Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2023 – 06:20 AM EDT

PDB ID	:	1NAA
Title	:	Cellobiose Dehydrogenase Flavoprotein Fragment in Complex with Cellobionolactam
Authors	:	Hallberg, B.M.; Henriksson, G.; Pettersson, G.; Vasella, A.; Divne, C.
Deposited on	:	2002-11-27
Resolution	:	1.80 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:

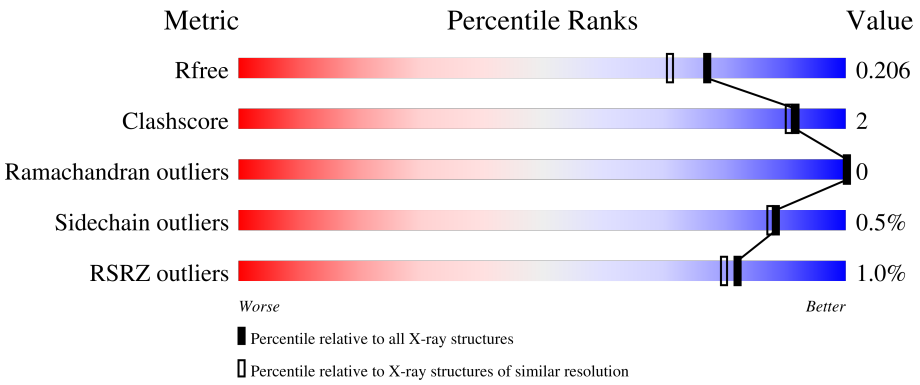
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	541	95% 5%
1	B	541	2% 95% 5%

2 Entry composition (i)

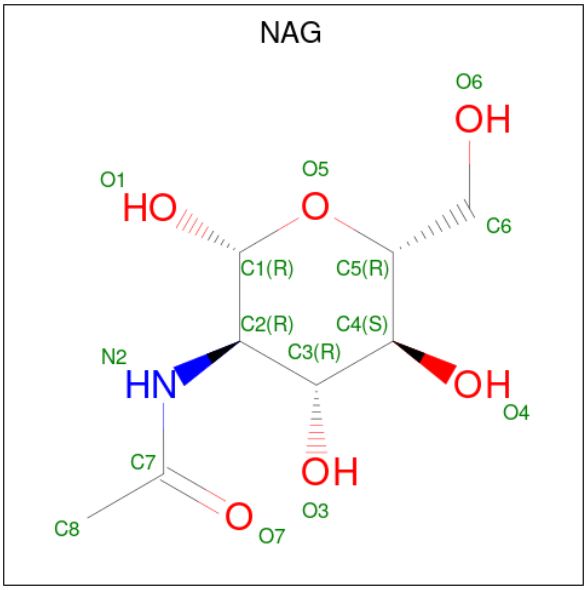
There are 5 unique types of molecules in this entry. The entry contains 9365 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cellobiose dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	541	4067	2583	691	785	8	0	0	0
1	B	541	4067	2583	691	785	8	0	0	0

- 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
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0
2	B	1	14	8	1	5	0	0

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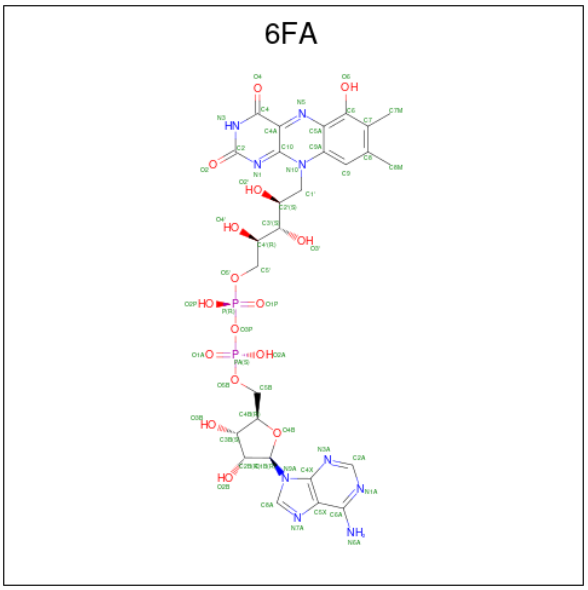
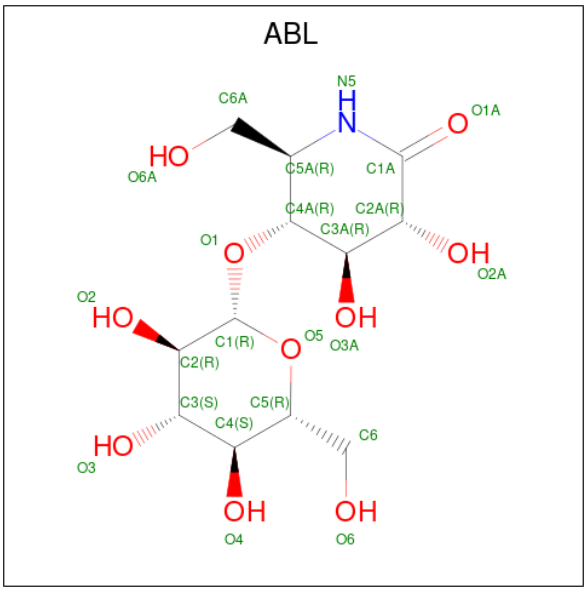
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	14	8	1	5	0	0

- Molecule 3 is 6-HYDROXY-FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: 6FA) (formula: $C_{27}H_{33}N_9O_{16}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	54	27	9	16	2	0	0
			Total	C	N	O	P		
3	B	1	54	27	9	16	2	0	0

- Molecule 4 is (2R,3R,4R,5R)-4,5-dihydroxy-2-(hydroxymethyl)-6-oxopiperidin-3-yl beta-D-glucopyranoside (three-letter code: ABL) (formula: $C_{12}H_{21}NO_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	23	12	1	10	0	0
			Total	C	N	O		
4	B	1	23	12	1	10	0	0

- Molecule 5 is water.

