Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 11:59 am BST

PDB ID	:	6ARJ
Title	:	Crystal structure of CARM1 with EPZ022302 and SAH
Authors	:	Boriack-Sjodin, P.A.; Jin, L.
Deposited on	:	2017-08-22
Resolution	:	1.92 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 following versions of software and data (see references ⓘ) were used in the production of this report:

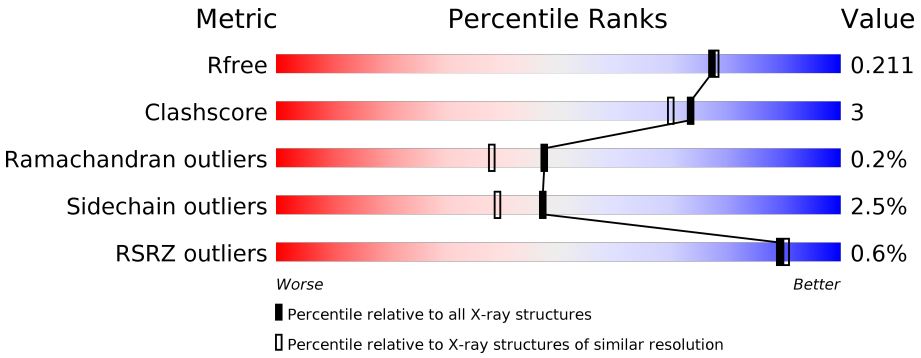
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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}	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 on 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	349	92% 7%
1	B	349	85% 13%
1	C	349	90% 8%
1	D	349	91% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12491 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.

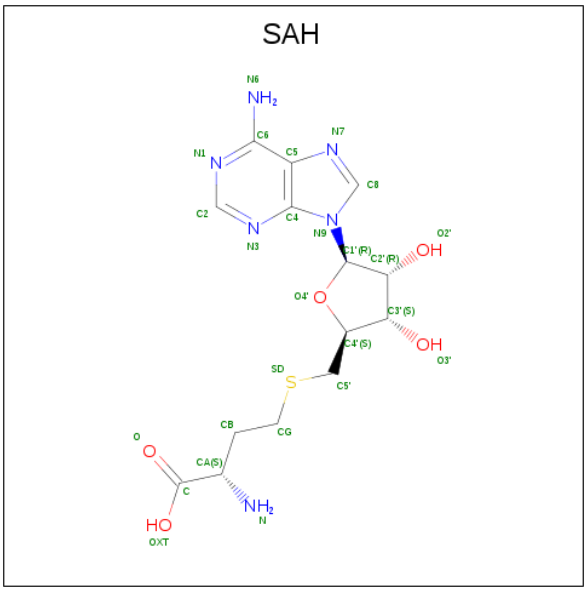
- Molecule 1 is a protein called Histone-arginine methyltransferase CARM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	8	0
			2819	1816	468	519	16			
1	B	344	Total	C	N	O	S	0	7	0
			2812	1811	468	517	16			
1	C	344	Total	C	N	O	S	0	2	0
			2778	1791	461	511	15			
1	D	343	Total	C	N	O	S	0	2	0
			2765	1784	456	510	15			

There are 12 discrepancies between the modelled and reference sequences:

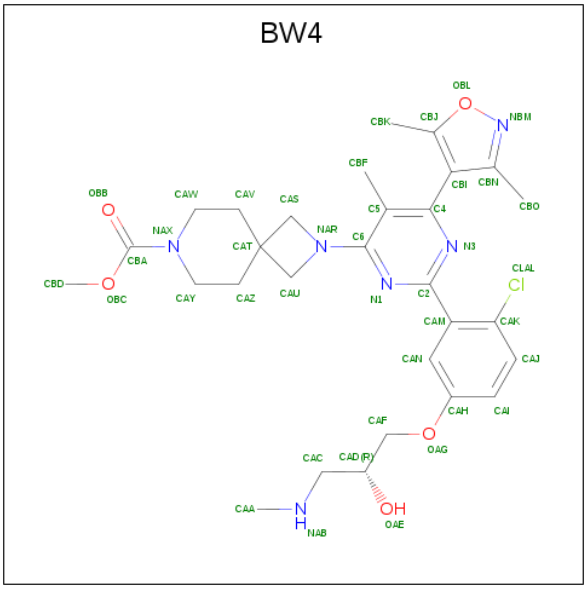
Chain	Residue	Modelled	Actual	Comment	Reference
A	131	SER	-	expression tag	UNP Q86X55
A	132	ILE	-	expression tag	UNP Q86X55
A	133	ALA	-	expression tag	UNP Q86X55
B	131	SER	-	expression tag	UNP Q86X55
B	132	ILE	-	expression tag	UNP Q86X55
B	133	ALA	-	expression tag	UNP Q86X55
C	131	SER	-	expression tag	UNP Q86X55
C	132	ILE	-	expression tag	UNP Q86X55
C	133	ALA	-	expression tag	UNP Q86X55
D	131	SER	-	expression tag	UNP Q86X55
D	132	ILE	-	expression tag	UNP Q86X55
D	133	ALA	-	expression tag	UNP Q86X55

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



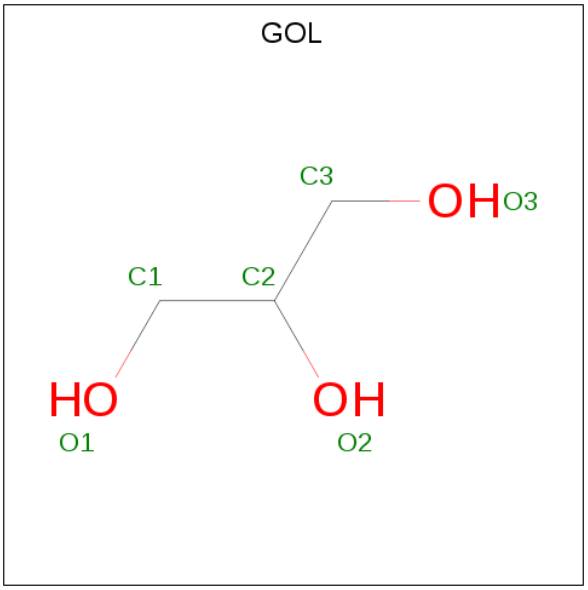
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is methyl 2-[2-{2-chloro-5-[(2R)-2-hydroxy-3-(methylamino)propoxy]phenyl}-6-(3,5-dimethyl-1,2-oxazol-4-yl)-5-methylpyrimidin-4-yl]-2,7-diazaspiro[3.5]nonane-7-carboxylate (three-letter code: BW4) (formula: $C_{29}H_{37}ClN_6O_5$).



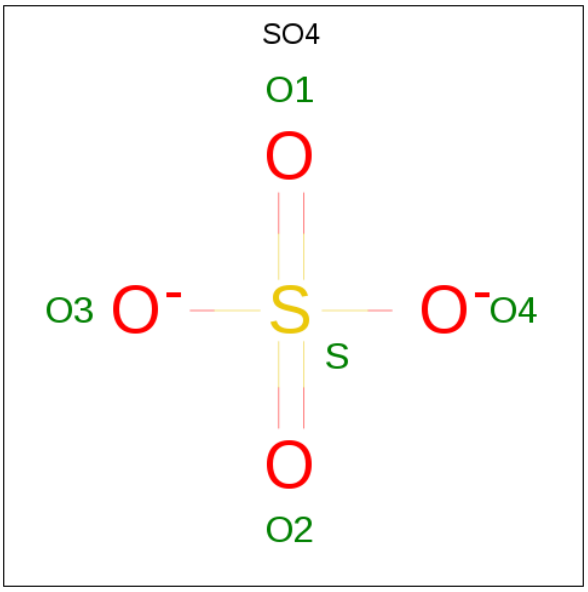
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	1
			82	58	2	12	10		
3	B	1	Total	C	Cl	N	O	0	1
			82	58	2	12	10		
3	C	1	Total	C	Cl	N	O	0	1
			82	58	2	12	10		
3	D	1	Total	C	Cl	N	O	0	1
			82	58	2	12	10		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	230	Total O 230 230	0	0
6	B	245	Total O 245 245	0	0
6	C	188	Total O 188 188	0	0
6	D	187	Total O 187 187	0	0

3 Residue-property plots (i)

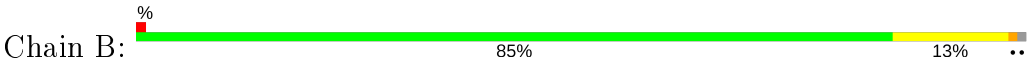
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

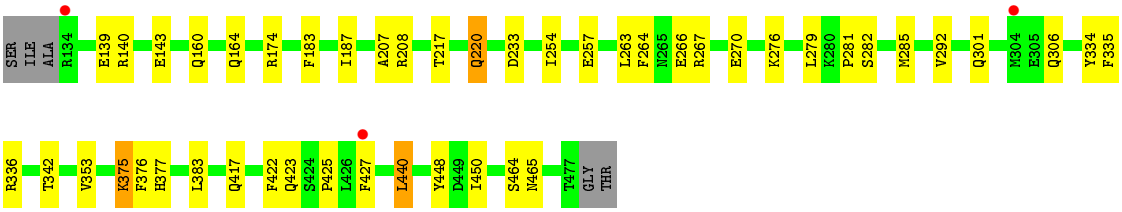
- Molecule 1: Histone-arginine methyltransferase CARM1

Chain A:

- Molecule 1: Histone-arginine methyltransferase CARM1

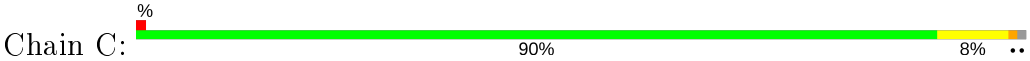
Chain B:

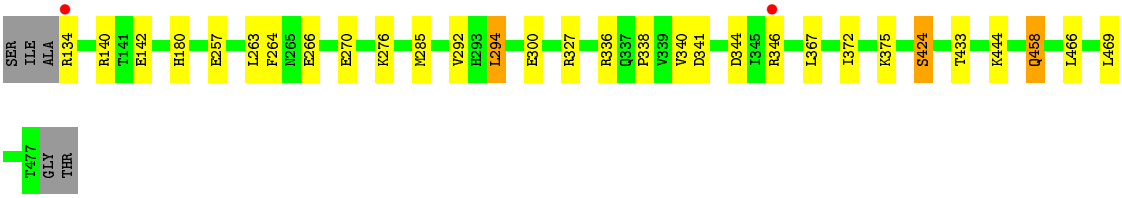




- Molecule 1: Histone-arginine methyltransferase CARM1

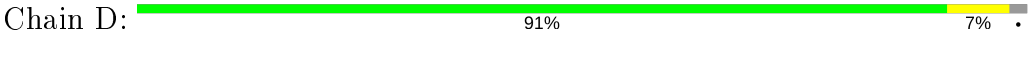
Chain C:

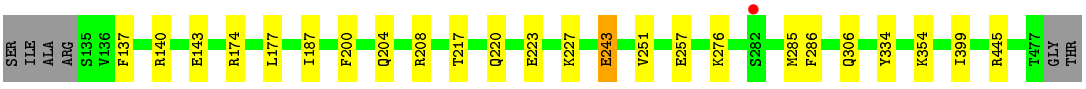




- Molecule 1: Histone-arginine methyltransferase CARM1

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	75.16Å 98.80Å 208.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.11 – 1.92 46.07 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.11-1.92) 99.8 (46.07-1.92)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.175 , 0.212 0.175 , 0.211	Depositor DCC
R_{free} test set	5909 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	24.3	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12491	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8537e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GOL, SAH, BW4, SO4

