Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 07:52 PM EDT

PDB ID	:	6XND
Title	:	Avidin-Biotin-Phenol
Authors	:	Ahmadvand, P.; Kang, C.
Deposited on	:	2020-07-02
Resolution	:	1.58 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

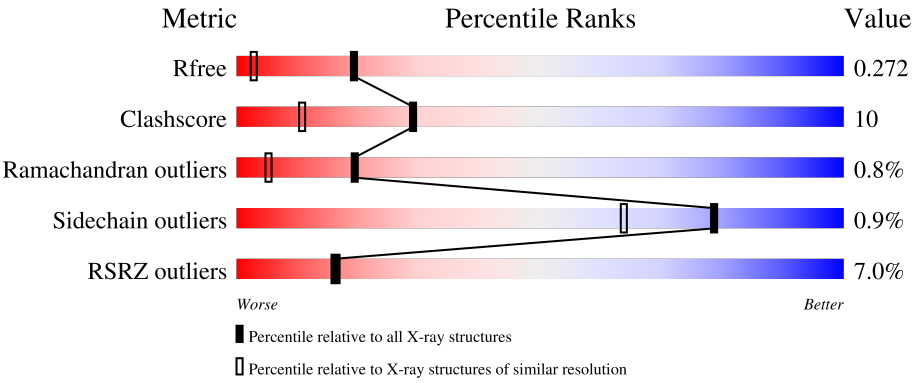
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.58 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	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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	128	10% 77% 13% • • 5%
1	B	128	7% 79% 15% • 5%
1	C	128	5% 81% 12% • 5%
1	D	128	4% 83% 12% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	201	X	-	-	-
3	V8M	B	202	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7799 atoms, of which 3847 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.

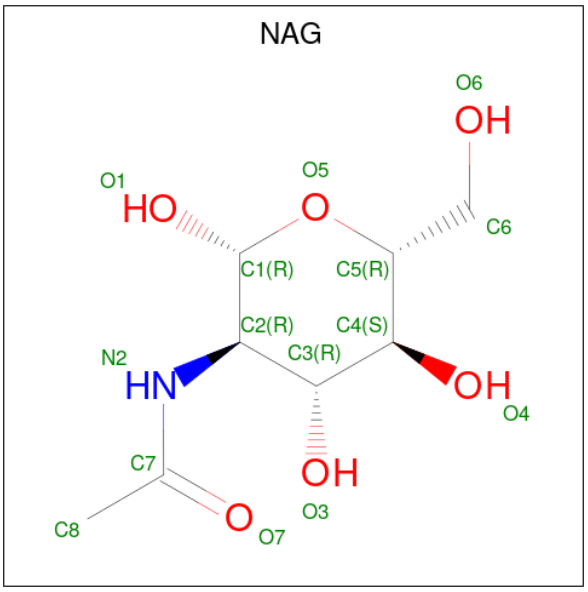
- Molecule 1 is a protein called Avidin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	121	Total	C	H	N	O	S	0	0	0
			1871	592	925	165	185	4			
1	B	121	Total	C	H	N	O	S	0	0	0
			1870	592	924	165	185	4			
1	C	121	Total	C	H	N	O	S	0	0	0
			1868	592	922	165	185	4			
1	D	121	Total	C	H	N	O	S	0	0	0
			1870	592	924	165	185	4			

There are 8 discrepancies between the modelled and reference sequences:

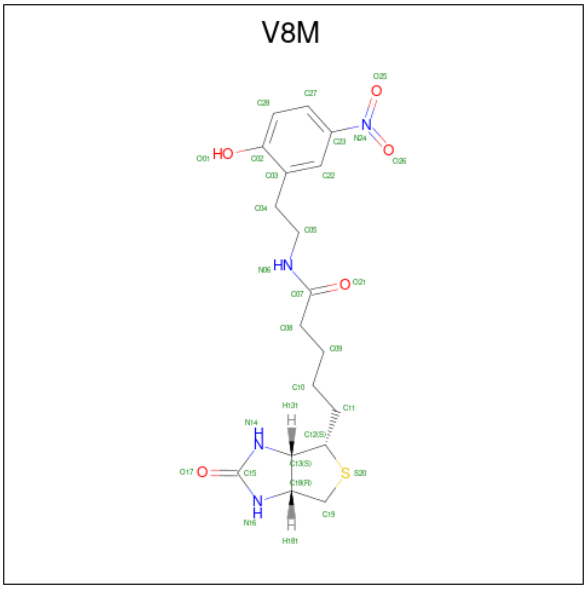
Chain	Residue	Modelled	Actual	Comment	Reference
A	34	THR	ILE	variant	UNP P02701
A	53	GLU	GLN	conflict	UNP P02701
B	34	THR	ILE	variant	UNP P02701
B	53	GLU	GLN	conflict	UNP P02701
C	34	THR	ILE	variant	UNP P02701
C	53	GLU	GLN	conflict	UNP P02701
D	34	THR	ILE	variant	UNP P02701
D	53	GLU	GLN	conflict	UNP P02701

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	28	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	28	0
			28	8	14	1	5		
2	C	1	Total	C	H	N	O	28	0
			28	8	14	1	5		
2	D	1	Total	C	H	N	O	28	0
			28	8	14	1	5		

- Molecule 3 is N-[2-(2-hydroxy-5-nitrophenyl)ethyl]-5-[(3aS,4S,6aS)-2-oxohexahydro-1H-thieno[3,4-d]imidazol-4-yl]pentanamide (three-letter code: V8M) (formula: $C_{18}H_{24}N_4O_5S$) (labeled as "Ligand of Interest" by depositor).



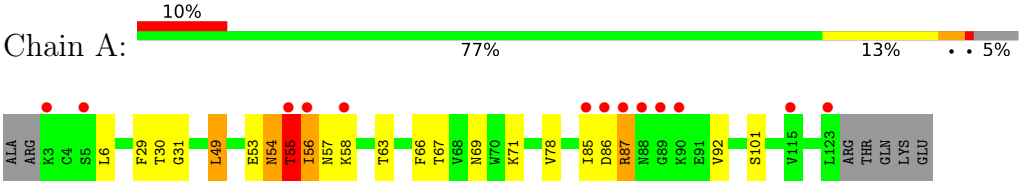
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			52	18	24	4	5	1		
3	B	1	Total	C	H	N	O	S	0	0
			52	18	24	4	5	1		
3	C	1	Total	C	H	N	O	S	0	0
			52	18	24	4	5	1		
3	D	1	Total	C	H	N	O	S	0	0
			52	18	24	4	5	1		

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.

