Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 02:32 PM EDT

PDB ID	:	2A5B
Title	:	Avidin complexed with 8-oxodeoxyguanosine
Authors	:	Conners, R.; Hooley, E.; Thomas, S.; Brady, R.L.
Deposited on	:	2005-06-30
Resolution	:	2.49 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:

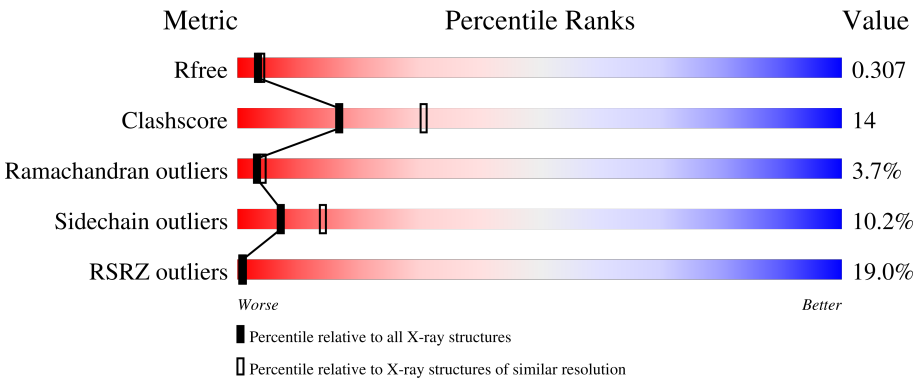
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	124	19% 64% 27% 9% •
1	B	124	19% 71% 23% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2040 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.

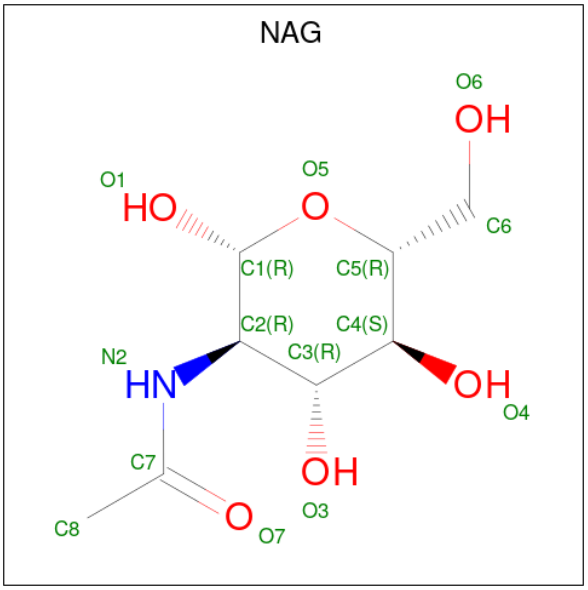
- Molecule 1 is a protein called Avidin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	124	974	607	174	189	4	24	0	0
1	B	124	974	607	174	189	4	40	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	THR	ILE	variant	UNP P02701
B	34	THR	ILE	variant	UNP P02701

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



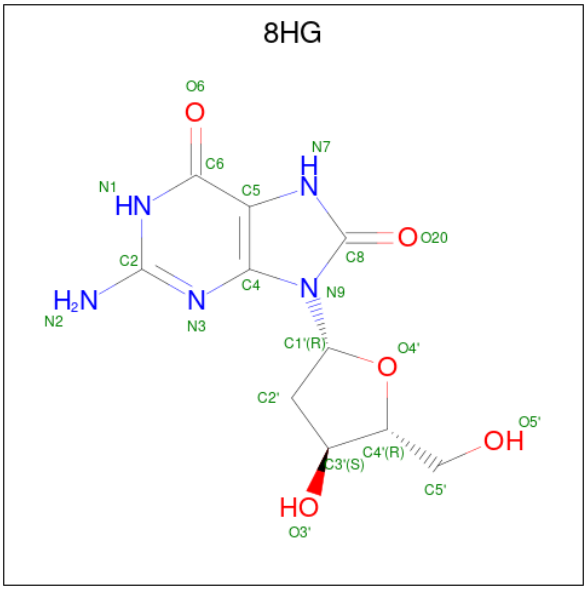
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	14	8	1	5	0	0

- Molecule 3 is 2'-DEOXY-8-OXOGUANOSINE (three-letter code: 8HG) (formula: $C_{10}H_{13}N_5O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	20	10	5	5	0	0

- Molecule 4 is water.