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	0.53	0/2899	0.66	1/3925 (0.0%)
1	B	0.56	0/2888	0.67	0/3910
1	C	0.48	0/2848	0.62	0/3858
1	D	0.51	0/2835	0.62	0/3841
All	All	0.52	0/11470	0.64	1/15534 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	247	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	464[B]	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2819	0	2765	10	0
1	B	2812	0	2763	29	0
1	C	2778	0	2726	17	0
1	D	2765	0	2711	13	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0
2	C	26	0	19	0	0
2	D	26	0	19	0	0
3	A	82	0	0	2	0
3	B	82	0	0	2	0
3	C	82	0	0	1	0
3	D	82	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	12	0	16	1	0
5	C	5	0	0	0	0
6	A	230	0	0	5	0
6	B	245	0	0	7	0
6	C	188	0	0	5	0
6	D	187	0	0	4	0
All	All	12491	0	11081	74	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (74) 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)
3:A:502[B]:BW4:CBD	3:A:502[B]:BW4:CAY	2.25	1.14
3:A:502[A]:BW4:CAW	3:A:502[A]:BW4:CBD	2.29	1.11
1:A:341[B]:ASP:OD1	6:A:601:HOH:O	1.75	1.03
1:C:424:SER:HB2	6:C:737:HOH:O	1.70	0.90
1:A:327:ARG:HD2	6:C:606:HOH:O	1.82	0.79
1:D:174:ARG:HD2	6:D:650:HOH:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:GLU:HG3	6:D:768:HOH:O	1.84	0.77
1:A:160:GLN:HE21	1:A:164:GLN:NE2	1.83	0.76
1:C:341:ASP:HB2	6:C:676:HOH:O	1.87	0.74
1:B:174:ARG:HD2	6:B:633:HOH:O	1.87	0.73
1:A:142:GLU:HG2	6:A:813:HOH:O	1.88	0.73
1:A:276:LYS:HD3	1:A:285[B]:MET:SD	2.31	0.70
1:B:160:GLN:O	1:B:164[A]:GLN:HG3	1.93	0.68
1:B:383:LEU:HD22	1:B:425:PRO:HB2	1.76	0.66
1:B:465[B]:ASN:CG	6:B:613:HOH:O	2.33	0.66
1:B:140[A]:ARG:HD3	1:B:267:ARG:CZ	2.26	0.65
1:A:186:LYS:NZ	6:A:602:HOH:O	2.23	0.65
1:B:270:GLU:OE1	6:B:601:HOH:O	2.14	0.65
1:C:344:ASP:OD1	1:C:346:ARG:HD3	1.99	0.63
1:B:375:LYS:HG3	6:B:826:HOH:O	1.98	0.63
1:A:369:ARG:HG3	1:A:441:ILE:CD1	2.34	0.58
1:C:180:HIS:HD2	6:C:770:HOH:O	1.87	0.57
1:D:223:GLU:OE1	1:D:227:LYS:HE2	2.05	0.57
1:C:458:GLN:H	1:C:458:GLN:HE21	1.52	0.57
1:C:263:LEU:HD23	1:C:292:VAL:HG22	1.87	0.57
1:B:342:THR:HA	1:B:417:GLN:NE2	2.21	0.56
1:B:217:THR:O	1:B:220:GLN:HG3	2.05	0.55
1:D:137:PHE:HB2	1:D:243:GLU:CG	2.35	0.55
1:D:445:ARG:HD3	6:D:694:HOH:O	2.05	0.55
1:D:399:ILE:HG12	6:D:636:HOH:O	2.05	0.55
1:B:336:ARG:HD3	6:B:819:HOH:O	2.09	0.53
1:D:177:LEU:HD13	4:D:504:GOL:H2	1.91	0.51
1:B:233:ASP:HB2	6:B:809:HOH:O	2.10	0.51
1:D:200:PHE:O	1:D:204:GLN:HG3	2.10	0.51
1:C:433:THR:H	1:C:458:GLN:HE22	1.58	0.51
1:B:342:THR:HA	1:B:417:GLN:HE21	1.75	0.50
1:C:336:ARG:HG2	1:C:466:LEU:O	2.12	0.50
1:B:264:PHE:CE2	1:B:292:VAL:HG21	2.47	0.49
1:C:458:GLN:H	1:C:458:GLN:NE2	2.09	0.49
1:D:217:THR:O	1:D:220:GLN:HG2	2.13	0.49
1:B:301:GLN:HG2	6:B:810:HOH:O	2.12	0.49
1:C:276:LYS:HE3	6:C:763:HOH:O	2.14	0.48
1:B:306:GLN:HE21	1:B:334:TYR:HB3	1.78	0.48
1:C:276:LYS:HD3	1:C:285[A]:MET:SD	2.54	0.48
1:B:375:LYS:HE2	1:B:375:LYS:HB3	1.63	0.47
1:B:375:LYS:HD2	1:B:377:HIS:CE1	2.50	0.47
1:B:335:PHE:CE2	1:B:423:GLN:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:LEU:HD23	1:B:292:VAL:CG2	2.45	0.46
1:A:267:ARG:CZ	1:A:442:ALA:HB1	2.46	0.46
1:B:383:LEU:HG	1:B:427:PHE:CE1	2.51	0.45
1:D:187:ILE:HG22	1:D:251:VAL:HG12	1.98	0.45
1:B:276:LYS:HD3	1:B:285[A]:MET:SD	2.57	0.45
1:C:264:PHE:CE2	1:C:292:VAL:HG21	2.51	0.45
1:D:137:PHE:HB2	1:D:243:GLU:HG2	1.97	0.45
1:B:353:VAL:HG13	1:B:376:PHE:CE1	2.52	0.45
1:D:306:GLN:HE21	1:D:334:TYR:HB3	1.81	0.45
1:B:254:ILE:HG13	1:B:279:LEU:HD13	2.00	0.44
1:A:270:GLU:HG3	6:A:654:HOH:O	2.17	0.44
1:B:440:LEU:HD12	1:B:450:ILE:HG12	1.99	0.44
1:A:342:THR:HG22	6:A:601:HOH:O	2.18	0.44
1:B:422:PHE:HA	1:B:465[A]:ASN:OD1	2.19	0.43
1:B:187:ILE:HD11	1:B:208:ARG:CZ	2.49	0.42
1:C:270:GLU:HG3	1:C:367:LEU:HD12	2.02	0.42
1:B:264:PHE:HB3	1:B:448:TYR:CE1	2.55	0.42
1:B:281:PRO:O	1:B:282:SER:HB2	2.20	0.42
1:C:338:PRO:HG2	1:C:469:LEU:HA	2.02	0.42
3:C:502[A]:BW4:CAU	3:C:502[A]:BW4:CBF	2.98	0.41
1:C:336:ARG:O	1:C:338:PRO:HD3	2.21	0.41
3:B:502[A]:BW4:CBF	3:B:502[A]:BW4:CAS	2.99	0.41
1:C:340:VAL:O	1:C:341:ASP:HB3	2.20	0.41
1:D:276:LYS:HD3	1:D:285[B]:MET:SD	2.60	0.41
3:B:502[B]:BW4:CBF	3:B:502[B]:BW4:CAS	2.99	0.41
1:B:183:PHE:O	1:B:207:ALA:HA	2.21	0.41
1:C:294:LEU:HD21	1:C:372:ILE:HG21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	350/349 (100%)	341 (97%)	8 (2%)	1 (0%)	41	31
1	B	349/349 (100%)	339 (97%)	9 (3%)	1 (0%)	41	31
1	C	344/349 (99%)	334 (97%)	9 (3%)	1 (0%)	41	31
1	D	343/349 (98%)	333 (97%)	10 (3%)	0	100	100
All	All	1386/1396 (99%)	1347 (97%)	36 (3%)	3 (0%)	47	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	GLU
1	B	266	GLU
1	C	266	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	308/303 (102%)	301 (98%)	7 (2%)	50	43
1	B	307/303 (101%)	301 (98%)	6 (2%)	55	49
1	C	302/303 (100%)	291 (96%)	11 (4%)	35	24
1	D	301/303 (99%)	295 (98%)	6 (2%)	55	49
All	All	1218/1212 (100%)	1188 (98%)	30 (2%)	47	39

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	257	GLU
1	A	294	LEU
1	A	346	ARG
1	A	360	LEU
1	A	417	GLN
1	A	444	LYS
1	B	139	GLU

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Mol	Chain	Res	Type
1	B	143	GLU
1	B	220	GLN
1	B	257	GLU
1	B	375	LYS
1	B	440	LEU
1	C	134	ARG
1	C	140	ARG
1	C	142	GLU
1	C	257	GLU
1	C	294	LEU
1	C	300	GLU
1	C	327	ARG
1	C	375	LYS
1	C	424	SER
1	C	444	LYS
1	C	458	GLN
1	D	140	ARG
1	D	208	ARG
1	D	243	GLU
1	D	257	GLU
1	D	286	PHE
1	D	354	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	164	GLN
1	A	265	ASN
1	A	311	ASN
1	A	417	GLN
1	B	148	GLN
1	B	161	ASN
1	B	180	HIS
1	B	220	GLN
1	B	265	ASN
1	B	306	GLN
1	B	417	GLN
1	B	446	GLN
1	C	160	GLN
1	C	161	ASN
1	C	164	GLN

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Mol	Chain	Res	Type
1	C	178	GLN
1	C	180	HIS
1	C	265	ASN
1	C	446	GLN
1	C	458	GLN
1	D	151	GLN
1	D	161	ASN
1	D	164	GLN
1	D	178	GLN
1	D	221	HIS
1	D	265	ASN
1	D	306	GLN
1	D	380	HIS
1	D	455	GLN
1	D	471	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

18 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	$\#\|Z\|>2$
3	BW4	A	502[A]	-	40,45,45	2.44	5 (12%)	47,66,66	2.00	14 (29%)
3	BW4	B	502[A]	-	40,45,45	2.38	5 (12%)	47,66,66	2.13	15 (31%)
3	BW4	C	502[A]	-	40,45,45	2.62	6 (15%)	47,66,66	2.00	14 (29%)
3	BW4	C	502[B]	-	40,45,45	2.62	6 (15%)	47,66,66	1.99	14 (29%)
3	BW4	B	502[B]	-	40,45,45	2.33	5 (12%)	47,66,66	2.15	15 (31%)
4	GOL	D	504	-	5,5,5	0.26	0	5,5,5	0.30	0
2	SAH	D	501	-	21,28,28	1.08	1 (4%)	20,40,40	1.57	4 (20%)
2	SAH	B	501	-	21,28,28	1.02	2 (9%)	20,40,40	1.57	3 (15%)
2	SAH	A	501	-	21,28,28	1.07	2 (9%)	20,40,40	1.57	4 (20%)
4	GOL	C	503	-	5,5,5	0.23	0	5,5,5	0.29	0
4	GOL	D	503	-	5,5,5	0.19	0	5,5,5	0.45	0
4	GOL	A	503	-	5,5,5	0.26	0	5,5,5	0.32	0
4	GOL	B	503	-	5,5,5	0.22	0	5,5,5	0.39	0
2	SAH	C	501	-	21,28,28	1.21	3 (14%)	20,40,40	1.36	3 (15%)
3	BW4	D	502[A]	-	40,45,45	2.52	5 (12%)	47,66,66	1.92	15 (31%)
5	SO4	C	504	-	4,4,4	0.34	0	6,6,6	0.10	0
3	BW4	D	502[B]	-	40,45,45	2.54	5 (12%)	47,66,66	1.92	15 (31%)
3	BW4	A	502[B]	-	40,45,45	2.48	5 (12%)	47,66,66	1.97	15 (31%)

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
3	BW4	A	502[A]	-	-	3/18/48/48	0/5/5/5
3	BW4	B	502[A]	-	-	2/18/48/48	0/5/5/5
3	BW4	C	502[A]	-	-	3/18/48/48	0/5/5/5
3	BW4	C	502[B]	-	-	4/18/48/48	0/5/5/5
3	BW4	B	502[B]	-	-	2/18/48/48	0/5/5/5
4	GOL	D	504	-	-	0/4/4/4	-
2	SAH	D	501	-	-	0/7/31/31	0/3/3/3
2	SAH	B	501	-	-	0/7/31/31	0/3/3/3
2	SAH	A	501	-	-	0/7/31/31	0/3/3/3
4	GOL	C	503	-	-	2/4/4/4	-
4	GOL	D	503	-	-	4/4/4/4	-
4	GOL	A	503	-	-	0/4/4/4	-
4	GOL	B	503	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	C	501	-	-	0/7/31/31	0/3/3/3
3	BW4	D	502[A]	-	-	0/18/48/48	0/5/5/5
3	BW4	D	502[B]	-	-	2/18/48/48	0/5/5/5
3	BW4	A	502[B]	-	-	3/18/48/48	0/5/5/5