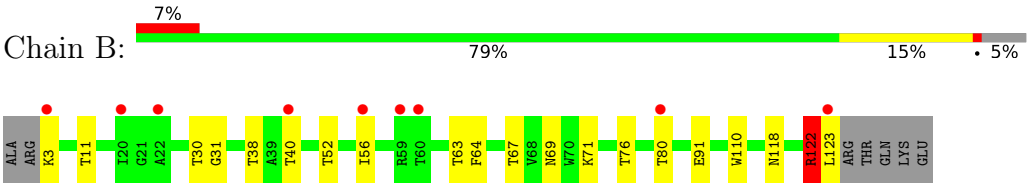
- Molecule 1: Avidin

Chain A:



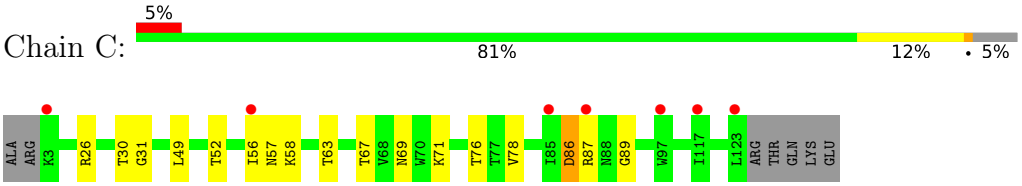
- Molecule 1: Avidin

Chain B:



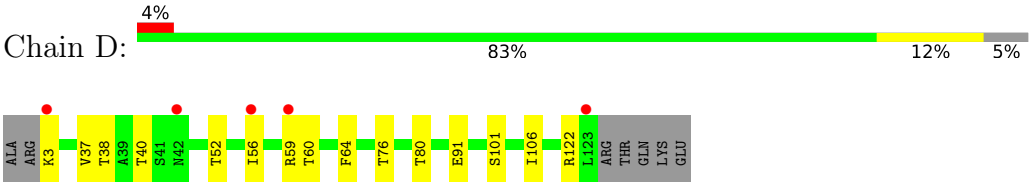
- Molecule 1: Avidin

Chain C:



- Molecule 1: Avidin

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.53Å 79.25Å 74.68Å 90.00° 105.46° 90.00°	Depositor
Resolution (Å)	44.84 – 1.58 44.84 – 1.58	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.84-1.58) 99.9 (44.84-1.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 1.58Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.234 , 0.272 0.234 , 0.272	Depositor DCC
R_{free} test set	1987 reflections (2.78%)	wwPDB-VP
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 36.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7799	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, V8M

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	0.55	0/964	0.80	1/1306 (0.1%)
1	B	0.54	0/964	0.76	1/1306 (0.1%)
1	C	0.56	0/964	0.76	0/1306
1	D	0.54	0/964	0.76	0/1306
All	All	0.55	0/3856	0.77	2/5224 (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	A	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	49	LEU	CA-CB-CG	9.37	136.85	115.30
1	B	122	ARG	NE-CZ-NH1	-5.85	117.38	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	54	ASN	Peptide
1	A	55	THR	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	946	925	925	25	0
1	B	946	924	927	24	0
1	C	946	922	927	21	0
1	D	946	924	927	18	0
2	A	14	14	13	0	0
2	B	14	14	13	0	0
2	C	14	14	13	0	0
2	D	14	14	13	0	0
3	A	28	24	0	1	0
3	B	28	24	0	5	0
3	C	28	24	0	1	0
3	D	28	24	0	2	0
All	All	3952	3847	3758	73	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 10.

