wwPDB X-ray Structure Validation Summary Report (i)

Nov 6, 2023 – 10:50 AM EST

PDB ID	:	4M49
Title	:	Lactate Dehydrogenase A in complex with a substituted pyrazine inhibitor compound 18
Authors	:	Eigenbrot, C.; Ultsch, M.
Deposited on	:	2013-08-06
Resolution	:	2.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

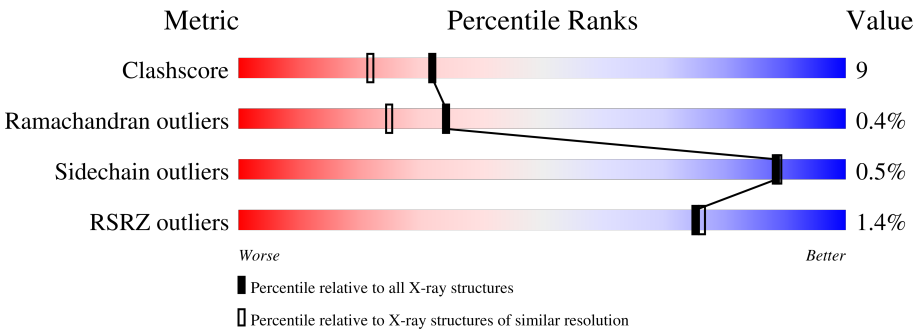
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.05 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))
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	331	2% 85% 14% •
1	B	331	% 86% 14%
1	C	331	% 82% 18%
1	D	331	2% 88% 11% •

2 Entry composition (i)

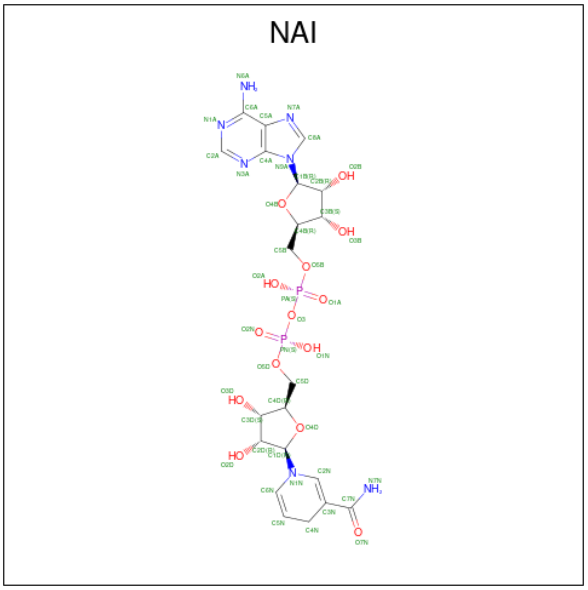
There are 7 unique types of molecules in this entry. The entry contains 11255 atoms, of which 7 are hydrogens and 0 are deuteriums.

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 L-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	331	2601	1662	440	484	15	0	7	0
1	B	331	2632	1691	445	482	14	0	10	0
1	C	331	2605	1666	443	482	14	0	7	0
1	D	331	2600	1667	440	478	15	0	6	0

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	44	21	7	14	2	0	0
2	B	1	44	21	7	14	2	0	0

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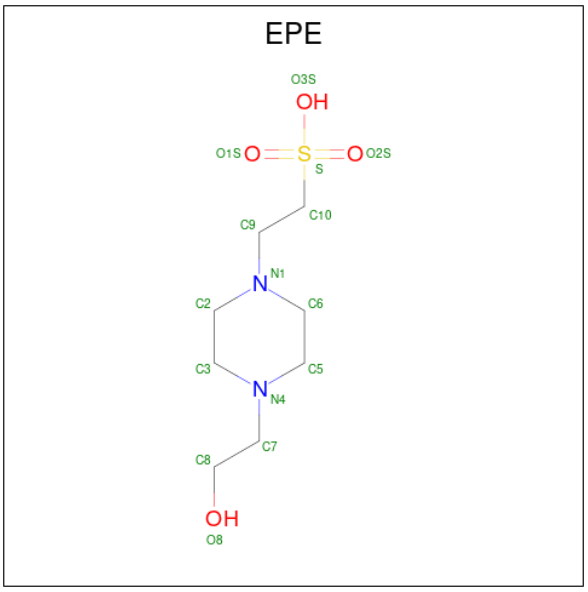
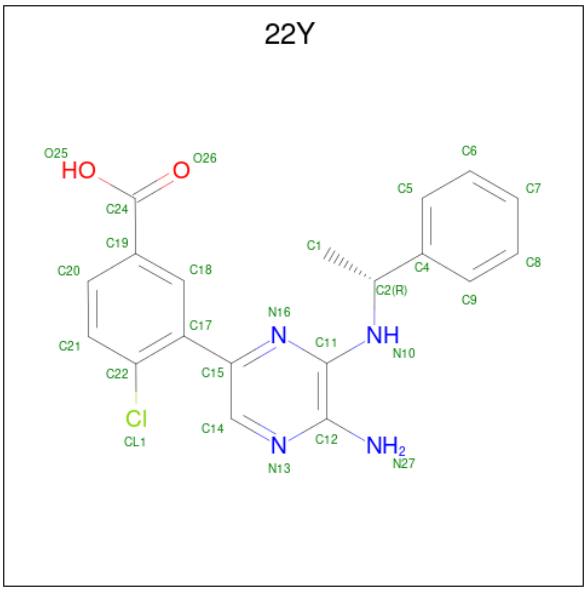
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	C	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
2	D	1	44	21	7	14	2	0	0