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502[B]	BW4	CBI-C4	-13.77	1.34	1.50
3	C	502[A]	BW4	CBI-C4	-13.70	1.34	1.50
3	A	502[B]	BW4	CBI-C4	-12.66	1.35	1.50
3	D	502[B]	BW4	CBI-C4	-12.60	1.36	1.50
3	D	502[A]	BW4	CBI-C4	-12.51	1.36	1.50
3	A	502[A]	BW4	CBI-C4	-12.34	1.36	1.50
3	B	502[A]	BW4	CBI-C4	-12.27	1.36	1.50
3	B	502[B]	BW4	CBI-C4	-11.98	1.36	1.50
3	D	502[B]	BW4	CBF-C5	-5.38	1.40	1.51
3	D	502[A]	BW4	CBF-C5	-5.37	1.40	1.51
3	B	502[A]	BW4	CBF-C5	-5.32	1.40	1.51
3	B	502[B]	BW4	CBF-C5	-5.29	1.40	1.51
3	C	502[A]	BW4	CBF-C5	-5.16	1.40	1.51
3	C	502[B]	BW4	CBF-C5	-5.12	1.41	1.51
3	D	502[A]	BW4	CAU-CAT	-4.76	1.50	1.54
3	A	502[B]	BW4	CBF-C5	-4.76	1.41	1.51
3	A	502[A]	BW4	CBF-C5	-4.73	1.41	1.51
3	D	502[B]	BW4	CAU-CAT	-4.69	1.50	1.54
3	A	502[A]	BW4	CBK-CBJ	3.92	1.53	1.48
3	D	502[B]	BW4	CBK-CBJ	3.84	1.53	1.48
3	A	502[B]	BW4	CAU-CAT	-3.66	1.51	1.54
3	D	502[A]	BW4	CBK-CBJ	3.49	1.53	1.48
3	D	502[B]	BW4	CAM-C2	-3.36	1.40	1.48
3	D	502[A]	BW4	CAM-C2	-3.35	1.40	1.48
3	A	502[A]	BW4	CAS-CAT	-3.35	1.51	1.54
3	B	502[B]	BW4	CAM-C2	-3.35	1.40	1.48
3	B	502[A]	BW4	CAM-C2	-3.34	1.40	1.48
3	C	502[A]	BW4	CAM-C2	-3.31	1.40	1.48
3	C	502[A]	BW4	CBK-CBJ	3.27	1.52	1.48
3	C	502[B]	BW4	CAM-C2	-3.26	1.41	1.48
3	C	502[B]	BW4	CBK-CBJ	3.15	1.52	1.48
3	A	502[B]	BW4	CAM-C2	-3.00	1.41	1.48
3	A	502[B]	BW4	CBK-CBJ	2.94	1.52	1.48
3	A	502[A]	BW4	CAM-C2	-2.90	1.41	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502[A]	BW4	CAS-CAT	-2.87	1.51	1.54
3	B	502[A]	BW4	CBK-CBJ	2.79	1.52	1.48
3	C	502[B]	BW4	CAU-CAT	-2.74	1.51	1.54
3	C	502[A]	BW4	CAU-CAT	-2.63	1.52	1.54
3	B	502[A]	BW4	CAU-CAT	-2.56	1.52	1.54
3	B	502[B]	BW4	CBK-CBJ	2.56	1.52	1.48
3	B	502[B]	BW4	CAU-CAT	-2.53	1.52	1.54
2	D	501	SAH	C5-C4	2.49	1.47	1.40
3	C	502[B]	BW4	CAS-CAT	-2.48	1.52	1.54
2	C	501	SAH	O4'-C1'	2.43	1.44	1.41
2	A	501	SAH	C5-C4	2.40	1.47	1.40
2	C	501	SAH	C5-C4	2.29	1.47	1.40
2	C	501	SAH	C2-N3	2.27	1.35	1.32
2	B	501	SAH	C5-C4	2.25	1.46	1.40
2	B	501	SAH	C2'-C1'	-2.04	1.50	1.53
2	A	501	SAH	C2-N3	2.03	1.35	1.32

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502[B]	BW4	C5-C4-N3	-6.18	117.18	123.06
3	B	502[A]	BW4	C5-C4-N3	-5.94	117.41	123.06
3	D	502[A]	BW4	C5-C4-N3	-5.31	118.00	123.06
3	D	502[B]	BW4	C5-C4-N3	-5.30	118.01	123.06
3	B	502[B]	BW4	CBD-OBC-CBA	-5.17	109.36	115.34
3	B	502[A]	BW4	CBD-OBC-CBA	-5.16	109.38	115.34
3	A	502[A]	BW4	C5-C4-N3	-4.77	118.52	123.06
3	B	502[B]	BW4	C4-N3-C2	4.75	123.43	117.09
3	A	502[B]	BW4	C5-C4-N3	-4.64	118.64	123.06
3	B	502[A]	BW4	C4-N3-C2	4.61	123.24	117.09
3	C	502[A]	BW4	C5-C4-N3	-4.40	118.87	123.06
3	C	502[B]	BW4	C5-C4-N3	-4.33	118.94	123.06
2	D	501	SAH	N3-C2-N1	-4.27	122.01	128.68
3	C	502[A]	BW4	C4-N3-C2	4.23	122.74	117.09
2	A	501	SAH	N3-C2-N1	-4.21	122.09	128.68
3	C	502[B]	BW4	C4-N3-C2	4.20	122.70	117.09
3	A	502[A]	BW4	CAU-NAR-C6	4.17	137.53	125.20
3	C	502[B]	BW4	CAW-NAX-CAY	4.13	120.58	112.62
3	C	502[A]	BW4	CAW-NAX-CAY	4.13	120.57	112.62
3	A	502[B]	BW4	CAS-NAR-C6	4.08	137.28	125.20
3	A	502[A]	BW4	C4-N3-C2	4.07	122.52	117.09
3	C	502[B]	BW4	N3-C2-N1	-4.06	118.66	125.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502[A]	BW4	N3-C2-N1	-4.02	118.72	125.23
3	C	502[B]	BW4	CAS-NAR-C6	4.00	137.02	125.20
3	A	502[B]	BW4	C4-N3-C2	3.99	122.42	117.09
3	C	502[A]	BW4	CBD-OBC-CBA	-3.98	110.74	115.34
3	A	502[A]	BW4	CAW-NAX-CAY	3.97	120.27	112.62
3	D	502[B]	BW4	CAS-NAR-C6	3.96	136.93	125.20
3	C	502[A]	BW4	CAU-NAR-C6	3.94	136.87	125.20
2	B	501	SAH	N3-C2-N1	-3.94	122.52	128.68
3	D	502[A]	BW4	C4-N3-C2	3.94	122.35	117.09
3	D	502[B]	BW4	C4-N3-C2	3.93	122.33	117.09
3	C	502[B]	BW4	CBD-OBC-CBA	-3.92	110.81	115.34
3	D	502[A]	BW4	CAS-NAR-C6	3.92	136.80	125.20
3	A	502[A]	BW4	C5-C6-NAR	3.91	125.38	118.78
3	A	502[A]	BW4	C5-C6-N1	-3.91	119.55	124.31
3	A	502[A]	BW4	N3-C2-N1	-3.86	118.98	125.23
3	A	502[B]	BW4	N3-C2-N1	-3.85	119.00	125.23
3	A	502[B]	BW4	CAW-NAX-CAY	3.85	120.04	112.62
3	A	502[B]	BW4	C5-C6-N1	-3.84	119.64	124.31
3	B	502[B]	BW4	N3-C2-N1	-3.78	119.11	125.23
3	B	502[A]	BW4	N3-C2-N1	-3.75	119.16	125.23
3	A	502[B]	BW4	C5-C6-NAR	3.72	125.05	118.78
3	B	502[A]	BW4	CAS-NAR-C6	3.66	136.03	125.20
3	B	502[B]	BW4	CAS-NAR-C6	3.66	136.03	125.20
3	C	502[A]	BW4	C5-C6-N1	-3.50	120.05	124.31
3	C	502[B]	BW4	C5-C6-N1	-3.50	120.05	124.31
3	D	502[A]	BW4	N3-C2-N1	-3.47	119.61	125.23
3	D	502[B]	BW4	N3-C2-N1	-3.47	119.62	125.23
3	D	502[A]	BW4	C5-C6-NAR	3.44	124.58	118.78
3	D	502[B]	BW4	C5-C6-NAR	3.43	124.56	118.78
2	C	501	SAH	N3-C2-N1	-3.40	123.37	128.68
3	B	502[B]	BW4	CAM-C2-N3	3.37	123.00	117.22
3	D	502[B]	BW4	C5-C6-N1	-3.36	120.22	124.31
3	D	502[A]	BW4	C5-C6-N1	-3.31	120.28	124.31
3	D	502[B]	BW4	CBD-OBC-CBA	-3.30	111.52	115.34
3	B	502[A]	BW4	CAM-C2-N3	3.26	122.82	117.22
3	A	502[A]	BW4	CAM-C2-N3	3.25	122.81	117.22
3	D	502[B]	BW4	CAW-NAX-CAY	3.25	118.89	112.62
3	B	502[B]	BW4	C5-C6-N1	-3.21	120.40	124.31
3	B	502[A]	BW4	C5-C6-N1	-3.21	120.40	124.31
3	A	502[B]	BW4	CAM-C2-N3	3.20	122.72	117.22
3	D	502[A]	BW4	CAW-NAX-CAY	3.20	118.78	112.62
3	D	502[A]	BW4	CBD-OBC-CBA	-3.12	111.73	115.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	SAH	C2-N1-C6	3.02	123.91	118.75
3	C	502[B]	BW4	C5-C6-NAR	3.01	123.86	118.78
3	B	502[B]	BW4	C5-C6-NAR	2.99	123.82	118.78
3	B	502[A]	BW4	C5-C6-NAR	2.96	123.77	118.78
2	B	501	SAH	C2-N1-C6	2.88	123.69	118.75
3	A	502[A]	BW4	OBC-CBA-OBB	-2.86	119.25	124.63
3	C	502[A]	BW4	C5-C6-NAR	2.85	123.58	118.78
3	D	502[A]	BW4	CAM-C2-N3	2.84	122.10	117.22
3	D	502[B]	BW4	CAM-C2-N3	2.81	122.05	117.22
3	B	502[A]	BW4	OBC-CBA-OBB	-2.79	119.38	124.63
3	B	502[B]	BW4	OBC-CBA-OBB	-2.78	119.41	124.63
3	A	502[A]	BW4	C6-N1-C2	2.75	122.39	116.35
3	A	502[B]	BW4	OBC-CBA-OBB	-2.72	119.50	124.63
3	A	502[B]	BW4	C6-N1-C2	2.72	122.31	116.35
3	C	502[B]	BW4	C6-N1-C2	2.70	122.27	116.35
3	A	502[B]	BW4	CBD-OBC-CBA	-2.69	112.23	115.34
3	C	502[B]	BW4	OBC-CBA-OBB	-2.67	119.60	124.63
3	C	502[A]	BW4	C6-N1-C2	2.66	122.18	116.35
3	B	502[B]	BW4	C4-C5-C6	2.66	118.55	115.54
3	B	502[B]	BW4	CAW-NAX-CAY	2.63	117.68	112.62
3	B	502[A]	BW4	CAW-NAX-CAY	2.62	117.67	112.62
3	C	502[A]	BW4	OBC-CBA-OBB	-2.61	119.72	124.63
3	D	502[A]	BW4	OBB-CBA-NAX	-2.59	119.98	124.32
3	D	502[B]	BW4	OBB-CBA-NAX	-2.59	119.98	124.32
3	D	502[B]	BW4	OBC-CBA-OBB	-2.59	119.75	124.63
2	D	501	SAH	C2-N1-C6	2.58	123.17	118.75
3	C	502[A]	BW4	CAS-CAT-CAU	2.57	89.69	85.68
3	C	502[B]	BW4	CAM-C2-N3	2.57	121.64	117.22
3	B	502[A]	BW4	C4-C5-C6	2.57	118.45	115.54
3	B	502[B]	BW4	OBB-CBA-NAX	-2.56	120.04	124.32
3	D	502[A]	BW4	OBC-CBA-OBB	-2.55	119.83	124.63
3	C	502[B]	BW4	CAS-CAT-CAU	2.53	89.62	85.68
3	B	502[A]	BW4	OBB-CBA-NAX	-2.51	120.12	124.32
2	B	501	SAH	C1'-N9-C4	-2.46	122.33	126.64
3	C	502[A]	BW4	CAM-C2-N3	2.44	121.41	117.22
3	D	502[B]	BW4	C6-N1-C2	2.42	121.64	116.35
3	C	502[A]	BW4	OBB-CBA-NAX	-2.41	120.28	124.32
3	D	502[A]	BW4	C6-N1-C2	2.41	121.62	116.35
3	D	502[A]	BW4	CAS-CAT-CAU	2.40	89.42	85.68
3	D	502[B]	BW4	CAS-CAT-CAU	2.37	89.37	85.68
3	A	502[B]	BW4	OBB-CBA-NAX	-2.34	120.41	124.32
2	A	501	SAH	O4'-C1'-C2'	-2.33	103.52	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	502[B]	BW4	C4-C5-C6	2.31	118.16	115.54
3	A	502[B]	BW4	CAS-CAT-CAU	2.29	89.25	85.68
3	D	502[A]	BW4	C4-C5-C6	2.29	118.13	115.54
3	A	502[A]	BW4	CBD-OBC-CBA	-2.28	112.70	115.34
3	B	502[A]	BW4	CAU-NAR-C6	2.28	131.93	125.20
3	B	502[B]	BW4	C6-N1-C2	2.27	121.32	116.35
3	B	502[B]	BW4	CAU-NAR-C6	2.27	131.92	125.20
3	B	502[A]	BW4	C6-N1-C2	2.27	121.32	116.35
2	D	501	SAH	C4-C5-N7	-2.25	107.06	109.40
3	C	502[B]	BW4	OBB-CBA-NAX	-2.25	120.56	124.32
3	A	502[A]	BW4	OBB-CBA-NAX	-2.22	120.61	124.32
3	A	502[A]	BW4	C4-C5-C6	2.20	118.03	115.54
2	C	501	SAH	C2-N1-C6	2.19	122.49	118.75
3	B	502[A]	BW4	CAS-CAT-CAU	2.18	89.08	85.68
3	C	502[A]	BW4	CAS-NAR-C6	2.18	131.64	125.20
3	B	502[B]	BW4	CAS-CAT-CAU	2.17	89.06	85.68
3	A	502[B]	BW4	C4-C5-C6	2.16	117.98	115.54
2	C	501	SAH	N6-C6-N1	2.13	123.00	118.57
2	A	501	SAH	C4-C5-N7	-2.12	107.19	109.40
3	C	502[B]	BW4	CAU-NAR-C6	2.12	131.47	125.20
3	A	502[A]	BW4	CAS-CAT-CAU	2.11	88.96	85.68
3	A	502[B]	BW4	CAU-NAR-C6	2.03	131.21	125.20
3	D	502[A]	BW4	CAU-NAR-C6	2.02	131.17	125.20
3	D	502[B]	BW4	CAU-NAR-C6	2.02	131.17	125.20
2	D	501	SAH	CB-CG-SD	-2.00	108.82	113.31