All (73) 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:D:202:V8M:C19	3:D:202:V8M:C18	1.74	1.41
3:B:202:V8M:C19	3:B:202:V8M:C18	1.91	1.32
3:C:202:V8M:C18	3:C:202:V8M:C19	1.74	1.26
1:A:101:SER:OG	3:A:202:V8M:O01	1.77	1.03
1:D:101:SER:OG	3:D:202:V8M:O01	1.81	0.98
1:B:118:ASN:OD1	3:B:202:V8M:O17	1.91	0.88
1:A:69:ASN:HB2	1:D:52:THR:HG21	1.58	0.85
3:B:202:V8M:C19	3:B:202:V8M:N16	2.40	0.84
3:B:202:V8M:C19	3:B:202:V8M:C15	2.66	0.72
1:A:63:THR:HG23	1:D:76:THR:OG1	1.90	0.71
1:B:52:THR:HG21	1:C:69:ASN:HB2	1.73	0.70
1:D:91:GLU:OE1	1:D:122:ARG:NH1	2.22	0.69
1:A:53:GLU:O	1:A:55:THR:HG23	1.93	0.69
1:B:91:GLU:OE1	1:B:122:ARG:NH1	2.23	0.69
1:D:38:THR:OG1	1:D:40:THR:HG22	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ILE:HG22	1:A:57:ASN:N	2.08	0.68
1:B:63:THR:HG22	1:C:76:THR:OG1	1.95	0.67
1:B:69:ASN:HB2	1:C:52:THR:HG21	1.77	0.65
1:A:85:ILE:O	1:A:87:ARG:NH1	2.33	0.61
1:B:71:LYS:HA	1:C:56:ILE:HD11	1.81	0.61
1:A:54:ASN:HB3	1:A:63:THR:HG22	1.81	0.61
1:C:26:ARG:HG3	1:C:26:ARG:HH11	1.66	0.61
1:B:38:THR:OG1	1:B:40:THR:HG22	2.01	0.61
1:B:91:GLU:CD	1:B:122:ARG:HH12	2.02	0.61
1:B:52:THR:HG22	1:C:67:THR:HG21	1.82	0.60
1:B:69:ASN:O	1:B:71:LYS:HE2	2.04	0.58
1:D:91:GLU:CD	1:D:122:ARG:HH12	2.05	0.58
1:A:30:THR:HG22	1:A:31:GLY:N	2.19	0.58
1:D:3:LYS:HD3	1:D:60:THR:HG22	1.84	0.57
1:A:30:THR:HG22	1:A:31:GLY:H	1.70	0.57
1:A:54:ASN:OD1	1:A:56:ILE:HG12	2.04	0.56
1:C:86:ASP:OD1	1:C:87:ARG:N	2.37	0.56
1:B:76:THR:OG1	1:C:63:THR:HG23	2.05	0.56
1:A:71:LYS:HA	1:D:56:ILE:HD11	1.89	0.54
1:B:30:THR:HG22	1:B:31:GLY:N	2.23	0.54
1:B:56:ILE:HD11	1:C:71:LYS:HA	1.89	0.54
1:B:110:TRP:HE1	1:D:37:VAL:HG21	1.72	0.54
1:A:30:THR:HG23	1:A:49:LEU:O	2.08	0.54
1:A:67:THR:HG21	1:D:52:THR:HG22	1.91	0.52
1:B:11:THR:HB	1:B:123:LEU:HD12	1.92	0.51
1:A:78:VAL:HG22	1:D:80:THR:OG1	2.10	0.51
1:B:67:THR:HG21	1:C:52:THR:HG22	1.94	0.50
1:A:92:VAL:HG11	1:D:106:ILE:HD12	1.93	0.50
1:C:30:THR:HG23	1:C:49:LEU:O	2.13	0.49
1:B:110:TRP:NE1	1:D:37:VAL:HG21	2.28	0.48
1:C:26:ARG:HG3	1:C:26:ARG:NH1	2.29	0.47
1:B:122:ARG:HH11	1:B:122:ARG:HG3	1.79	0.47
1:C:56:ILE:HD13	1:C:56:ILE:HA	1.78	0.47
1:C:30:THR:HG22	1:C:31:GLY:H	1.81	0.45
1:B:52:THR:HG22	1:C:67:THR:CG2	2.46	0.44
1:A:54:ASN:OD1	1:A:56:ILE:CG1	2.65	0.44
1:D:64:PHE:O	1:D:80:THR:HG23	2.18	0.43
1:A:78:VAL:CG2	1:D:80:THR:OG1	2.66	0.43
1:B:56:ILE:HD13	1:B:56:ILE:HA	1.86	0.43
1:B:80:THR:OG1	1:C:78:VAL:HG22	2.18	0.43
1:A:87:ARG:HA	1:A:87:ARG:HD3	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:PHE:O	1:B:80:THR:HG23	2.18	0.42
1:D:56:ILE:HD13	1:D:56:ILE:HA	1.77	0.42
1:A:6:LEU:HD23	1:A:29:PHE:CE2	2.55	0.42
1:A:30:THR:CG2	1:A:31:GLY:N	2.83	0.42
1:B:67:THR:CG2	1:C:52:THR:HG22	2.50	0.42
1:A:54:ASN:OD1	1:A:54:ASN:O	2.39	0.41
1:A:67:THR:CG2	1:D:52:THR:HG22	2.50	0.41
1:D:3:LYS:HD2	1:D:60:THR:HA	2.02	0.41
1:B:122:ARG:NH1	1:B:122:ARG:HG3	2.35	0.41
3:B:202:V8M:C19	3:B:202:V8M:N14	2.66	0.41
1:C:30:THR:HG22	1:C:31:GLY:N	2.35	0.41
1:A:57:ASN:O	1:A:58:LYS:C	2.59	0.41
1:A:30:THR:CG2	1:A:31:GLY:H	2.32	0.41
1:C:87:ARG:C	1:C:89:GLY:H	2.24	0.41
1:A:49:LEU:HG	1:A:66:PHE:CD1	2.56	0.40
1:C:57:ASN:O	1:C:58:LYS:C	2.60	0.40
1:C:49:LEU:HA	1:C:67:THR: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	119/128 (93%)	114 (96%)	2 (2%)	3 (2%)	5 0
1	B	119/128 (93%)	118 (99%)	1 (1%)	0	100 100
1	C	119/128 (93%)	116 (98%)	2 (2%)	1 (1%)	19 5
1	D	119/128 (93%)	118 (99%)	1 (1%)	0	100 100
All	All	476/512 (93%)	466 (98%)	6 (1%)	4 (1%)	19 5

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	THR
1	A	56	ILE
1	C	86	ASP
1	A	86	ASP

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	106/112 (95%)	105 (99%)	1 (1%)	78	64
1	B	106/112 (95%)	104 (98%)	2 (2%)	57	31
1	C	106/112 (95%)	106 (100%)	0	100	100
1	D	106/112 (95%)	105 (99%)	1 (1%)	78	64
All	All	424/448 (95%)	420 (99%)	4 (1%)	78	64

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	ARG
1	B	3	LYS
1	B	122	ARG
1	D	59	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	42	ASN
1	B	118	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)

8 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	A	201	1	14,14,15	0.73	0	17,19,21	1.19	1 (5%)
2	NAG	C	201	-	14,14,15	0.88	0	17,19,21	1.71	2 (11%)
3	V8M	C	202	-	30,30,30	5.07	15 (50%)	41,41,41	4.44	22 (53%)
3	V8M	D	202	-	30,30,30	4.99	15 (50%)	41,41,41	4.57	16 (39%)
2	NAG	B	201	-	14,14,15	0.87	0	17,19,21	1.62	3 (17%)
3	V8M	B	202	-	30,30,30	5.89	14 (46%)	41,41,41	6.49	15 (36%)
2	NAG	D	201	-	14,14,15	0.82	0	17,19,21	1.87	4 (23%)
3	V8M	A	202	-	30,30,30	4.92	13 (43%)	41,41,41	4.62	13 (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
2	NAG	A	201	1	1/1/7/7	2/6/23/26	0/1/1/1
2	NAG	C	201	-	-	2/6/23/26	0/1/1/1
3	V8M	C	202	-	-	6/17/38/38	0/3/3/3
3	V8M	D	202	-	-	4/17/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	201	-	-	2/6/23/26	0/1/1/1
3	V8M	B	202	-	2/2/9/9	2/17/38/38	0/3/3/3
2	NAG	D	201	-	-	2/6/23/26	0/1/1/1
3	V8M	A	202	-	-	4/17/38/38	0/3/3/3

