Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 01:36 AM EDT

PDB ID	:	3K5K
Title	:	Discovery of a 2,4-Diamino-7-aminoalkoxy-quinazoline as a Potent Inhibitor of Histone Lysine Methyltransferase, G9a
Authors	:	Dong, A.; Wasney, G.A.; Liu, F.; Chen, X.; Allali-Hassani, A.; Senisterra, G.; Chau, I.; Bountra, C.; Weigelt, J.; Edwards, A.M.; Arrowsmith, C.H.; Frye, S.V.; Bochkarev, A.; Brown, P.J.; Jin, J.; Vedadi, M.; Structural Genomics Consortium (SGC)
Deposited on	:	2009-10-07
Resolution	:	1.70 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

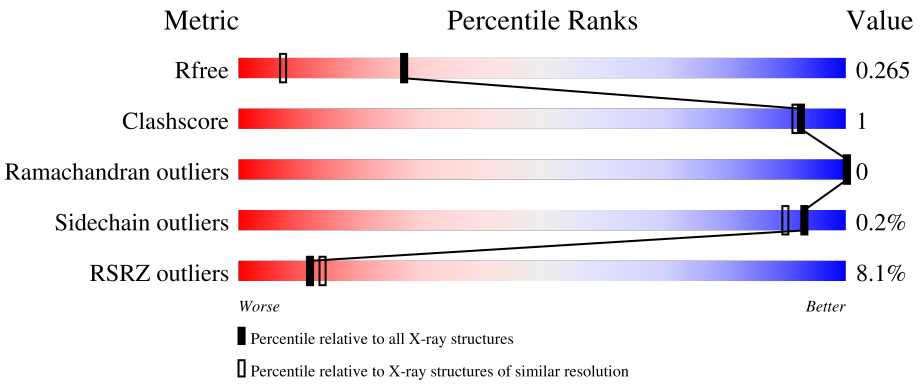
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	283	6% 92%
1	B	283	9% 93% 5%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 4816 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-lysine N-methyltransferase, H3 lysine-9 specific 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	272	2126	1329	370	404	23	11	3	0
1	B	269	2095	1307	362	403	23	6	1	0

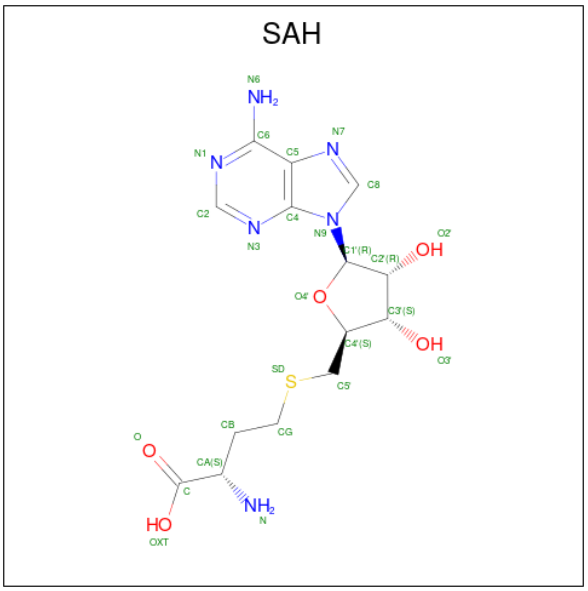
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	911	GLY	-	expression tag	UNP Q96KQ7
A	912	SER	-	expression tag	UNP Q96KQ7
B	911	GLY	-	expression tag	UNP Q96KQ7
B	912	SER	-	expression tag	UNP Q96KQ7

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

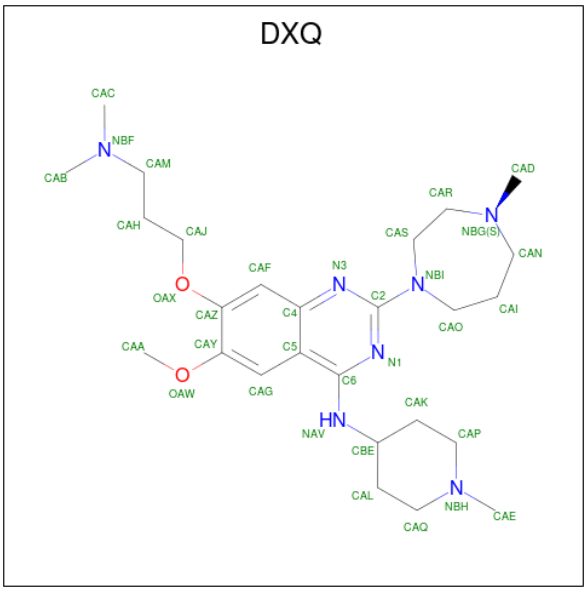
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	4	4	4	0	0
2	B	4	4	4	0	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

- Molecule 4 is 7-[3-(dimethylamino)propoxy]-6-methoxy-2-(4-methyl-1,4-diazepan-1-yl)-N-(1-methylpiperidin-4-yl)quinazolin-4-amine (three-letter code: DXQ) (formula: $C_{26}H_{43}N_7O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	35	26	7	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	35	26	7	2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	2	2	2	0	0
5	B	2	2	2	0	0

- Molecule 6 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	X		
6	A	1	1	1	0	0
6	B	1	1	1	0	0

- Molecule 7 is water.