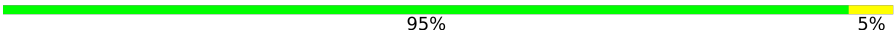
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	533	533	533	0	0
			Total	O		
5	B	474	474	474	0	0

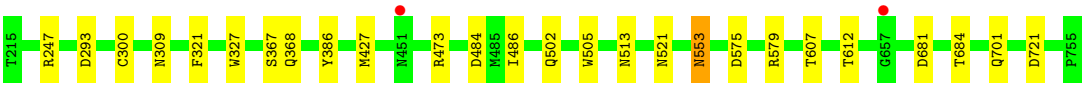
3 Residue-property plots (i)

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: Cellobiose dehydrogenase

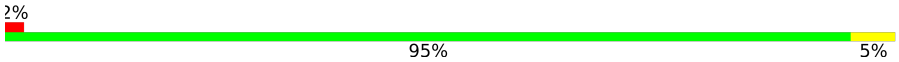
Chain A:

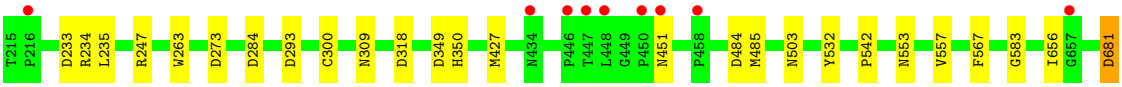


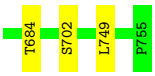


• Molecule 1: Cellobiose dehydrogenase

Chain B:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	185.95Å 185.95Å 81.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.80 29.95 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.80) 97.6 (29.95-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 1.80Å)	Xtriage
Refinement program	REFMAC, CNS	Depositor
R, R_{free}	0.146 , 0.185 0.180 , 0.206	Depositor DCC
R_{free} test set	1894 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å^2)	16.1	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9365	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: 6FA, ABL, NAG

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	1.02	4/4179 (0.1%)	0.92	4/5728 (0.1%)
1	B	0.98	2/4179 (0.0%)	0.94	11/5728 (0.2%)
All	All	1.00	6/8358 (0.1%)	0.93	15/11456 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	427	MET	CG-SD	-9.64	1.56	1.81
1	A	427	MET	CG-SD	-8.65	1.58	1.81
1	A	368	GLN	CG-CD	5.94	1.64	1.51
1	A	386	TYR	CD2-CE2	5.64	1.47	1.39
1	A	367	SER	CB-OG	-5.49	1.35	1.42
1	B	702	SER	CB-OG	-5.00	1.35	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	484	ASP	CB-CG-OD1	7.94	125.45	118.30
1	B	681	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	473	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	B	233	ASP	CB-CG-OD2	6.43	124.09	118.30
1	B	484	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	293	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	234	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	318	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	485	MET	CG-SD-CE	5.14	108.43	100.20
1	B	273	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	284	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	293	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	427	MET	CA-CB-CG	-5.11	104.61	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	349	ASP	CB-CG-OD1	5.05	122.84	118.30

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	4067	0	3945	13	0
1	B	4067	0	3946	13	0
2	A	42	0	39	0	0
2	B	28	0	26	0	0
3	A	54	0	26	3	0
3	B	54	0	26	2	0
4	A	23	0	16	0	0
4	B	23	0	16	0	0
5	A	533	0	0	2	0
5	B	474	0	0	4	0
All	All	9365	0	8040	26	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 2.

All (26) 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:503:ASN:OD1	5:B:2246:HOH:O	2.12	0.67
1:B:309:ASN:HB2	3:B:1801:6FA:C5A	2.25	0.67
1:B:681:ASP:OD1	5:B:2324:HOH:O	2.13	0.66
1:A:513:ASN:OD1	5:A:1498:HOH:O	2.15	0.65
1:A:309:ASN:HB2	3:A:801:6FA:C5A	2.34	0.57
1:A:684:THR:HG21	5:A:1473:HOH:O	2.04	0.56
1:A:247:ARG:HD3	1:A:300:CYS:SG	2.48	0.54
1:B:235:LEU:HD23	1:B:749:LEU:HD21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:HIS:HD2	5:B:2091:HOH:O	1.93	0.51
1:A:521:ASN:ND2	1:A:607:THR:OG1	2.44	0.51
1:B:684:THR:HG21	5:B:2443:HOH:O	2.14	0.48
1:B:247:ARG:HD3	1:B:300:CYS:SG	2.56	0.45
1:A:553:ASN:HD22	1:A:553:ASN:C	2.21	0.44
1:B:309:ASN:HB2	3:B:1801:6FA:N5	2.32	0.44
1:A:502:GLN:HA	1:A:505:TRP:CE2	2.53	0.43
1:A:309:ASN:HB2	3:A:801:6FA:N5	2.33	0.43
1:A:681:ASP:HB3	1:A:684:THR:HG23	2.00	0.43
1:A:321:PHE:HA	1:A:327:TRP:CD1	2.54	0.43
1:B:532:TYR:CZ	1:B:557:VAL:HG11	2.55	0.42
1:A:721:ASP:HB2	3:A:801:6FA:O2P	2.19	0.42
1:B:263:TRP:CD1	1:B:542:PRO:HG3	2.55	0.41
1:B:567:PHE:CE2	1:B:583:GLY:HA3	2.55	0.41
1:A:486:ILE:HG21	1:A:505:TRP:CD2	2.55	0.41
1:B:656:ILE:HG21	1:B:656:ILE:HD13	1.68	0.41
1:A:579:ARG:HA	1:A:612:THR:O	2.21	0.41
1:B:350:HIS:CD2	1:B:350:HIS:O	2.74	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	539/541 (100%)	524 (97%)	15 (3%)	0	100	100
1	B	539/541 (100%)	521 (97%)	18 (3%)	0	100	100
All	All	1078/1082 (100%)	1045 (97%)	33 (3%)	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	439/439 (100%)	437 (100%)	2 (0%)	88 87
1	B	439/439 (100%)	437 (100%)	2 (0%)	88 87
All	All	878/878 (100%)	874 (100%)	4 (0%)	88 87