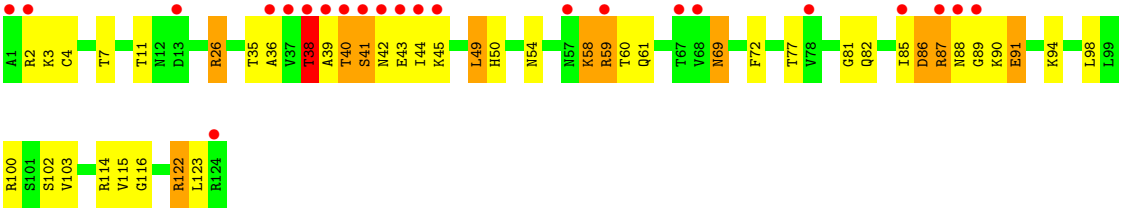
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	19	19	19	0	0
			Total	O		
4	B	25	25	25	0	0

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.

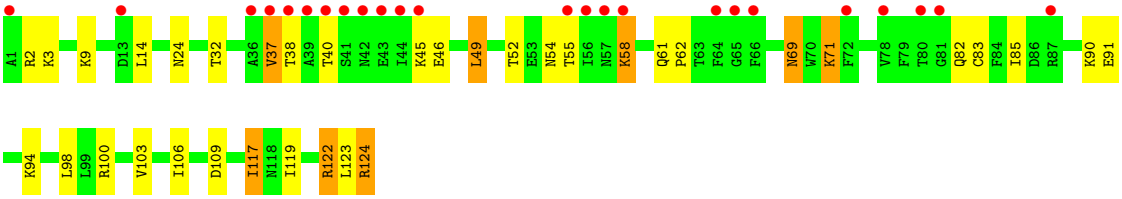
- Molecule 1: Avidin

Chain A:



- Molecule 1: Avidin

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	70.02Å 79.49Å 42.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.70 – 2.49 25.67 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.5 (52.70-2.49) 98.6 (25.67-2.49)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.219 , 0.310 0.215 , 0.307	Depositor DCC
R_{free} test set	413 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	48.4	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 40.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	2040	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.16% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 8HG

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	1.03	3/992 (0.3%)	1.08	4/1341 (0.3%)
1	B	1.04	4/992 (0.4%)	1.19	9/1341 (0.7%)
All	All	1.03	7/1984 (0.4%)	1.13	13/2682 (0.5%)

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	A	1	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	9	LYS	CD-CE	-10.64	1.24	1.51
1	A	90	LYS	CA-CB	-10.28	1.31	1.53
1	B	71	LYS	CA-CB	-8.65	1.34	1.53
1	A	26	ARG	CG-CD	-8.59	1.30	1.51
1	A	58	LYS	CA-CB	-6.89	1.38	1.53
1	B	58	LYS	CA-CB	-5.39	1.42	1.53
1	B	45	LYS	CG-CD	-5.18	1.34	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	90	LYS	N-CA-CB	15.39	138.30	110.60
1	B	124	ARG	N-CA-CB	-14.13	85.16	110.60
1	B	124	ARG	CA-CB-CG	14.04	144.29	113.40
1	B	45	LYS	CB-CG-CD	13.11	145.70	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	90	LYS	CA-CB-CG	9.73	134.81	113.40
1	B	49	LEU	CA-CB-CG	7.89	133.44	115.30
1	B	45	LYS	CG-CD-CE	7.64	134.83	111.90
1	A	49	LEU	CA-CB-CG	7.62	132.83	115.30
1	B	3	LYS	CA-CB-CG	6.49	127.69	113.40
1	B	90	LYS	CB-CG-CD	-6.13	95.65	111.60
1	B	117	ILE	CB-CA-C	-5.54	100.52	111.60
1	A	114	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	69	ASN	N-CA-CB	-5.17	101.30	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	90	LYS	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	59	ARG	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	974	0	959	36	0
1	B	974	0	960	28	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	20	0	13	3	0
4	A	19	0	0	1	0
4	B	25	0	0	0	0
All	All	2040	0	1958	53	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 14.