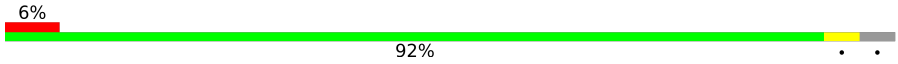
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	236	236	236	0	0
7	B	223	223	223	0	0

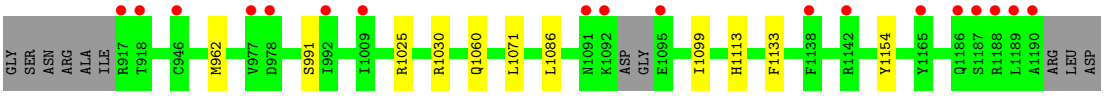
3 Residue-property plots (i)

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: Histone-lysine N-methyltransferase, H3 lysine-9 specific 3

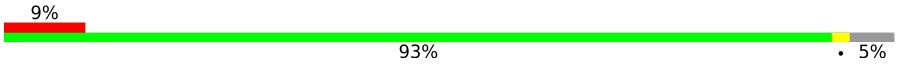
Chain A:

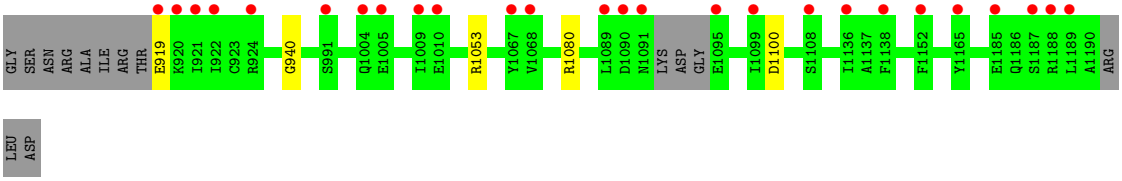




• Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-9 specific 3

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.67Å 78.07Å 72.51Å 90.00° 91.81° 90.00°	Depositor
Resolution (Å)	29.58 – 1.70 28.32 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.58-1.70) 97.0 (28.32-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.209 , 0.264 0.209 , 0.265	Depositor DCC
R_{free} test set	1372 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4816	wwPDB-VP
Average B, all atoms (Å^2)	35.0	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 21.86 % 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 6.4178e-03. 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, DXQ, SAH, CL, UNX

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	0.54	0/2171	0.60	0/2946
1	B	0.54	0/2140	0.60	0/2906
All	All	0.54	0/4311	0.60	0/5852

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	2126	0	1928	7	0
1	B	2095	0	1895	3	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	26	0	19	0	0
3	B	26	0	19	0	0
4	A	35	0	43	1	0
4	B	35	0	43	2	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	A	236	0	0	1	0
7	B	223	0	0	2	0
All	All	4816	0	3947	12	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 1.

All (12) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:919:GLU:HG3	1:B:940:GLY:HA3	1.75	0.68
1:B:919:GLU:CD	1:B:1053:ARG:HH22	2.15	0.49
1:A:1060:GLN:HG2	7:A:208:HOH:O	2.13	0.48
4:B:2001:DXQ:HAP	7:B:344:HOH:O	2.13	0.47
1:A:962:MET:HE3	1:A:1133:PHE:CE1	2.53	0.44
1:A:1025:ARG:O	1:A:1030:ARG:HD2	2.19	0.43
1:A:962:MET:HE3	1:A:1133:PHE:HE1	1.84	0.43
1:A:1086:LEU:O	4:A:2000:DXQ:HAJ	2.20	0.41
1:A:1113:HIS:HB2	1:A:1154:TYR:CG	2.56	0.41
1:A:1071:LEU:HD23	1:A:1099:ILE:HG12	2.03	0.40
1:B:1080:ARG:HD2	1:B:1100:ASP:OD2	2.21	0.40
4:B:2001:DXQ:HABB	7:B:310:HOH:O	2.22	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	271/283 (96%)	261 (96%)	10 (4%)	0	100 100
1	B	266/283 (94%)	253 (95%)	13 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	537/566 (95%)	514 (96%)	23 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	220/253 (87%)	219 (100%)	1 (0%)	88	83
1	B	221/253 (87%)	221 (100%)	0	100	100
All	All	441/506 (87%)	440 (100%)	1 (0%)	93	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	991	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	972	GLN
1	A	1060	GLN
1	B	1091	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 12 are monoatomic and 2 are unknown - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SAH	A	1198	-	24,28,28	1.14	3 (12%)	25,40,40	1.52	7 (28%)
4	DXQ	B	2001	-	37,38,38	1.20	3 (8%)	45,52,52	2.50	16 (35%)
3	SAH	B	1198	-	24,28,28	1.16	2 (8%)	25,40,40	1.39	5 (20%)
4	DXQ	A	2000	-	37,38,38	1.14	3 (8%)	45,52,52	2.46	13 (28%)

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	SAH	A	1198	-	-	3/11/31/31	0/3/3/3
4	DXQ	B	2001	-	-	1/17/38/38	0/4/4/4
3	SAH	B	1198	-	-	2/11/31/31	0/3/3/3
4	DXQ	A	2000	-	-	1/17/38/38	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2001	DXQ	C6-C5	-4.04	1.39	1.44
4	A	2000	DXQ	C6-C5	-3.46	1.40	1.44
3	A	1198	SAH	C5-C4	2.68	1.48	1.40
3	B	1198	SAH	C2-N3	2.65	1.36	1.32
3	B	1198	SAH	C5-C4	2.53	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2000	DXQ	CAF-CAZ	2.42	1.40	1.36
3	A	1198	SAH	O4'-C1'	2.16	1.44	1.41
4	A	2000	DXQ	CAG-CAY	2.15	1.40	1.36
3	A	1198	SAH	C2-N3	2.08	1.35	1.32
4	B	2001	DXQ	CAF-CAZ	2.05	1.40	1.36
4	B	2001	DXQ	CAG-CAY	2.01	1.40	1.36