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

Mol	Chain	Res	Type
1	A	553	ASN
1	A	701	GLN
1	B	451	ASN
1	B	553	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	333	ASN
1	A	350	HIS
1	A	356	GLN
1	A	373	GLN
1	A	377	GLN
1	A	513	ASN
1	A	521	ASN
1	A	553	ASN
1	A	566	ASN
1	A	602	GLN
1	A	671	GLN
1	B	333	ASN
1	B	350	HIS
1	B	373	GLN
1	B	377	GLN
1	B	502	GLN
1	B	503	ASN
1	B	521	ASN

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Mol	Chain	Res	Type
1	B	553	ASN
1	B	566	ASN
1	B	602	GLN
1	B	701	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)

9 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	802	1	14,14,15	0.76	0	17,19,21	1.58	3 (17%)
3	6FA	A	801	-	54,59,59	2.21	14 (25%)	68,91,91	1.50	14 (20%)
2	NAG	A	803	1	14,14,15	0.68	0	17,19,21	1.38	2 (11%)
4	ABL	B	1901	-	24,24,24	1.01	2 (8%)	32,35,35	1.32	4 (12%)
2	NAG	A	804	1	14,14,15	0.88	0	17,19,21	1.75	4 (23%)
4	ABL	A	901	-	24,24,24	0.92	0	32,35,35	1.19	4 (12%)
3	6FA	B	1801	-	54,59,59	2.27	13 (24%)	68,91,91	1.78	17 (25%)
2	NAG	B	1803	1	14,14,15	0.96	1 (7%)	17,19,21	1.79	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	B	1804	1	14,14,15	1.10	2 (14%)	17,19,21	2.37	5 (29%)

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	802	1	-	0/6/23/26	0/1/1/1
3	6FA	A	801	-	-	5/30/50/50	0/6/6/6
2	NAG	A	803	1	-	1/6/23/26	0/1/1/1
4	ABL	B	1901	-	-	1/8/48/48	0/2/2/2
2	NAG	A	804	1	-	3/6/23/26	0/1/1/1
4	ABL	A	901	-	-	1/8/48/48	0/2/2/2
3	6FA	B	1801	-	-	3/30/50/50	0/6/6/6
2	NAG	B	1803	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1804	1	-	4/6/23/26	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1801	6FA	C2B-C1B	-9.32	1.39	1.53
3	A	801	6FA	C2B-C1B	-6.40	1.44	1.53
3	A	801	6FA	O6-C6	-5.11	1.25	1.37
3	A	801	6FA	O3B-C3B	-4.99	1.31	1.43
3	B	1801	6FA	C3B-C4B	-4.83	1.40	1.53
3	A	801	6FA	C2B-C3B	-4.69	1.40	1.53
3	A	801	6FA	C4A-N5	4.58	1.39	1.30
3	B	1801	6FA	C2B-C3B	-4.41	1.41	1.53
3	B	1801	6FA	O2B-C2B	-4.11	1.33	1.43
3	A	801	6FA	C3B-C4B	-4.11	1.42	1.53
3	B	1801	6FA	O3B-C3B	-4.06	1.33	1.43
3	B	1801	6FA	O6-C6	-4.06	1.27	1.37
3	A	801	6FA	C9A-C5A	-3.92	1.35	1.41
3	A	801	6FA	C6-C5A	3.88	1.48	1.38
3	A	801	6FA	O2B-C2B	-3.46	1.34	1.43
3	B	1801	6FA	C6-C5A	3.27	1.46	1.38
3	B	1801	6FA	C8-C7	3.19	1.46	1.40
3	A	801	6FA	C6-C7	3.13	1.46	1.40
3	B	1801	6FA	C4A-N5	2.90	1.36	1.30
3	B	1801	6FA	C5X-C4X	2.79	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1804	NAG	O5-C1	-2.73	1.39	1.43
3	A	801	6FA	C8-C7	2.59	1.45	1.40
2	B	1803	NAG	C2-N2	-2.56	1.42	1.46
3	B	1801	6FA	C4-N3	-2.56	1.34	1.38
3	A	801	6FA	C5X-C4X	2.50	1.47	1.40
4	B	1901	ABL	C2A-C1A	-2.44	1.51	1.52
3	B	1801	6FA	C4A-C10	-2.36	1.37	1.44
3	B	1801	6FA	C10-N1	2.33	1.38	1.33
4	B	1901	ABL	O3A-C3A	2.29	1.48	1.43
3	A	801	6FA	C4-N3	-2.08	1.35	1.38
2	B	1804	NAG	C2-N2	-2.02	1.42	1.46
3	A	801	6FA	C4A-C10	-2.00	1.38	1.44