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	202	V8M	C19-C18	21.01	1.91	1.53
3	D	202	V8M	C19-C18	11.99	1.74	1.53
3	C	202	V8M	C19-C18	11.94	1.74	1.53
3	C	202	V8M	C19-S20	-11.43	1.47	1.81
3	A	202	V8M	C19-C18	11.17	1.73	1.53
3	D	202	V8M	C18-N16	-10.32	1.30	1.46
3	B	202	V8M	C12-S20	-10.05	1.66	1.82
3	A	202	V8M	C18-N16	-9.63	1.31	1.46
3	A	202	V8M	C19-S20	-9.52	1.53	1.81
3	B	202	V8M	C19-S20	-9.37	1.53	1.81
3	A	202	V8M	C12-S20	-8.88	1.68	1.82
3	B	202	V8M	C12-C13	8.67	1.72	1.53
3	C	202	V8M	C18-N16	-8.63	1.32	1.46
3	B	202	V8M	C18-N16	-8.55	1.33	1.46
3	C	202	V8M	C18-C13	-8.50	1.32	1.55
3	C	202	V8M	C12-S20	-8.42	1.69	1.82
3	D	202	V8M	C19-S20	-8.27	1.57	1.81
3	D	202	V8M	C12-C13	8.11	1.71	1.53
3	C	202	V8M	O25-N24	7.73	1.41	1.22
3	D	202	V8M	O25-N24	7.52	1.40	1.22
3	D	202	V8M	C13-N14	-7.49	1.32	1.45
3	D	202	V8M	C18-C13	-7.43	1.35	1.55
3	A	202	V8M	O25-N24	7.43	1.40	1.22
3	A	202	V8M	C13-N14	-7.41	1.32	1.45
3	B	202	V8M	O25-N24	7.36	1.40	1.22
3	A	202	V8M	C12-C13	7.12	1.69	1.53
3	C	202	V8M	C15-N14	7.02	1.47	1.35
3	A	202	V8M	C18-C13	-6.79	1.36	1.55
3	C	202	V8M	C12-C13	6.73	1.68	1.53
3	D	202	V8M	C12-S20	-6.64	1.72	1.82
3	A	202	V8M	C15-N16	6.25	1.45	1.35
3	D	202	V8M	C15-N16	6.20	1.45	1.35
3	B	202	V8M	C15-N14	6.03	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	202	V8M	C07-N06	5.97	1.47	1.33
3	C	202	V8M	C07-N06	5.88	1.46	1.33
3	B	202	V8M	O17-C15	-5.88	1.11	1.23
3	B	202	V8M	C18-C13	-5.88	1.39	1.55
3	D	202	V8M	C15-N14	5.86	1.45	1.35
3	A	202	V8M	C15-N14	5.46	1.44	1.35
3	A	202	V8M	C07-N06	5.16	1.45	1.33
3	B	202	V8M	C15-N16	4.92	1.43	1.35
3	C	202	V8M	C15-N16	4.84	1.43	1.35
3	C	202	V8M	C13-N14	-4.74	1.37	1.45
3	B	202	V8M	C13-N14	-4.46	1.37	1.45
3	C	202	V8M	C11-C12	-4.12	1.43	1.52
3	B	202	V8M	C11-C12	-3.71	1.44	1.52
3	B	202	V8M	O01-C02	3.67	1.43	1.36
3	B	202	V8M	C07-N06	3.64	1.41	1.33
3	A	202	V8M	C11-C12	-3.52	1.44	1.52
3	D	202	V8M	O21-C07	-3.00	1.17	1.23
3	C	202	V8M	C04-C03	2.83	1.57	1.51
3	D	202	V8M	C11-C12	-2.76	1.46	1.52
3	A	202	V8M	O17-C15	-2.48	1.18	1.23
3	D	202	V8M	C08-C07	2.37	1.55	1.51
3	C	202	V8M	O01-C02	2.25	1.41	1.36
3	C	202	V8M	C08-C07	2.21	1.55	1.51
3	D	202	V8M	O01-C02	2.17	1.40	1.36

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	202	V8M	C19-C18-C13	-24.17	87.68	108.66
3	B	202	V8M	C13-C18-N16	18.40	121.97	102.43
3	B	202	V8M	C19-C18-N16	-14.61	94.46	113.03
3	A	202	V8M	C12-C13-N14	13.13	124.89	113.13
3	B	202	V8M	C18-N16-C15	-12.96	95.57	112.46
3	C	202	V8M	C13-C12-S20	-12.55	93.25	105.20
3	D	202	V8M	C12-C13-N14	12.18	124.04	113.13
3	B	202	V8M	C13-C12-S20	-11.92	93.84	105.20
3	A	202	V8M	C18-C19-S20	-11.77	96.22	106.31
3	C	202	V8M	C13-C18-N16	11.68	114.84	102.43
3	D	202	V8M	C13-C18-N16	11.34	114.48	102.43
3	D	202	V8M	C13-C12-S20	-10.74	94.97	105.20
3	A	202	V8M	C13-C12-S20	-10.36	95.34	105.20
3	A	202	V8M	C19-C18-N16	10.21	126.00	113.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	202	V8M	C13-N14-C15	-9.79	103.50	112.62
3	C	202	V8M	C13-N14-C15	-8.89	104.34	112.62
3	D	202	V8M	C19-C18-N16	8.88	124.31	113.03
3	D	202	V8M	C08-C07-N06	8.87	131.35	116.42
3	B	202	V8M	C13-N14-C15	-8.87	104.36	112.62
3	A	202	V8M	C13-C18-N16	8.83	111.81	102.43
3	A	202	V8M	C18-C13-N14	8.73	112.05	102.67
3	C	202	V8M	C19-C18-N16	8.62	123.99	113.03
3	D	202	V8M	C18-C19-S20	-8.51	99.02	106.31
3	B	202	V8M	C18-C19-S20	8.39	113.50	106.31
3	C	202	V8M	C19-C18-C13	-7.75	101.94	108.66
3	C	202	V8M	C12-C13-N14	7.13	119.51	113.13
3	A	202	V8M	C18-N16-C15	-6.60	103.86	112.46
3	D	202	V8M	C13-N14-C15	-6.40	106.65	112.62
3	D	202	V8M	C18-N16-C15	-6.39	104.14	112.46
3	C	202	V8M	C18-C19-S20	-6.37	100.85	106.31
3	C	202	V8M	C18-N16-C15	-6.29	104.26	112.46
3	C	202	V8M	C18-C13-N14	6.14	109.27	102.67
3	B	202	V8M	N16-C15-N14	5.66	114.08	108.76
3	D	202	V8M	C18-C13-N14	5.54	108.63	102.67
3	D	202	V8M	O21-C07-N06	-5.42	112.79	123.01
2	C	201	NAG	O5-C1-C2	4.45	118.31	111.29
2	D	201	NAG	C1-O5-C5	4.29	118.00	112.19
3	D	202	V8M	C19-C18-C13	-4.25	104.97	108.66
2	B	201	NAG	C1-C2-N2	4.02	117.36	110.49
2	D	201	NAG	O5-C5-C6	-3.79	101.26	107.20
2	C	201	NAG	C4-C3-C2	-3.77	105.49	111.02
3	C	202	V8M	C12-C13-C18	3.73	113.26	108.94
3	B	202	V8M	C22-C03-C02	3.72	122.64	118.17
3	B	202	V8M	O17-C15-N16	-3.69	120.63	125.94
2	A	201	NAG	C1-O5-C5	3.47	116.89	112.19
3	D	202	V8M	N16-C15-N14	-3.45	105.53	108.76
3	D	202	V8M	O21-C07-C08	-3.37	115.85	122.02
3	C	202	V8M	C05-N06-C07	-3.28	116.74	122.84
2	D	201	NAG	O5-C1-C2	3.25	116.42	111.29
3	D	202	V8M	C04-C05-N06	-3.18	102.40	111.99
3	C	202	V8M	C08-C07-N06	3.16	121.75	116.42
3	A	202	V8M	C05-C04-C03	-3.03	106.03	112.93
3	A	202	V8M	C19-S20-C12	3.00	96.05	89.89
3	C	202	V8M	C04-C05-N06	2.99	121.01	111.99
3	C	202	V8M	C27-C23-C22	-2.90	118.70	122.40
3	C	202	V8M	C04-C03-C02	2.81	125.87	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	202	V8M	C19-S20-C12	2.77	95.58	89.89
3	B	202	V8M	C28-C02-C03	-2.77	117.06	120.41
3	D	202	V8M	C05-N06-C07	2.69	127.83	122.84
3	C	202	V8M	O17-C15-N14	2.69	129.79	125.94
3	C	202	V8M	O21-C07-N06	-2.68	117.96	123.01
2	B	201	NAG	O5-C1-C2	2.63	115.44	111.29
3	B	202	V8M	C12-C13-N14	2.61	115.46	113.13
3	B	202	V8M	C04-C03-C22	-2.57	114.22	119.41
3	C	202	V8M	C27-C23-N24	2.51	122.61	118.92
3	C	202	V8M	C23-C22-C03	2.48	122.05	119.54
3	B	202	V8M	C04-C05-N06	-2.46	104.57	111.99
3	B	202	V8M	C11-C12-C13	-2.29	108.06	114.73
2	B	201	NAG	C4-C3-C2	-2.28	107.67	111.02
2	D	201	NAG	C4-C3-C2	-2.18	107.82	111.02
3	A	202	V8M	C05-N06-C07	-2.15	118.85	122.84
3	D	202	V8M	C19-S20-C12	2.11	94.22	89.89
3	C	202	V8M	C04-C03-C22	-2.10	115.16	119.41
3	C	202	V8M	C10-C11-C12	-2.07	109.67	113.86
3	A	202	V8M	C10-C11-C12	-2.06	109.69	113.86
3	A	202	V8M	C27-C23-N24	2.04	121.92	118.92