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2000	DXQ	CAQ-NBH-CAP	6.54	118.67	109.52
4	A	2000	DXQ	C6-C5-C4	5.76	119.51	115.88
4	B	2001	DXQ	C6-C5-C4	5.68	119.46	115.88
4	A	2000	DXQ	CAR-CAS-NBI	-5.65	106.79	113.30
4	B	2001	DXQ	CAQ-NBH-CAP	5.62	117.38	109.52
4	B	2001	DXQ	CAR-CAS-NBI	-5.37	107.11	113.30
4	B	2001	DXQ	C5-C6-NAV	-5.37	115.56	120.63
4	B	2001	DXQ	CAG-C5-C6	-5.19	120.20	124.88
4	A	2000	DXQ	CAG-C5-C6	-5.16	120.22	124.88
4	B	2001	DXQ	C6-NAV-CBE	4.75	133.20	124.16
4	A	2000	DXQ	C6-NAV-CBE	4.61	132.92	124.16
4	A	2000	DXQ	C5-C6-NAV	-4.53	116.36	120.63
4	A	2000	DXQ	C5-C4-N3	-4.00	118.56	122.81
3	B	1198	SAH	N3-C2-N1	-3.76	122.80	128.68
3	A	1198	SAH	N3-C2-N1	-3.70	122.90	128.68
4	B	2001	DXQ	C5-C4-N3	-3.52	119.08	122.81
4	A	2000	DXQ	CAK-CBE-NAV	3.23	115.63	110.60
4	B	2001	DXQ	CAI-CAN-NBG	-3.13	109.35	117.34
4	B	2001	DXQ	CAS-NBI-CAO	3.09	122.99	117.47
4	B	2001	DXQ	OAW-CAY-CAG	-3.08	121.26	125.24
4	B	2001	DXQ	NAV-C6-N1	3.07	125.42	118.90
3	A	1198	SAH	C2-N1-C6	2.79	123.53	118.75
3	B	1198	SAH	OXT-C-O	-2.78	117.78	124.09
4	B	2001	DXQ	N1-C2-NBI	2.76	120.52	117.11
4	A	2000	DXQ	OAW-CAY-CAG	-2.75	121.68	125.24
4	B	2001	DXQ	CAL-CBE-NAV	2.68	114.77	110.60
4	B	2001	DXQ	CAK-CBE-NAV	2.66	114.74	110.60
4	A	2000	DXQ	NAV-C6-N1	2.63	124.48	118.90
4	B	2001	DXQ	OAW-CAY-CAZ	2.54	118.95	115.41
3	B	1198	SAH	OXT-C-CA	2.49	121.87	113.38
3	B	1198	SAH	N6-C6-N1	2.37	123.49	118.57
3	A	1198	SAH	O4'-C1'-C2'	-2.32	103.53	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1198	SAH	OXT-C-CA	2.32	121.30	113.38
4	B	2001	DXQ	CAP-CAK-CBE	-2.21	106.63	110.50
3	B	1198	SAH	C2-N1-C6	2.20	122.51	118.75
3	A	1198	SAH	C4-C5-N7	-2.18	107.13	109.40
4	A	2000	DXQ	CAS-NBI-CAO	2.18	121.36	117.47
4	A	2000	DXQ	CAQ-CAL-CBE	-2.13	106.76	110.50
3	A	1198	SAH	OXT-C-O	-2.11	119.30	124.09
3	A	1198	SAH	C3'-C2'-C1'	2.06	104.08	100.98
4	A	2000	DXQ	OAW-CAY-CAZ	2.00	118.20	115.41

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2000	DXQ	CAK-CBE-NAV-C6
4	B	2001	DXQ	CAK-CBE-NAV-C6
3	A	1198	SAH	CB-CG-SD-C5'
3	A	1198	SAH	OXT-C-CA-CB
3	B	1198	SAH	CB-CG-SD-C5'
3	A	1198	SAH	O-C-CA-CB
3	B	1198	SAH	O-C-CA-CB

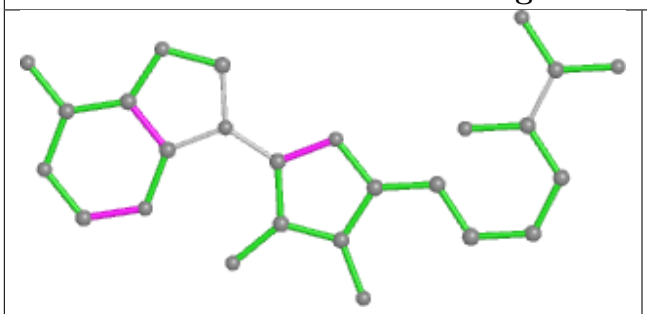
There are no ring outliers.

2 monomers are involved in 3 short contacts:

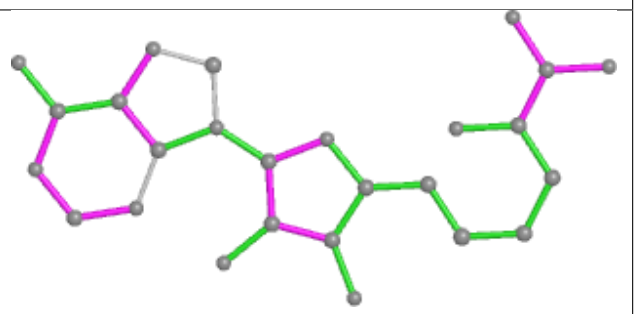
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2001	DXQ	2	0
4	A	2000	DXQ	1	0

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.

