.41	0.42
1:H:26:LYS:N	1:H:43:THR:O	2.47	0.42
1:M:64:ASP:OD1	3:M:203:HOH:O	2.22	0.42
1:N:89:LEU:HD23	1:O:57:TYR:CG	2.54	0.42
1:S:81:LYS:NZ	3:S:4304:HOH:O	2.45	0.42
1:N:5:ALA:HB1	1:N:22:GLU:OE2	2.20	0.42
1:Q:25:VAL:HG13	1:Q:42:VAL:HG13	2.02	0.42
1:I:11:LEU:HD22	1:I:18:ARG:HA	2.02	0.42
2:R:101:4BW:H15	2:R:101:4BW:H9	2.00	0.42
1:G:64:ASP:O	1:G:68:ARG:HG3	2.20	0.42
1:F:43:THR:HG22	1:F:49:GLU:HG2	2.01	0.41
1:Q:15:LYS:HD3	1:Q:18:ARG:HH21	1.85	0.41
1:Q:52:GLY:CA	1:Q:74:GLN:HG2	2.49	0.41
1:S:39:VAL:HG22	1:S:53:THR:HG22	2.02	0.41
1:J:91:ASP:O	3:J:203:HOH:O	2.21	0.41
1:N:43:THR:HG22	1:N:49:GLU:HG2	2.02	0.41
1:P:64:ASP:HB3	1:P:68:ARG:NH1	2.35	0.41
1:C:15:LYS:HB3	3:I:225:HOH:O	2.20	0.41
1:I:41:VAL:HG11	1:J:34:SER:HB3	2.03	0.41
2:K:101:4BW:H15	2:K:101:4BW:H9	2.02	0.41
1:S:17:LYS:NZ	3:S:4301:HOH:O	2.51	0.41
1:E:78:SER:OG	3:E:201:HOH:O	2.20	0.41
2:C:101:4BW:NAT	1:D:49:GLU:O	2.45	0.41
1:P:6:GLU:O	1:P:12:ARG:NH1	2.42	0.41
2:S:4201:4BW:H15	2:S:4201:4BW:H9	2.02	0.41
1:N:76:LEU:O	1:N:80:ILE:HG12	2.21	0.41
1:R:18:ARG:NH2	3:R:209:HOH:O	2.52	0.40
1:L:64:ASP:HB3	1:L:68:ARG:NH1	2.37	0.40
1:N:15:LYS:HE3	1:Q:9:GLU:OE2	2.22	0.40
1:C:49:GLU:OE1	1:D:34:SER:OG	2.26	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:SER:HB3	1:F:17:LYS:HB2	2.03	0.40

All (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
3:G:247:HOH:O	3:Q:213:HOH:O[1_556]	2.02	0.18
3:B:355:HOH:O	3:F:206:HOH:O[1_655]	2.08	0.12
3:D:478:HOH:O	3:I:260:HOH:O[1_645]	2.11	0.09
3:F:203:HOH:O	3:H:208:HOH:O[1_545]	2.13	0.07
3:G:218:HOH:O	3:R:209:HOH:O[1_546]	2.13	0.07
3:B:330:HOH:O	3:F:228:HOH:O[1_655]	2.16	0.04
3:B:333:HOH:O	3:F:234:HOH:O[1_655]	2.17	0.03

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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 (i)

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	PHE
1	C	88	GLU
1	E	79	PHE
1	H	4	ASN
1	H	79	PHE
1	L	3	ILE
1	O	60	GLU
1	O	79	PHE

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 (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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
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

All (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
2	N	101	4BW	OAX-CBO	20.64	1.68	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	101	4BW	OAX-CBO	20.60	1.67	1.40
2	P	101	4BW	OAX-CBO	20.60	1.67	1.40
2	F	101	4BW	OAX-CBO	20.60	1.67	1.40
2	L	101	4BW	OAX-CBO	20.58	1.67	1.40
2	O	101	4BW	OAX-CBO	20.57	1.67	1.40
2	J	101	4BW	OAX-CBO	20.57	1.67	1.40
2	B	201	4BW	OAX-CBO	20.56	1.67	1.40
2	E	101	4BW	OAX-CBO	20.55	1.67	1.40
2	G	101	4BW	OAX-CBO	20.54	1.67	1.40
2	H	101	4BW	OAX-CBO	20.53	1.67	1.40
2	A	201	4BW	OAX-CBO	20.51	1.67	1.40
2	D	301	4BW	OAX-CBO	20.50	1.67	1.40
2	I	101	4BW	OAX-CBO	20.48	1.67	1.40
2	C	101	4BW	OAX-CBO	20.47	1.67	1.40
2	T	101	4BW	C2'-C3'	-13.13	1.24	1.53
2	K	101	4BW	C2'-C3'	-13.12	1.24	1.53
2	H	101	4BW	C2'-C3'	-13.11	1.24	1.53
2	B	201	4BW	C2'-C3'	-13.09	1.24	1.53
2	I	101	4BW	C2'-C3'	-13.08	1.24	1.53
2	A	201	4BW	C2'-C3'	-13.06	1.24	1.53
2	R	101	4BW	C2'-C3'	-13.06	1.24	1.53
2	Q	101	4BW	C2'-C3'	-13.05	1.24	1.53
2	C	101	4BW	C2'-C3'	-13.04	1.24	1.53
2	S	4201	4BW	C2'-C3'	-13.04	1.24	1.53
2	O	101	4BW	C2'-C3'	-13.04	1.24	1.53
2	G	101	4BW	C2'-C3'	-13.03	1.24	1.53
2	F	101	4BW	C2'-C3'	-13.01	1.24	1.53
2	L	101	4BW	C2'-C3'	-13.00	1.24	1.53
2	J	101	4BW	C2'-C3'	-13.00	1.24	1.53
2	M	101	4BW	C2'-C3'	-13.00	1.24	1.53
2	P	101	4BW	C2'-C3'	-13.00	1.24	1.53
2	N	101	4BW	C2'-C3'	-13.00	1.24	1.53
2	E	101	4BW	C2'-C3'	-12.99	1.24	1.53
2	D	301	4BW	C2'-C3'	-12.98	1.24	1.53
2	L	101	4BW	O4'-C1'	8.24	1.51	1.40
2	Q	101	4BW	O4'-C1'	8.22	1.51	1.40
2	K	101	4BW	O4'-C1'	8.20	1.51	1.40
2	I	101	4BW	O4'-C1'	8.19	1.51	1.40
2	J	101	4BW	O4'-C1'	8.14	1.51	1.40
2	G	101	4BW	O4'-C1'	8.14	1.51	1.40
2	R	101	4BW	O4'-C1'	8.14	1.51	1.40
2	E	101	4BW	O4'-C1'	8.13	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	101	4BW	O4'-C1'	8.12	1.51	1.40
2	F	101	4BW	O4'-C1'	8.12	1.51	1.40
2	T	101	4BW	O4'-C1'	8.12	1.51	1.40
2	S	4201	4BW	O4'-C1'	8.11	1.51	1.40
2	B	201	4BW	O4'-C1'	8.11	1.51	1.40
2	D	301	4BW	O4'-C1'	8.11	1.51	1.40
2	C	101	4BW	O4'-C1'	8.10	1.51	1.40
2	A	201	4BW	O4'-C1'	8.10	1.51	1.40
2	M	101	4BW	O4'-C1'	8.09	1.51	1.40
2	N	101	4BW	O4'-C1'	8.06	1.51	1.40
2	P	101	4BW	O4'-C1'	8.06	1.51	1.40
2	O	101	4BW	O4'-C1'	8.01	1.51	1.40
2	D	301	4BW	O4'-C4'	-8.01	1.27	1.45
2	H	101	4BW	O4'-C4'	-8.01	1.27	1.45
2	R	101	4BW	O4'-C4'	-8.00	1.27	1.45
2	N	101	4BW	O4'-C4'	-7.99	1.27	1.45
2	J	101	4BW	O4'-C4'	-7.97	1.27	1.45
2	I	101	4BW	O4'-C4'	-7.97	1.27	1.45
2	S	4201	4BW	O4'-C4'	-7.96	1.27	1.45
2	G	101	4BW	O4'-C4'	-7.96	1.27	1.45
2	M	101	4BW	O4'-C4'	-7.95	1.27	1.45
2	T	101	4BW	O4'-C4'	-7.95	1.27	1.45
2	B	201	4BW	O4'-C4'	-7.95	1.27	1.45
2	C	101	4BW	O4'-C4'	-7.95	1.27	1.45
2	K	101	4BW	O4'-C4'	-7.94	1.27	1.45
2	E	101	4BW	O4'-C4'	-7.94	1.27	1.45
2	L	101	4BW	O4'-C4'	-7.94	1.27	1.45
2	P	101	4BW	O4'-C4'	-7.94	1.27	1.45
2	A	201	4BW	O4'-C4'	-7.93	1.27	1.45
2	F	101	4BW	O4'-C4'	-7.93	1.27	1.45
2	Q	101	4BW	O4'-C4'	-7.91	1.27	1.45
2	O	101	4BW	O4'-C4'	-7.86	1.27	1.45
2	T	101	4BW	C1'-N9	-6.90	1.32	1.49
2	M	101	4BW	C1'-N9	-6.84	1.33	1.49
2	R	101	4BW	C1'-N9	-6.84	1.33	1.49
2	A	201	4BW	C1'-N9	-6.83	1.33	1.49
2	J	101	4BW	C1'-N9	-6.83	1.33	1.49
2	N	101	4BW	C1'-N9	-6.83	1.33	1.49
2	S	4201	4BW	C1'-N9	-6.81	1.33	1.49
2	E	101	4BW	C1'-N9	-6.81	1.33	1.49
2	I	101	4BW	C1'-N9	-6.80	1.33	1.49
2	P	101	4BW	C1'-N9	-6.80	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	101	4BW	C1'-N9	-6.79	1.33	1.49
2	D	301	4BW	C1'-N9	-6.79	1.33	1.49
2	H	101	4BW	C1'-N9	-6.78	1.33	1.49
2	Q	101	4BW	C1'-N9	-6.77	1.33	1.49
2	F	101	4BW	C1'-N9	-6.77	1.33	1.49
2	L	101	4BW	C1'-N9	-6.76	1.33	1.49
2	B	201	4BW	C1'-N9	-6.76	1.33	1.49
2	G	101	4BW	C1'-N9	-6.75	1.33	1.49
2	C	101	4BW	C1'-N9	-6.74	1.33	1.49
2	O	101	4BW	C1'-N9	-6.59	1.33	1.49
2	D	301	4BW	OAX-CBK	-6.48	1.30	1.45
2	S	4201	4BW	OAX-CBK	-6.47	1.30	1.45
2	O	101	4BW	OAX-CBK	-6.46	1.30	1.45
2	P	101	4BW	OAX-CBK	-6.45	1.30	1.45
2	J	101	4BW	OAX-CBK	-6.45	1.30	1.45
2	Q	101	4BW	OAX-CBK	-6.43	1.30	1.45
2	B	201	4BW	OAX-CBK	-6.43	1.30	1.45
2	F	101	4BW	OAX-CBK	-6.43	1.30	1.45
2	L	101	4BW	OAX-CBK	-6.42	1.30	1.45
2	G	101	4BW	OAX-CBK	-6.42	1.30	1.45
2	A	201	4BW	OAX-CBK	-6.41	1.30	1.45
2	R	101	4BW	OAX-CBK	-6.41	1.30	1.45
2	M	101	4BW	OAX-CBK	-6.41	1.30	1.45
2	K	101	4BW	OAX-CBK	-6.40	1.30	1.45
2	H	101	4BW	OAX-CBK	-6.40	1.30	1.45
2	T	101	4BW	OAX-CBK	-6.38	1.30	1.45
2	I	101	4BW	OAX-CBK	-6.32	1.31	1.45
2	N	101	4BW	OAX-CBK	-6.27	1.31	1.45
2	C	101	4BW	OAX-CBK	-6.26	1.31	1.45
2	E	101	4BW	OAX-CBK	-6.24	1.31	1.45
2	T	101	4BW	CBA-NAS	5.06	1.45	1.33
2	M	101	4BW	CBA-NAS	5.06	1.45	1.33
2	N	101	4BW	CBA-NAS	5.05	1.45	1.33
2	R	101	4BW	CBA-NAS	5.04	1.45	1.33
2	J	101	4BW	CBA-NAS	5.04	1.45	1.33
2	Q	101	4BW	CBA-NAS	5.03	1.45	1.33
2	B	201	4BW	CBA-NAS	5.02	1.45	1.33
2	O	101	4BW	CBA-NAS	5.02	1.45	1.33
2	K	101	4BW	CBA-NAS	5.02	1.45	1.33
2	F	101	4BW	CBA-NAS	5.01	1.45	1.33
2	L	101	4BW	CBA-NAS	5.01	1.45	1.33
2	E	101	4BW	CBA-NAS	5.01	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	4201	4BW	CBA-NAS	5.01	1.45	1.33
2	G	101	4BW	CBA-NAS	4.99	1.45	1.33
2	A	201	4BW	CBA-NAS	4.98	1.45	1.33
2	P	101	4BW	CBA-NAS	4.97	1.45	1.33
2	C	101	4BW	CBA-NAS	4.95	1.45	1.33
2	H	101	4BW	CBA-NAS	4.95	1.45	1.33
2	D	301	4BW	CBA-NAS	4.93	1.45	1.33
2	I	101	4BW	CBA-NAS	4.91	1.45	1.33
2	P	101	4BW	CBA-NAA	4.80	1.45	1.34
2	T	101	4BW	CBA-NAA	4.79	1.45	1.34
2	H	101	4BW	CBA-NAA	4.79	1.45	1.34
2	G	101	4BW	CBA-NAA	4.79	1.45	1.34
2	O	101	4BW	CBA-NAA	4.78	1.45	1.34
2	B	201	4BW	CBA-NAA	4.78	1.45	1.34
2	N	101	4BW	CBA-NAA	4.78	1.45	1.34
2	M	101	4BW	CBA-NAA	4.77	1.45	1.34
2	K	101	4BW	CBA-NAA	4.77	1.45	1.34
2	C	101	4BW	CBA-NAA	4.77	1.45	1.34
2	R	101	4BW	CBA-NAA	4.77	1.45	1.34
2	A	201	4BW	CBA-NAA	4.77	1.45	1.34
2	L	101	4BW	CBA-NAA	4.76	1.45	1.34
2	I	101	4BW	CBA-NAA	4.75	1.45	1.34
2	D	301	4BW	CBA-NAA	4.75	1.45	1.34
2	S	4201	4BW	CBA-NAA	4.74	1.45	1.34
2	Q	101	4BW	CBA-NAA	4.74	1.45	1.34
2	F	101	4BW	CBA-NAA	4.73	1.45	1.34
2	J	101	4BW	CBA-NAA	4.73	1.45	1.34
2	E	101	4BW	CBA-NAA	4.72	1.45	1.34
2	O	101	4BW	C3'-C4'	4.11	1.63	1.52
2	P	101	4BW	C3'-C4'	4.05	1.63	1.52
2	N	101	4BW	C3'-C4'	4.03	1.63	1.52
2	C	101	4BW	C3'-C4'	4.01	1.63	1.52
2	F	101	4BW	C3'-C4'	4.01	1.63	1.52
2	T	101	4BW	C3'-C4'	4.00	1.63	1.52
2	B	201	4BW	C3'-C4'	4.00	1.63	1.52
2	E	101	4BW	C3'-C4'	4.00	1.63	1.52
2	D	301	4BW	C3'-C4'	4.00	1.63	1.52
2	A	201	4BW	C3'-C4'	3.99	1.63	1.52
2	M	101	4BW	C3'-C4'	3.99	1.63	1.52
2	L	101	4BW	C3'-C4'	3.98	1.63	1.52
2	S	4201	4BW	C3'-C4'	3.97	1.63	1.52
2	R	101	4BW	C3'-C4'	3.97	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	101	4BW	C3'-C4'	3.96	1.63	1.52
2	K	101	4BW	C3'-C4'	3.95	1.63	1.52
2	G	101	4BW	C3'-C4'	3.92	1.63	1.52
2	I	101	4BW	C3'-C4'	3.92	1.63	1.52
2	J	101	4BW	C3'-C4'	3.92	1.63	1.52
2	H	101	4BW	C3'-C4'	3.90	1.63	1.52
2	O	101	4BW	OAZ-CBM	-3.80	1.31	1.44
2	D	301	4BW	O2'-C2'	3.74	1.52	1.43
2	C	101	4BW	O2'-C2'	3.73	1.52	1.43
2	I	101	4BW	O2'-C2'	3.71	1.52	1.43
2	P	101	4BW	O2'-C2'	3.70	1.52	1.43
2	G	101	4BW	O2'-C2'	3.68	1.52	1.43
2	B	201	4BW	O2'-C2'	3.68	1.52	1.43
2	N	101	4BW	O2'-C2'	3.68	1.52	1.43
2	M	101	4BW	O2'-C2'	3.67	1.52	1.43
2	P	101	4BW	OAZ-CBM	-3.67	1.31	1.44
2	H	101	4BW	O2'-C2'	3.67	1.52	1.43
2	N	101	4BW	OAZ-CBM	-3.66	1.31	1.44
2	S	4201	4BW	O2'-C2'	3.66	1.52	1.43
2	O	101	4BW	O2'-C2'	3.66	1.52	1.43
2	S	4201	4BW	OAZ-CBM	-3.66	1.31	1.44
2	T	101	4BW	OAZ-CBM	-3.66	1.31	1.44
2	F	101	4BW	O2'-C2'	3.65	1.52	1.43
2	E	101	4BW	O2'-C2'	3.65	1.52	1.43
2	K	101	4BW	OAZ-CBM	-3.65	1.31	1.44
2	L	101	4BW	O2'-C2'	3.65	1.52	1.43
2	T	101	4BW	O2'-C2'	3.64	1.52	1.43
2	J	101	4BW	O2'-C2'	3.64	1.52	1.43
2	K	101	4BW	O2'-C2'	3.64	1.52	1.43
2	M	101	4BW	OAZ-CBM	-3.63	1.31	1.44
2	Q	101	4BW	O2'-C2'	3.63	1.51	1.43
2	Q	101	4BW	OAZ-CBM	-3.63	1.31	1.44
2	R	101	4BW	O2'-C2'	3.63	1.51	1.43
2	A	201	4BW	O2'-C2'	3.63	1.51	1.43
2	F	101	4BW	OAZ-CBM	-3.62	1.31	1.44
2	D	301	4BW	OAZ-CBM	-3.61	1.31	1.44
2	G	101	4BW	OAZ-CBM	-3.61	1.31	1.44
2	E	101	4BW	OAZ-CBM	-3.59	1.31	1.44
2	R	101	4BW	CBG-NAS	3.59	1.45	1.37
2	L	101	4BW	OAZ-CBM	-3.59	1.31	1.44
2	T	101	4BW	CBG-NAS	3.58	1.45	1.37
2	R	101	4BW	OAZ-CBM	-3.58	1.31	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	101	4BW	CBG-NAS	3.57	1.45	1.37
2	B	201	4BW	OAZ-CBM	-3.57	1.31	1.44
2	J	101	4BW	OAZ-CBM	-3.57	1.31	1.44
2	O	101	4BW	CBG-NAS	3.57	1.45	1.37
2	E	101	4BW	CBG-NAS	3.57	1.45	1.37
2	N	101	4BW	CBG-NAS	3.57	1.45	1.37
2	B	201	4BW	CBG-NAS	3.56	1.45	1.37
2	A	201	4BW	OAZ-CBM	-3.56	1.31	1.44
2	J	101	4BW	CBG-NAS	3.55	1.45	1.37
2	C	101	4BW	OAZ-CBM	-3.55	1.32	1.44
2	H	101	4BW	OAZ-CBM	-3.55	1.32	1.44
2	S	4201	4BW	CBG-NAS	3.55	1.45	1.37
2	F	101	4BW	CBG-NAS	3.55	1.45	1.37
2	K	101	4BW	CBG-NAS	3.53	1.45	1.37
2	Q	101	4BW	CBG-NAS	3.52	1.45	1.37
2	J	101	4BW	CBI-CBM	3.52	1.60	1.53
2	P	101	4BW	CBG-NAS	3.51	1.45	1.37
2	C	101	4BW	CBG-NAS	3.51	1.45	1.37
2	L	101	4BW	CBG-NAS	3.51	1.45	1.37
2	G	101	4BW	CBG-NAS	3.50	1.45	1.37
2	D	301	4BW	CBG-NAS	3.50	1.45	1.37
2	I	101	4BW	OAZ-CBM	-3.49	1.32	1.44
2	C	101	4BW	CBI-CBM	3.49	1.60	1.53
2	I	101	4BW	CBI-CBM	3.48	1.60	1.53
2	L	101	4BW	CBI-CBM	3.48	1.60	1.53
2	H	101	4BW	CBI-CBM	3.46	1.60	1.53
2	R	101	4BW	CBI-CBM	3.46	1.60	1.53
2	A	201	4BW	CBG-NAS	3.45	1.45	1.37
2	I	101	4BW	CBG-NAS	3.43	1.45	1.37
2	N	101	4BW	CBI-CBM	3.43	1.60	1.53
2	Q	101	4BW	CBI-CBM	3.43	1.60	1.53
2	M	101	4BW	CBI-CBM	3.41	1.60	1.53
2	H	101	4BW	CBG-NAS	3.40	1.45	1.37
2	P	101	4BW	CBI-CBM	3.40	1.60	1.53
2	E	101	4BW	CBI-CBM	3.40	1.60	1.53
2	B	201	4BW	CBI-CBM	3.40	1.60	1.53
2	S	4201	4BW	CBI-CBM	3.35	1.60	1.53
2	K	101	4BW	CBI-CBM	3.34	1.60	1.53
2	G	101	4BW	CBI-CBM	3.34	1.60	1.53
2	O	101	4BW	CBI-CBM	3.33	1.60	1.53
2	D	301	4BW	CBI-CBM	3.33	1.60	1.53
2	F	101	4BW	CBI-CBM	3.33	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	4BW	CBI-CBM	3.31	1.60	1.53
2	T	101	4BW	CBI-CBM	3.28	1.60	1.53
2	T	101	4BW	CBA-NAT	3.00	1.44	1.37
2	I	101	4BW	CBA-NAT	2.98	1.44	1.37
2	D	301	4BW	CBA-NAT	2.96	1.44	1.37
2	C	101	4BW	CBA-NAT	2.95	1.44	1.37
2	O	101	4BW	CBA-NAT	2.94	1.44	1.37
2	N	101	4BW	CBA-NAT	2.94	1.44	1.37
2	K	101	4BW	CBA-NAT	2.94	1.44	1.37
2	R	101	4BW	CBA-NAT	2.94	1.44	1.37
2	B	201	4BW	CBA-NAT	2.94	1.44	1.37
2	P	101	4BW	CBA-NAT	2.93	1.44	1.37
2	L	101	4BW	CBA-NAT	2.92	1.44	1.37
2	H	101	4BW	CBA-NAT	2.91	1.44	1.37
2	E	101	4BW	CBA-NAT	2.91	1.44	1.37
2	M	101	4BW	CBA-NAT	2.91	1.44	1.37
2	J	101	4BW	CBA-NAT	2.90	1.44	1.37
2	F	101	4BW	CBA-NAT	2.90	1.44	1.37
2	S	4201	4BW	CBA-NAT	2.89	1.44	1.37
2	A	201	4BW	CBA-NAT	2.85	1.44	1.37
2	Q	101	4BW	CBA-NAT	2.85	1.44	1.37
2	G	101	4BW	CBA-NAT	2.85	1.44	1.37
2	I	101	4BW	C6-N6	2.82	1.44	1.34
2	R	101	4BW	C6-N6	2.81	1.44	1.34
2	L	101	4BW	C6-N6	2.81	1.44	1.34
2	F	101	4BW	C6-N6	2.81	1.44	1.34
2	N	101	4BW	C6-N6	2.81	1.44	1.34
2	O	101	4BW	C6-N6	2.81	1.44	1.34
2	K	101	4BW	C6-N6	2.80	1.44	1.34
2	C	101	4BW	C6-N6	2.80	1.44	1.34
2	S	4201	4BW	C6-N6	2.80	1.44	1.34
2	B	201	4BW	C6-N6	2.80	1.44	1.34
2	E	101	4BW	C6-N6	2.79	1.44	1.34
2	J	101	4BW	C6-N6	2.79	1.44	1.34
2	H	101	4BW	C6-N6	2.79	1.44	1.34
2	Q	101	4BW	C6-N6	2.79	1.44	1.34
2	M	101	4BW	C6-N6	2.78	1.44	1.34
2	D	301	4BW	C6-N6	2.78	1.44	1.34
2	T	101	4BW	C6-N6	2.78	1.44	1.34
2	G	101	4BW	C6-N6	2.77	1.44	1.34
2	A	201	4BW	C6-N6	2.76	1.44	1.34
2	P	101	4BW	C6-N6	2.76	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	101	4BW	CBC-NAT	2.55	1.41	1.37
2	T	101	4BW	CBO-NBQ	-2.51	1.43	1.50
2	I	101	4BW	CBC-NAT	2.49	1.41	1.37
2	R	101	4BW	CBC-NAT	2.49	1.41	1.37
2	B	201	4BW	CBC-NAT	2.49	1.41	1.37
2	K	101	4BW	CBC-NAT	2.47	1.41	1.37
2	N	101	4BW	CBC-NAT	2.45	1.41	1.37
2	F	101	4BW	CBC-NAT	2.45	1.41	1.37
2	S	4201	4BW	CBC-NAT	2.44	1.41	1.37
2	P	101	4BW	CBC-NAT	2.44	1.41	1.37
2	J	101	4BW	CBC-NAT	2.43	1.41	1.37
2	O	101	4BW	CBC-NAT	2.43	1.41	1.37
2	E	101	4BW	CBC-NAT	2.43	1.41	1.37
2	M	101	4BW	CBC-NAT	2.43	1.41	1.37
2	L	101	4BW	CBC-NAT	2.43	1.41	1.37
2	C	101	4BW	CBC-NAT	2.42	1.41	1.37
2	H	101	4BW	CBC-NAT	2.42	1.41	1.37
2	A	201	4BW	CBC-NAT	2.39	1.41	1.37
2	G	101	4BW	CBC-NAT	2.38	1.41	1.37
2	O	101	4BW	OAG-CBI	2.35	1.48	1.43
2	R	101	4BW	OAG-CBI	2.35	1.48	1.43
2	Q	101	4BW	OAG-CBI	2.34	1.48	1.43
2	I	101	4BW	OAG-CBI	2.34	1.48	1.43
2	M	101	4BW	OAG-CBI	2.34	1.48	1.43
2	J	101	4BW	OAG-CBI	2.34	1.48	1.43
2	S	4201	4BW	OAG-CBI	2.34	1.48	1.43
2	N	101	4BW	OAG-CBI	2.33	1.48	1.43
2	K	101	4BW	OAG-CBI	2.33	1.48	1.43
2	H	101	4BW	OAG-CBI	2.33	1.48	1.43
2	O	101	4BW	CBO-NBQ	-2.33	1.43	1.50
2	Q	101	4BW	CBC-NAT	2.33	1.41	1.37
2	L	101	4BW	OAG-CBI	2.32	1.48	1.43
2	P	101	4BW	OAG-CBI	2.31	1.48	1.43
2	D	301	4BW	CBC-NAT	2.31	1.41	1.37
2	G	101	4BW	OAG-CBI	2.31	1.48	1.43
2	B	201	4BW	OAG-CBI	2.30	1.48	1.43
2	E	101	4BW	OAG-CBI	2.28	1.48	1.43
2	F	101	4BW	OAG-CBI	2.28	1.48	1.43
2	D	301	4BW	OAG-CBI	2.27	1.48	1.43
2	C	101	4BW	OAG-CBI	2.27	1.48	1.43
2	T	101	4BW	OAG-CBI	2.26	1.48	1.43
2	A	201	4BW	OAG-CBI	2.26	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	101	4BW	CBO-NBQ	-2.20	1.44	1.50
2	L	101	4BW	CBO-NBQ	-2.19	1.44	1.50
2	G	101	4BW	CBO-NBQ	-2.19	1.44	1.50
2	Q	101	4BW	CBO-NBQ	-2.18	1.44	1.50
2	S	4201	4BW	CBO-NBQ	-2.18	1.44	1.50
2	R	101	4BW	CBO-NBQ	-2.18	1.44	1.50
2	M	101	4BW	CBO-NBQ	-2.16	1.44	1.50
2	A	201	4BW	CBO-NBQ	-2.16	1.44	1.50
2	K	101	4BW	CBO-NBQ	-2.15	1.44	1.50
2	N	101	4BW	CBO-NBQ	-2.15	1.44	1.50
2	F	101	4BW	CBO-NBQ	-2.15	1.44	1.50
2	J	101	4BW	CBO-NBQ	-2.14	1.44	1.50
2	D	301	4BW	CBO-NBQ	-2.14	1.44	1.50
2	B	201	4BW	CBO-NBQ	-2.12	1.44	1.50
2	I	101	4BW	CBO-NBQ	-2.11	1.44	1.50
2	C	101	4BW	CBO-NBQ	-2.11	1.44	1.50
2	H	101	4BW	CBO-NBQ	-2.11	1.44	1.50
2	P	101	4BW	O3'-C3'	2.06	1.51	1.44
2	N	101	4BW	O3'-C3'	2.04	1.51	1.44
2	O	101	4BW	O3'-C3'	2.04	1.51	1.44
2	M	101	4BW	O3'-C3'	2.02	1.51	1.44
2	R	101	4BW	O3'-C3'	2.02	1.51	1.44
2	G	101	4BW	O3'-C3'	2.02	1.51	1.44
2	B	201	4BW	O3'-C3'	2.01	1.50	1.44
2	T	101	4BW	O3'-C3'	2.00	1.50	1.44