All (53) 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:A:39:ALA:O	1:A:40:THR:OG1	1.70	1.09
3:A:255:8HG:H2'2	4:A:273:HOH:O	1.60	1.01
1:A:2:ARG:HG2	1:A:85:ILE:HD12	1.51	0.93
1:B:122:ARG:HH11	1:B:122:ARG:HG3	1.32	0.93
1:B:61:GLN:HE21	1:B:85:ILE:H	1.15	0.90
1:A:36:ALA:HB1	1:A:40:THR:HG22	1.60	0.82
1:A:39:ALA:C	1:A:40:THR:HG1	1.82	0.82
1:B:61:GLN:NE2	1:B:85:ILE:H	1.80	0.79
1:A:86:ASP:O	1:A:87:ARG:O	2.02	0.78
1:A:40:THR:O	1:A:41:SER:HB3	1.84	0.75
1:A:69:ASN:HD21	1:B:54:ASN:HA	1.58	0.69
1:A:82:GLN:HE22	1:B:103:VAL:H	1.41	0.67
1:A:7:THR:O	1:A:122:ARG:NH2	2.28	0.67
1:B:122:ARG:HH11	1:B:122:ARG:CG	2.08	0.66
1:B:122:ARG:HG3	1:B:122:ARG:NH1	2.09	0.65
1:A:40:THR:O	1:A:41:SER:CB	2.46	0.63
1:A:4:CYS:SG	1:A:91:GLU:HG2	2.42	0.59
1:A:61:GLN:HE21	1:A:85:ILE:H	1.51	0.58
1:A:103:VAL:H	1:B:82:GLN:HE22	1.51	0.57
1:A:2:ARG:HD2	1:A:85:ILE:HG21	1.84	0.57
1:A:82:GLN:HE22	1:B:103:VAL:HG22	1.72	0.55
1:B:62:PRO:HD2	1:B:83:CYS:HB3	1.87	0.55
1:B:32:THR:HG21	1:B:46:GLU:OE1	2.06	0.54
1:B:94:LYS:HD2	1:B:119:ILE:HG12	1.91	0.53
1:A:59:ARG:HB3	1:A:60:THR:O	2.09	0.53
1:B:91:GLU:OE1	1:B:122:ARG:NH1	2.42	0.51
1:A:100:ARG:HH21	1:B:82:GLN:NE2	2.10	0.50
1:A:36:ALA:CB	1:A:40:THR:HG22	2.34	0.50
1:A:54:ASN:HA	1:B:69:ASN:HD21	1.75	0.50
1:A:38:THR:HG22	1:A:39:ALA:H	1.77	0.49
1:A:86:ASP:O	1:A:87:ARG:C	2.50	0.49
1:A:86:ASP:OD2	1:A:87:ARG:N	2.46	0.49
1:A:100:ARG:HH21	1:B:82:GLN:HE21	1.59	0.48
1:B:100:ARG:NH2	1:B:109:ASP:OD1	2.41	0.47
1:B:32:THR:HG23	1:B:46:GLU:HG3	1.97	0.45
1:B:61:GLN:NE2	1:B:85:ILE:N	2.58	0.45
1:A:50:HIS:CD2	1:B:52:THR:HG21	2.52	0.45
1:B:24:ASN:OD1	1:B:24:ASN:C	2.56	0.44
1:A:11:THR:HB	1:A:123:LEU:HD13	1.99	0.44
1:B:117:ILE:O	1:B:117:ILE:HG13	2.18	0.44
1:A:88:ASN:N	1:A:89:GLY:HA3	2.31	0.43
1:A:77:THR:OG1	3:A:255:8HG:N2	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:GLN:HE21	1:B:100:ARG:HH21	1.67	0.43
1:A:82:GLN:NE2	1:B:103:VAL:H	2.12	0.42
1:A:42:ASN:CG	1:A:43:GLU:H	2.22	0.42
1:A:81:GLY:HA2	1:B:100:ARG:HD3	2.02	0.42
1:B:91:GLU:CD	1:B:122:ARG:HH12	2.21	0.42
1:A:115:VAL:HG22	1:A:116:GLY:N	2.35	0.41
1:A:98:LEU:HG	1:B:98:LEU:HG	2.01	0.41
1:A:45:LYS:HD3	1:A:72:PHE:CG	2.55	0.41
1:A:39:ALA:O	1:A:40:THR:CB	2.65	0.41
1:A:72:PHE:CE1	3:A:255:8HG:H4'	2.56	0.41
1:B:122:ARG:CG	1:B:122:ARG:NH1	2.72	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	122/124 (98%)	106 (87%)	11 (9%)	5 (4%)	3 3
1	B	122/124 (98%)	108 (88%)	10 (8%)	4 (3%)	4 5
All	All	244/248 (98%)	214 (88%)	21 (9%)	9 (4%)	3 4