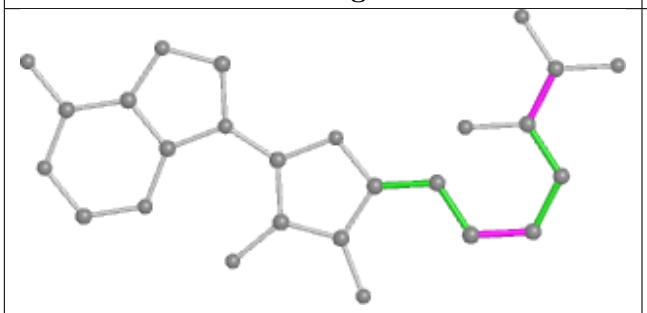
Ligand SAH A 1198



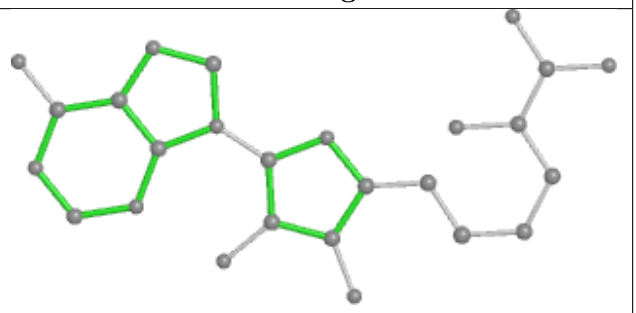
Bond lengths



Bond angles

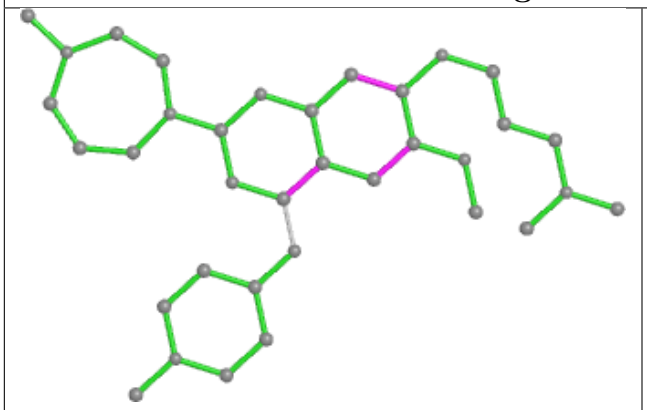


Torsions

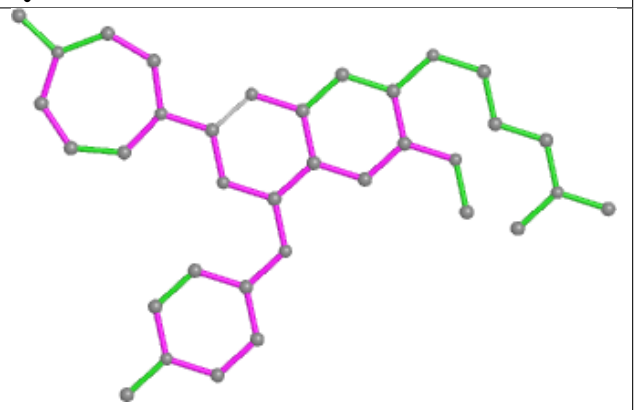


Rings

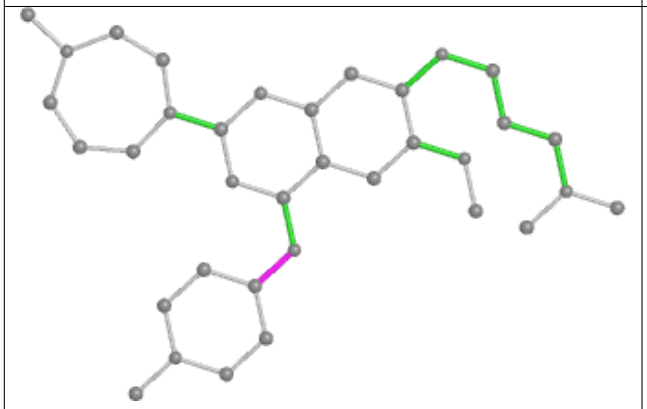
Ligand DXQ B 2001



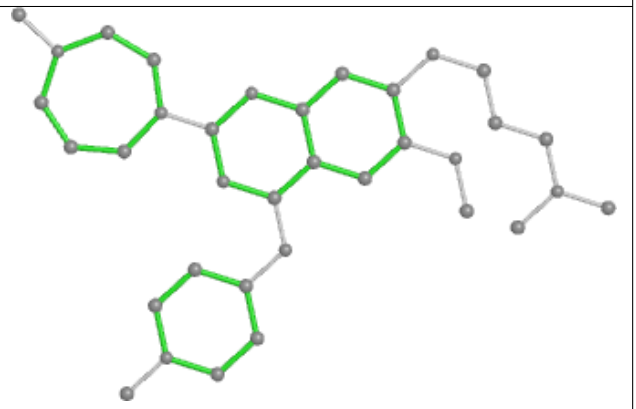
Bond lengths



Bond angles

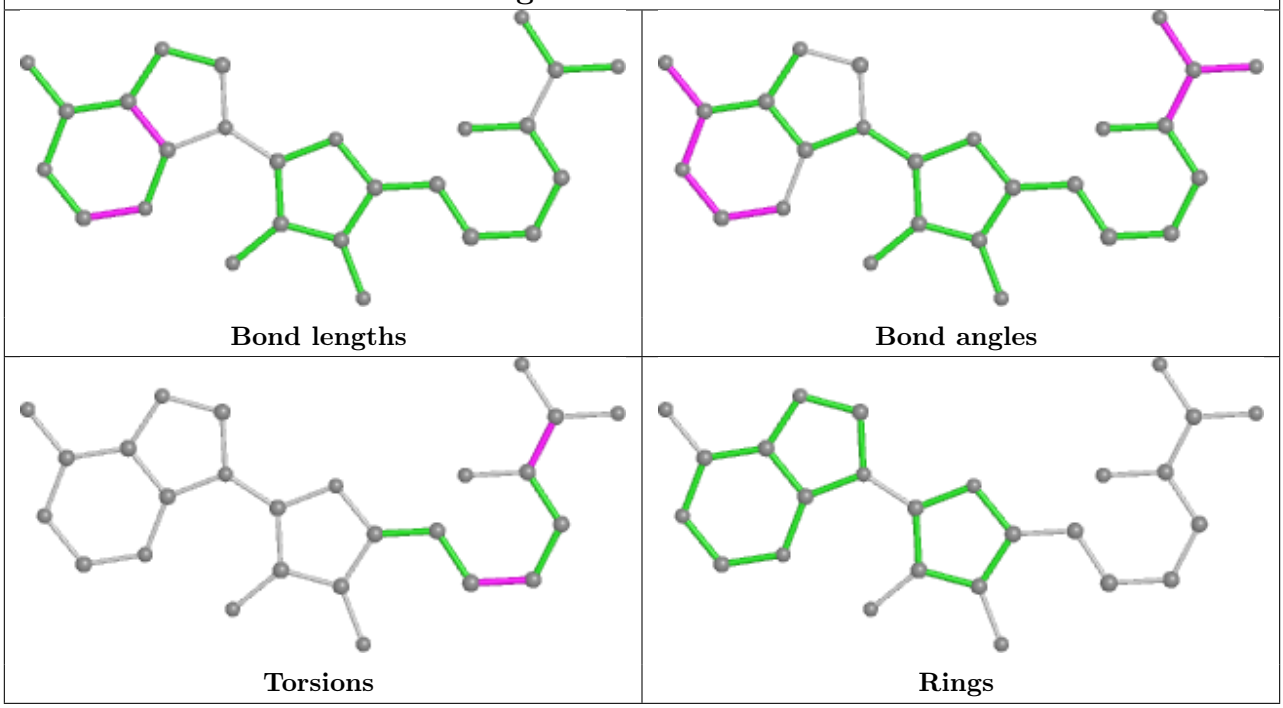


Torsions

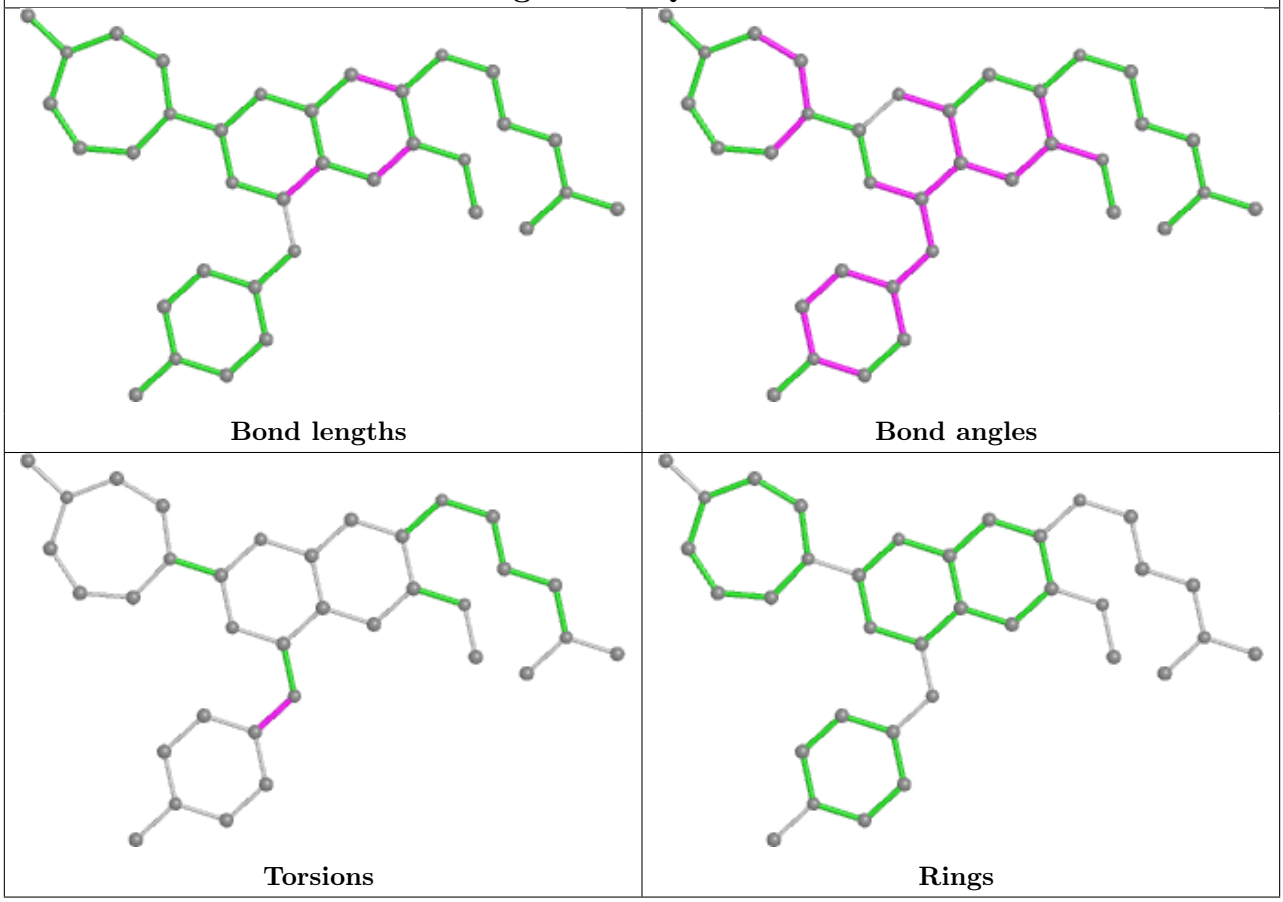


Rings

Ligand SAH B 1198



Ligand DXQ A 2000



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	272/283 (96%)	0.40	18 (6%)	18	20	23, 33, 48, 68	2 (0%)
1	B	269/283 (95%)	0.44	26 (9%)	7	8	19, 33, 52, 67	1 (0%)
All	All	541/566 (95%)	0.42	44 (8%)	12	14	19, 33, 51, 68	3 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1108[A]	SER	9.3
1	A	946	CYS	8.4
1	A	1189	LEU	7.3
1	A	977	VAL	6.7
1	A	1091	ASN	6.0