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502[A]	BW4	OBB-CBA-OBC-CBD
3	A	502[A]	BW4	NAX-CBA-OBC-CBD
3	C	502[A]	BW4	OBB-CBA-OBC-CBD
3	C	502[A]	BW4	NAX-CBA-OBC-CBD
3	C	502[B]	BW4	OBB-CBA-OBC-CBD
3	C	502[B]	BW4	NAX-CBA-OBC-CBD
4	C	503	GOL	C1-C2-C3-O3
4	D	503	GOL	O1-C1-C2-C3
4	D	503	GOL	C1-C2-C3-O3
4	B	503	GOL	C1-C2-C3-O3
3	A	502[B]	BW4	OBB-CBA-OBC-CBD
3	A	502[B]	BW4	NAX-CBA-OBC-CBD

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Mol	Chain	Res	Type	Atoms
4	D	503	GOL	O1-C1-C2-O2
3	B	502[A]	BW4	NAX-CBA-OBC-CBD
3	B	502[A]	BW4	OBB-CBA-OBC-CBD
4	D	503	GOL	O2-C2-C3-O3
3	B	502[B]	BW4	OBB-CBA-OBC-CBD
3	B	502[B]	BW4	NAX-CBA-OBC-CBD
4	C	503	GOL	O2-C2-C3-O3
4	B	503	GOL	O2-C2-C3-O3
3	D	502[B]	BW4	NAX-CBA-OBC-CBD
3	D	502[B]	BW4	OBB-CBA-OBC-CBD
3	A	502[A]	BW4	N1-C2-CAM-CAN
3	C	502[A]	BW4	N1-C2-CAM-CAN
3	C	502[B]	BW4	N1-C2-CAM-CAN
3	C	502[B]	BW4	N3-C2-CAM-CAN
3	A	502[B]	BW4	N1-C2-CAM-CAN

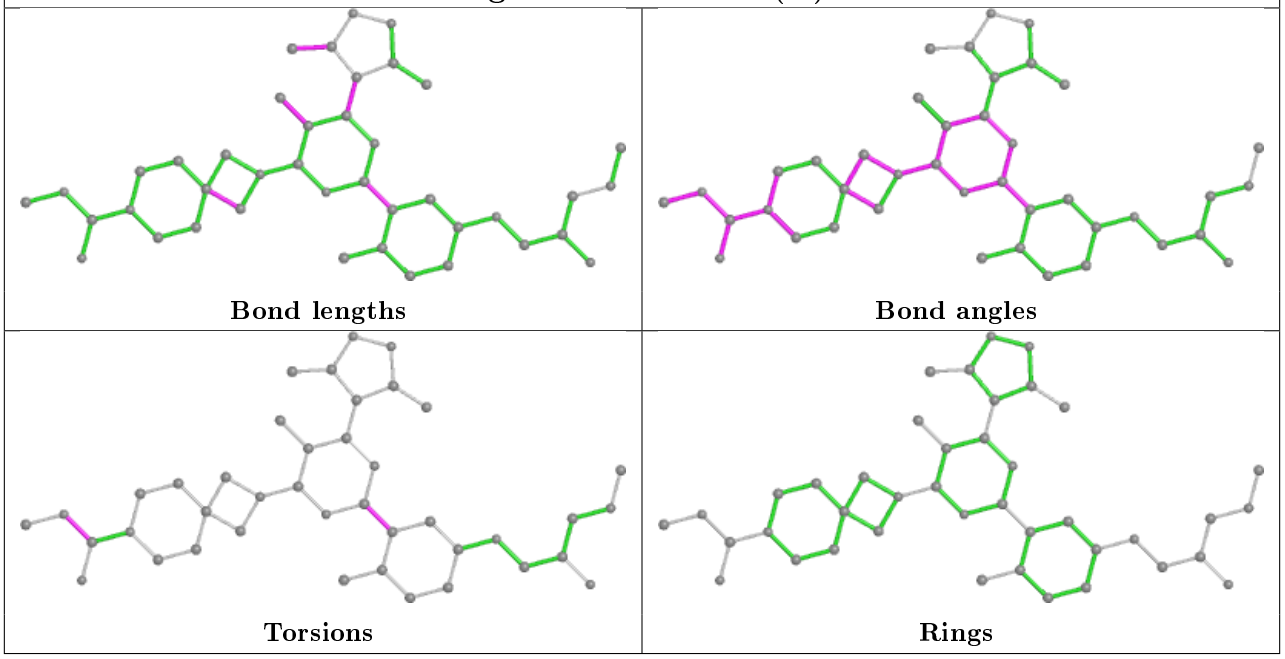
There are no ring outliers.

6 monomers are involved in 6 short contacts:

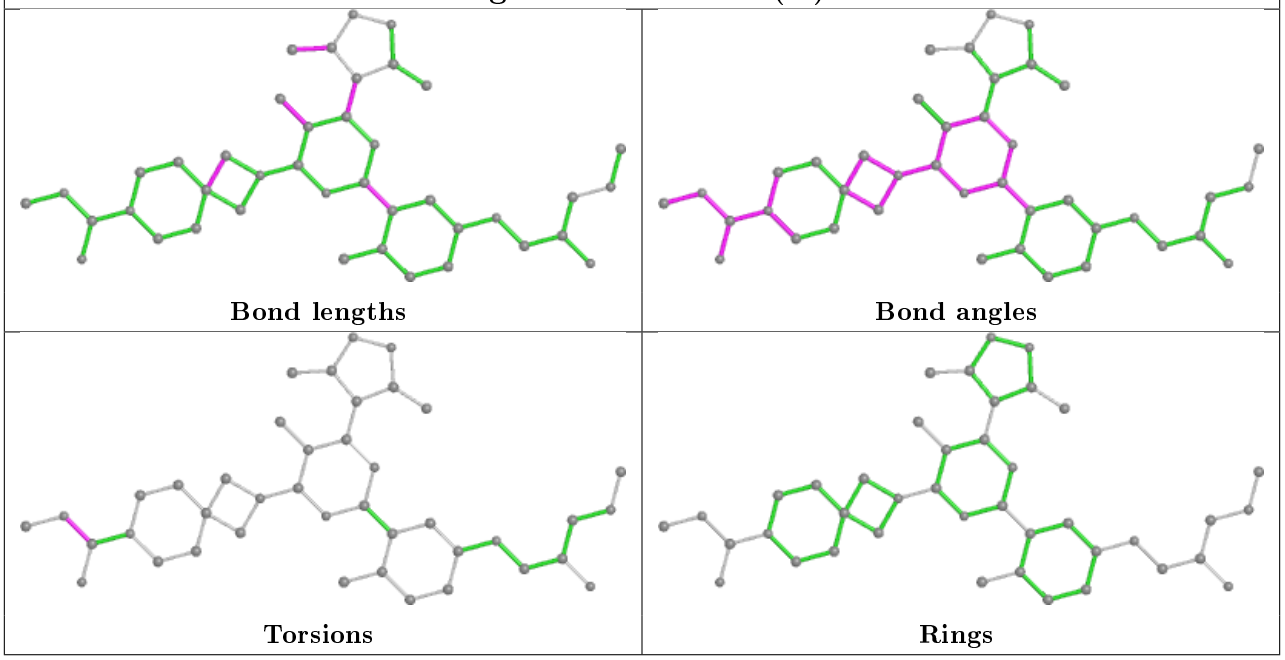
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502[A]	BW4	1	0
3	B	502[A]	BW4	1	0
3	C	502[A]	BW4	1	0
3	B	502[B]	BW4	1	0
4	D	504	GOL	1	0
3	A	502[B]	BW4	1	0

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.