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	A	41	SER
1	A	87	ARG
1	B	58	LYS
1	A	58	LYS
1	B	38	THR
1	B	40	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	40	THR
1	B	37	VAL

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	108/108 (100%)	96 (89%)	12 (11%)	6 11
1	B	108/108 (100%)	98 (91%)	10 (9%)	9 17
All	All	216/216 (100%)	194 (90%)	22 (10%)	7 14

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	26	ARG
1	A	35	THR
1	A	38	THR
1	A	44	ILE
1	A	49	LEU
1	A	69	ASN
1	A	86	ASP
1	A	91	GLU
1	A	94	LYS
1	A	102	SER
1	A	122	ARG
1	B	2	ARG
1	B	14	LEU
1	B	37	VAL
1	B	49	LEU
1	B	55	THR
1	B	71	LYS
1	B	106	ILE
1	B	122	ARG
1	B	123	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	124	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	61	GLN
1	A	69	ASN
1	A	82	GLN
1	B	61	GLN
1	B	69	ASN
1	B	82	GLN

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)

3 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	NAG	B	201	1	14,14,15	0.61	0	17,19,21	1.36	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	A	201	1	14,14,15	0.78	0	17,19,21	2.35	8 (47%)
3	8HG	A	255	-	22,22,22	1.67	5 (22%)	30,33,33	3.59	16 (53%)

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	NAG	B	201	1	-	2/6/23/26	0/1/1/1
2	NAG	A	201	1	-	0/6/23/26	0/1/1/1
3	8HG	A	255	-	-	4/6/18/18	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	255	8HG	C8-N9	-3.29	1.35	1.40
3	A	255	8HG	O20-C8	3.24	1.29	1.23
3	A	255	8HG	C4-N9	-2.99	1.33	1.39
3	A	255	8HG	C5-C4	2.90	1.41	1.37
3	A	255	8HG	C6-N1	-2.61	1.34	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	255	8HG	O4'-C1'-N9	11.32	119.68	108.29
3	A	255	8HG	C5-C4-N3	-7.73	119.82	127.80
3	A	255	8HG	N7-C8-N9	6.97	114.85	106.58
3	A	255	8HG	C2'-C1'-N9	-6.16	108.72	116.01
3	A	255	8HG	N9-C4-N3	3.96	130.34	125.81
2	A	201	NAG	C4-C3-C2	3.84	116.64	111.02
3	A	255	8HG	C2-N3-C4	3.76	118.99	112.30
2	A	201	NAG	C1-O5-C5	3.73	117.24	112.19
2	A	201	NAG	C3-C4-C5	3.68	116.81	110.24
3	A	255	8HG	C5-N7-C8	-3.62	104.26	109.47
2	A	201	NAG	O5-C5-C4	3.61	119.60	110.83
2	A	201	NAG	C2-N2-C7	-3.51	117.90	122.90
3	A	255	8HG	O4'-C4'-C5'	2.90	115.47	109.21
2	B	201	NAG	C1-O5-C5	2.82	116.02	112.19
3	A	255	8HG	C2-N1-C6	-2.82	119.96	125.10
3	A	255	8HG	C4'-O4'-C1'	-2.75	102.80	109.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	255	8HG	N2-C2-N3	-2.66	114.56	119.73
2	A	201	NAG	O3-C3-C4	-2.45	104.68	110.35
3	A	255	8HG	C5-C6-N1	2.43	119.54	112.31
3	A	255	8HG	O20-C8-N9	-2.38	122.66	125.99
3	A	255	8HG	N2-C2-N1	2.33	121.67	116.71
3	A	255	8HG	O20-C8-N7	-2.29	122.49	126.64
2	A	201	NAG	C1-C2-N2	2.24	114.31	110.49
2	B	201	NAG	C2-N2-C7	-2.13	119.86	122.90
2	A	201	NAG	C6-C5-C4	-2.03	108.25	113.00
3	A	255	8HG	O6-C6-C5	-2.02	122.62	127.24