1	B	921	ILE	5.4
1	A	1190	ALA	4.5
1	A	1187	SER	4.4
1	B	1091	ASN	4.3
1	B	920	LYS	4.0
1	A	1186	GLN	3.7
1	A	1165	TYR	3.6
1	A	917	ARG	3.5
1	A	1142[A]	ARG	3.4
1	A	1188	ARG	3.4
1	B	1095	GLU	3.3
1	B	1099	ILE	3.2
1	A	1009	ILE	3.1
1	A	978	ASP	3.0
1	B	1165	TYR	2.9
1	B	1152	PHE	2.8
1	B	1005	GLU	2.7
1	B	1004	GLN	2.7
1	A	992	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1187	SER	2.6
1	A	1095	GLU	2.5
1	A	918	THR	2.5
1	B	1189	LEU	2.5
1	B	991	SER	2.5
1	B	1188	ARG	2.4
1	A	1138	PHE	2.4
1	B	1138	PHE	2.4
1	B	1067	TYR	2.4
1	B	1068	VAL	2.3
1	B	1185	GLU	2.3
1	B	922	ILE	2.3
1	B	924	ARG	2.2
1	B	1009	ILE	2.2
1	A	1092	LYS	2.1
1	B	1010	GLU	2.1
1	B	1136	ILE	2.1
1	B	1089	LEU	2.1
1	B	1090	ASP	2.0
1	B	919	GLU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DXQ	B	2001	35/35	0.81	0.15	37,40,51,53	0
6	UNX	B	1199	1/1	0.83	0.34	30,30,30,30	0
5	CL	A	3004	1/1	0.88	0.10	59,59,59,59	0