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
2	J	101	4BW	N3-C2-N1	-5.37	121.39	128.67
2	Q	101	4BW	N3-C2-N1	-5.36	121.39	128.67
2	D	301	4BW	N3-C2-N1	-5.35	121.41	128.67
2	K	101	4BW	N3-C2-N1	-5.34	121.43	128.67
2	O	101	4BW	N3-C2-N1	-5.31	121.47	128.67
2	B	201	4BW	N3-C2-N1	-5.31	121.47	128.67
2	I	101	4BW	N3-C2-N1	-5.31	121.47	128.67
2	N	101	4BW	N3-C2-N1	-5.31	121.47	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	101	4BW	N3-C2-N1	-5.31	121.47	128.67
2	M	101	4BW	N3-C2-N1	-5.30	121.47	128.67
2	E	101	4BW	N3-C2-N1	-5.30	121.48	128.67
2	C	101	4BW	N3-C2-N1	-5.29	121.49	128.67
2	L	101	4BW	N3-C2-N1	-5.29	121.50	128.67
2	G	101	4BW	N3-C2-N1	-5.25	121.55	128.67
2	T	101	4BW	N3-C2-N1	-5.24	121.56	128.67
2	I	101	4BW	C4'-O4'-C1'	-5.21	105.15	109.92
2	A	201	4BW	C4'-O4'-C1'	-5.13	105.23	109.92
2	S	4201	4BW	N3-C2-N1	-5.12	121.72	128.67
2	N	101	4BW	C4'-O4'-C1'	-5.10	105.25	109.92
2	P	101	4BW	CBK-OAX-CBO	-5.04	105.31	109.92
2	T	101	4BW	C4'-O4'-C1'	-5.00	105.34	109.92
2	L	101	4BW	C4'-O4'-C1'	-4.96	105.39	109.92
2	K	101	4BW	C4'-O4'-C1'	-4.94	105.40	109.92
2	M	101	4BW	C4'-O4'-C1'	-4.89	105.44	109.92
2	B	201	4BW	C4'-O4'-C1'	-4.87	105.46	109.92
2	G	101	4BW	C4'-O4'-C1'	-4.79	105.54	109.92
2	D	301	4BW	C4'-O4'-C1'	-4.77	105.56	109.92
2	O	101	4BW	CBK-OAX-CBO	-4.77	105.56	109.92
2	J	101	4BW	C4'-O4'-C1'	-4.76	105.57	109.92
2	H	101	4BW	C4'-O4'-C1'	-4.75	105.58	109.92
2	P	101	4BW	C4'-O4'-C1'	-4.71	105.61	109.92
2	Q	101	4BW	C4'-O4'-C1'	-4.68	105.64	109.92
2	C	101	4BW	C4'-O4'-C1'	-4.59	105.72	109.92
2	F	101	4BW	C4'-O4'-C1'	-4.53	105.78	109.92
2	S	4201	4BW	CBK-OAX-CBO	-4.41	105.89	109.92
2	B	201	4BW	CBK-OAX-CBO	-4.38	105.91	109.92
2	E	101	4BW	C4'-O4'-C1'	-4.34	105.95	109.92
2	K	101	4BW	CBK-OAX-CBO	-4.34	105.95	109.92
2	D	301	4BW	CBK-OAX-CBO	-4.33	105.96	109.92
2	Q	101	4BW	CBK-OAX-CBO	-4.23	106.05	109.92
2	S	4201	4BW	C4'-O4'-C1'	-4.22	106.06	109.92
2	A	201	4BW	CBK-OAX-CBO	-4.08	106.19	109.92
2	G	101	4BW	CBK-OAX-CBO	-4.05	106.22	109.92
2	F	101	4BW	CBK-OAX-CBO	-4.04	106.23	109.92
2	R	101	4BW	CBK-OAX-CBO	-3.98	106.28	109.92
2	J	101	4BW	CBK-OAX-CBO	-3.98	106.28	109.92
2	L	101	4BW	CBK-OAX-CBO	-3.96	106.30	109.92
2	M	101	4BW	CBK-OAX-CBO	-3.90	106.35	109.92
2	T	101	4BW	CBK-OAX-CBO	-3.66	106.57	109.92
2	H	101	4BW	CBK-OAX-CBO	-3.37	106.84	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	101	4BW	C4'-O4'-C1'	-3.36	106.84	109.92
2	J	101	4BW	CAL-NAR-CBE	3.34	108.24	102.55
2	S	4201	4BW	CAL-NAR-CBE	3.30	108.17	102.55
2	P	101	4BW	CAL-NAR-CBE	3.30	108.17	102.55
2	H	101	4BW	CAL-NAR-CBE	3.30	108.16	102.55
2	G	101	4BW	CAL-NAR-CBE	3.29	108.15	102.55
2	M	101	4BW	CAL-NAR-CBE	3.28	108.14	102.55
2	K	101	4BW	CAL-NAR-CBE	3.28	108.13	102.55
2	R	101	4BW	CAL-NAR-CBE	3.28	108.13	102.55
2	L	101	4BW	CAL-NAR-CBE	3.27	108.12	102.55
2	T	101	4BW	CBE-CBC-NAT	3.27	120.30	114.07
2	D	301	4BW	CAL-NAR-CBE	3.27	108.11	102.55
2	F	101	4BW	CAL-NAR-CBE	3.26	108.10	102.55
2	I	101	4BW	CAL-NAR-CBE	3.24	108.07	102.55
2	Q	101	4BW	CAL-NAR-CBE	3.24	108.07	102.55
2	A	201	4BW	CAL-NAR-CBE	3.24	108.06	102.55
2	O	101	4BW	CAL-NAR-CBE	3.23	108.04	102.55
2	E	101	4BW	CAL-NAR-CBE	3.22	108.04	102.55
2	B	201	4BW	CAL-NAR-CBE	3.22	108.03	102.55
2	N	101	4BW	CAL-NAR-CBE	3.21	108.02	102.55
2	C	101	4BW	CAL-NAR-CBE	3.20	108.00	102.55
2	G	101	4BW	CBE-CBC-NAT	3.19	120.15	114.07
2	L	101	4BW	CBM-CBI-CBO	3.17	106.87	99.89
2	N	101	4BW	CBM-CBI-CBO	3.15	106.81	99.89
2	L	101	4BW	CBE-CBC-NAT	3.14	120.07	114.07
2	H	101	4BW	CBE-CBC-NAT	3.13	120.05	114.07
2	M	101	4BW	CBE-CBC-NAT	3.13	120.04	114.07
2	S	4201	4BW	CBE-CBC-NAT	3.13	120.03	114.07
2	J	101	4BW	CBE-CBC-NAT	3.11	120.01	114.07
2	R	101	4BW	CBE-CBC-NAT	3.11	120.00	114.07
2	N	101	4BW	CBE-CBC-NAT	3.11	120.00	114.07
2	T	101	4BW	CAL-NAR-CBE	3.11	107.84	102.55
2	A	201	4BW	CBE-CBC-NAT	3.10	119.99	114.07
2	K	101	4BW	CBE-CBC-NAT	3.09	119.97	114.07
2	A	201	4BW	CBM-CBI-CBO	3.09	106.69	99.89
2	P	101	4BW	CBE-CBC-NAT	3.08	119.95	114.07
2	C	101	4BW	CBM-CBI-CBO	3.07	106.64	99.89
2	Q	101	4BW	CBE-CBC-NAT	3.07	119.93	114.07
2	F	101	4BW	CBE-CBC-NAT	3.07	119.92	114.07
2	H	101	4BW	CBM-CBI-CBO	3.07	106.63	99.89
2	I	101	4BW	CBM-CBI-CBO	3.06	106.62	99.89
2	O	101	4BW	CBE-CBC-NAT	3.06	119.91	114.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	101	4BW	CBE-CBC-NAT	3.05	119.88	114.07
2	D	301	4BW	CBE-CBC-NAT	3.03	119.86	114.07
2	T	101	4BW	CBA-NAT-CBC	-3.03	119.56	125.11
2	B	201	4BW	CBE-CBC-NAT	3.02	119.83	114.07
2	C	101	4BW	CBE-CBC-NAT	3.01	119.81	114.07
2	H	101	4BW	CBA-NAT-CBC	-3.00	119.61	125.11
2	J	101	4BW	CBM-CBI-CBO	2.99	106.47	99.89
2	I	101	4BW	CBE-CBC-NAT	2.98	119.75	114.07
2	R	101	4BW	CBM-CBI-CBO	2.97	106.42	99.89
2	Q	101	4BW	CBM-CBI-CBO	2.96	106.40	99.89
2	L	101	4BW	CBA-NAT-CBC	-2.96	119.69	125.11
2	B	201	4BW	CBM-CBI-CBO	2.96	106.39	99.89
2	F	101	4BW	CBM-CBI-CBO	2.96	106.39	99.89
2	T	101	4BW	OAC-CBC-CBE	-2.95	118.46	124.32
2	E	101	4BW	CBM-CBI-CBO	2.95	106.38	99.89
2	J	101	4BW	CBA-NAT-CBC	-2.95	119.71	125.11
2	M	101	4BW	CBM-CBI-CBO	2.95	106.37	99.89
2	O	101	4BW	CBM-CBI-CBO	2.94	106.36	99.89
2	P	101	4BW	CBM-CBI-CBO	2.93	106.32	99.89
2	K	101	4BW	CBA-NAT-CBC	-2.92	119.77	125.11
2	N	101	4BW	CBA-NAT-CBC	-2.91	119.78	125.11
2	R	101	4BW	CBA-NAT-CBC	-2.91	119.79	125.11
2	Q	101	4BW	CBA-NAT-CBC	-2.90	119.80	125.11
2	M	101	4BW	CBA-NAT-CBC	-2.90	119.80	125.11
2	E	101	4BW	CBA-NAT-CBC	-2.90	119.81	125.11
2	S	4201	4BW	CBA-NAT-CBC	-2.90	119.81	125.11
2	G	101	4BW	CBA-NAT-CBC	-2.87	119.85	125.11
2	A	201	4BW	CBA-NAT-CBC	-2.86	119.87	125.11
2	K	101	4BW	CBM-CBI-CBO	2.86	106.17	99.89
2	F	101	4BW	CBA-NAT-CBC	-2.86	119.88	125.11
2	P	101	4BW	CBA-NAT-CBC	-2.85	119.90	125.11
2	C	101	4BW	CBA-NAT-CBC	-2.84	119.91	125.11
2	O	101	4BW	CBA-NAT-CBC	-2.83	119.92	125.11
2	D	301	4BW	CBM-CBI-CBO	2.83	106.11	99.89
2	B	201	4BW	CBA-NAT-CBC	-2.83	119.94	125.11
2	D	301	4BW	CBA-NAT-CBC	-2.82	119.94	125.11
2	G	101	4BW	CBM-CBI-CBO	2.81	106.08	99.89
2	I	101	4BW	CBA-NAT-CBC	-2.81	119.96	125.11
2	S	4201	4BW	CBM-CBI-CBO	2.76	105.96	99.89
2	D	301	4BW	C4-C5-N7	-2.69	106.49	109.34
2	I	101	4BW	OAX-CBO-NBQ	2.68	112.30	108.75
2	T	101	4BW	CBM-CBI-CBO	2.67	105.76	99.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	101	4BW	C4-C5-N7	-2.66	106.52	109.34
2	S	4201	4BW	C4-C5-N7	-2.65	106.53	109.34
2	J	101	4BW	C4-C5-N7	-2.65	106.53	109.34
2	F	101	4BW	C4-C5-N7	-2.64	106.55	109.34
2	L	101	4BW	C4-C5-N7	-2.63	106.55	109.34
2	B	201	4BW	C4-C5-N7	-2.63	106.56	109.34
2	C	101	4BW	C4-C5-N7	-2.61	106.57	109.34
2	I	101	4BW	C4-C5-N7	-2.61	106.58	109.34
2	R	101	4BW	C4-C5-N7	-2.61	106.58	109.34
2	M	101	4BW	C4-C5-N7	-2.60	106.59	109.34
2	K	101	4BW	C4-C5-N7	-2.60	106.59	109.34
2	T	101	4BW	C4-C5-N7	-2.58	106.61	109.34
2	G	101	4BW	C4-C5-N7	-2.58	106.61	109.34
2	A	201	4BW	C4-C5-N7	-2.55	106.64	109.34
2	N	101	4BW	C4-C5-N7	-2.54	106.66	109.34
2	E	101	4BW	C4-C5-N7	-2.52	106.67	109.34
2	Q	101	4BW	C4-C5-N7	-2.51	106.68	109.34
2	P	101	4BW	C4-C5-N7	-2.51	106.69	109.34
2	O	101	4BW	C4-C5-N7	-2.42	106.78	109.34
2	O	101	4BW	O4'-C1'-N9	2.37	111.89	108.75
2	N	101	4BW	C3'-C2'-C1'	2.31	104.96	99.89
2	O	101	4BW	OAC-CBC-CBE	-2.27	119.82	124.32
2	M	101	4BW	C3'-C2'-C1'	2.25	104.85	99.89
2	N	101	4BW	OAC-CBC-CBE	-2.23	119.89	124.32
2	K	101	4BW	OAC-CBC-CBE	-2.15	120.05	124.32
2	R	101	4BW	OAC-CBC-CBE	-2.15	120.06	124.32
2	S	4201	4BW	C3'-C2'-C1'	2.14	104.59	99.89
2	B	201	4BW	OAC-CBC-CBE	-2.13	120.10	124.32
2	P	101	4BW	OAC-CBC-CBE	-2.13	120.11	124.32
2	L	101	4BW	OAC-CBC-CBE	-2.13	120.11	124.32
2	F	101	4BW	C3'-C2'-C1'	2.11	104.53	99.89
2	C	101	4BW	OAC-CBC-CBE	-2.11	120.14	124.32
2	E	101	4BW	C3'-C2'-C1'	2.10	104.51	99.89
2	M	101	4BW	OAC-CBC-CBE	-2.09	120.18	124.32
2	H	101	4BW	OAC-CBC-CBE	-2.08	120.20	124.32
2	I	101	4BW	OAC-CBC-CBE	-2.08	120.21	124.32
2	C	101	4BW	C3'-C2'-C1'	2.07	104.43	99.89
2	G	101	4BW	OAC-CBC-CBE	-2.06	120.23	124.32
2	J	101	4BW	OAC-CBC-CBE	-2.06	120.24	124.32
2	P	101	4BW	C3'-C2'-C1'	2.06	104.41	99.89
2	R	101	4BW	C3'-C2'-C1'	2.05	104.41	99.89
2	D	301	4BW	OAC-CBC-CBE	-2.03	120.29	124.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	4201	4BW	OAC-CBC-CBE	-2.03	120.30	124.32
2	Q	101	4BW	OAC-CBC-CBE	-2.03	120.30	124.32
2	E	101	4BW	CBK-OAX-CBO	-2.02	108.08	109.92
2	E	101	4BW	OAC-CBC-CBE	-2.01	120.34	124.32