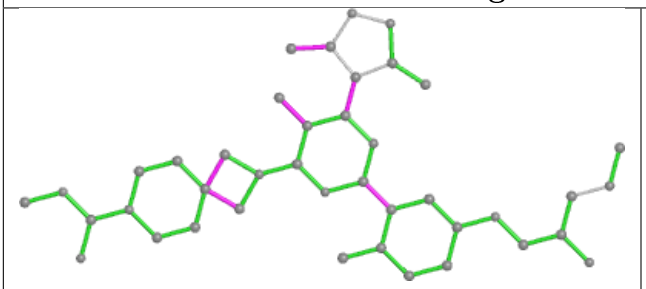
Ligand BW4 A 502 (A)



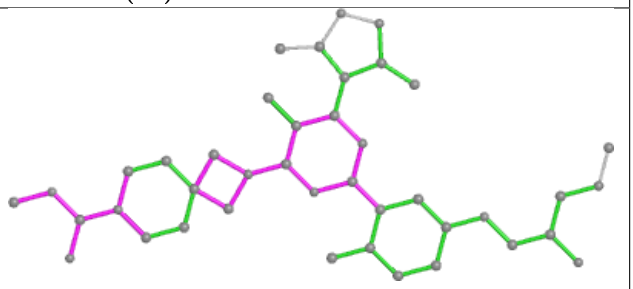
Ligand BW4 B 502 (A)



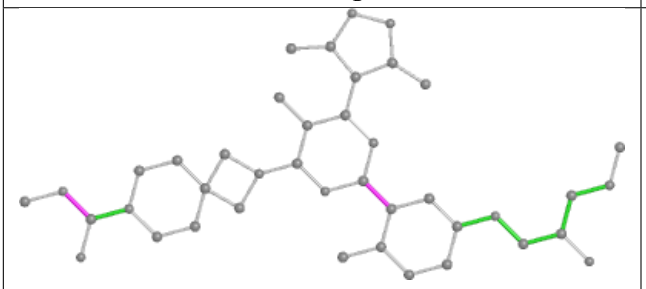
Ligand BW4 C 502 (A)



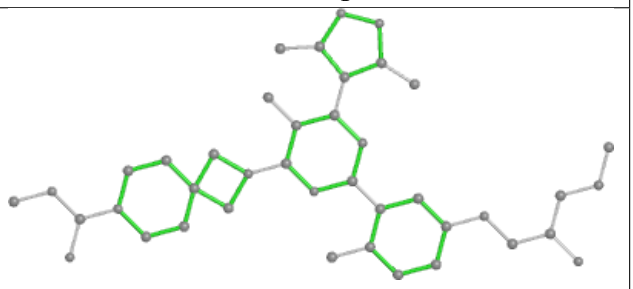
Bond lengths



Bond angles

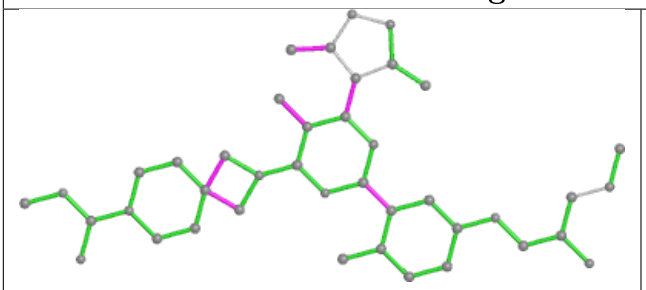


Torsions

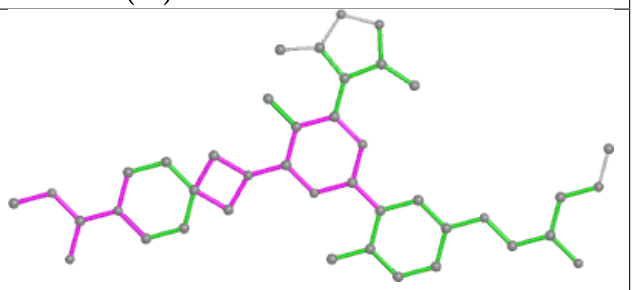


Rings

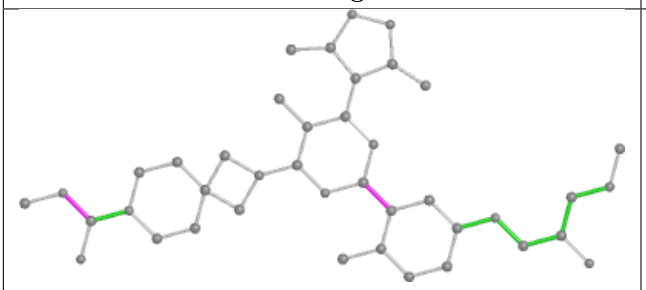
Ligand BW4 C 502 (B)



Bond lengths



Bond angles



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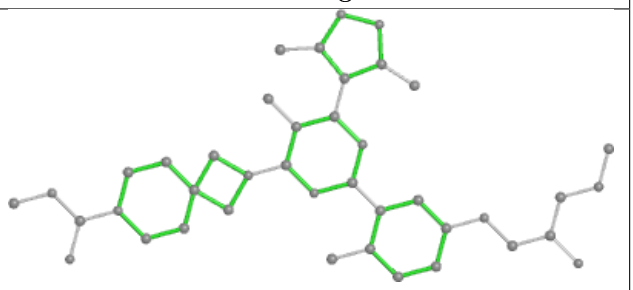
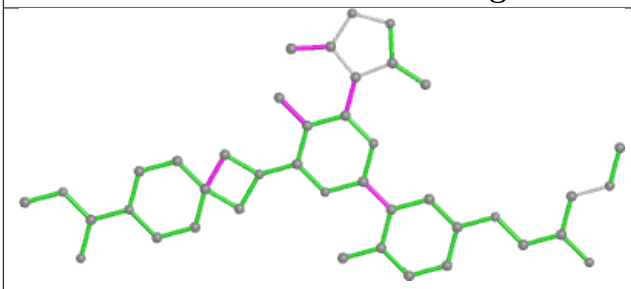
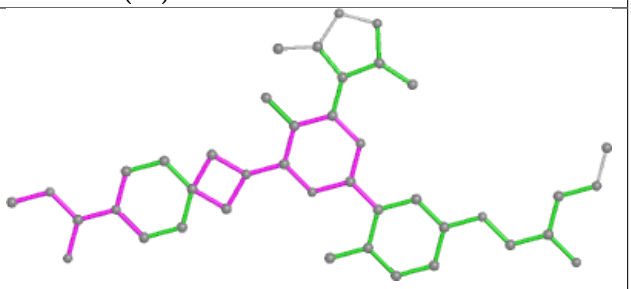


Rings

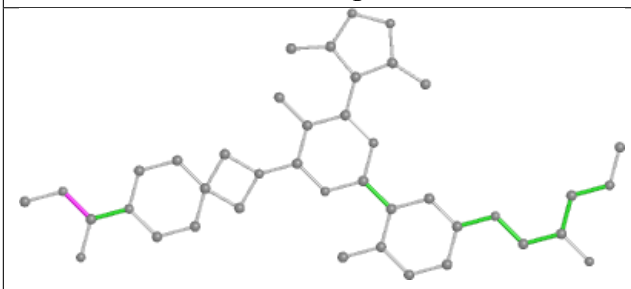
Ligand BW4 B 502 (B)



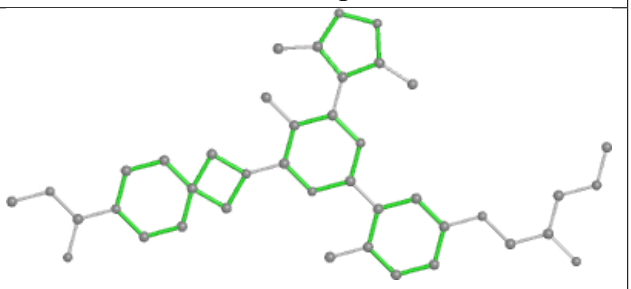
Bond lengths



Bond angles

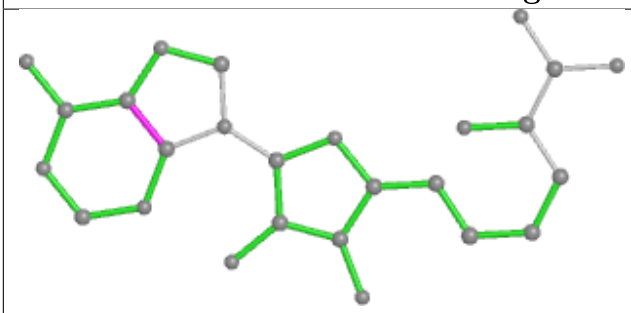


Torsions

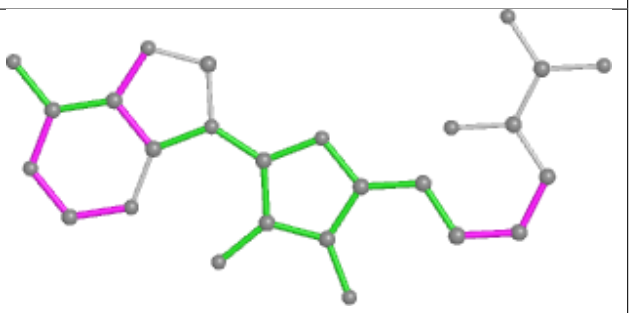


Rings

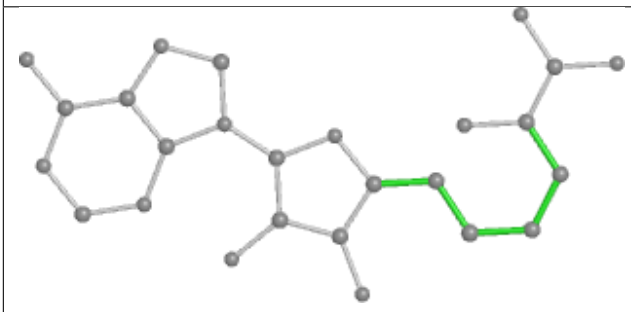
Ligand SAH D 501



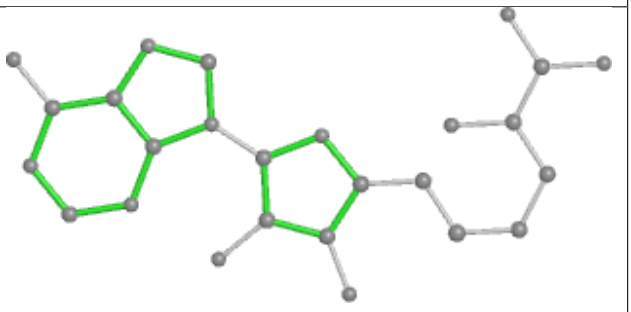
Bond lengths



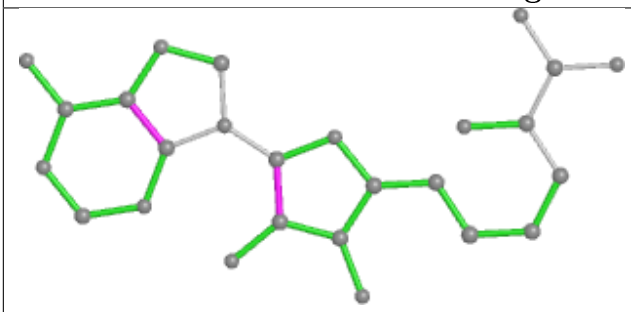
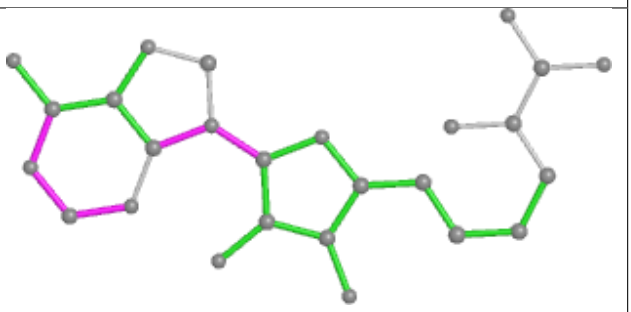
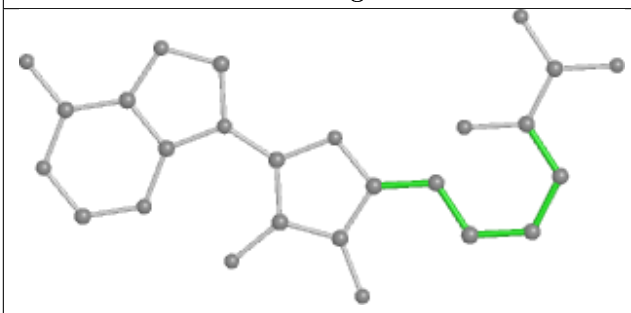
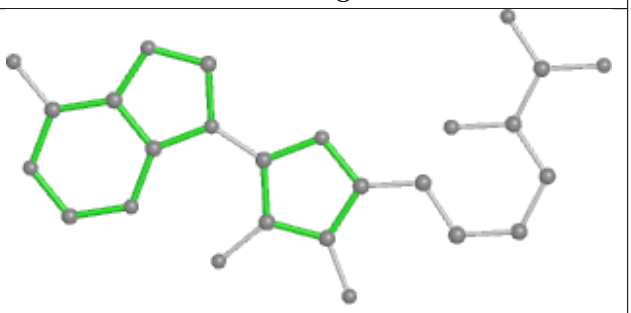
Bond angles