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1804	NAG	O5-C1-C2	-6.82	100.52	111.29
3	B	1801	6FA	C1B-N9A-C4X	4.23	134.07	126.64
2	B	1804	NAG	O5-C5-C6	4.09	113.61	107.20
3	B	1801	6FA	C9A-N10-C10	-4.06	114.44	120.77
3	A	801	6FA	C3B-C2B-C1B	4.04	107.07	100.98
3	A	801	6FA	O2B-C2B-C3B	3.83	124.21	111.82
3	B	1801	6FA	C3B-C2B-C1B	3.67	106.50	100.98
2	A	804	NAG	O5-C1-C2	-3.53	105.72	111.29
2	A	802	NAG	O5-C1-C2	-3.51	105.75	111.29
2	B	1803	NAG	C2-N2-C7	3.51	127.90	122.90
3	B	1801	6FA	N3A-C2A-N1A	-3.45	123.28	128.68
2	A	804	NAG	C4-C3-C2	-3.45	105.96	111.02
2	B	1803	NAG	C4-C3-C2	-3.43	106.00	111.02
3	B	1801	6FA	C5B-C4B-C3B	3.40	127.94	115.18
3	B	1801	6FA	O3B-C3B-C4B	3.40	120.87	111.05
3	B	1801	6FA	C4A-C10-N10	3.39	121.44	116.48
2	B	1804	NAG	C4-C3-C2	3.38	115.97	111.02
3	A	801	6FA	C9A-N10-C10	-3.22	115.76	120.77
3	B	1801	6FA	O2B-C2B-C3B	3.21	122.20	111.82
3	A	801	6FA	N3A-C2A-N1A	-3.11	123.81	128.68
3	A	801	6FA	C5B-C4B-C3B	2.98	126.36	115.18
4	B	1901	ABL	O3-C3-C4	2.91	117.07	110.35
4	A	901	ABL	C3A-C4A-C5A	-2.86	106.19	111.18
3	B	1801	6FA	O4B-C1B-C2B	2.86	111.11	106.93
3	B	1801	6FA	O4-C4-N3	2.86	125.59	120.12
3	B	1801	6FA	C2A-N1A-C6A	2.84	123.61	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1901	ABL	O1-C4A-C3A	2.81	114.76	107.28
3	B	1801	6FA	C9-C9A-N10	-2.66	118.23	121.84
3	B	1801	6FA	C5X-C6A-N6A	2.64	124.36	120.35
3	B	1801	6FA	C4-C4A-C10	2.61	121.17	116.79
4	A	901	ABL	O3A-C3A-C2A	-2.56	104.79	109.68
3	A	801	6FA	O4-C4-C4A	-2.55	119.84	126.60
2	A	804	NAG	O5-C5-C6	2.48	111.10	107.20
2	A	803	NAG	O4-C4-C3	-2.45	104.68	110.35
2	A	802	NAG	C1-C2-N2	-2.41	106.37	110.49
3	B	1801	6FA	O2B-C2B-C1B	2.39	119.68	110.85
2	A	804	NAG	C1-O5-C5	2.34	115.36	112.19
2	B	1803	NAG	O6-C6-C5	-2.33	103.30	111.29
3	A	801	6FA	O4-C4-N3	2.31	124.54	120.12
3	A	801	6FA	O4B-C4B-C3B	2.30	109.66	105.11
3	A	801	6FA	O2'-C2'-C3'	2.26	114.58	109.10
2	A	803	NAG	O7-C7-N2	2.25	126.09	121.95
4	A	901	ABL	C6A-C5A-N5	-2.25	105.14	109.56
2	B	1804	NAG	O3-C3-C4	-2.24	105.16	110.35
3	A	801	6FA	C2A-N1A-C6A	2.17	122.47	118.75
4	B	1901	ABL	O1-C1-O5	-2.12	104.75	110.67
4	A	901	ABL	C1-O5-C5	2.12	117.85	113.69
2	B	1804	NAG	C6-C5-C4	-2.12	108.03	113.00
3	B	1801	6FA	C10-C4A-N5	-2.10	120.40	124.86
4	B	1901	ABL	O3A-C3A-C2A	-2.07	105.72	109.68
2	A	802	NAG	O5-C5-C6	2.07	110.45	107.20
3	A	801	6FA	C1B-N9A-C4X	2.02	130.20	126.64
3	B	1801	6FA	C5A-C6-C7	-2.02	117.11	120.21
3	A	801	6FA	C4-N3-C2	-2.02	121.91	125.64
2	B	1803	NAG	C6-C5-C4	-2.01	108.30	113.00
3	A	801	6FA	O3B-C3B-C4B	2.01	116.86	111.05
3	A	801	6FA	O2B-C2B-C1B	2.00	118.24	110.85

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	6FA	N10-C1'-C2'-O2'
2	B	1804	NAG	C8-C7-N2-C2
2	B	1804	NAG	O7-C7-N2-C2
2	B	1804	NAG	O5-C5-C6-O6
2	A	804	NAG	C8-C7-N2-C2
2	B	1804	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	804	NAG	O7-C7-N2-C2
4	B	1901	ABL	C3A-C4A-O1-C1
3	A	801	6FA	P-O3P-PA-O1A
4	A	901	ABL	C3A-C4A-O1-C1
3	A	801	6FA	PA-O3P-P-O5'
3	B	1801	6FA	PA-O3P-P-O5'
3	A	801	6FA	P-O3P-PA-O2A
3	A	801	6FA	O4B-C4B-C5B-O5B
3	B	1801	6FA	O4B-C4B-C5B-O5B
3	B	1801	6FA	P-O3P-PA-O1A
2	A	804	NAG	O5-C5-C6-O6
2	A	803	NAG	O5-C5-C6-O6