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	201	NAG	C1
3	B	202	V8M	C13
3	B	202	V8M	C18

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	202	V8M	C02-C03-C04-C05
3	C	202	V8M	C03-C04-C05-N06
3	D	202	V8M	C10-C11-C12-S20
3	A	202	V8M	C22-C23-N24-O26
3	A	202	V8M	C27-C23-N24-O25
3	A	202	V8M	C27-C23-N24-O26
3	A	202	V8M	C22-C23-N24-O25
2	B	201	NAG	O5-C5-C6-O6
3	D	202	V8M	C08-C07-N06-C05
2	A	201	NAG	O5-C5-C6-O6
2	D	201	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	D	202	V8M	C03-C04-C05-N06
2	B	201	NAG	C4-C5-C6-O6
3	D	202	V8M	O21-C07-N06-C05
2	D	201	NAG	C4-C5-C6-O6
2	A	201	NAG	C4-C5-C6-O6
2	C	201	NAG	O5-C5-C6-O6
2	C	201	NAG	C4-C5-C6-O6
3	C	202	V8M	C27-C23-N24-O25
3	C	202	V8M	C22-C23-N24-O25
3	C	202	V8M	C27-C23-N24-O26
3	C	202	V8M	C22-C23-N24-O26
3	B	202	V8M	C22-C03-C04-C05
3	B	202	V8M	C02-C03-C04-C05

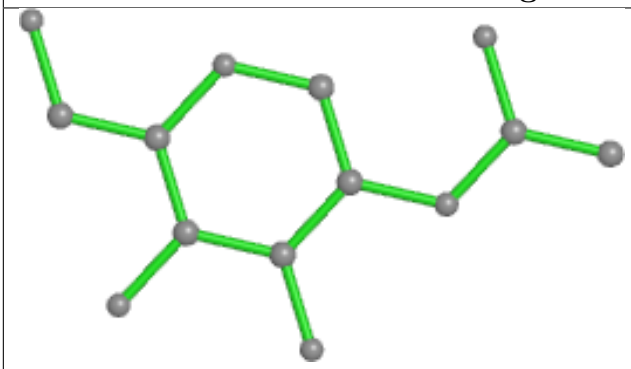
There are no ring outliers.

4 monomers are involved in 9 short contacts:

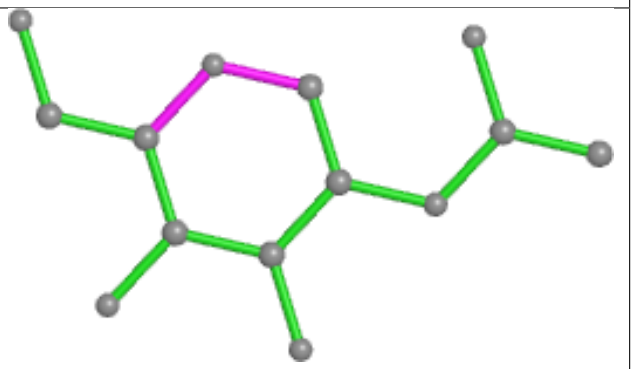
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	202	V8M	1	0
3	D	202	V8M	2	0
3	B	202	V8M	5	0
3	A	202	V8M	1	0

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.