There are no chirality outliers.

All (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
2	B	201	4BW	C5'-O5'-PBS-OAI
2	F	101	4BW	CAN-OAV-PBR-OAD
2	I	101	4BW	CAN-OAV-PBR-O3'
2	I	101	4BW	CAN-OAV-PBR-OAH
2	I	101	4BW	CAN-OAV-PBR-OAD
2	J	101	4BW	CAN-OAV-PBR-OAD
2	J	101	4BW	C5'-O5'-PBS-OAI
2	L	101	4BW	CAN-OAV-PBR-OAD
2	L	101	4BW	C5'-O5'-PBS-OAI
2	O	101	4BW	C5'-O5'-PBS-OAZ
2	O	101	4BW	O4'-C4'-C5'-O5'
2	O	101	4BW	C3'-C4'-C5'-O5'
2	P	101	4BW	CAN-OAV-PBR-O3'
2	R	101	4BW	CAN-OAV-PBR-OAD
2	S	4201	4BW	CAN-OAV-PBR-OAD
2	T	101	4BW	CAN-OAV-PBR-OAD
2	C	101	4BW	OAV-CAN-CBK-CBM
2	N	101	4BW	OAV-CAN-CBK-CBM
2	N	101	4BW	OAV-CAN-CBK-OAX
2	E	101	4BW	OAV-CAN-CBK-CBM
2	I	101	4BW	OAV-CAN-CBK-OAX
2	C	101	4BW	OAV-CAN-CBK-OAX
2	P	101	4BW	OAV-CAN-CBK-OAX
2	E	101	4BW	OAV-CAN-CBK-OAX
2	C	101	4BW	C3'-O3'-PBR-OAD
2	E	101	4BW	C3'-O3'-PBR-OAD
2	N	101	4BW	C3'-O3'-PBR-OAD
2	P	101	4BW	C3'-O3'-PBR-OAD
2	A	201	4BW	C5'-O5'-PBS-OAI
2	B	201	4BW	C5'-O5'-PBS-OAZ
2	D	301	4BW	CAN-OAV-PBR-OAD

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Mol	Chain	Res	Type	Atoms
2	G	101	4BW	C5'-O5'-PBS-OAI
2	H	101	4BW	CAN-OAV-PBR-OAD
2	H	101	4BW	C5'-O5'-PBS-OAI
2	I	101	4BW	C5'-O5'-PBS-OAI
2	J	101	4BW	C5'-O5'-PBS-OAZ
2	M	101	4BW	C5'-O5'-PBS-OAI
2	N	101	4BW	CAN-OAV-PBR-OAD
2	N	101	4BW	C5'-O5'-PBS-OAI
2	O	101	4BW	CAN-OAV-PBR-OAD
2	O	101	4BW	C5'-O5'-PBS-OAI
2	P	101	4BW	CAN-OAV-PBR-OAH
2	P	101	4BW	CAN-OAV-PBR-OAD
2	P	101	4BW	C5'-O5'-PBS-OAE
2	Q	101	4BW	CAN-OAV-PBR-OAD
2	R	101	4BW	C5'-O5'-PBS-OAI
2	T	101	4BW	C5'-O5'-PBS-OAI
2	I	101	4BW	OAV-CAN-CBK-CBM
2	L	101	4BW	C3'-O3'-PBR-OAD
2	N	101	4BW	C3'-O3'-PBR-OAH
2	O	101	4BW	C3'-O3'-PBR-OAD
2	J	101	4BW	O4'-C4'-C5'-O5'

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

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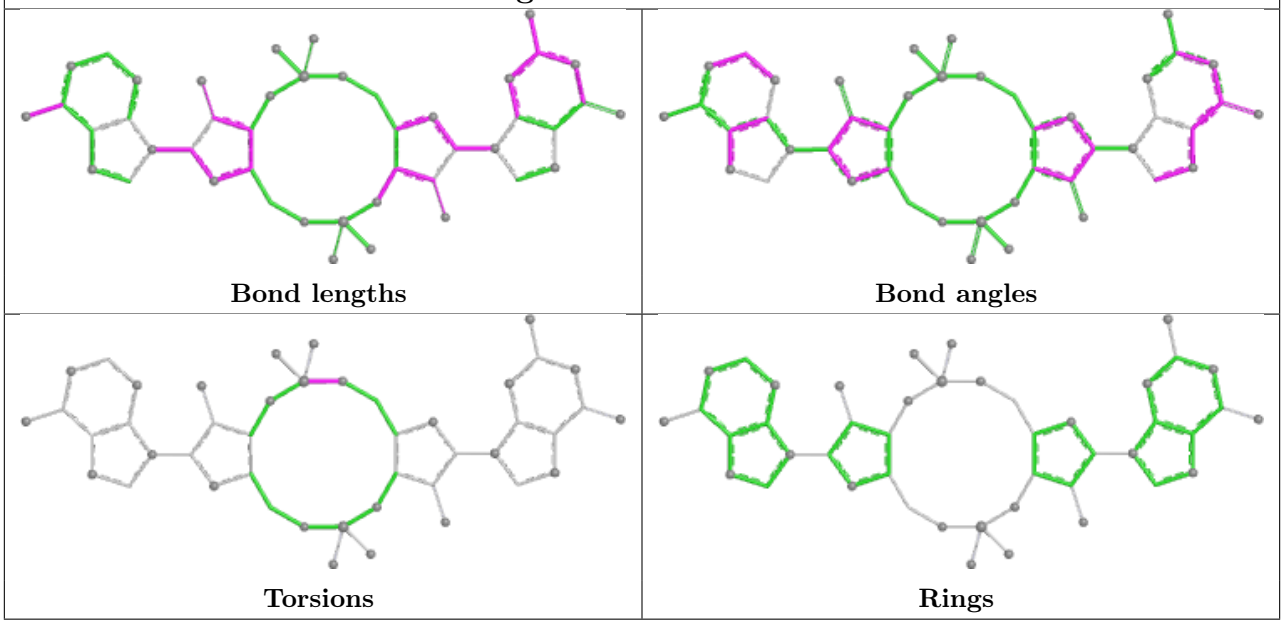
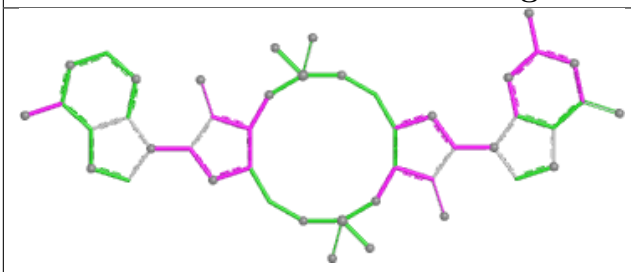
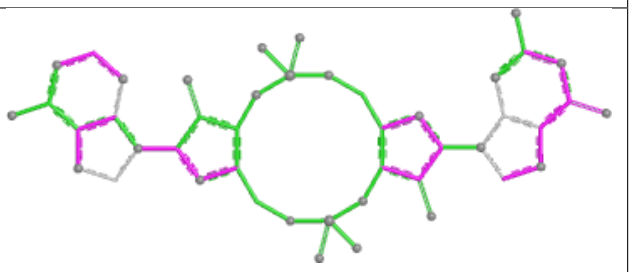
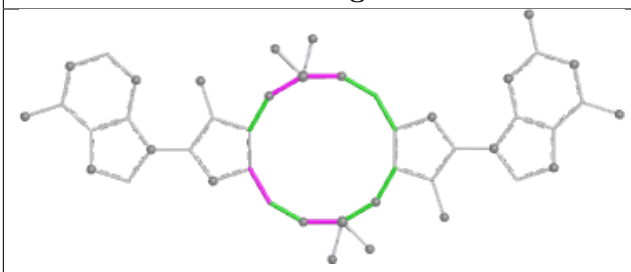
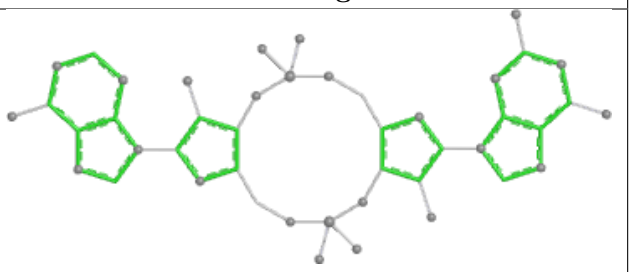
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	4BW	1	0
2	J	101	4BW	2	0
2	P	101	4BW	2	0
2	N	101	4BW	2	0

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 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 4BW S 4201



Ligand 4BW O 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

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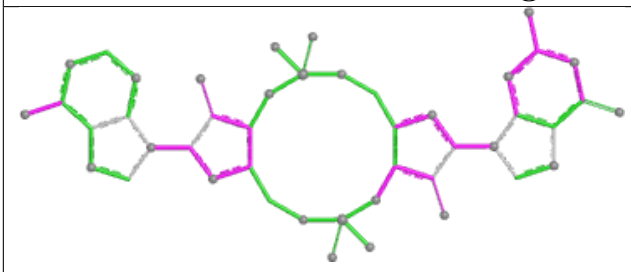
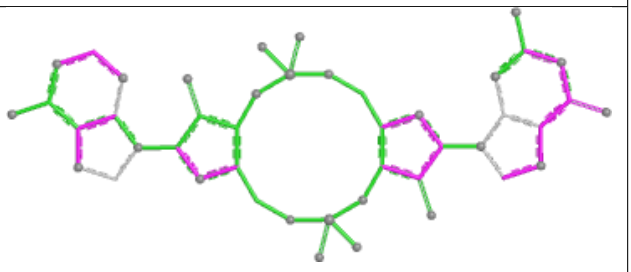
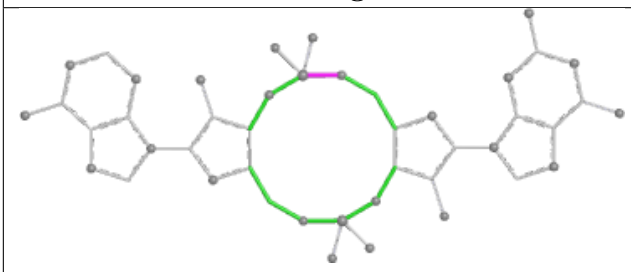
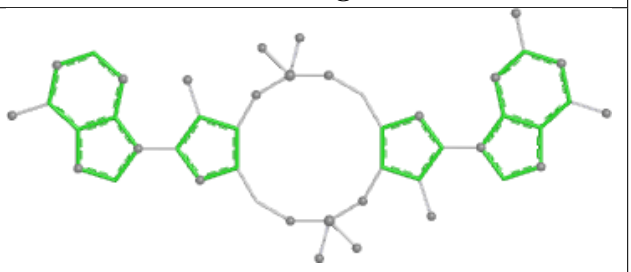
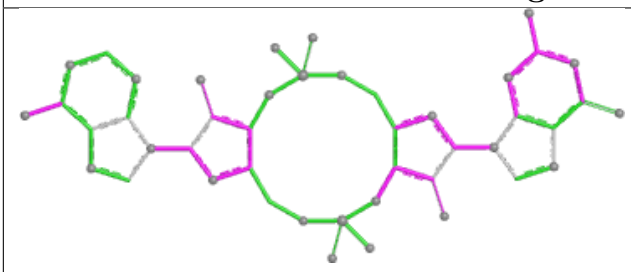
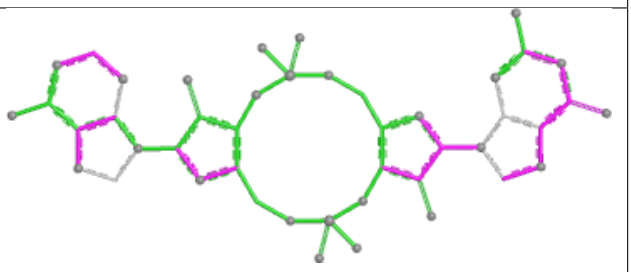
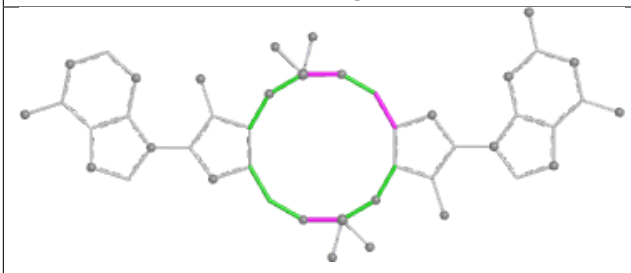
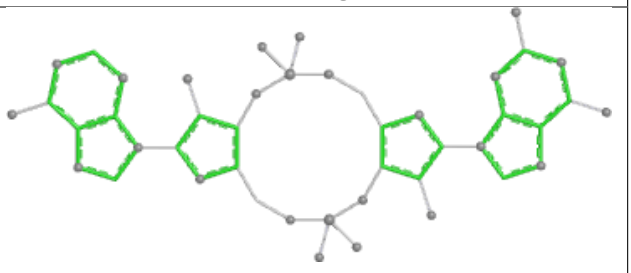
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 4BW I 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