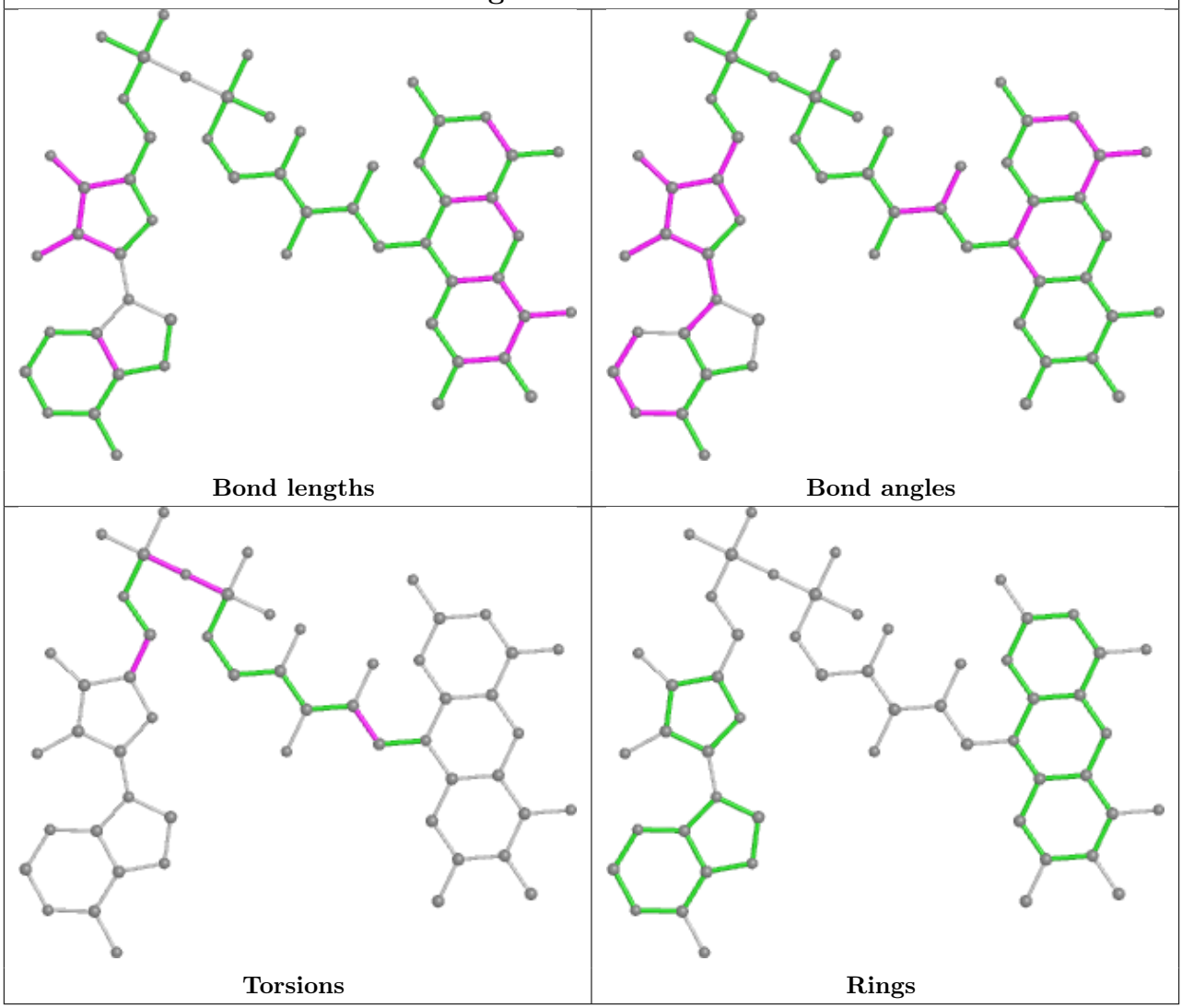
There are no ring outliers.

2 monomers are involved in 5 short contacts:

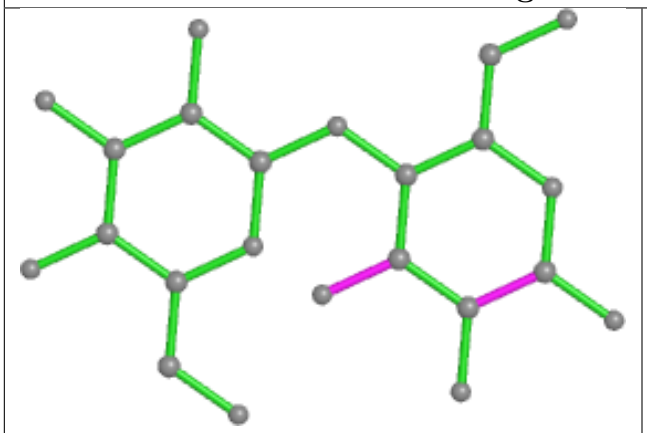
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	6FA	3	0
3	B	1801	6FA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