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	255	8HG	O4'-C1'-N9-C4
3	A	255	8HG	C3'-C4'-C5'-O5'
3	A	255	8HG	O4'-C4'-C5'-O5'
2	B	201	NAG	C4-C5-C6-O6
2	B	201	NAG	O5-C5-C6-O6
3	A	255	8HG	C2'-C1'-N9-C8

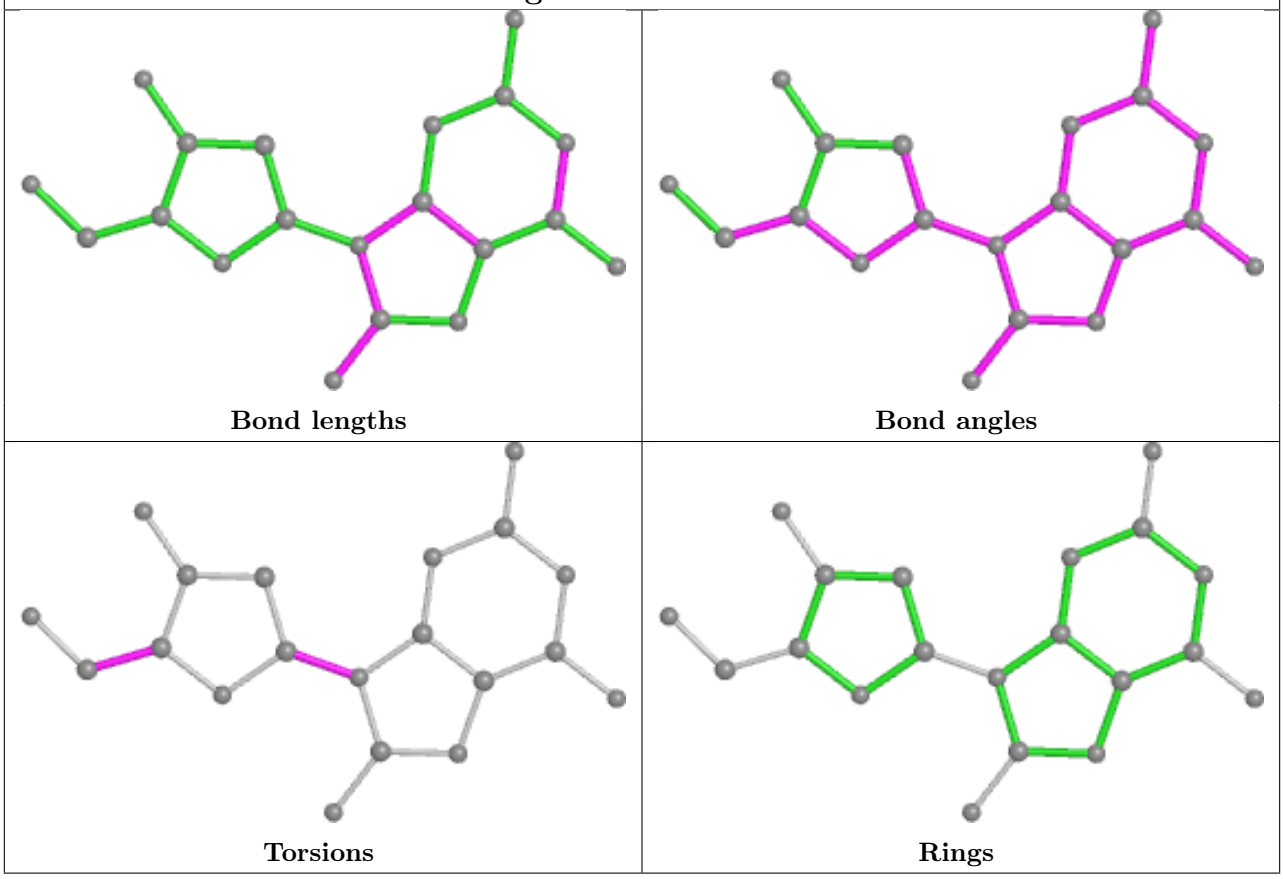
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	255	8HG	3	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 8HG A 255