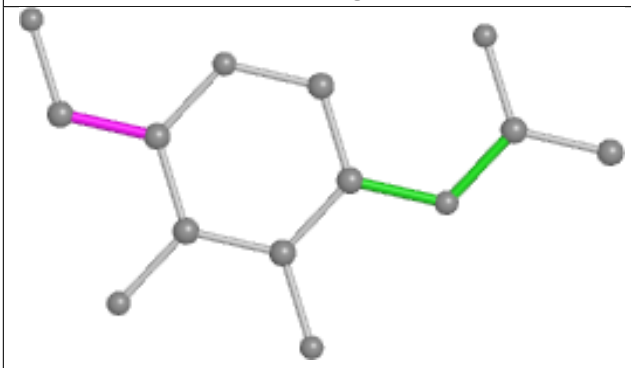
Ligand NAG A 201



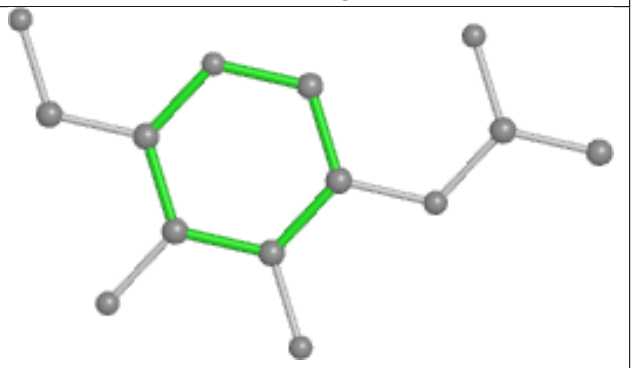
Bond lengths



Bond angles

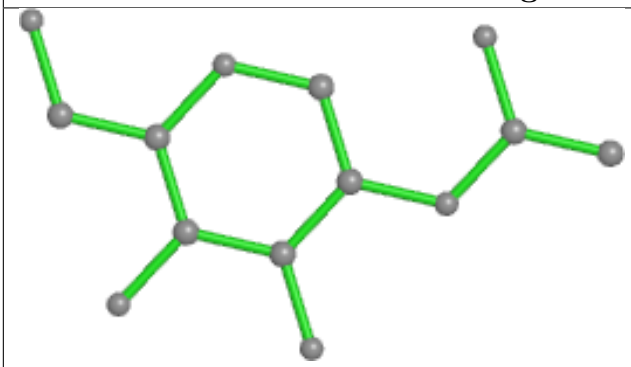


Torsions

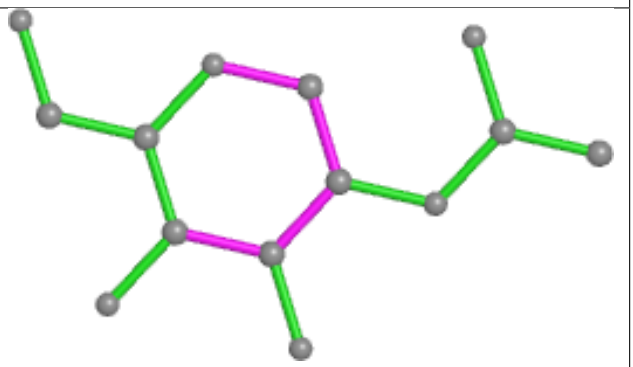


Rings

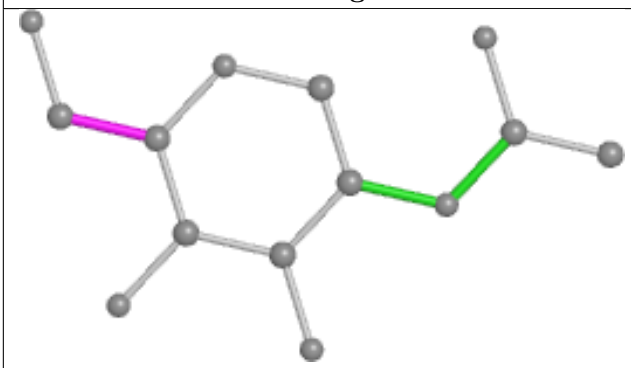
Ligand NAG C 201



Bond lengths



Bond angles



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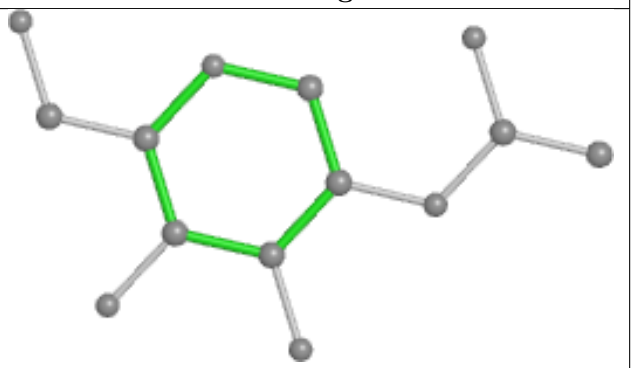
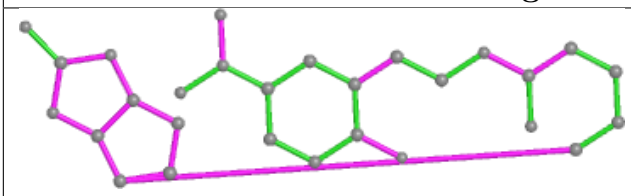
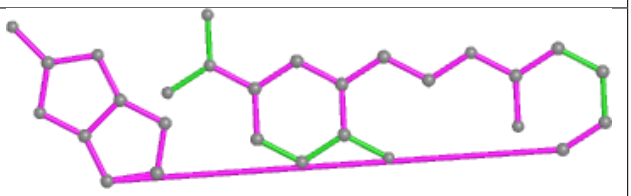
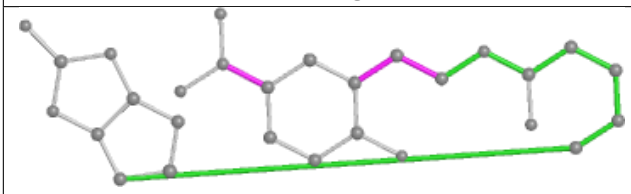
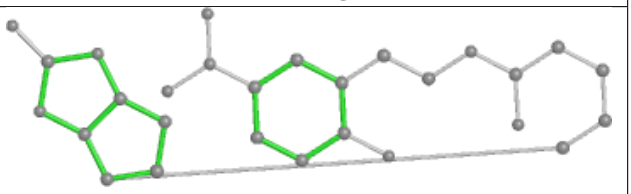