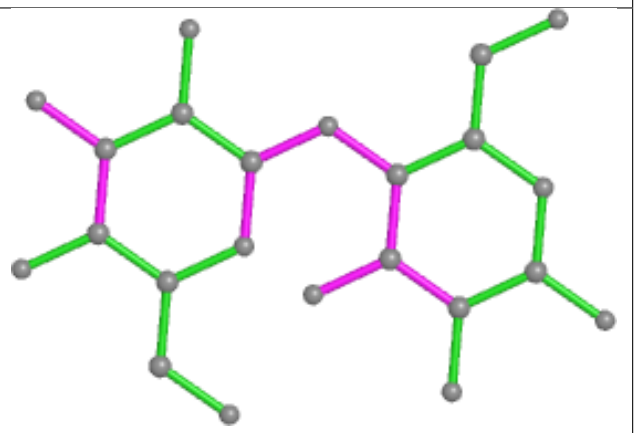
Ligand 6FA A 801



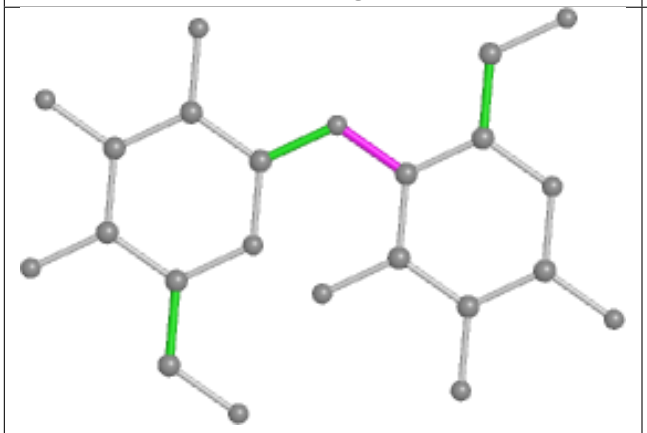
Ligand ABL B 1901



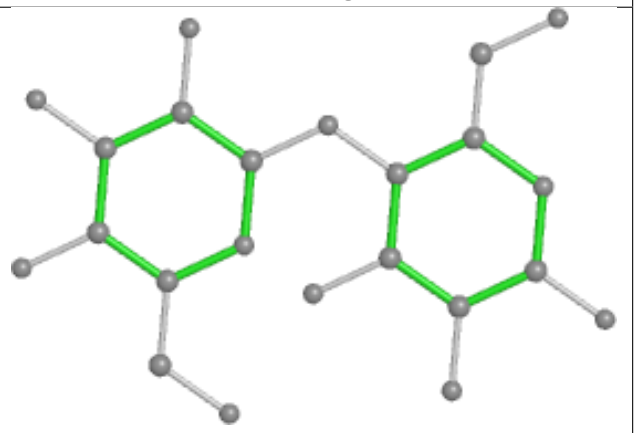
Bond lengths



Bond angles

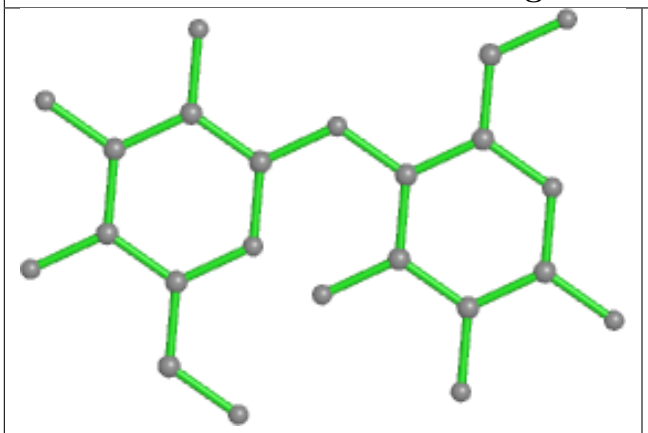


Torsions

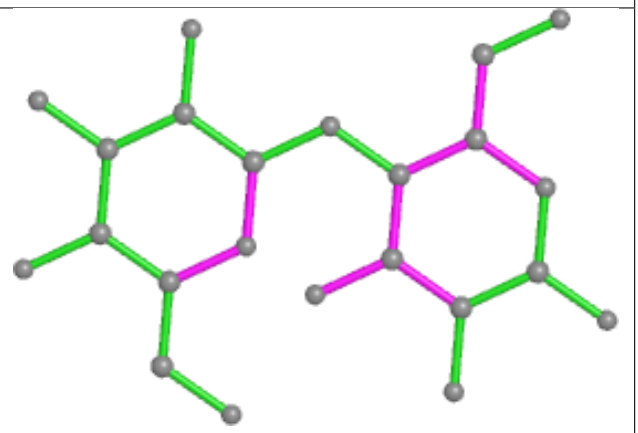


Rings

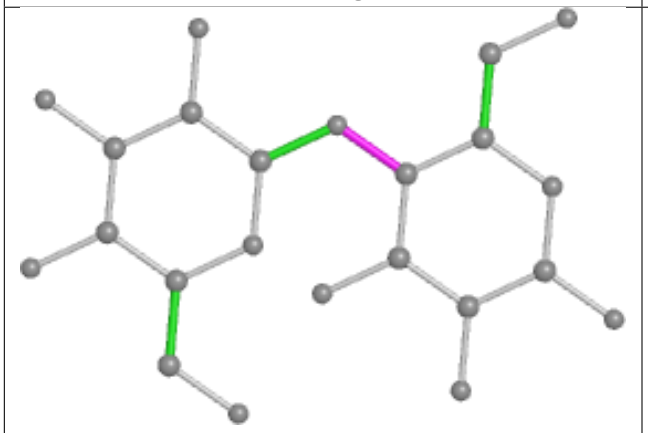
Ligand ABL A 901



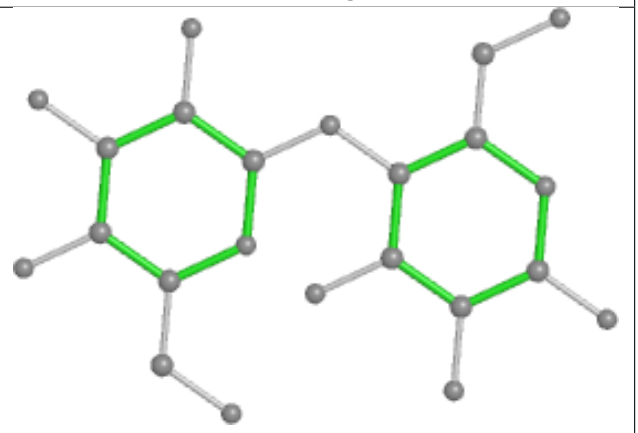
Bond lengths



Bond angles

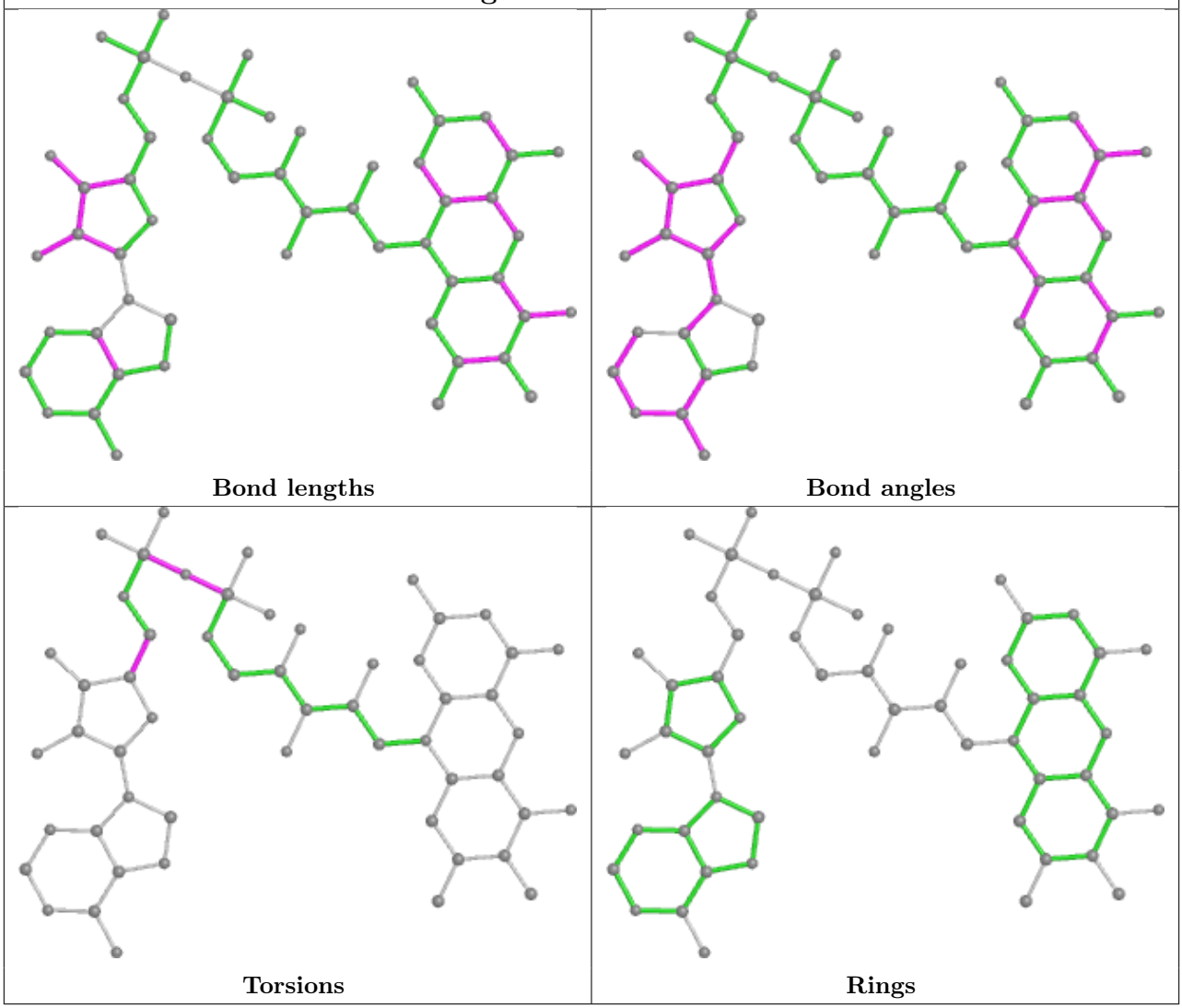


Torsions



Rings

Ligand 6FA B 1801



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	541/541 (100%)	-0.23	2 (0%)	92	90	6, 8, 12, 26	0
1	B	541/541 (100%)	-0.16	9 (1%)	70	66	6, 8, 12, 31	0
All	All	1082/1082 (100%)	-0.19	11 (1%)	82	80	6, 8, 12, 31	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	448	LEU	3.2