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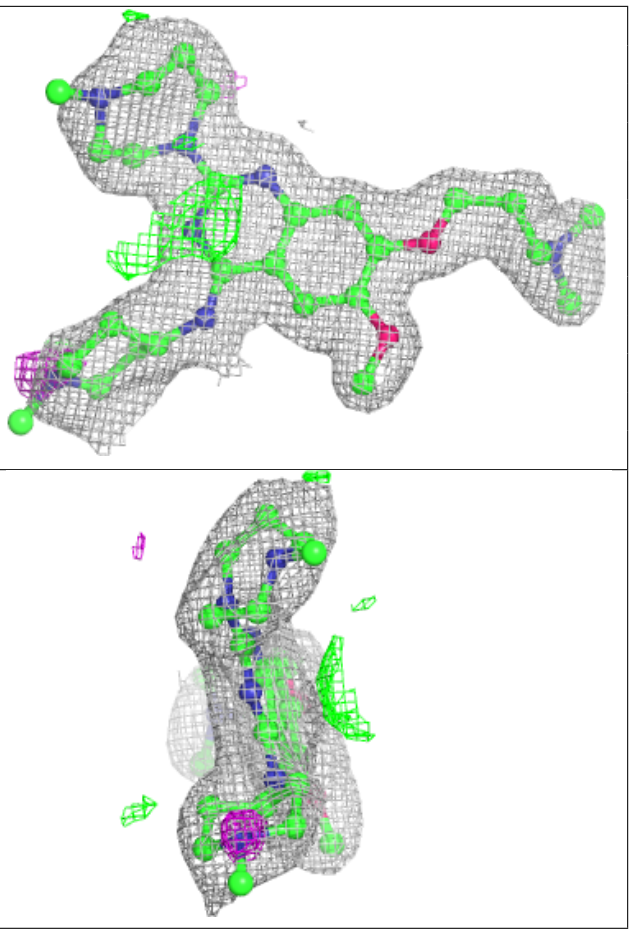
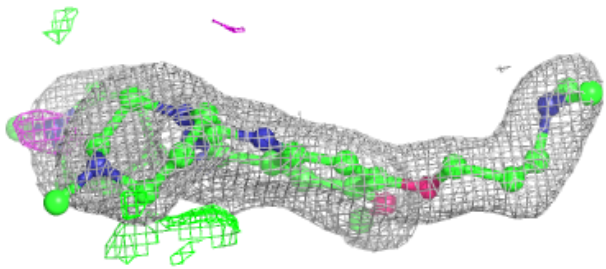
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	UNX	A	1199	1/1	0.88	0.34	30,30,30,30	0
4	DXQ	A	2000	35/35	0.88	0.11	35,43,52,53	0
5	CL	B	3005	1/1	0.90	0.08	68,68,68,68	0
3	SAH	B	1198	26/26	0.93	0.11	29,31,33,34	0
3	SAH	A	1198	26/26	0.94	0.08	29,31,34,35	0
5	CL	B	3003	1/1	0.98	0.10	28,28,28,28	0
2	ZN	B	1197	1/1	0.98	0.04	37,37,37,37	0
2	ZN	A	1197	1/1	0.99	0.03	37,37,37,37	0
2	ZN	B	1194	1/1	0.99	0.06	27,27,27,27	0
5	CL	A	3001	1/1	0.99	0.14	23,23,23,23	0
2	ZN	B	1195	1/1	0.99	0.05	27,27,27,27	0
2	ZN	B	1196	1/1	0.99	0.07	29,29,29,29	0
2	ZN	A	1194	1/1	0.99	0.06	33,33,33,33	0
2	ZN	A	1195	1/1	0.99	0.04	32,32,32,32	0
2	ZN	A	1196	1/1	0.99	0.02	35,35,35,35	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 DXQ B 2001:

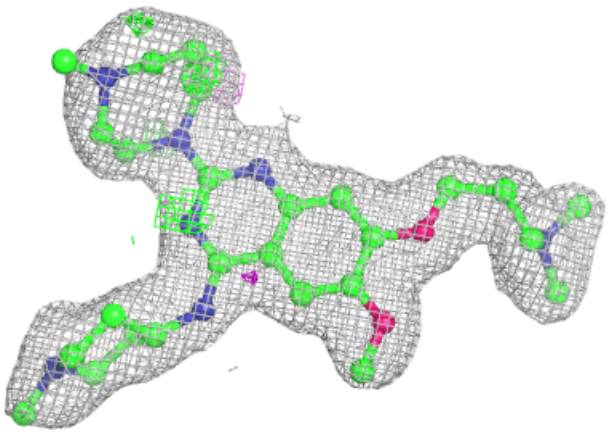
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

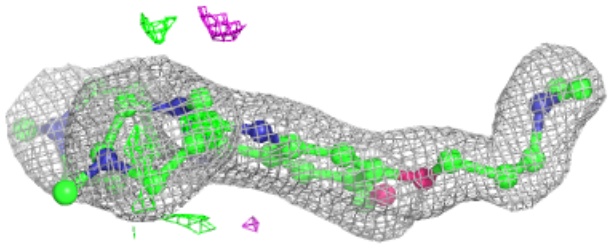


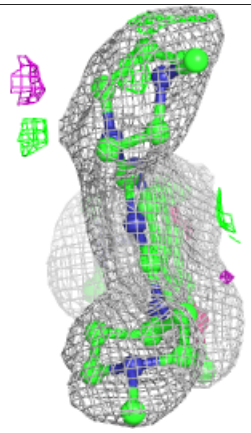


Electron density around DXQ A 2000:

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

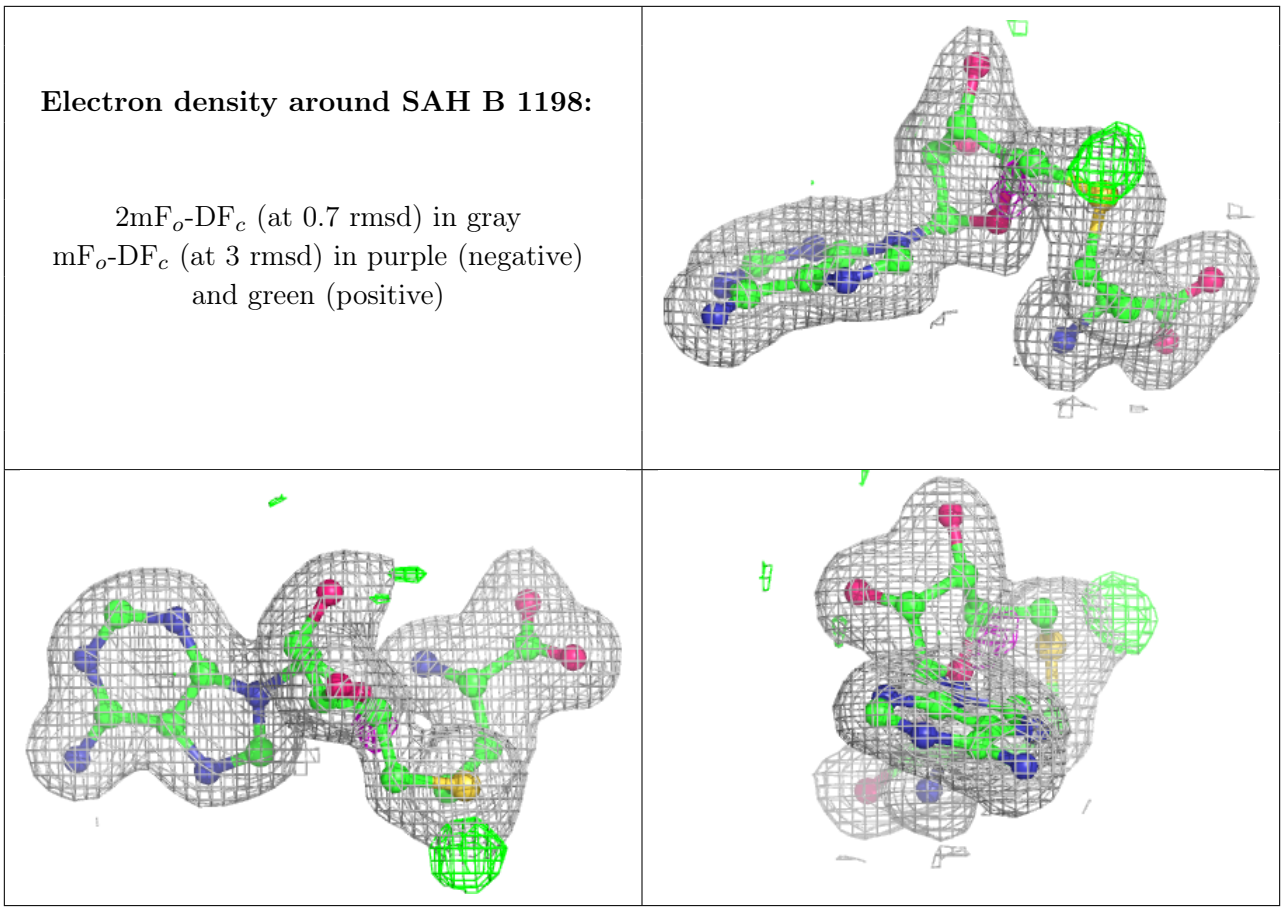






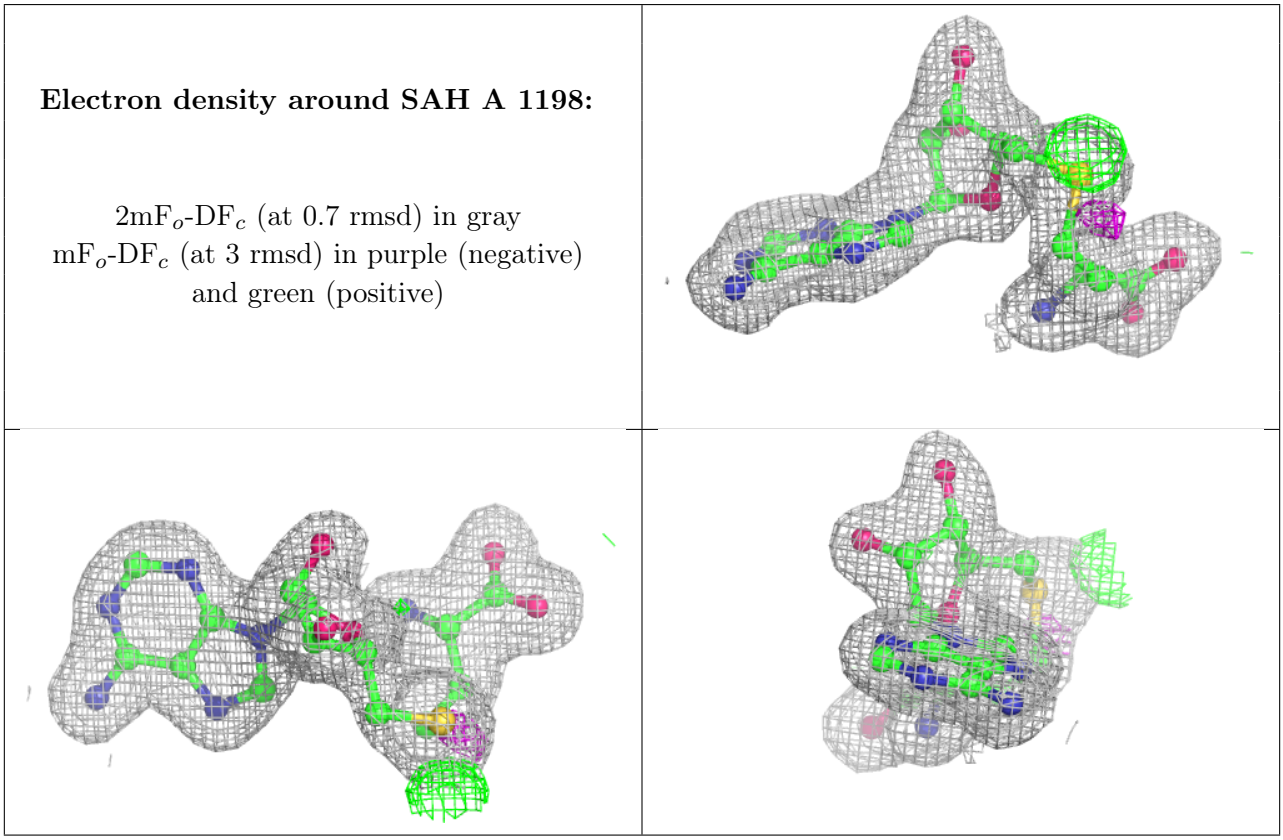
Electron density around SAH B 1198:

$2mF_o$-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 1198:

$2mF_o$-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.