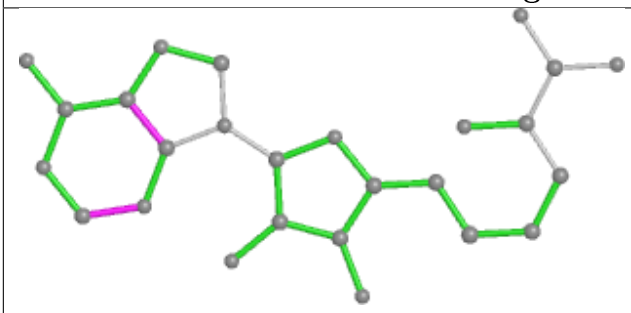
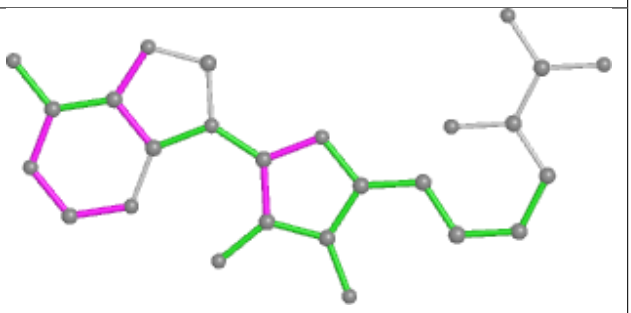
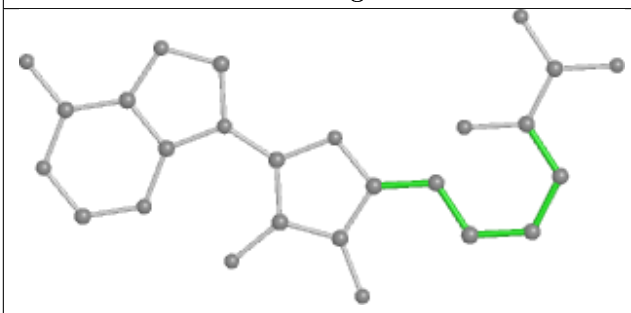
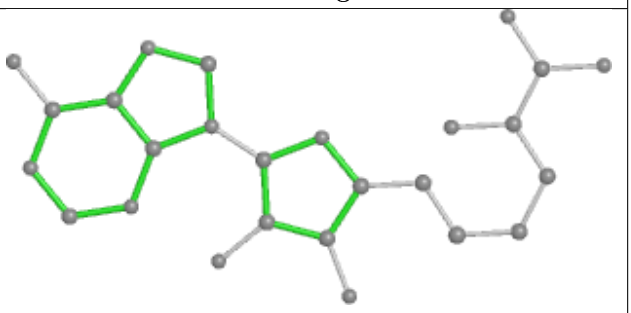


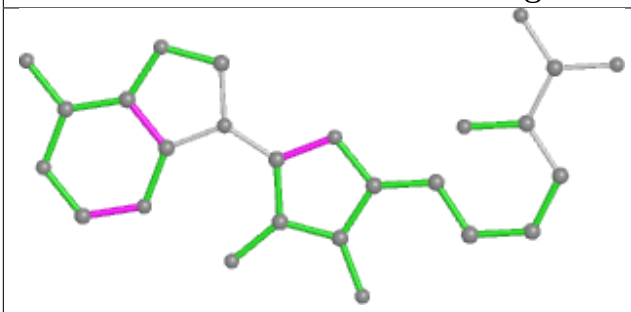
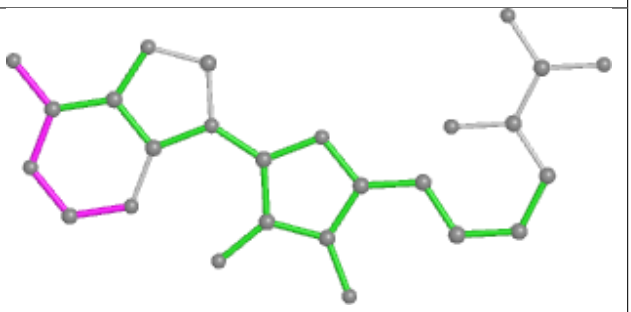
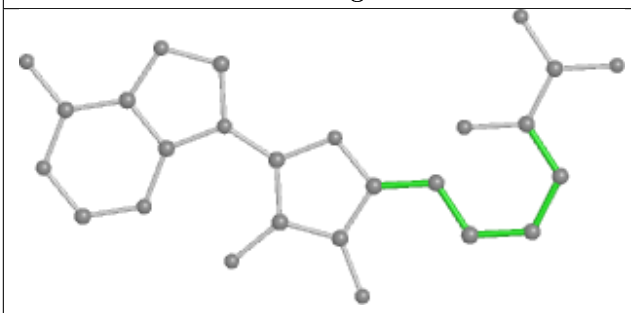
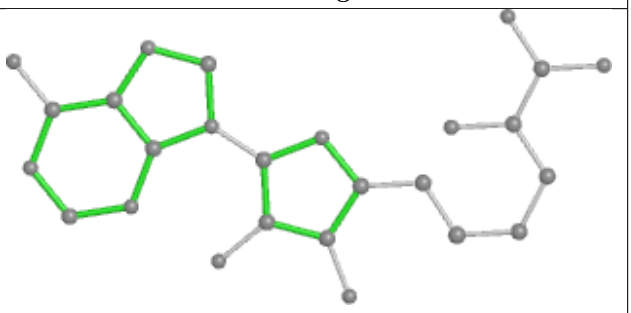
Torsions

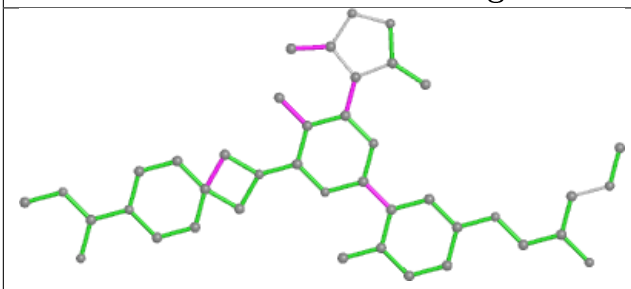
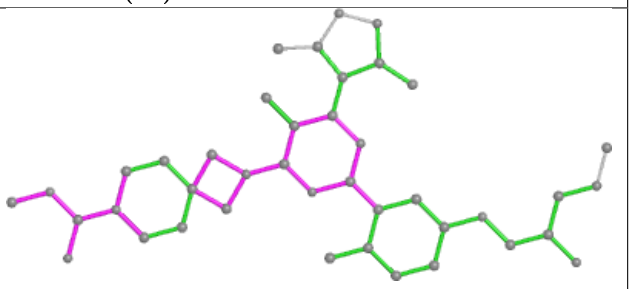
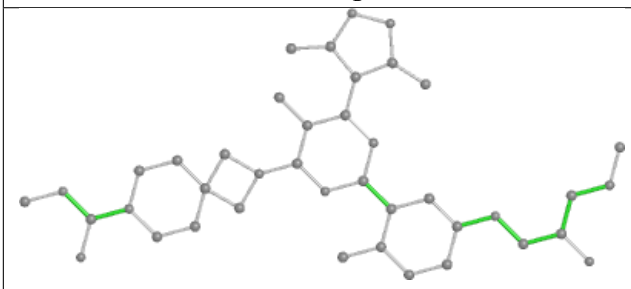
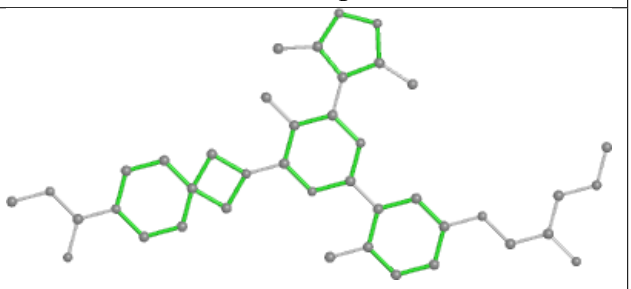


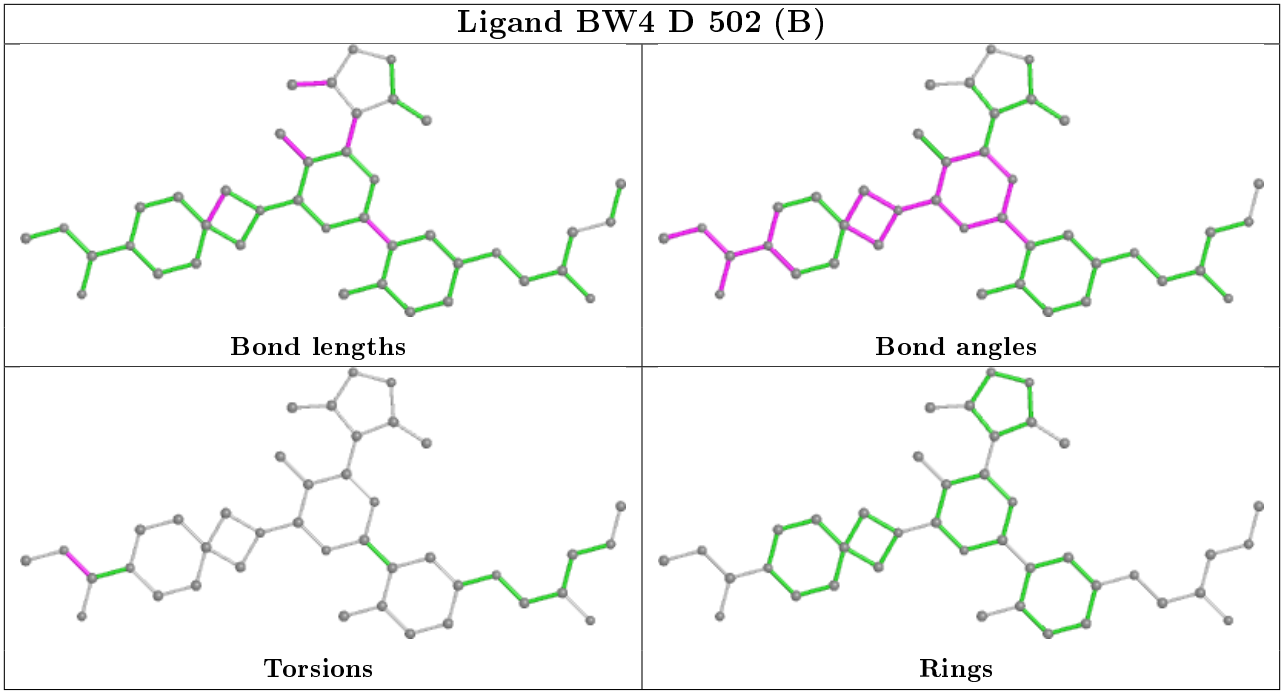
Rings

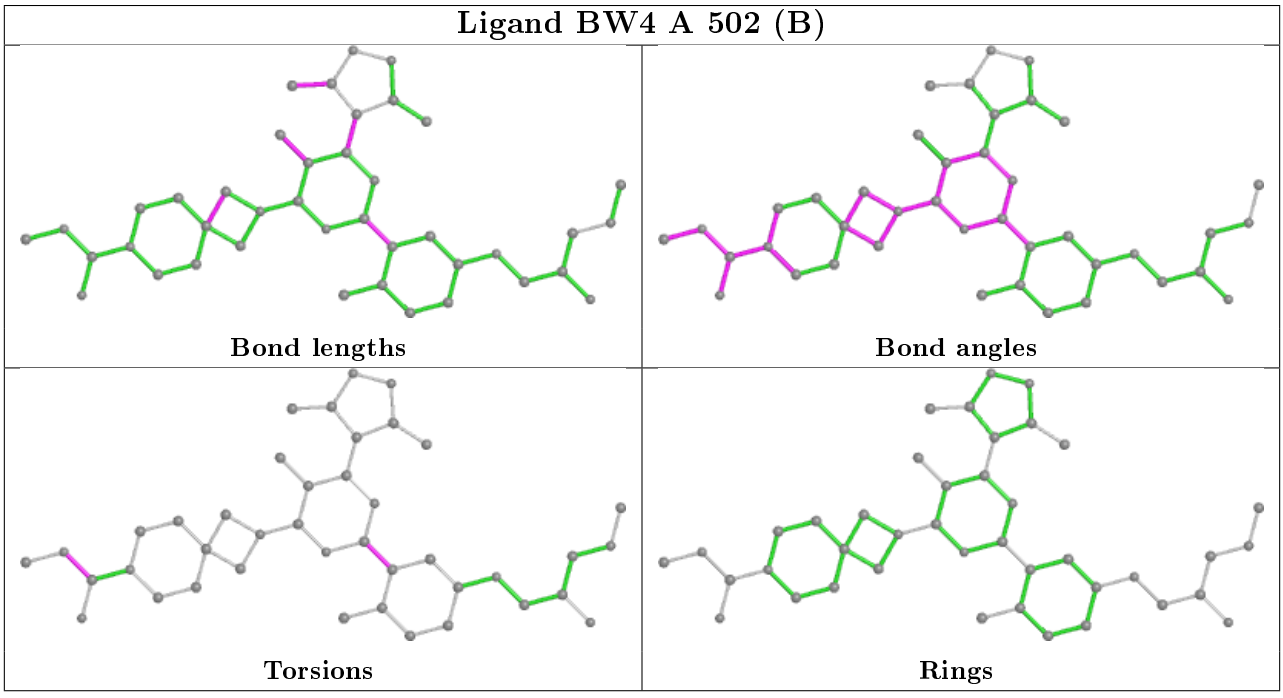
Ligand SAH B 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH A 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH C 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BW4 D 502 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	344/349 (98%)	-0.35	2 (0%)	89	90	14, 22, 33, 58	0
1	B	344/349 (98%)	-0.36	3 (0%)	84	85	13, 21, 33, 60	0
1	C	344/349 (98%)	-0.32	2 (0%)	89	90	20, 27, 39, 77	0
1	D	343/349 (98%)	-0.29	1 (0%)	94	94	20, 28, 40, 56	0
All	All	1375/1396 (98%)	-0.33	8 (0%)	89	90	13, 25, 38, 77	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	134	ARG	4.0
1	B	134	ARG	3.5
1	C	346	ARG	2.5
1	B	427	PHE	2.5
1	B	304[A]	MET	2.3
1	A	134	ARG	2.2
1	A	346	ARG	2.2
1	D	282	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