1	B	446	PRO	3.0
1	B	450	PRO	2.9
1	B	447	THR	2.6
1	B	458	PRO	2.3
1	B	434	ASN	2.3
1	B	216	PRO	2.3
1	B	657	GLY	2.2
1	B	451	ASN	2.2
1	A	657	GLY	2.1
1	A	451	ASN	2.1

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)

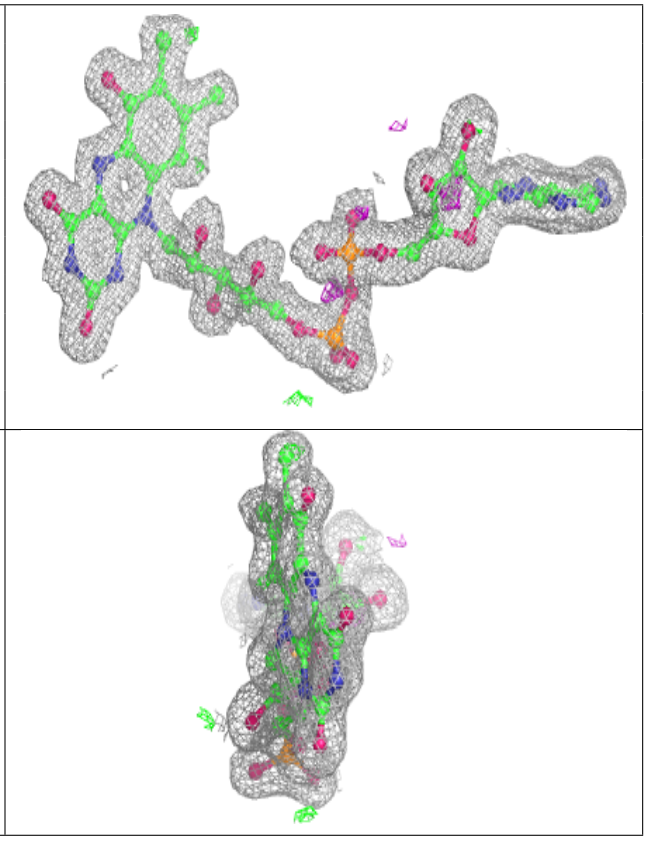
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	A	804	14/15	0.82	0.35	9,13,16,18	0
2	NAG	B	1804	14/15	0.82	0.32	10,13,18,18	0
2	NAG	B	1803	14/15	0.93	0.12	6,9,11,11	0
2	NAG	A	803	14/15	0.94	0.13	7,10,11,12	0
2	NAG	A	802	14/15	0.94	0.09	7,8,12,13	0
3	6FA	B	1801	54/54	0.96	0.10	5,8,9,11	0
3	6FA	A	801	54/54	0.97	0.12	5,8,10,11	0
4	ABL	B	1901	23/23	0.97	0.10	4,8,9,10	0
4	ABL	A	901	23/23	0.98	0.12	6,8,9,10	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.