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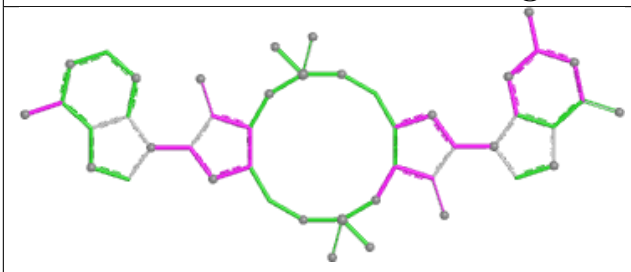
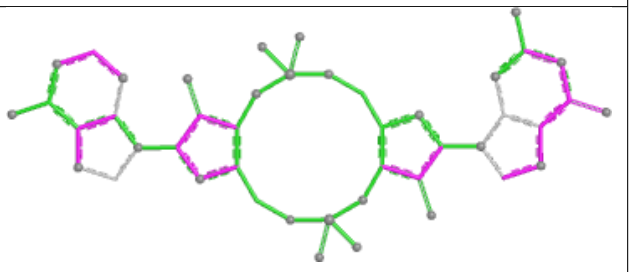
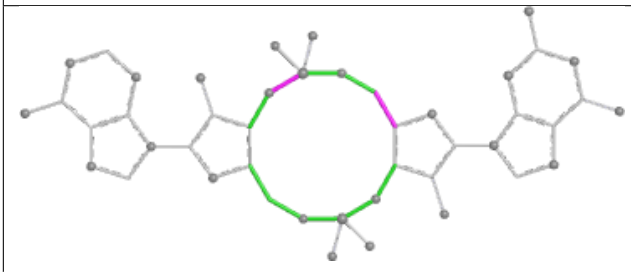
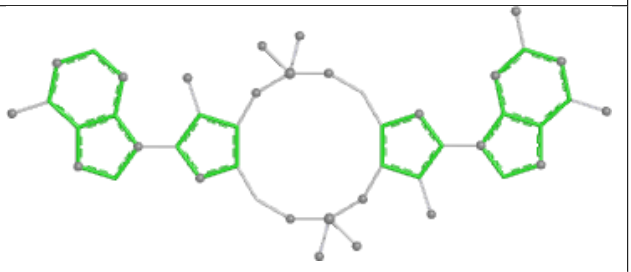
 Bond lengths	 Bond angles
 Torsions	 Rings

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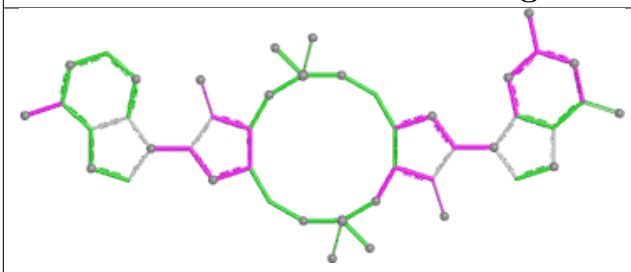
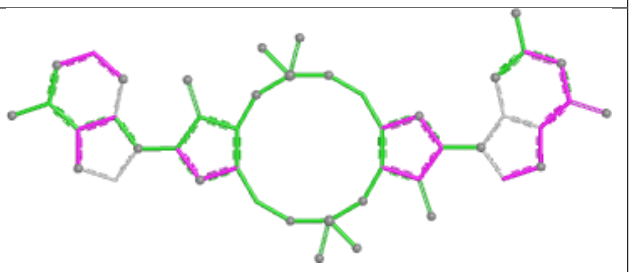
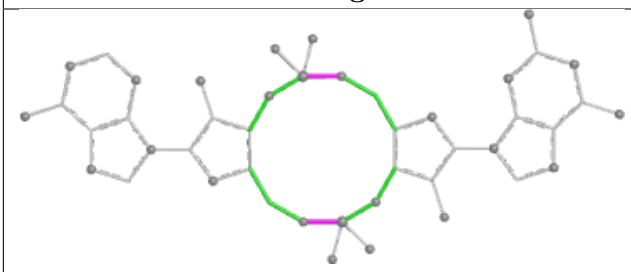
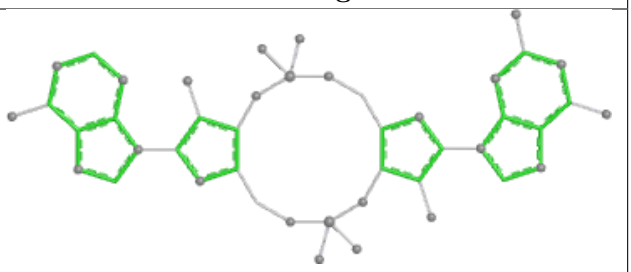
 Bond lengths	 Bond angles
 Torsions	 Rings

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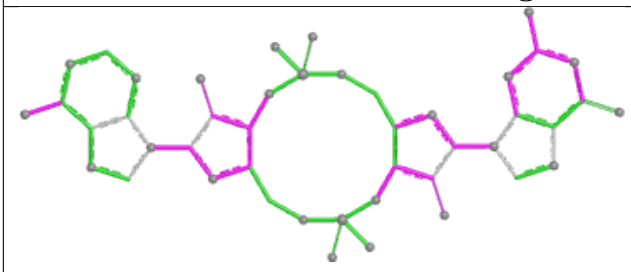
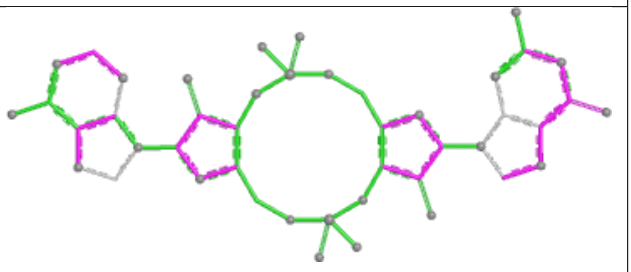
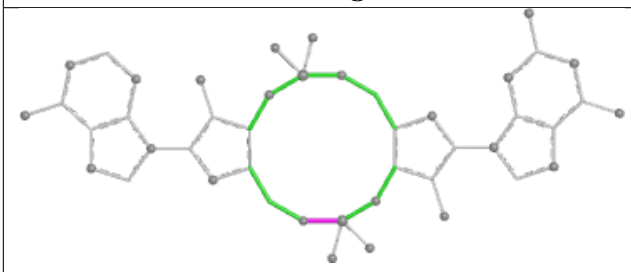
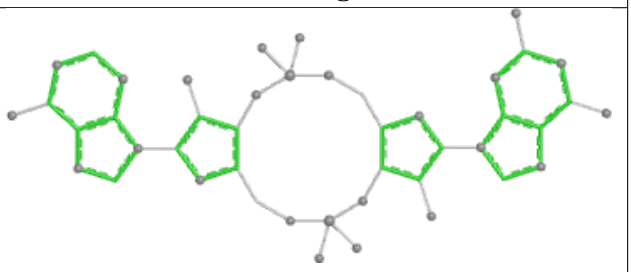
 Bond lengths	 Bond angles
 Torsions	 Rings

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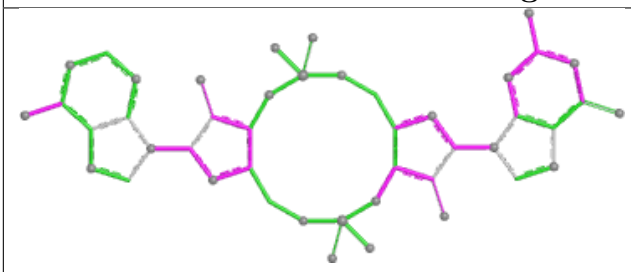
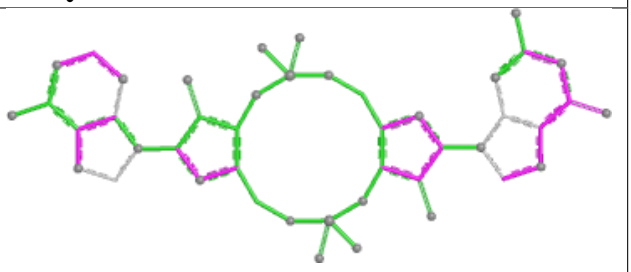
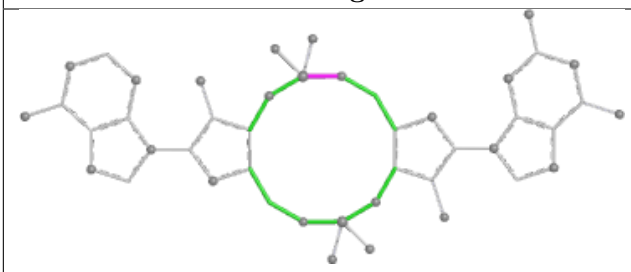
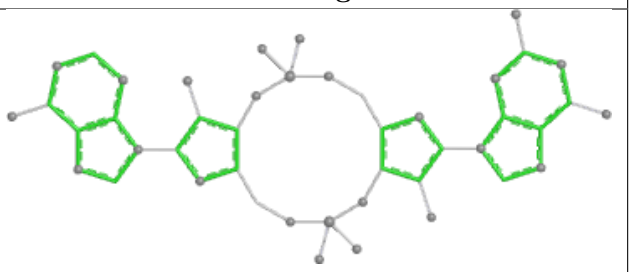
 Bond lengths	 Bond angles
 Torsions	 Rings

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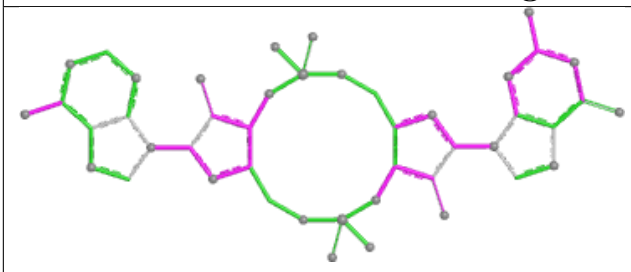
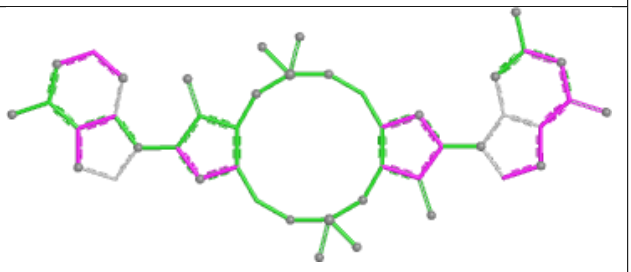
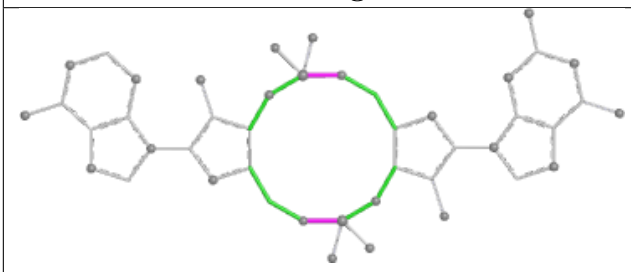
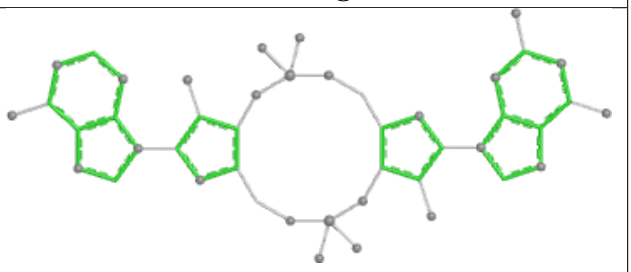
 Bond lengths	 Bond angles
 Torsions	 Rings

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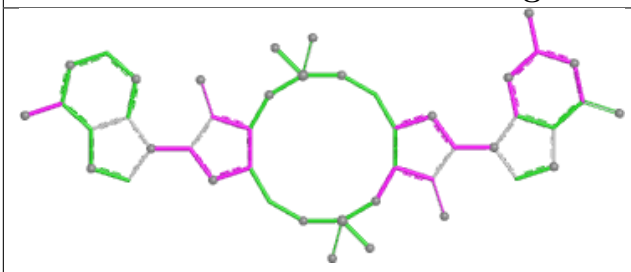
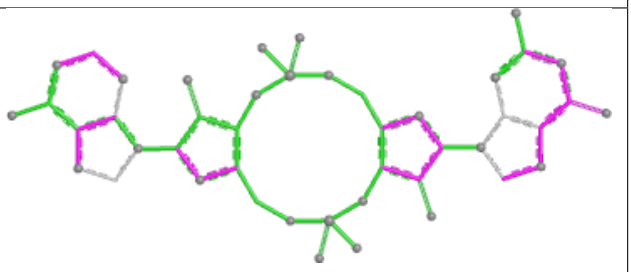
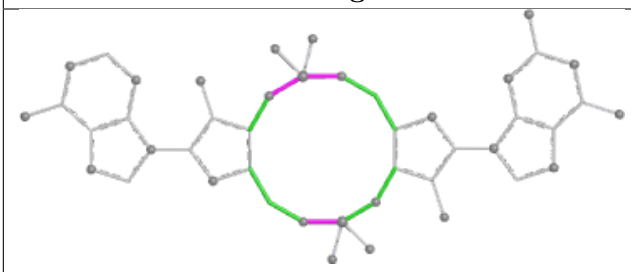
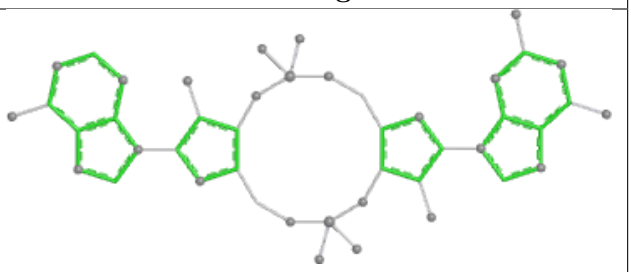
 Bond lengths	 Bond angles
 Torsions	 Rings

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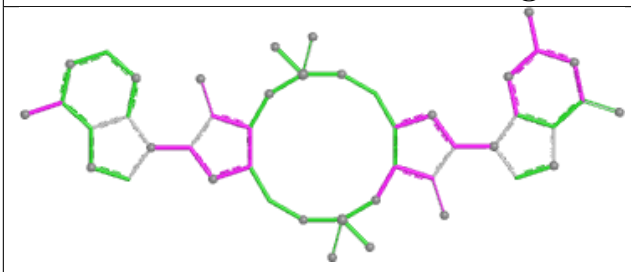
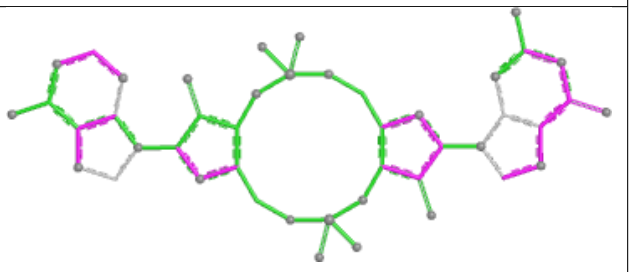
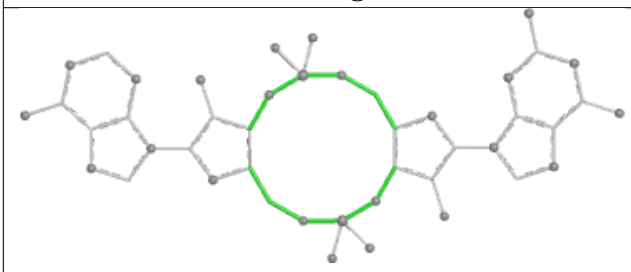
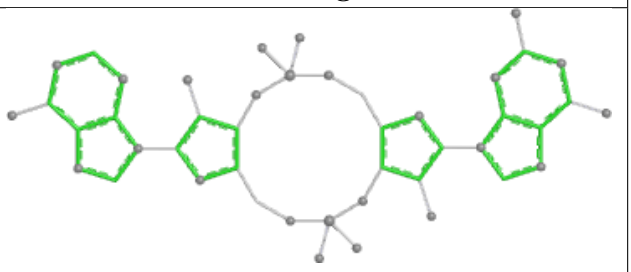
 Bond lengths	 Bond angles
 Torsions	 Rings