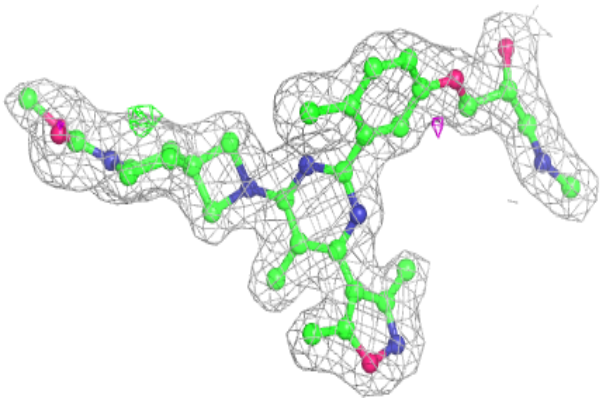
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

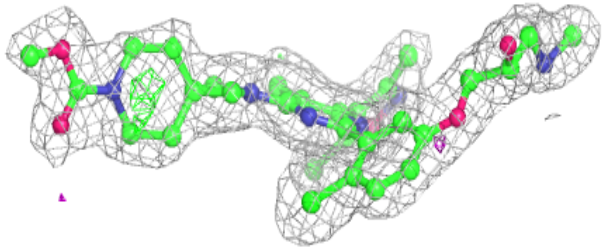
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	D	504	6/6	0.80	0.22	50,51,54,56	0
4	GOL	A	503	6/6	0.84	0.11	47,51,54,59	0
4	GOL	B	503	6/6	0.84	0.17	56,58,60,61	0
4	GOL	C	503	6/6	0.85	0.15	48,51,52,58	0
4	GOL	D	503	6/6	0.85	0.17	60,62,64,68	0
5	SO4	C	504	5/5	0.86	0.27	82,83,87,87	0
3	BW4	D	502[A]	41/41	0.95	0.10	21,24,41,44	41
3	BW4	A	502[A]	41/41	0.95	0.13	15,16,34,39	41
3	BW4	D	502[B]	41/41	0.95	0.10	21,25,44,46	41
3	BW4	A	502[B]	41/41	0.95	0.13	16,18,40,45	41
3	BW4	C	502[A]	41/41	0.96	0.11	22,25,46,48	41
3	BW4	C	502[B]	41/41	0.96	0.11	22,24,41,44	41
3	BW4	B	502[B]	41/41	0.96	0.10	14,17,35,38	41
3	BW4	B	502[A]	41/41	0.96	0.10	14,18,36,39	41
2	SAH	D	501	26/26	0.97	0.07	23,26,29,29	0
2	SAH	C	501	26/26	0.97	0.08	21,23,24,25	0
2	SAH	A	501	26/26	0.98	0.09	14,15,17,18	0
2	SAH	B	501	26/26	0.98	0.07	15,16,18,19	0

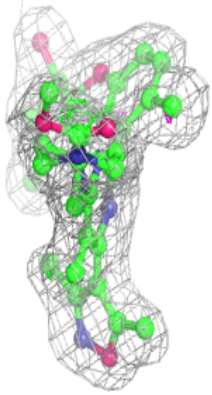
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BW4 D 502 (A):

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

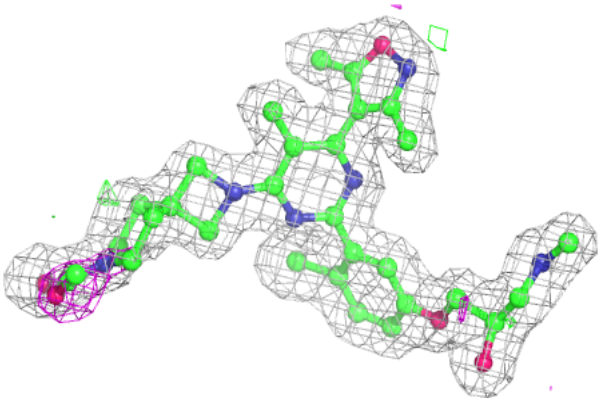


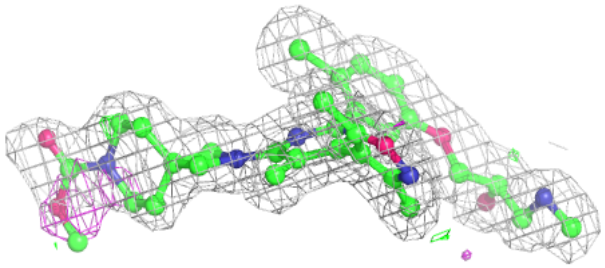


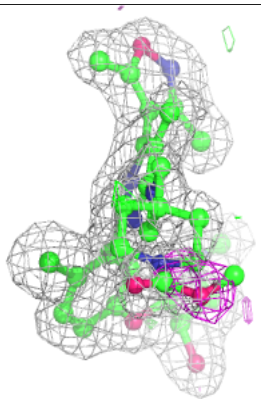


Electron density around BW4 A 502 (A):

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

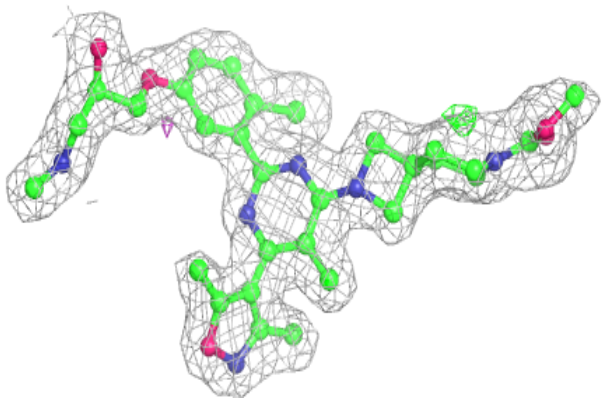


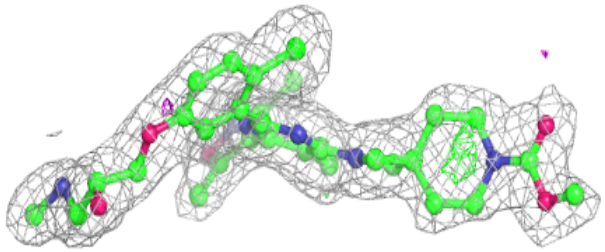


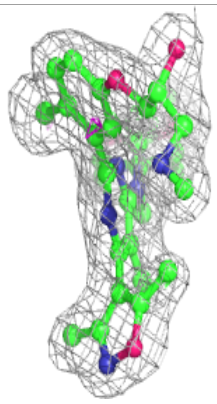


Electron density around BW4 D 502 (B):

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

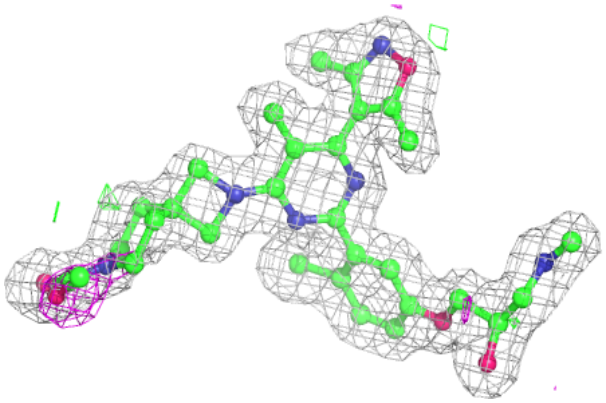


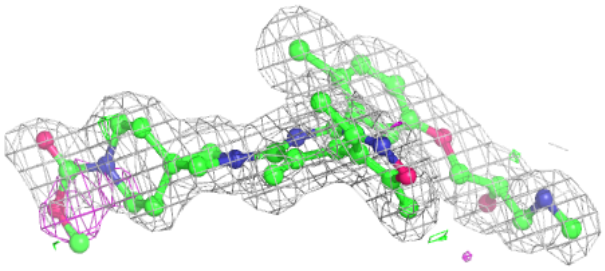


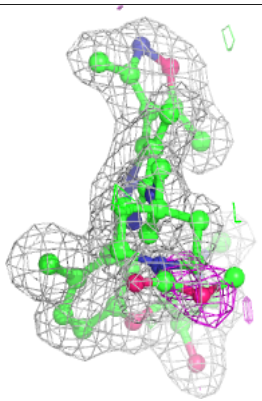


Electron density around BW4 A 502 (B):

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

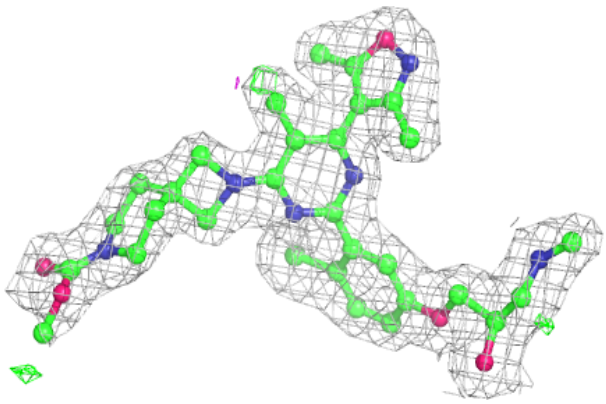


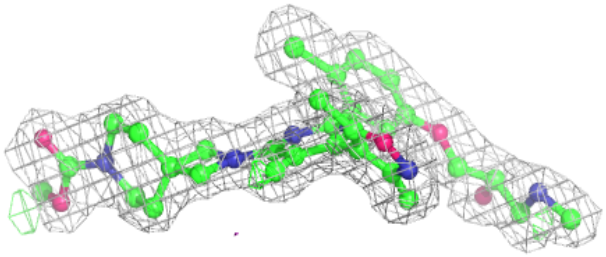


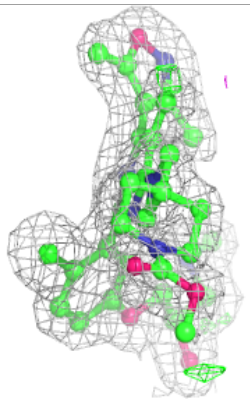


Electron density around BW4 C 502 (A):