Rings

Ligand V8M C 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

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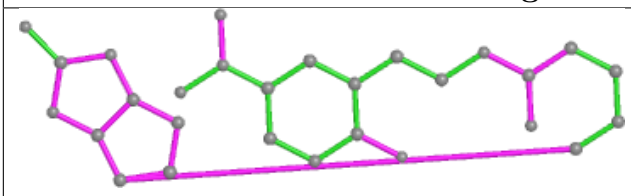
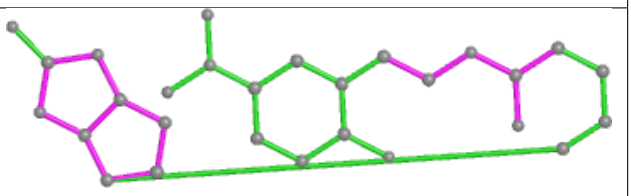
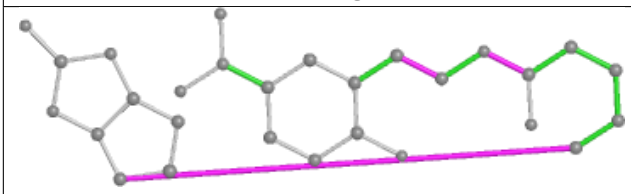
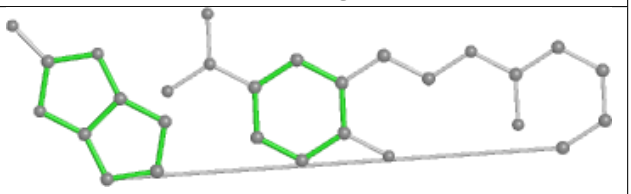
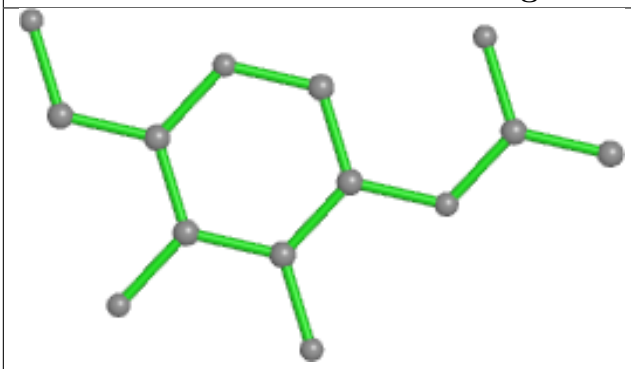
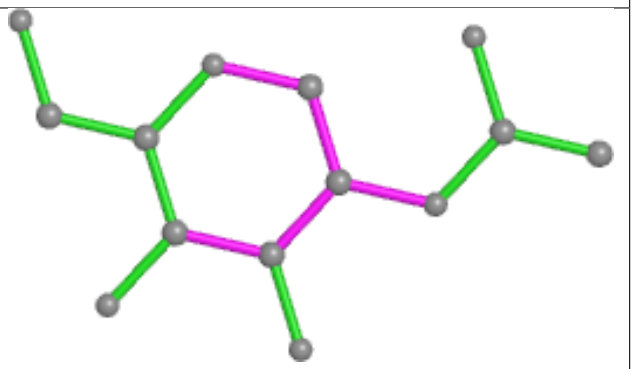
	