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	124/124 (100%)	1.83	23 (18%)	1	1	19, 34, 50, 59	21 (16%)
1	B	124/124 (100%)	1.04	24 (19%)	1	1	20, 34, 61, 66	18 (14%)
All	All	248/248 (100%)	1.43	47 (18%)	1	1	19, 34, 55, 66	39 (15%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	VAL	24.4
1	A	42	ASN	23.1
1	A	38	THR	21.6
1	A	1	ALA	21.3
1	A	36	ALA	20.2
1	B	38	THR	15.4
1	A	40	THR	14.4
1	B	39	ALA	13.3
1	B	41	SER	13.1
1	B	40	THR	12.4
1	A	43	GLU	12.2
1	A	124	ARG	12.1
1	A	39	ALA	11.7
1	A	2	ARG	10.4
1	A	88	ASN	8.8
1	A	87	ARG	7.0
1	A	41	SER	6.6
1	B	1	ALA	5.4
1	A	78	VAL	3.7
1	B	45	LYS	3.5
1	A	44	ILE	3.5
1	B	44	ILE	3.2
1	A	67	THR	3.2
1	B	78	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	57	ASN	2.9
1	B	80	THR	2.9
1	B	55	THR	2.9
1	B	43	GLU	2.8
1	B	57	ASN	2.8
1	B	37	VAL	2.7
1	B	66	PHE	2.7
1	B	56	ILE	2.6
1	B	58	LYS	2.6
1	A	59	ARG	2.6
1	B	64	PHE	2.5
1	B	81	GLY	2.5
1	B	13	ASP	2.5
1	A	89	GLY	2.4
1	B	42	ASN	2.4
1	B	36	ALA	2.3
1	B	65	GLY	2.3
1	A	85	ILE	2.3
1	B	72	PHE	2.3
1	B	87	ARG	2.2
1	A	45	LYS	2.2
1	A	68	VAL	2.1
1	A	13	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, 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.

Continued on next page...

Continued from previous page...

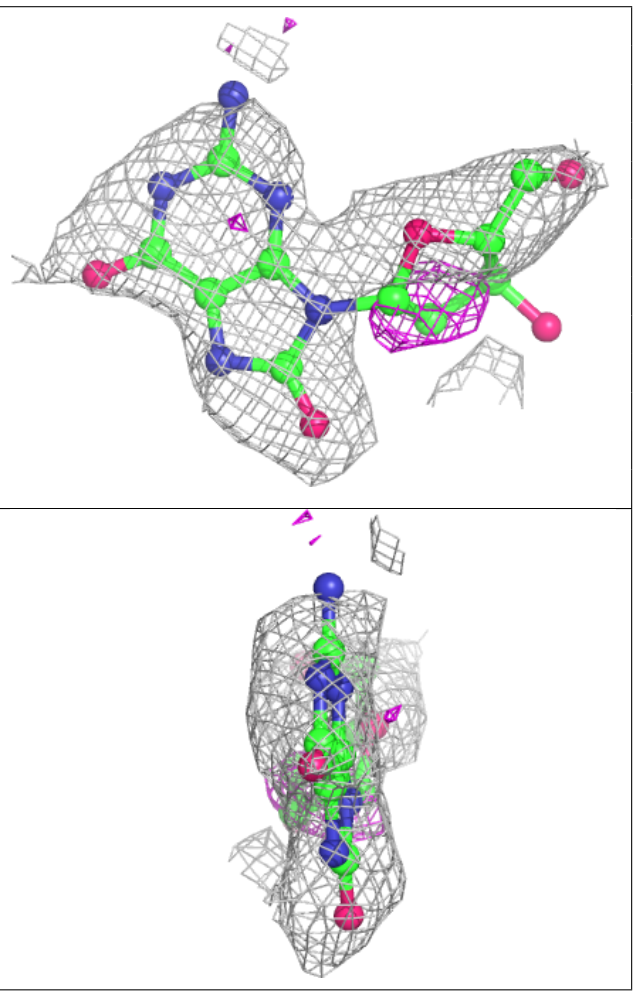
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	8HG	A	255	20/20	0.58	0.36	71,72,75,75	0
2	NAG	B	201	14/15	0.87	0.31	58,62,64,67	0
2	NAG	A	201	14/15	0.88	0.26	46,50,56,57	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 8HG A 255:

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.