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

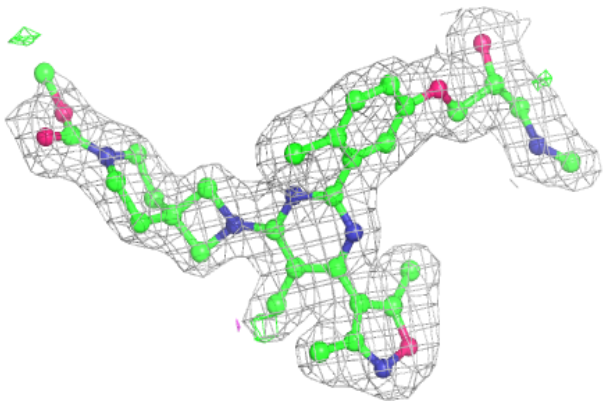


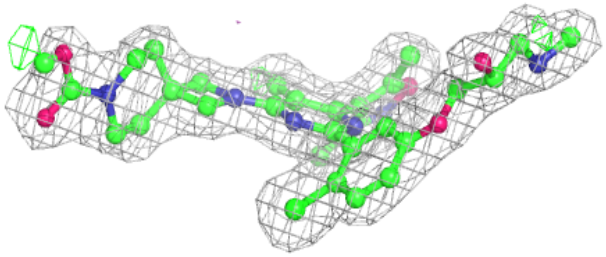


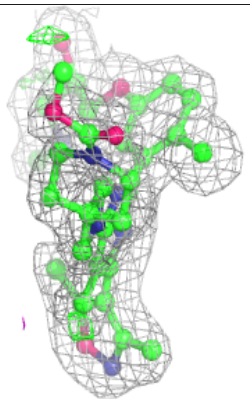


Electron density around BW4 C 502 (B):

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

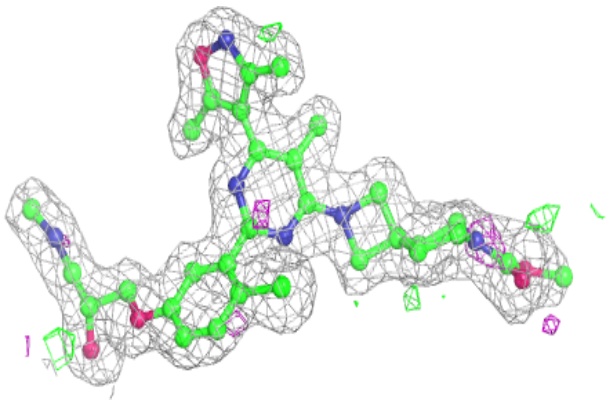


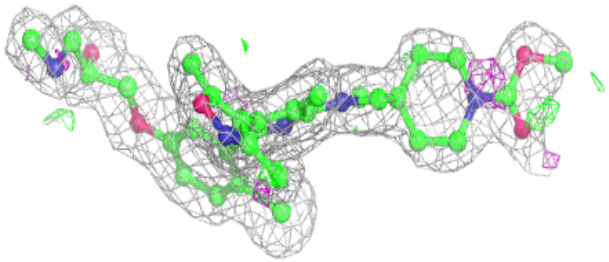


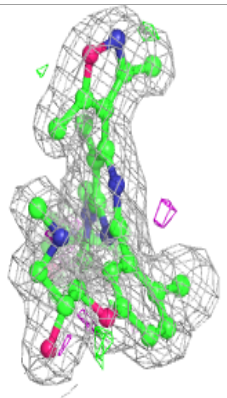


Electron density around BW4 B 502 (B):

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

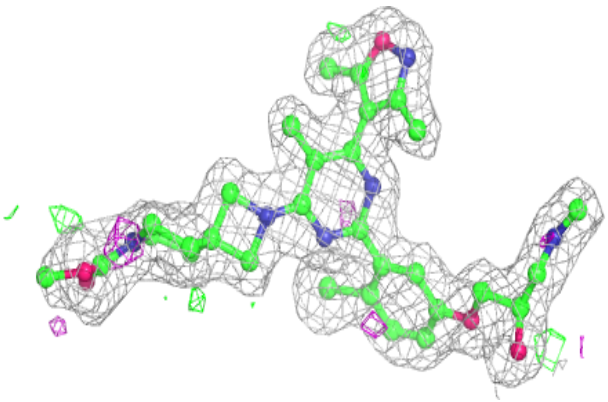


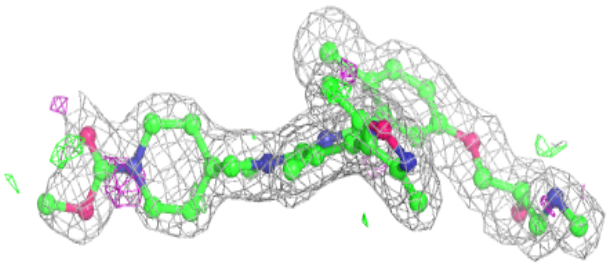


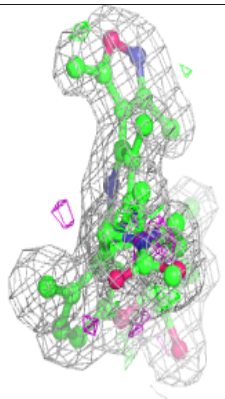


Electron density around BW4 B 502 (A):

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

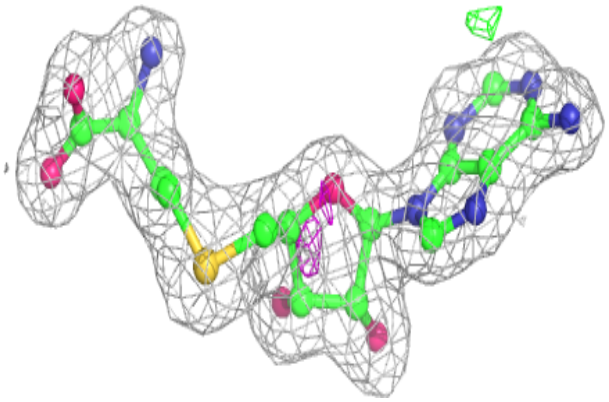


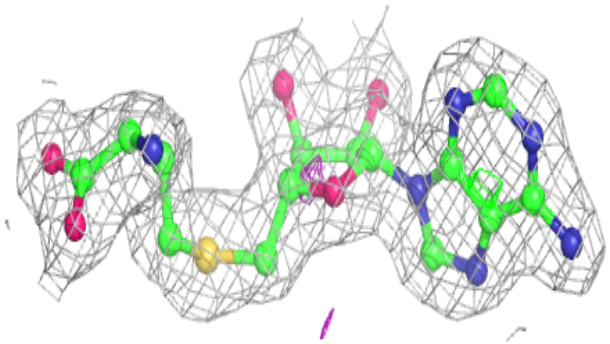


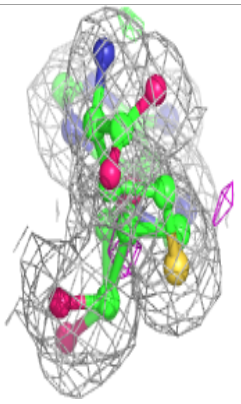


Electron density around SAH D 501:

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

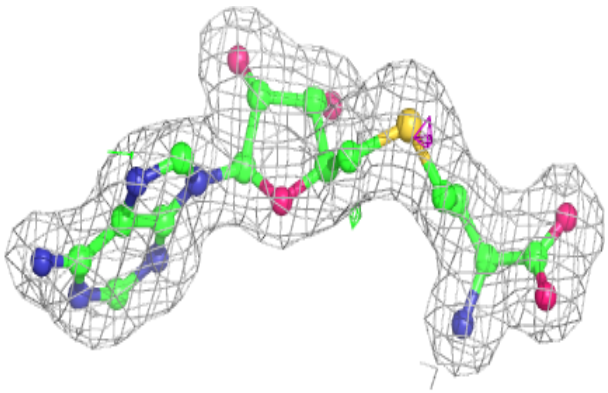


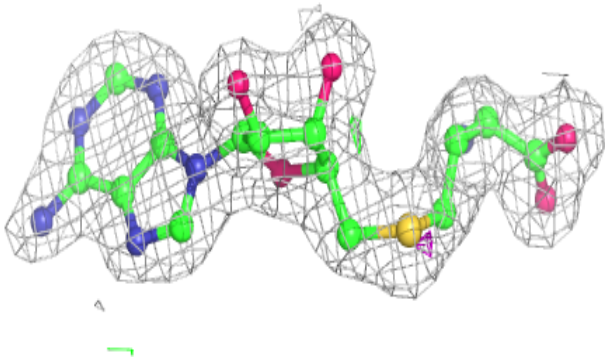


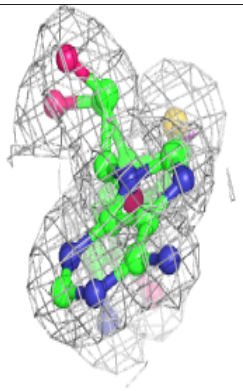


Electron density around SAH C 501:

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

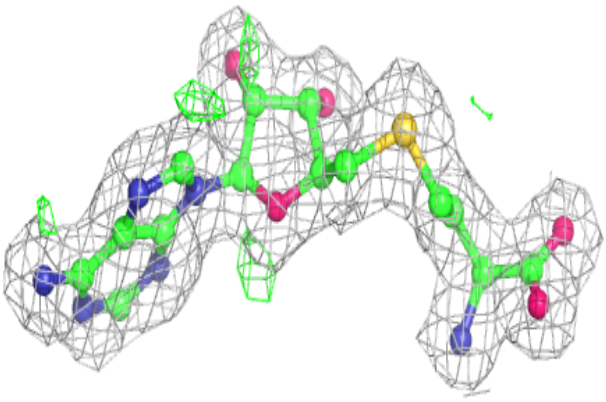


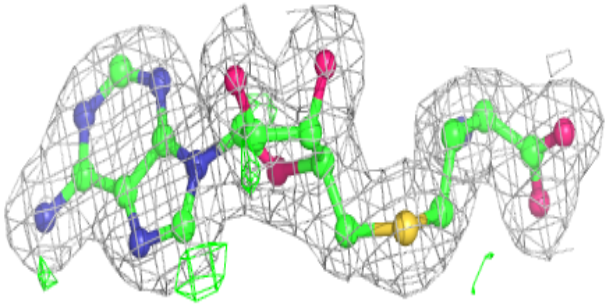


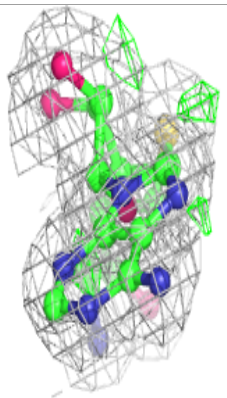


Electron density around SAH A 501:

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

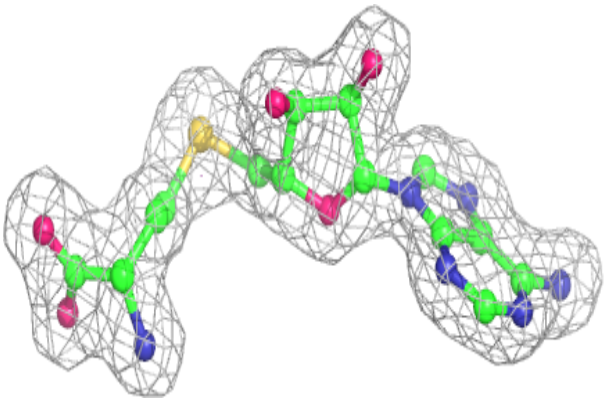


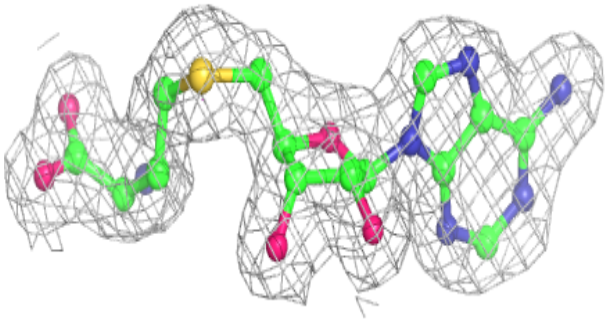


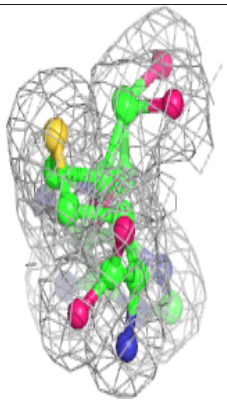


Electron density around SAH B 501:

$2mF_o$-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 (i)

There are no such residues in this entry.