Bond lengths	Bond angles
	
Torsions	Rings

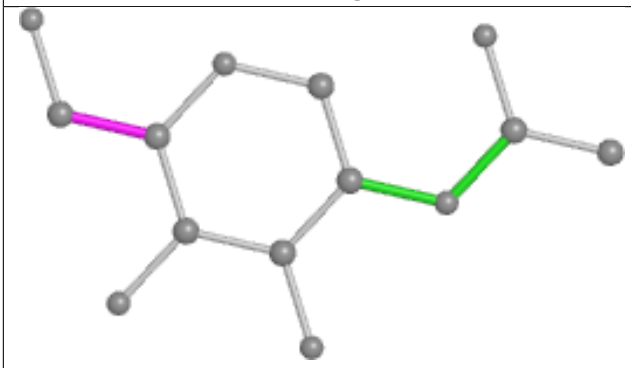
Ligand NAG B 201



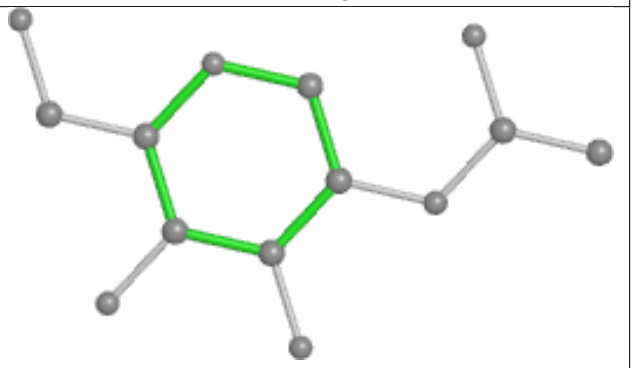
Bond lengths



Bond angles

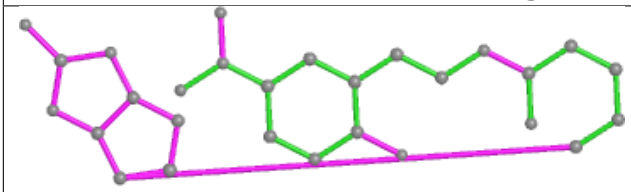


Torsions

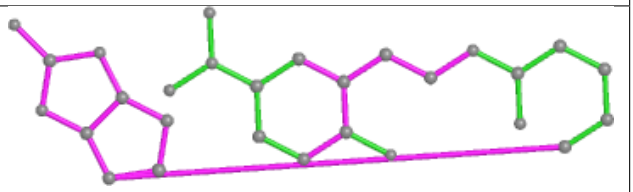


Rings

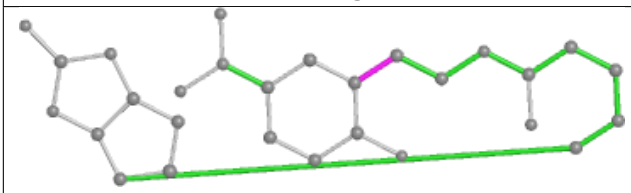
Ligand V8M B 202



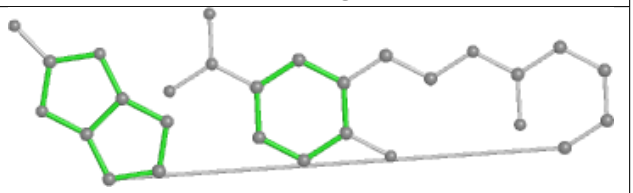
Bond lengths



Bond angles

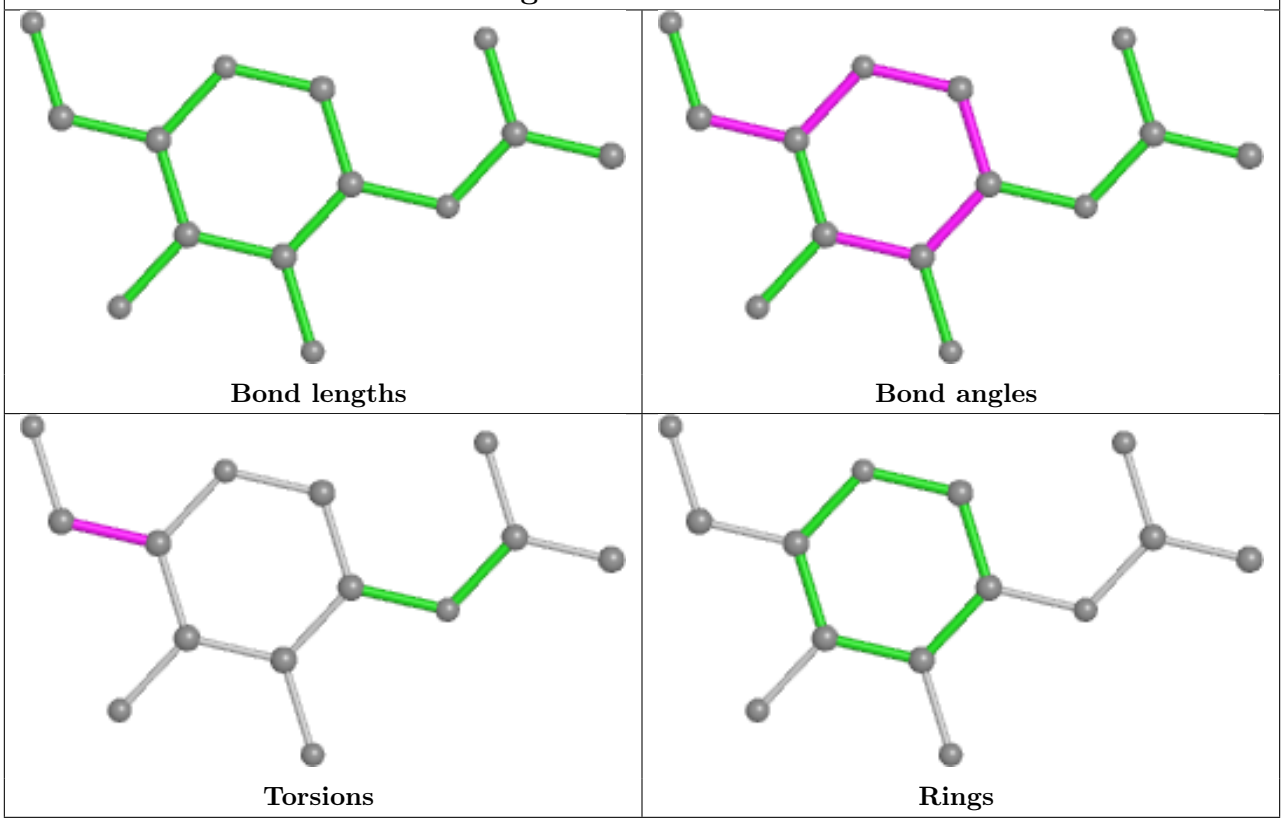


Torsions

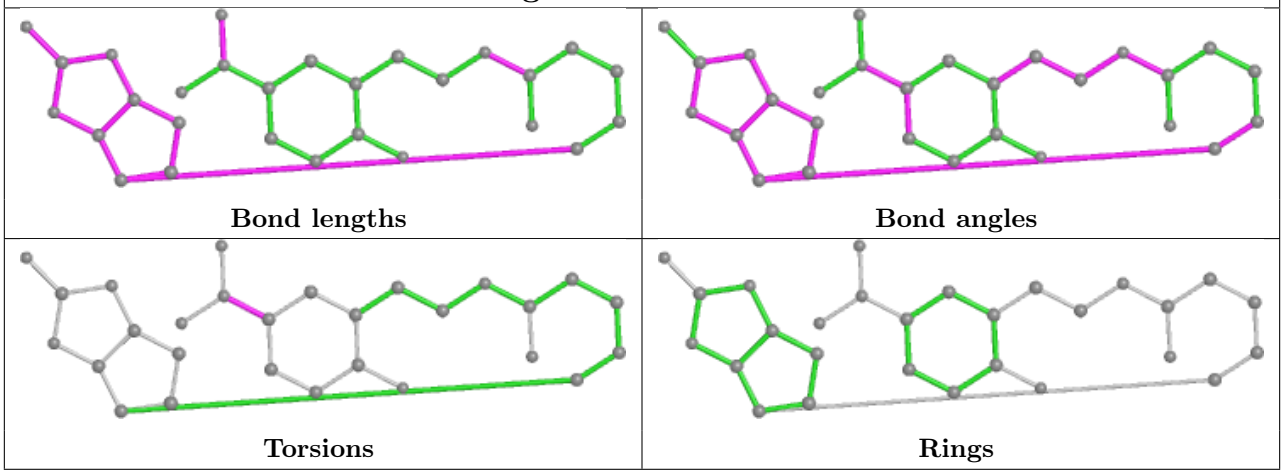


Rings

Ligand NAG D 201



Ligand V8M A 202



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	121/128 (94%)	0.69	13 (10%) 6 5	20, 28, 59, 75	0
1	B	121/128 (94%)	0.59	9 (7%) 14 14	20, 29, 44, 56	0
1	C	121/128 (94%)	0.34	7 (5%) 23 23	19, 27, 45, 62	0
1	D	121/128 (94%)	0.41	5 (4%) 37 37	20, 29, 44, 53	0
All	All	484/512 (94%)	0.51	34 (7%) 16 16	19, 28, 48, 75	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	ILE	8.1
1	A	87	ARG	7.4
1	A	58	LYS	6.3
1	A	55	THR	6.0
1	A	88	ASN	5.7
1	D	123	LEU	5.0
1	B	56	ILE	4.2
1	D	56	ILE	3.7
1	B	59	ARG	3.4
1	C	3	LYS	3.1
1	A	3	LYS	2.8
1	A	5	SER	2.8
1	B	123	LEU	2.8
1	C	123	LEU	2.8
1	C	97	TRP	2.8
1	D	59	ARG	2.6
1	B	3	LYS	2.5
1	C	56	ILE	2.5
1	C	85	ILE	2.3
1	C	87	ARG	2.3
1	D	3	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	60	THR	2.2
1	A	86	ASP	2.2
1	A	85	ILE	2.2
1	A	90	LYS	2.2
1	A	123	LEU	2.2
1	B	80	THR	2.1
1	C	117	ILE	2.1
1	A	115	VAL	2.1
1	B	40	THR	2.1
1	B	20	ILE	2.1
1	B	22	ALA	2.1
1	D	42	ASN	2.0
1	A	89	GLY	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)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.