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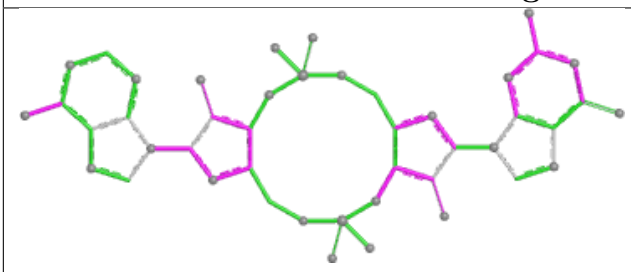
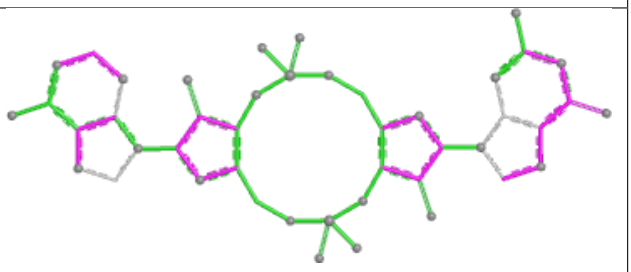
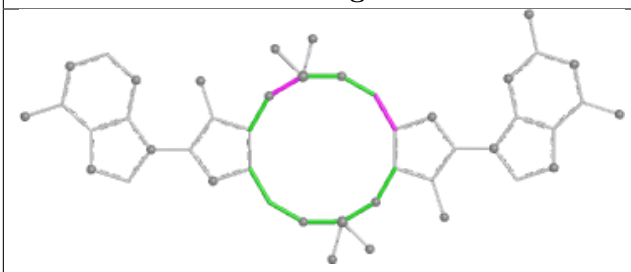
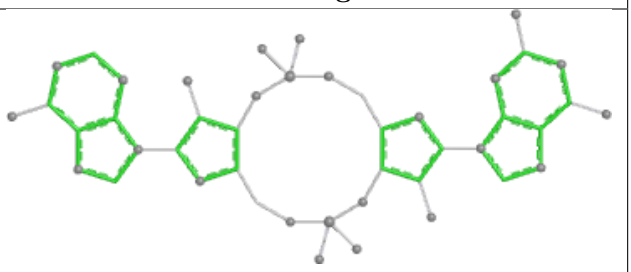
 Bond lengths	 Bond angles
 Torsions	 Rings

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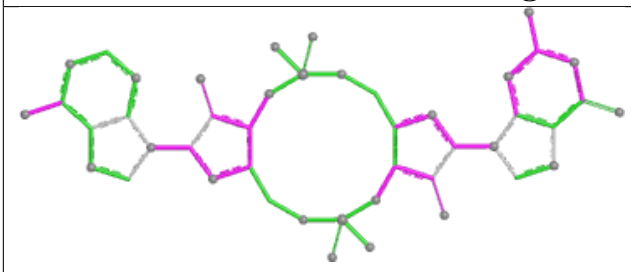
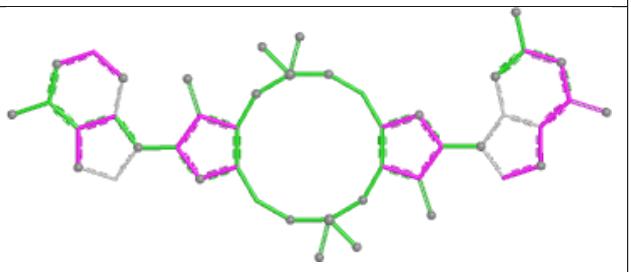
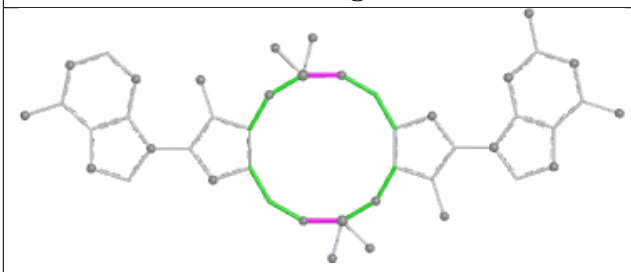
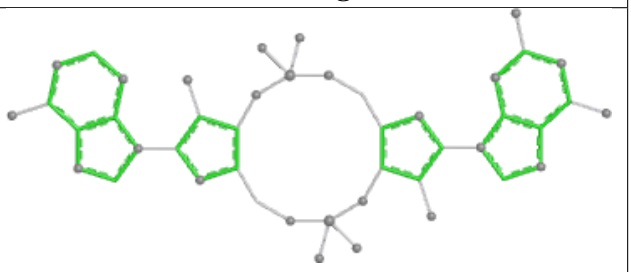
 Bond lengths	 Bond angles
 Torsions	 Rings

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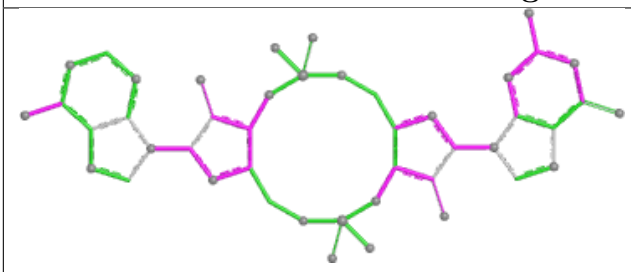
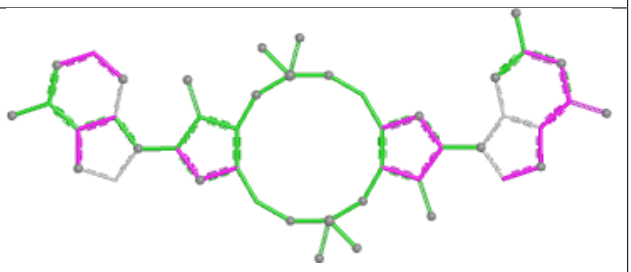
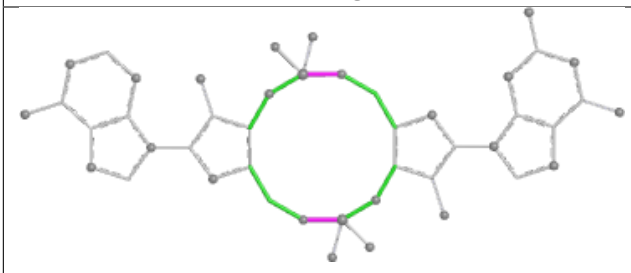
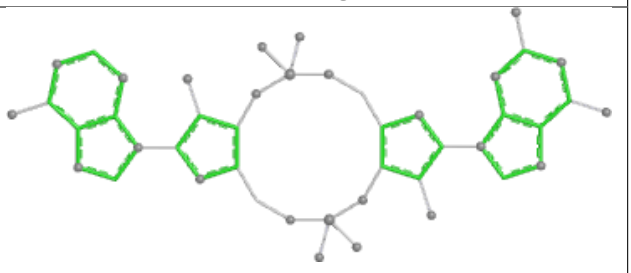
 Bond lengths	 Bond angles
 Torsions	 Rings

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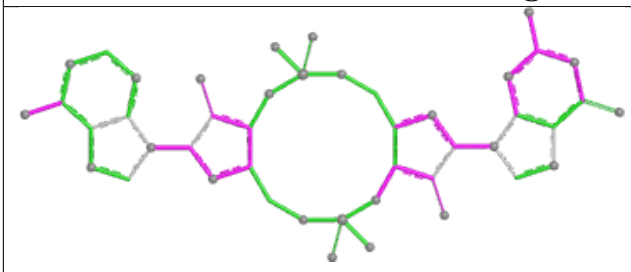
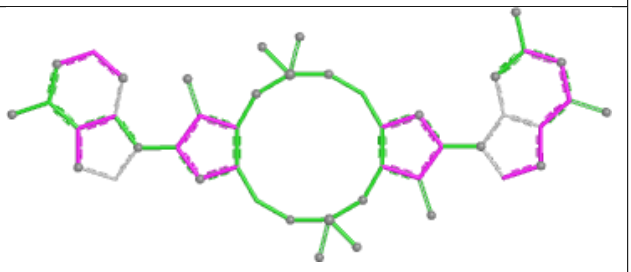
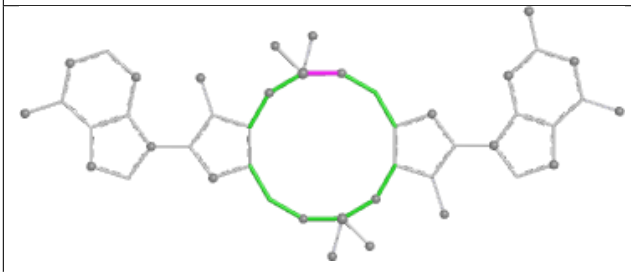
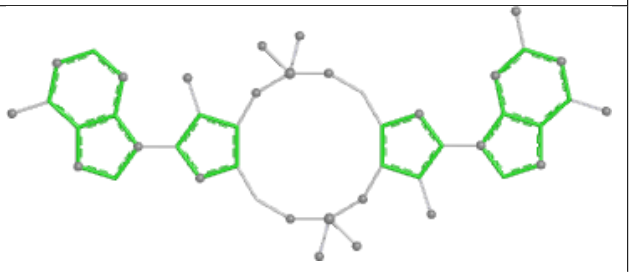
 Bond lengths	 Bond angles
 Torsions	 Rings

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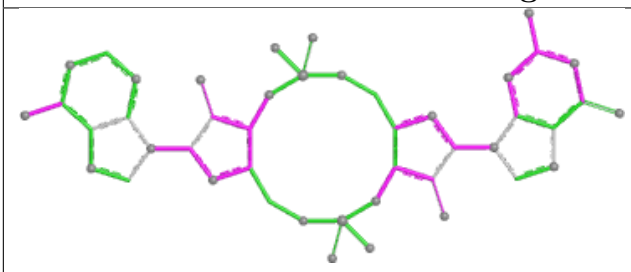
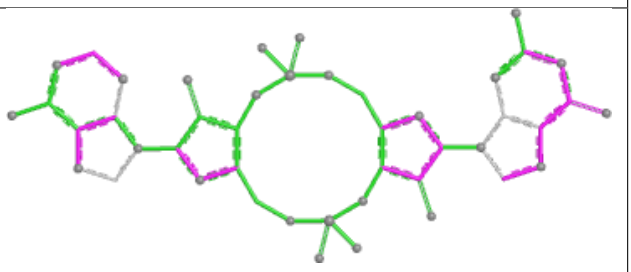
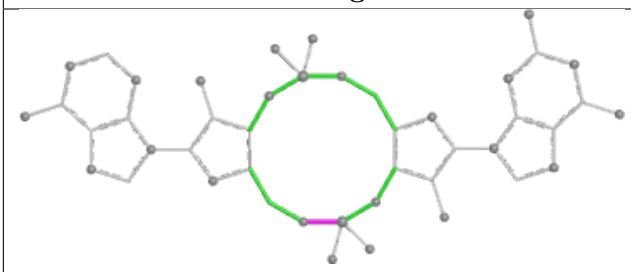
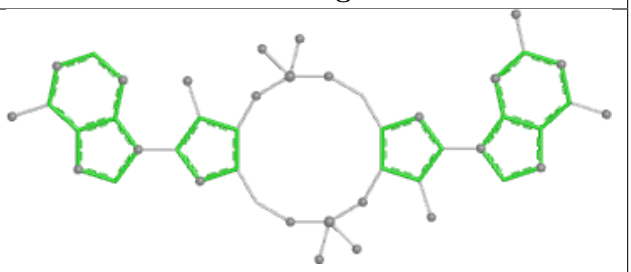
 Bond lengths	 Bond angles
 Torsions	 Rings

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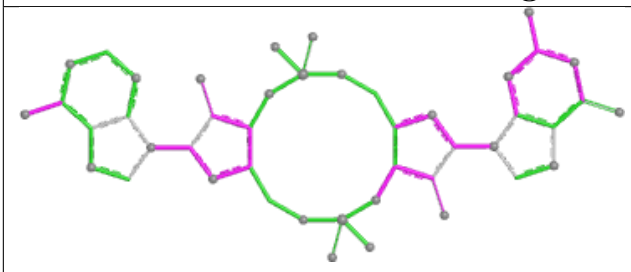
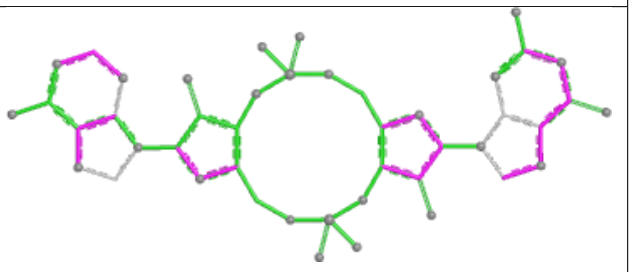
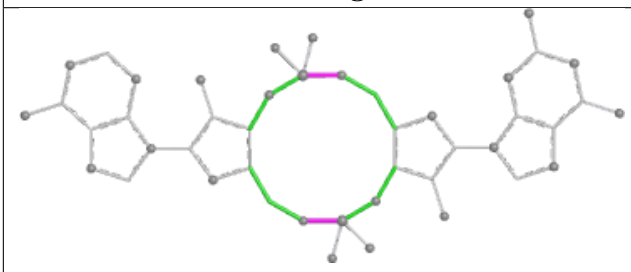
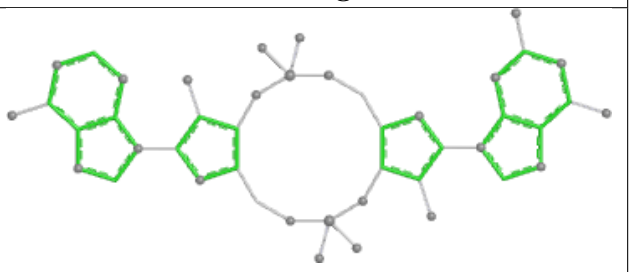
 Bond lengths	 Bond angles
 Torsions	 Rings

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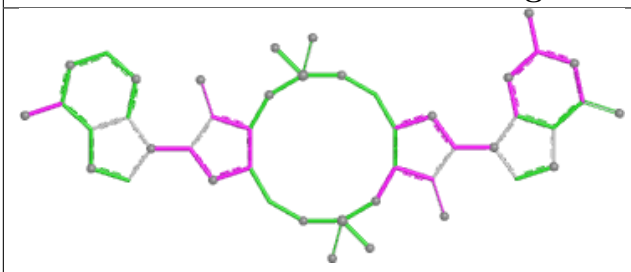
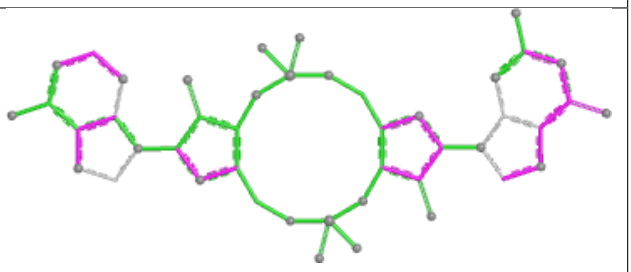
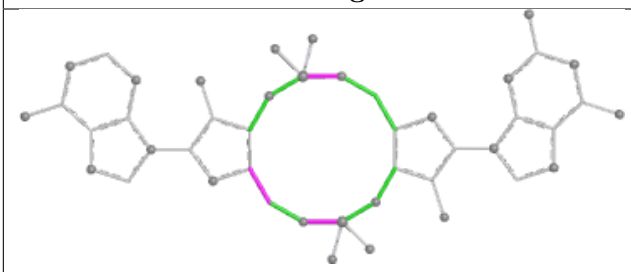
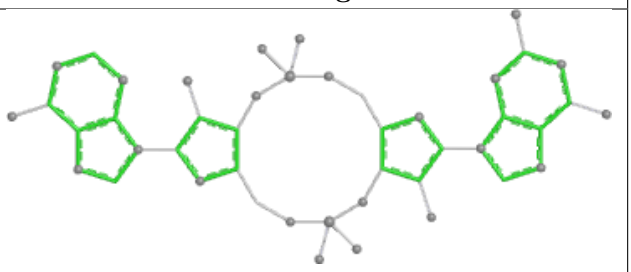
 Bond lengths	 Bond angles
 Torsions	 Rings

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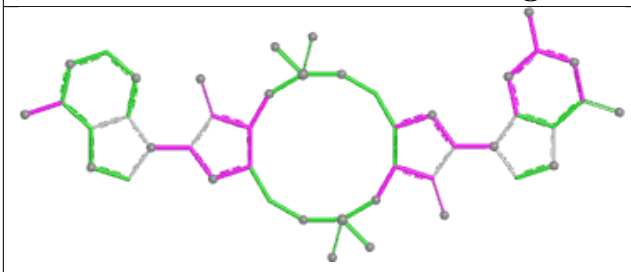
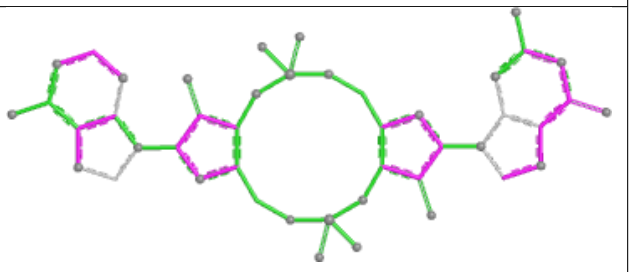
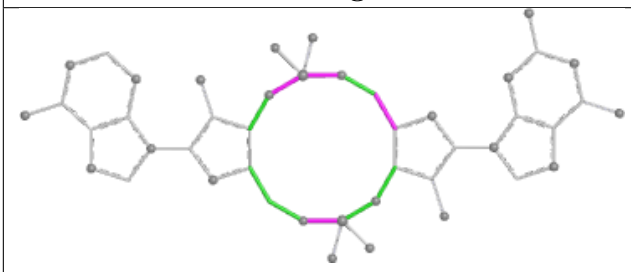
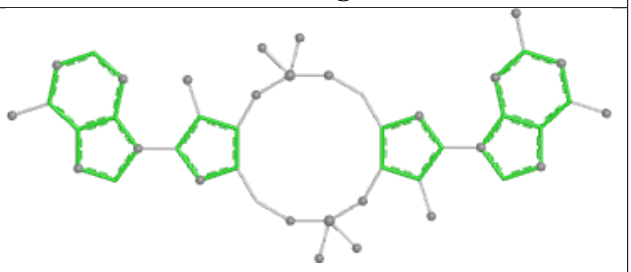
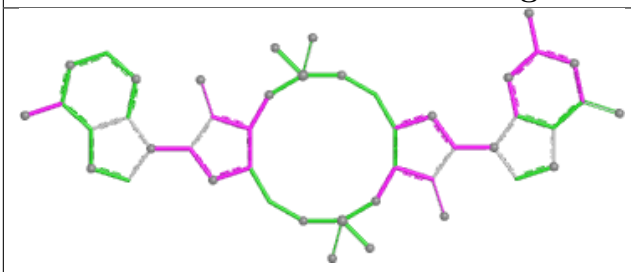
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 4BW N 101