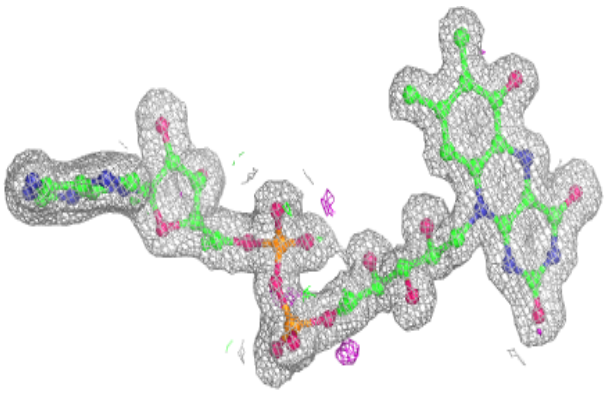
Electron density around 6FA B 1801:

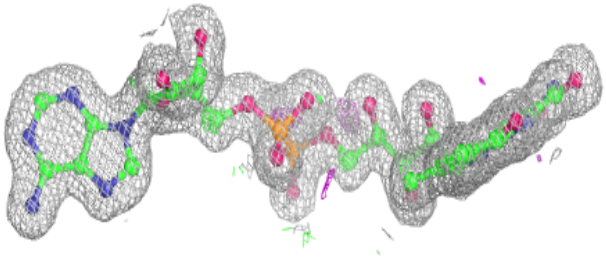
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

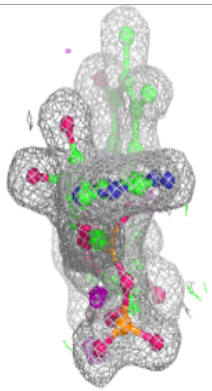


Electron density around 6FA A 801:

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

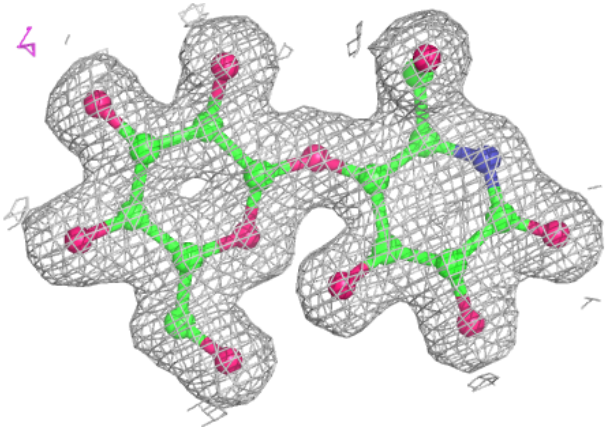


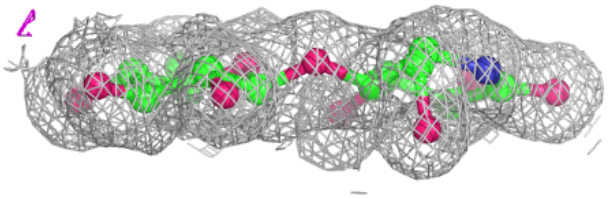


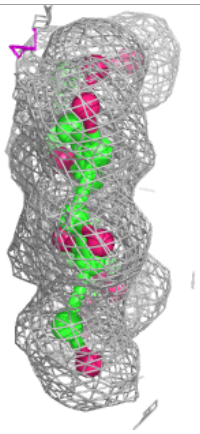


Electron density around ABL B 1901:

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

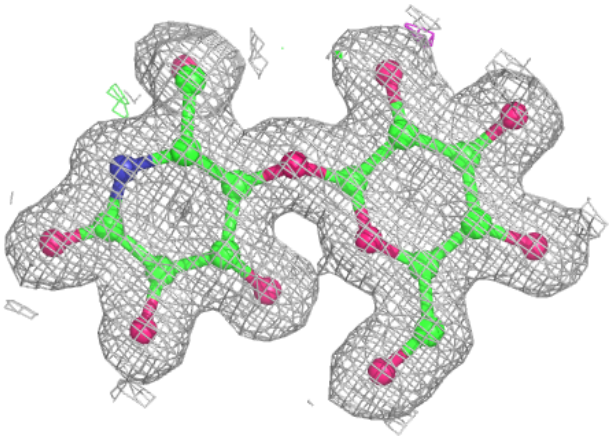


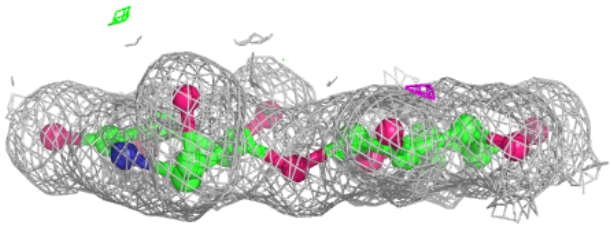


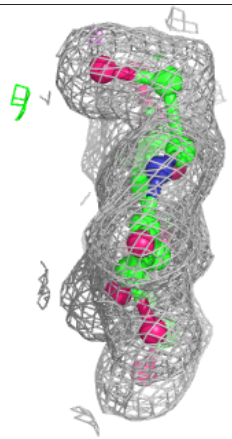


Electron density around ABL A 901:

$2mF_o$-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.