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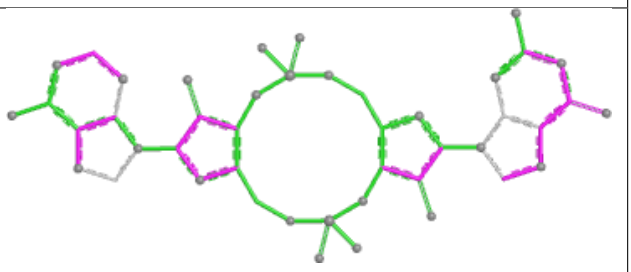

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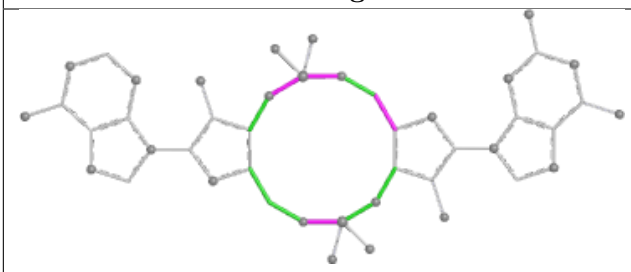

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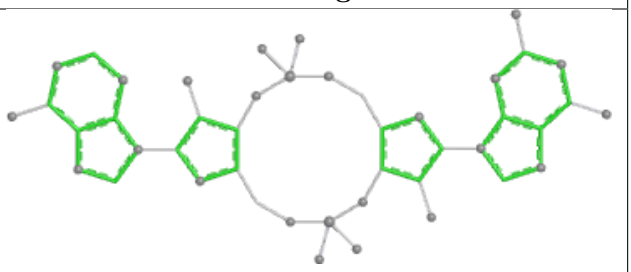

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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

All (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
1	P	33	VAL	4.8
1	D	96	ILE	4.7
1	M	21	TYR	4.6
1	L	3	ILE	4.5
1	N	5	ALA	4.3
1	O	44	ASP	4.2
1	O	41	VAL	4.2
1	O	5	ALA	4.1
1	N	21	TYR	3.9
1	N	65	GLU	3.9
1	O	28	ALA	3.8
1	L	87	GLY	3.8
1	O	42	VAL	3.7
1	O	10	CYS	3.7
1	G	1	MET	3.6
1	E	3	ILE	3.6
1	O	20	VAL	3.6
1	P	39	VAL	3.6
1	O	24	LEU	3.5
1	O	54	SER	3.5
1	P	30	PHE	3.5
1	M	24	LEU	3.4
1	O	22	GLU	3.4
1	O	67	GLY	3.3
1	O	30	PHE	3.3
1	O	59	VAL	3.2
1	O	51	ILE	3.1
1	L	2	LYS	3.1
1	N	90	SER	3.1
1	Q	15	LYS	3.0
1	O	90	SER	3.0
1	O	43	THR	3.0
1	P	87	GLY	2.9
1	O	11	LEU	2.9
1	M	91	ASP	2.9
1	O	71	ALA	2.9
1	M	89	LEU	2.9
1	N	89	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	12	ARG	2.9
1	M	16	LEU	2.8
1	N	41	VAL	2.8
1	O	55	SER	2.8
1	O	68	ARG	2.8
1	N	73	SER	2.8
1	M	61	ASN	2.8
1	N	46	ASN	2.8
1	T	15	LYS	2.7
1	M	85	TYR	2.7
1	P	42	VAL	2.7
1	O	40	CYS	2.7
1	S	15	LYS	2.7
1	O	7	ASN	2.7
1	Q	92	VAL	2.7
1	M	51	ILE	2.7
1	P	88	GLU	2.7
1	O	72	LEU	2.6
1	M	50	VAL	2.6
1	K	8	PHE	2.6
1	M	10	CYS	2.6
1	P	45	HIS	2.6
1	M	84	ALA	2.6
1	P	80	ILE	2.6
1	M	25	VAL	2.5
1	M	8	PHE	2.5
1	N	8	PHE	2.5
1	N	22	GLU	2.5
1	O	89	LEU	2.5
1	K	2	LYS	2.5
1	N	55	SER	2.5
1	P	27	GLU	2.5
1	O	15	LYS	2.5
1	M	5	ALA	2.5
1	O	84	ALA	2.5
1	P	57	TYR	2.5
1	O	60	GLU	2.5
1	Q	45	HIS	2.5
1	G	15	LYS	2.5
1	O	76	LEU	2.5
1	M	65	GLU	2.4
1	O	45	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	O	27	GLU	2.4
1	O	56	VAL	2.4
1	N	57	TYR	2.4
1	N	62	PHE	2.4
1	N	87	GLY	2.4
1	S	43	THR	2.4
1	M	48	PHE	2.4
1	K	9	GLU	2.3
1	R	95	ASN	2.3
1	M	33	VAL	2.3
1	N	79	PHE	2.3
1	Q	3	ILE	2.3
1	O	35	PRO	2.3
1	M	22	GLU	2.3
1	O	9	GLU	2.3
1	O	39	VAL	2.3
1	N	85	TYR	2.3
1	M	11	LEU	2.3
1	O	53	THR	2.3
1	O	62	PHE	2.2
1	T	23	ASP	2.2
1	M	42	VAL	2.2
1	O	50	VAL	2.2
1	T	4	ASN	2.2
1	K	3	ILE	2.2
1	L	94	GLU	2.2
1	S	14	SER	2.2
1	P	40	CYS	2.2
1	Q	48	PHE	2.2
1	M	87	GLY	2.2
1	D	4	ASN	2.2
1	P	82	PHE	2.1
1	N	86	SER	2.1
1	Q	28	ALA	2.1
1	M	45	HIS	2.1
1	P	3	ILE	2.1
1	P	34	SER	2.1
1	E	45	HIS	2.1
1	P	35	PRO	2.1
1	O	88	GLU	2.1
1	T	59	VAL	2.1
1	K	15	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	90	SER	2.1
1	O	38	THR	2.1
1	O	87	GLY	2.1
1	O	23	ASP	2.1
1	O	64	ASP	2.1
1	N	72	LEU	2.1
1	O	16	LEU	2.1
1	O	29	THR	2.1
1	O	80	ILE	2.1
1	P	48	PHE	2.1
1	O	74	GLN	2.1
1	L	63	ASN	2.0
1	T	35	PRO	2.0
1	R	21	TYR	2.0
1	N	20	VAL	2.0
1	N	31	VAL	2.0
1	P	56	VAL	2.0
1	Q	24	LEU	2.0
1	G	3	ILE	2.0
1	S	3	ILE	2.0
1	R	22	GLU	2.0
1	M	28	ALA	2.0
1	S	91	ASP	2.0

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, 95^{th} 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.

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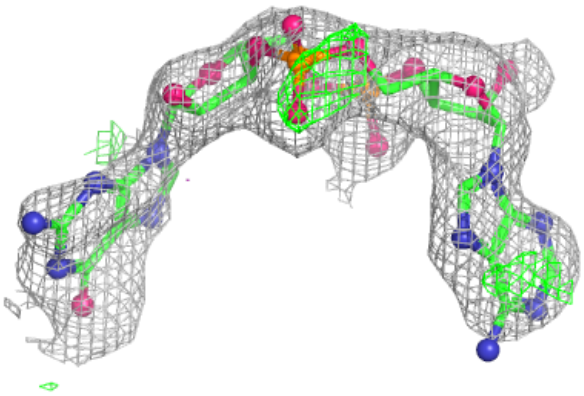
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

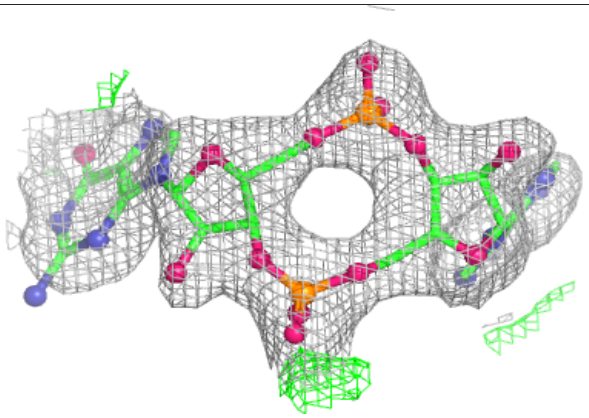
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	4BW	O	101	45/45	0.80	0.14	42,52,58,65	0
2	4BW	N	101	45/45	0.85	0.13	40,48,53,61	0
2	4BW	P	101	45/45	0.88	0.12	35,42,47,49	0
2	4BW	T	101	45/45	0.90	0.12	31,41,47,51	0
2	4BW	Q	101	45/45	0.91	0.09	19,28,31,38	0
2	4BW	M	101	45/45	0.92	0.09	30,34,40,41	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
2	4BW	B	201	45/45	0.96	0.06	9,15,18,18	0

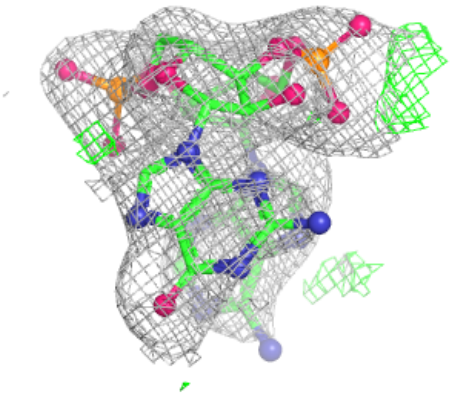
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

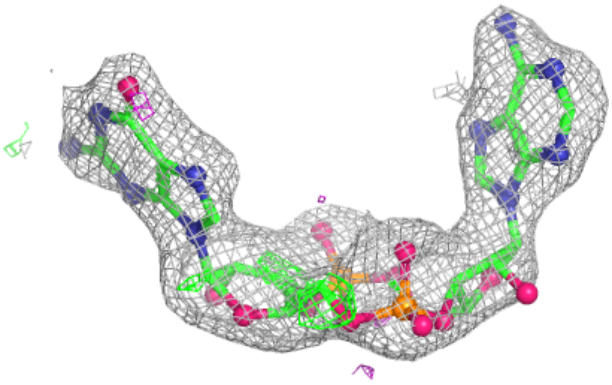


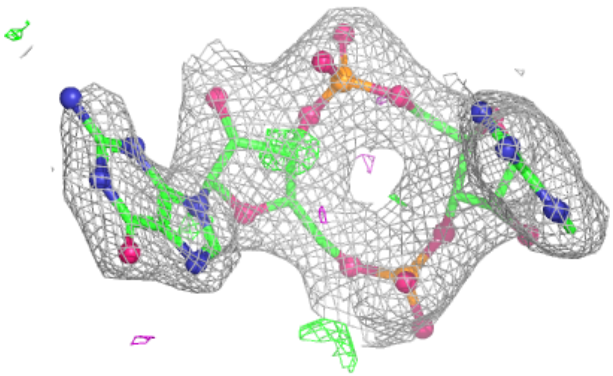


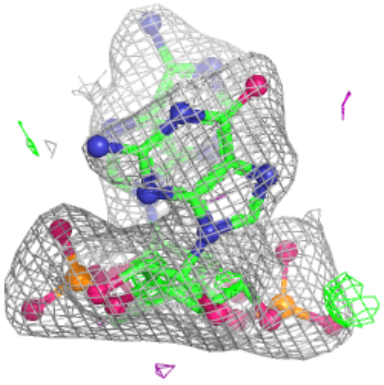


Electron density around 4BW N 101:

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

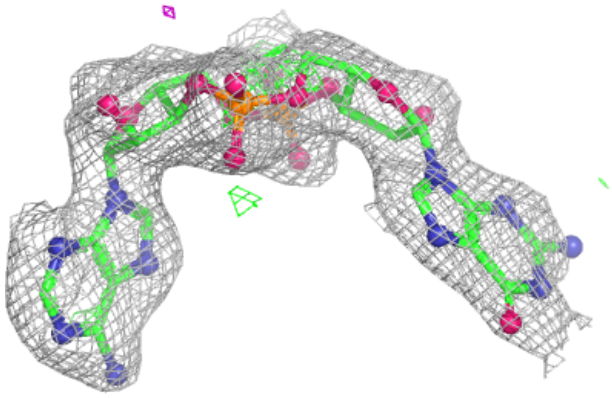


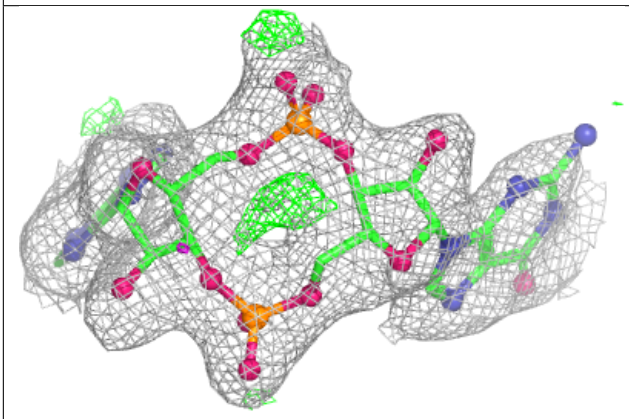


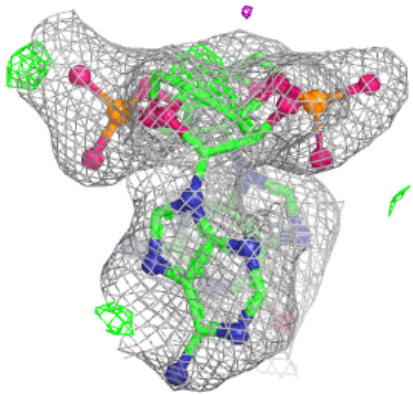


Electron density around 4BW P 101:

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

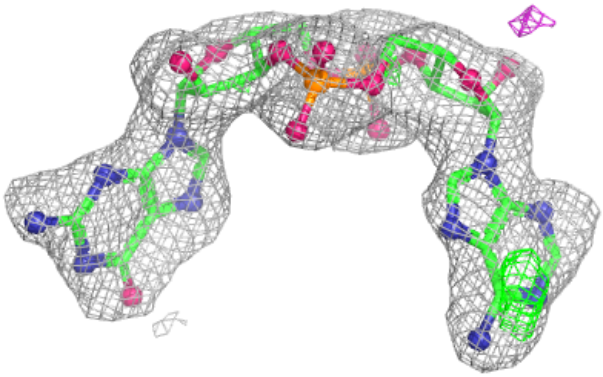


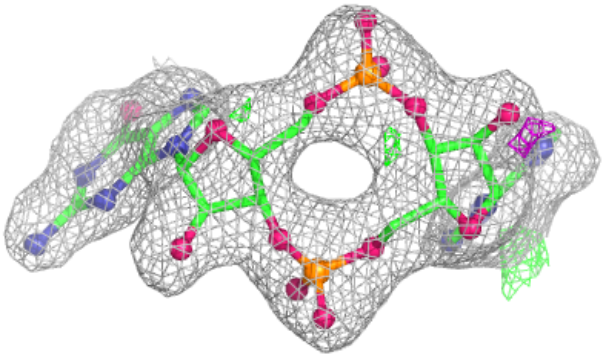


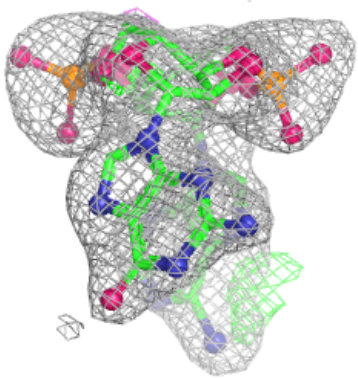


Electron density around 4BW T 101:

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

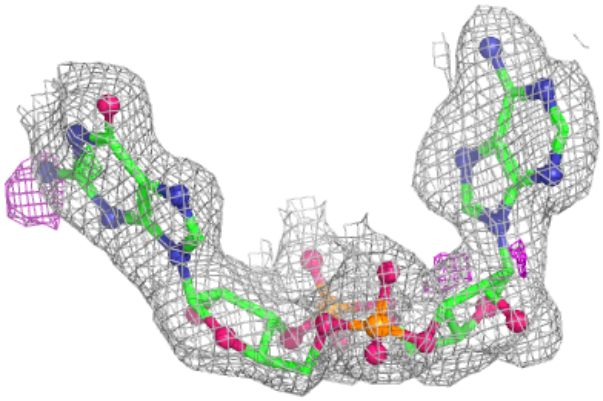


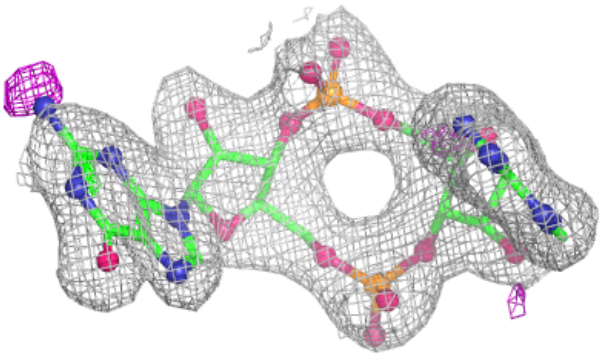


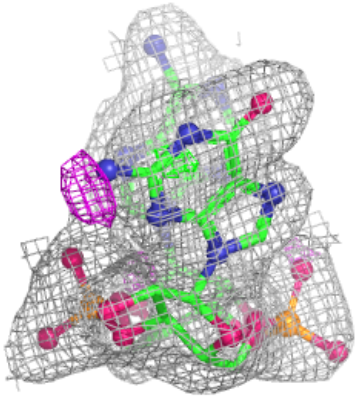


Electron density around 4BW Q 101:

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

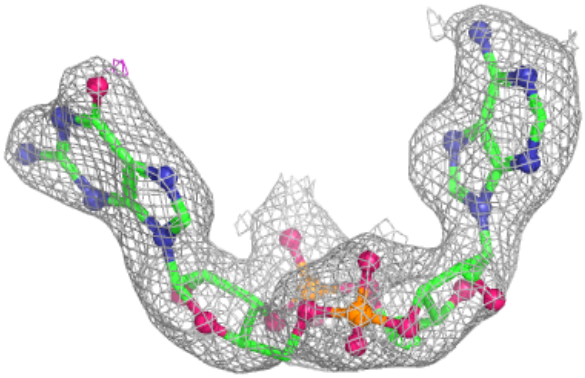


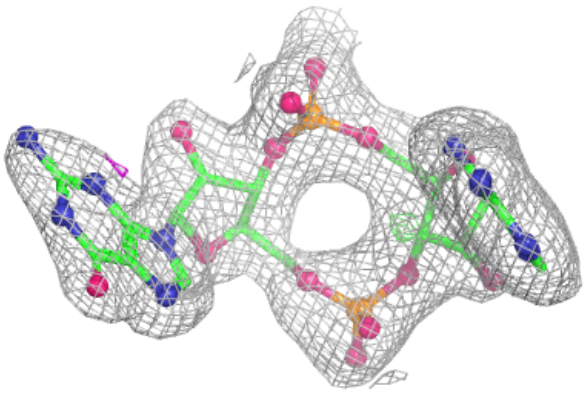


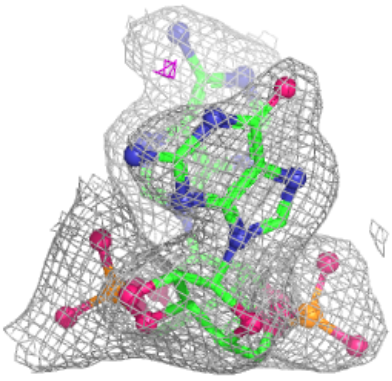


Electron density around 4BW M 101:

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

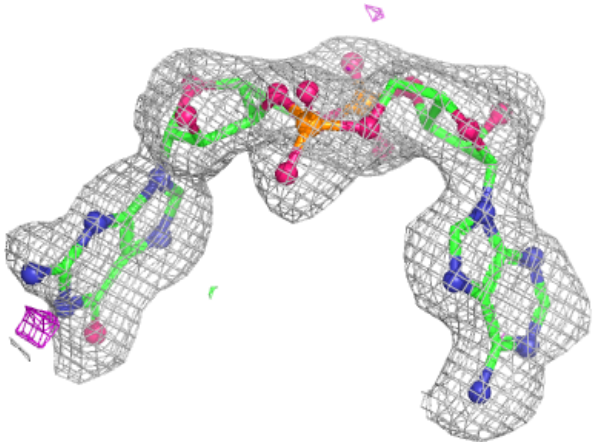


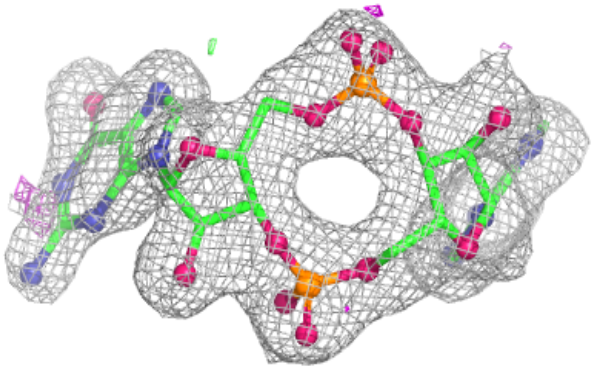


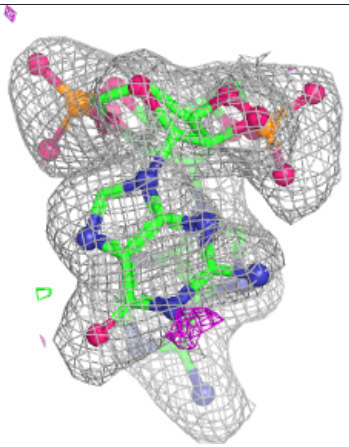


Electron density around 4BW I 101:

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

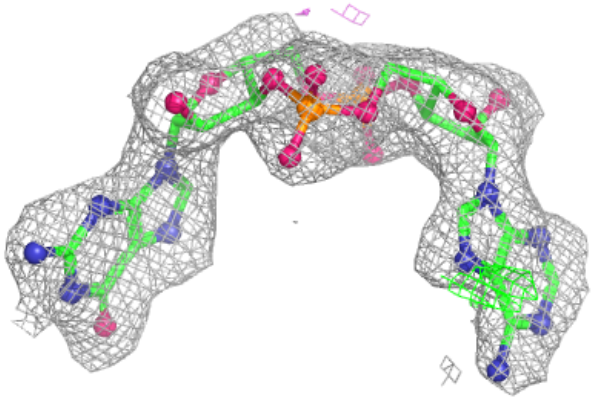


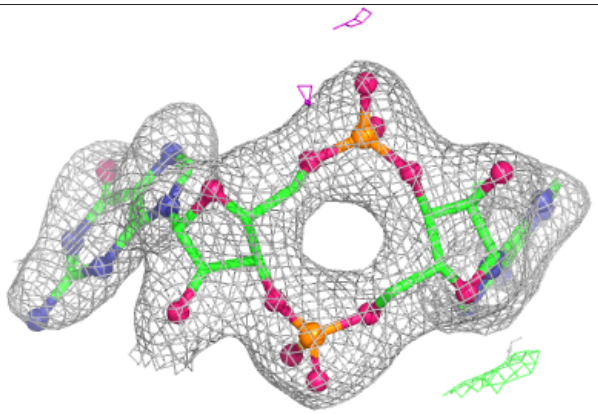


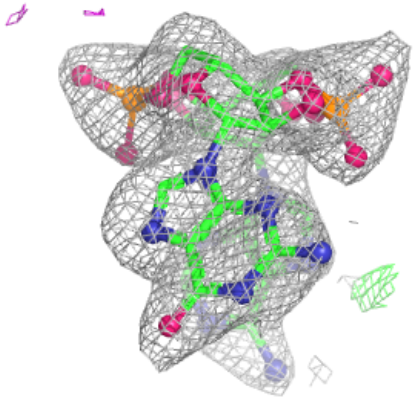


Electron density around 4BW R 101:

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

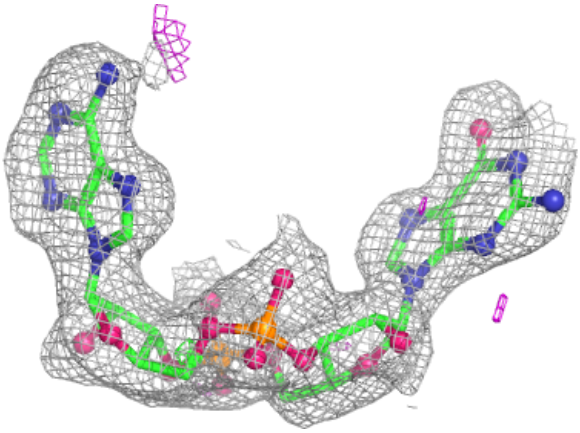


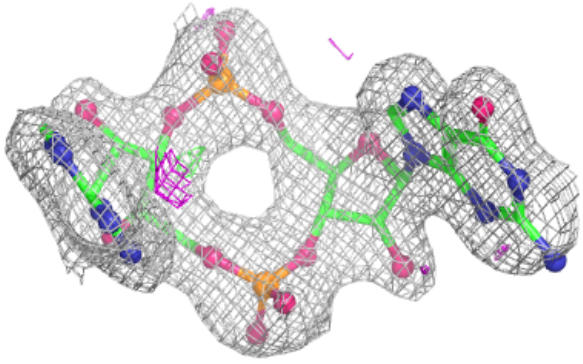


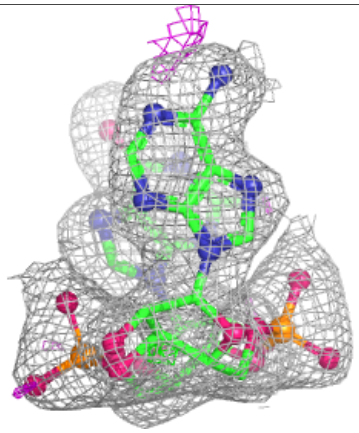


Electron density around 4BW S 4201:

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

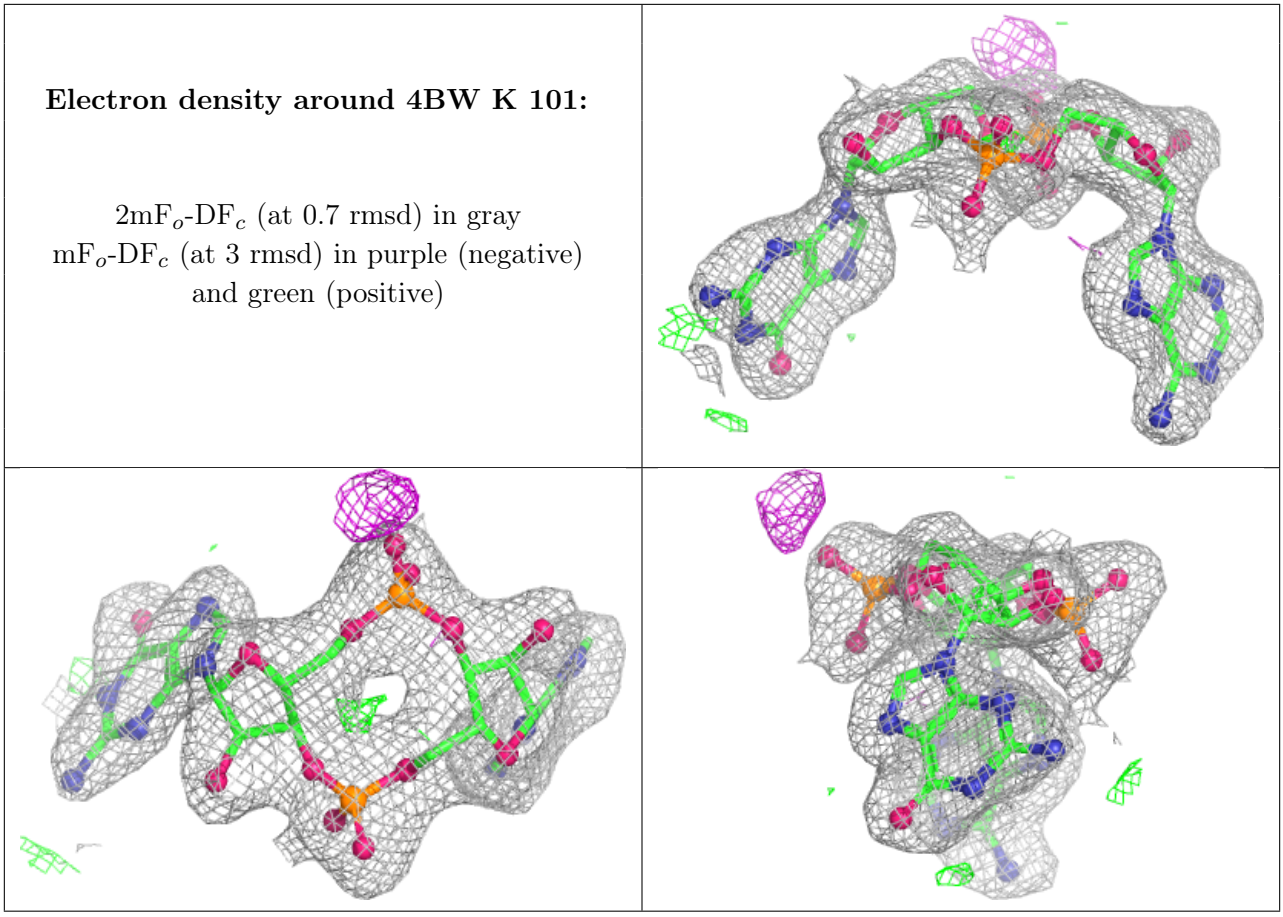






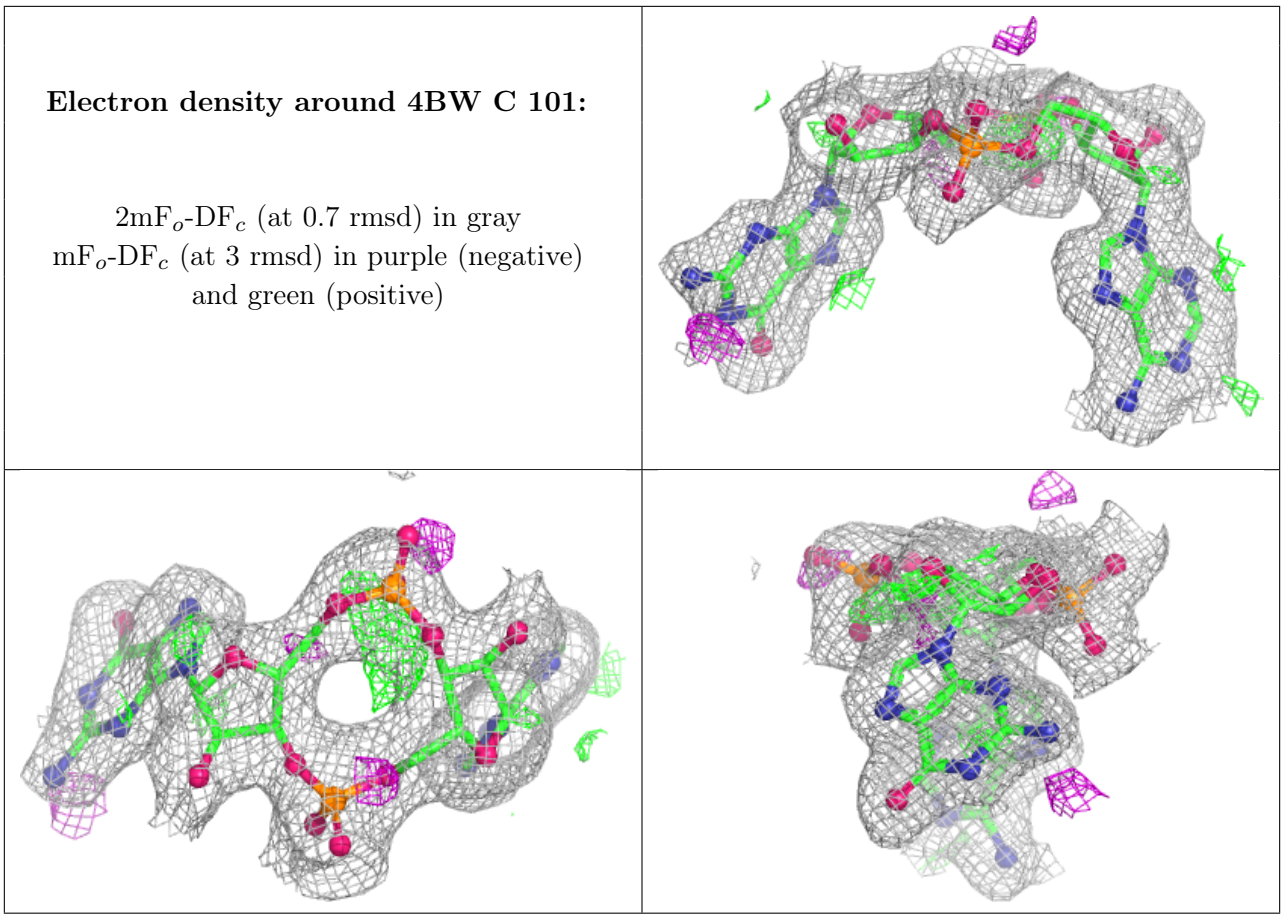
Electron density around 4BW K 101:

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



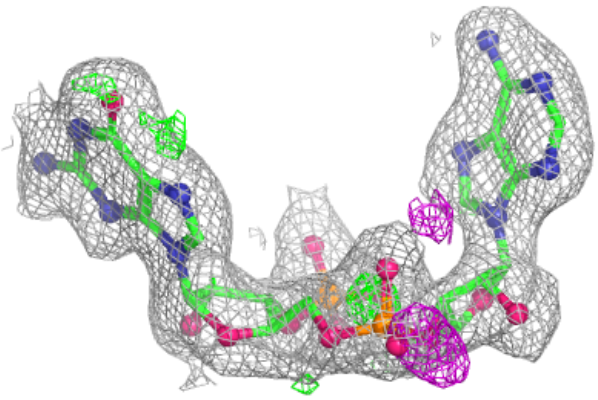
Electron density around 4BW C 101:

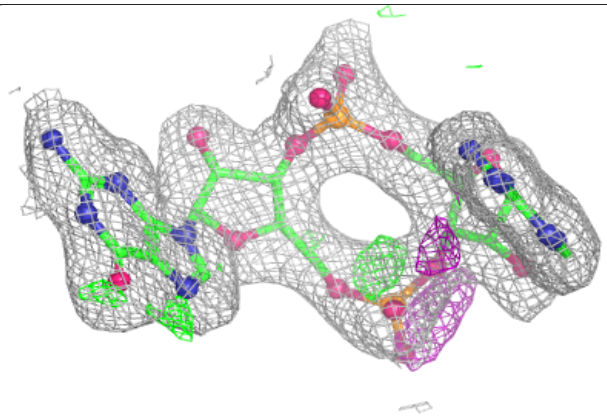
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

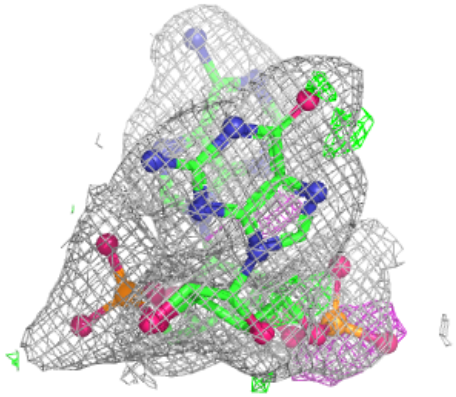


Electron density around 4BW E 101:

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

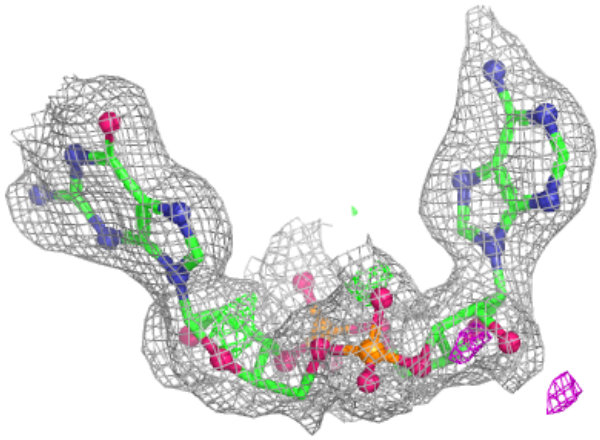


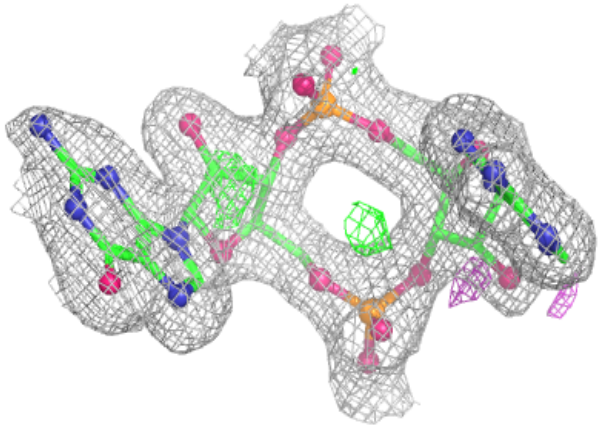


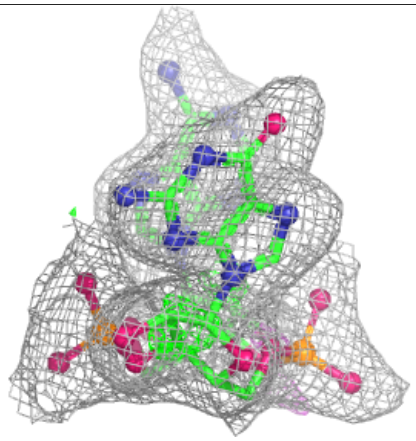


Electron density around 4BW D 301:

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

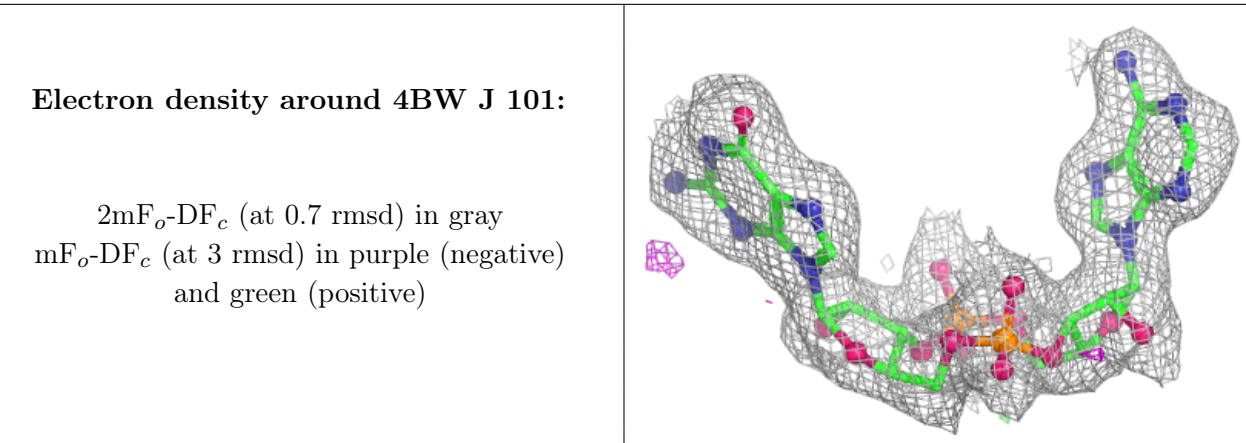






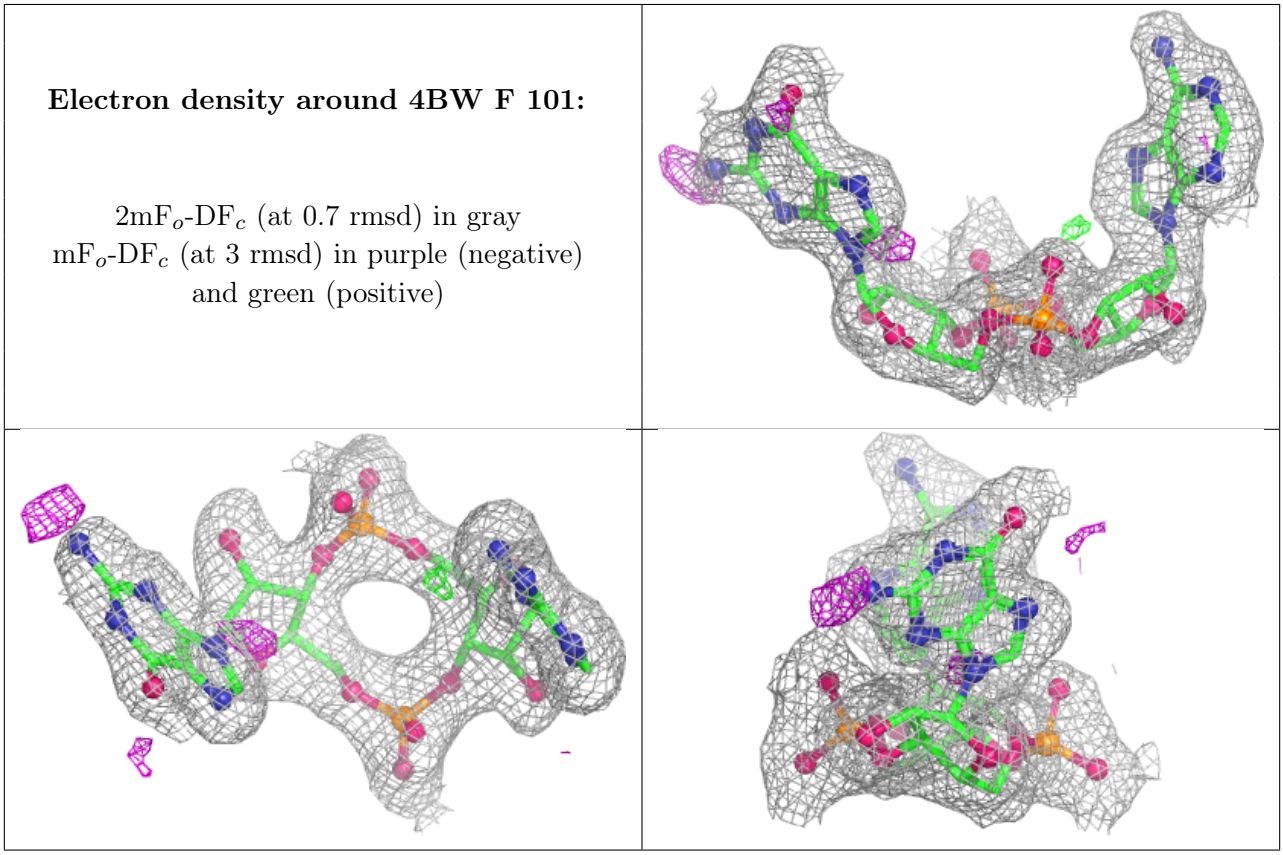
Electron density around 4BW J 101:

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



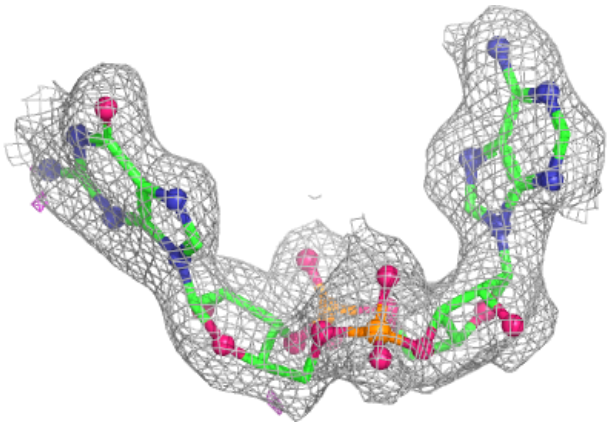
Electron density around 4BW F 101:

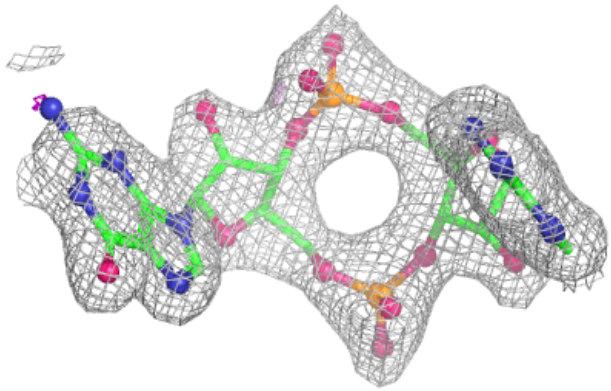
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

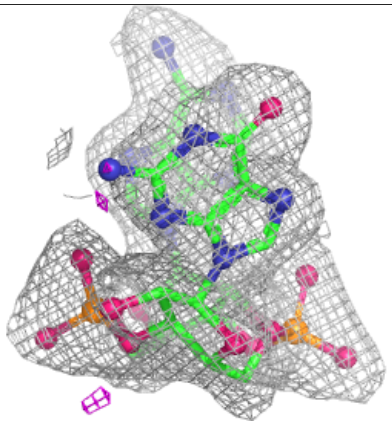


Electron density around 4BW L 101:

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

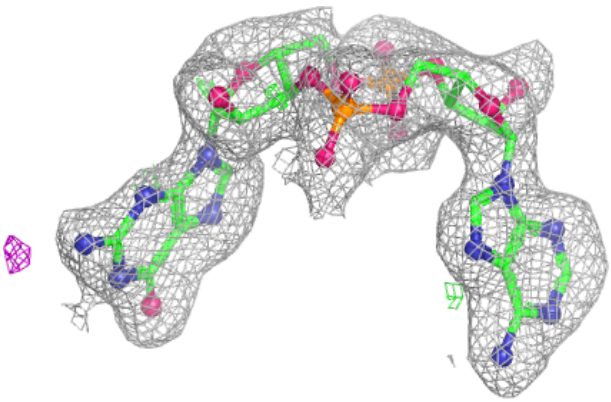


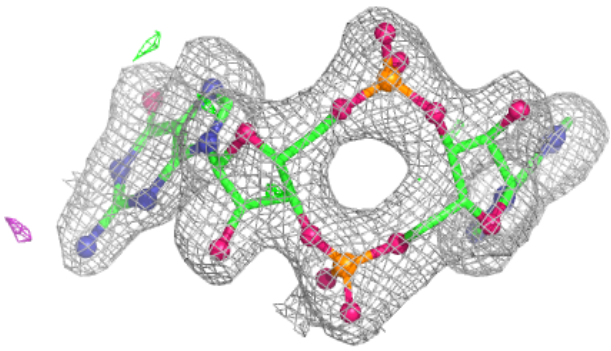


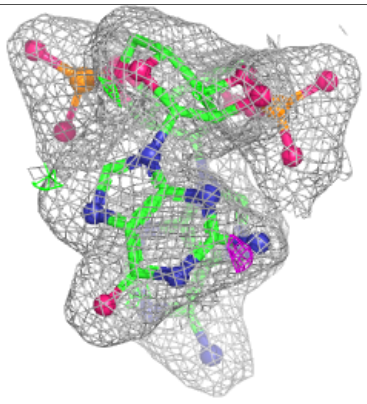


Electron density around 4BW G 101:

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

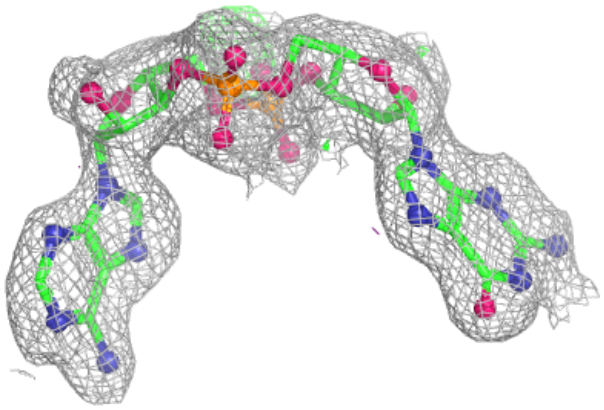


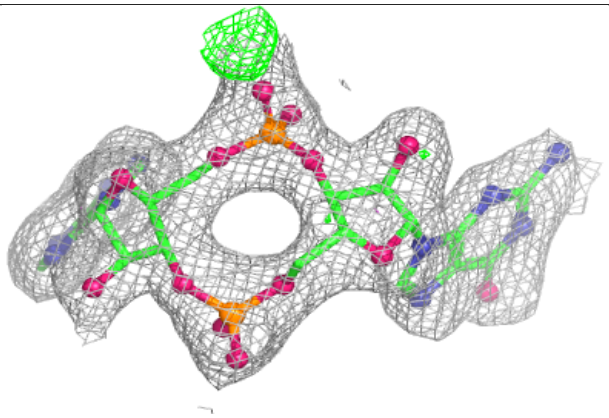


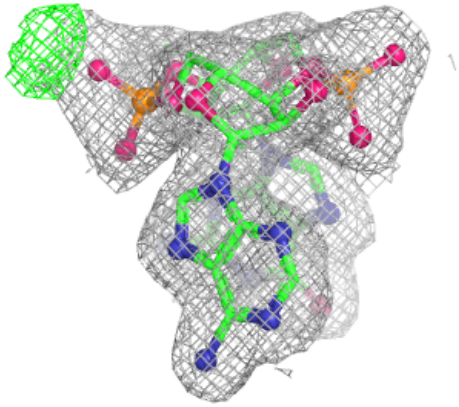


Electron density around 4BW H 101:

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

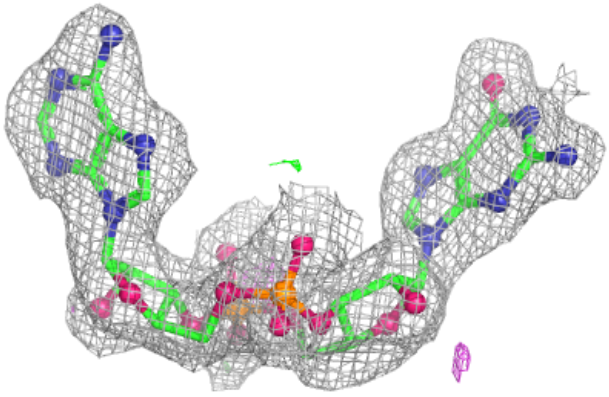


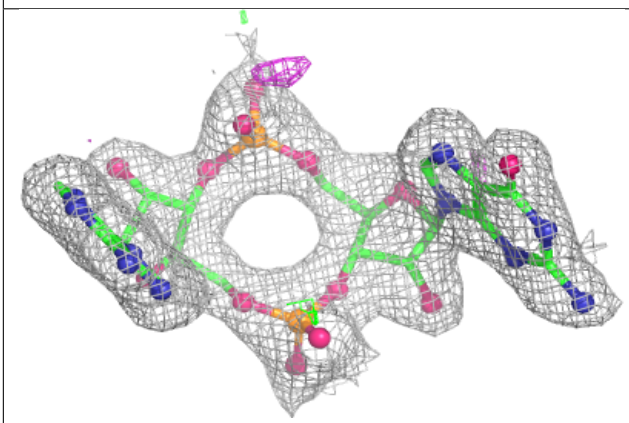


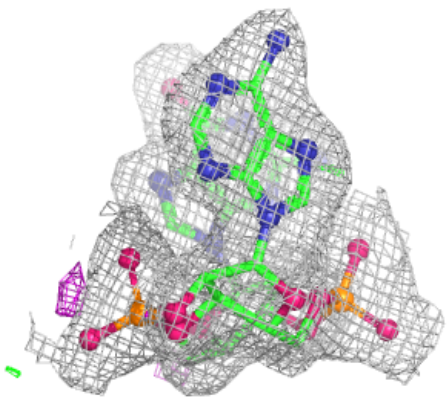


Electron density around 4BW A 201:

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

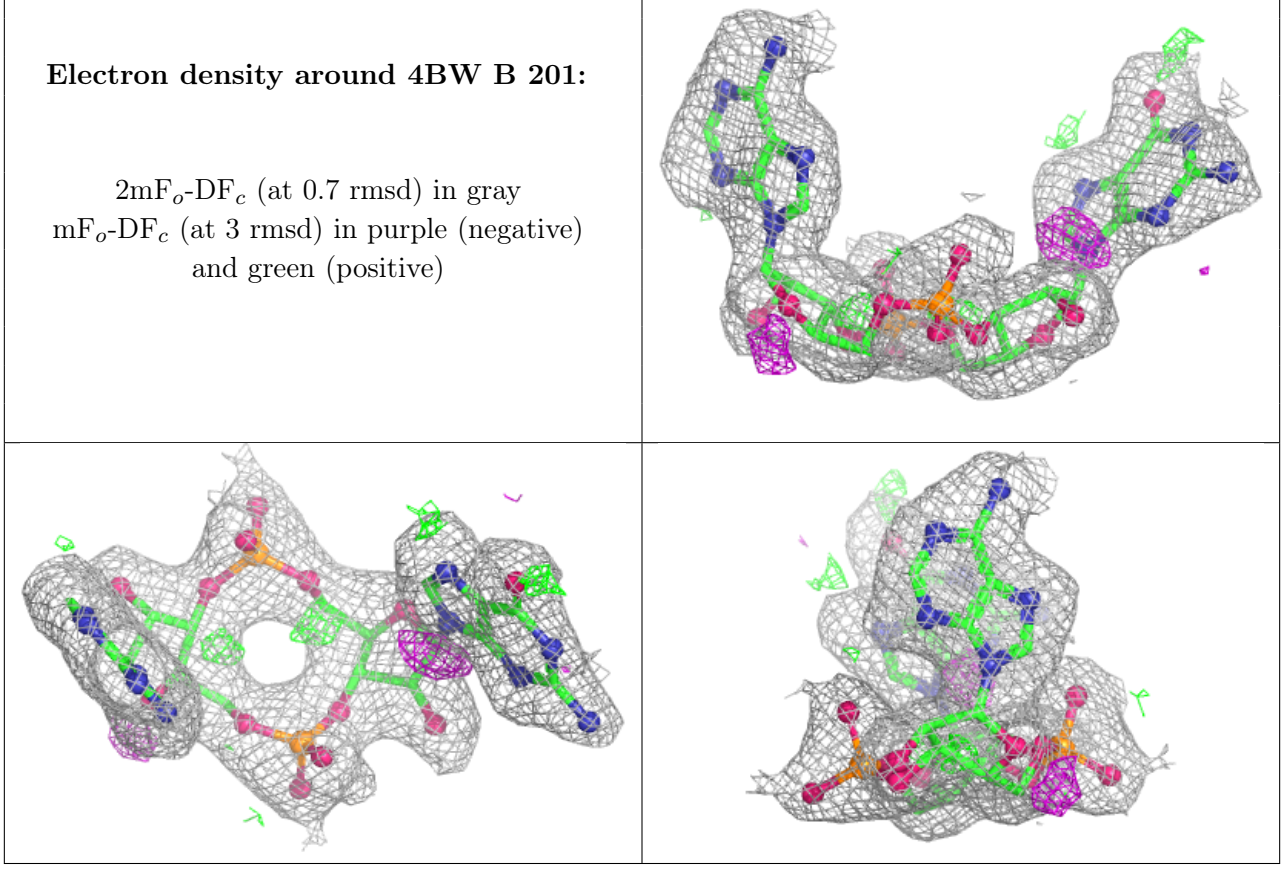






Electron density around 4BW B 201:

$2mF_o$-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.