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



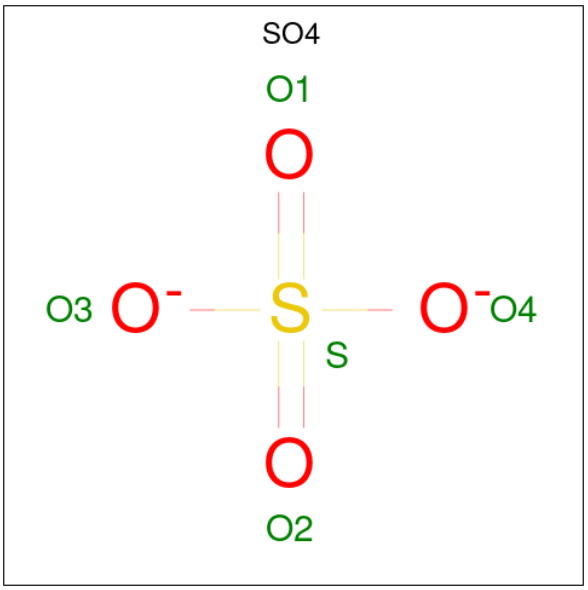
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	15	8	2	4	1	0	0
			Total	C	N	O	S		
3	B	1	15	8	2	4	1	0	0
			Total	C	N	O	S		
3	C	1	15	8	2	4	1	0	0

- Molecule 4 is 3-(5-amino-6-{[(1R)-1-phenylethyl]amino}pyrazin-2-yl)-4-chlorobenzoic acid (three-letter code: 22Y) (formula: $C_{19}H_{17}ClN_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Cl H N O 27 19 1 1 4 2	0	0
4	C	1	Total C Cl H N O 27 19 1 1 4 2	0	0
4	D	1	Total C Cl N O 26 19 1 4 2	0	0

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



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

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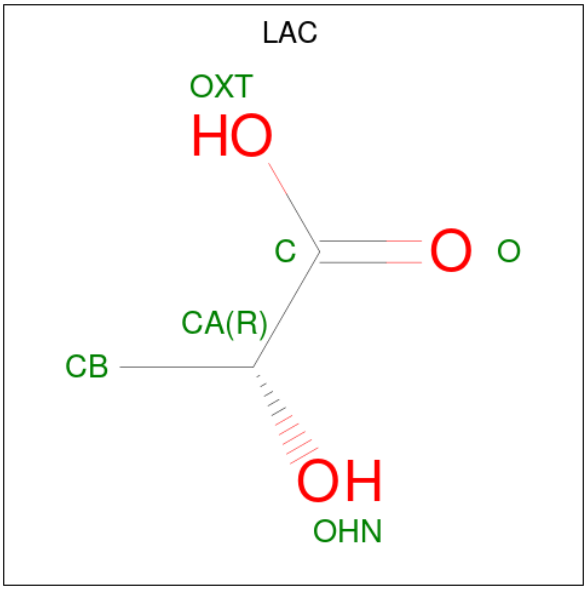
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	C	1	5	4	1	0	0
			Total	O	S		
5	D	1	5	4	1	0	0

- Molecule 6 is LACTIC ACID (three-letter code: LAC) (formula: $C_3H_6O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	B	1	11	3	5	3	0	0

- Molecule 7 is water.

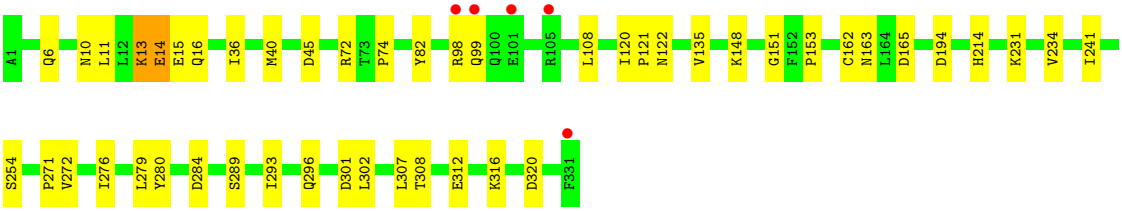
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	109	109	109	0	0
			Total	O		
7	B	166	166	166	0	0
			Total	O		
7	C	76	76	76	0	0
			Total	O		
7	D	139	139	139	0	0

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.

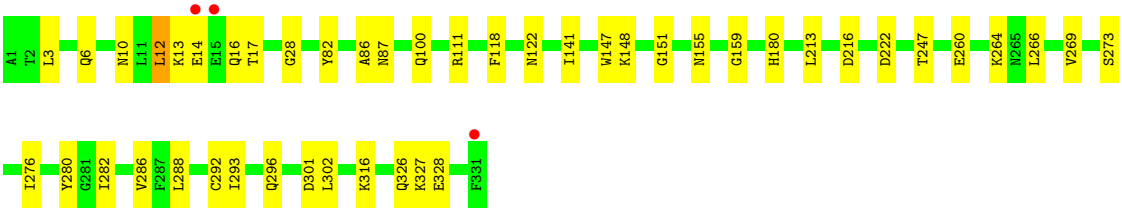
• Molecule 1: L-lactate dehydrogenase A chain

Chain A:



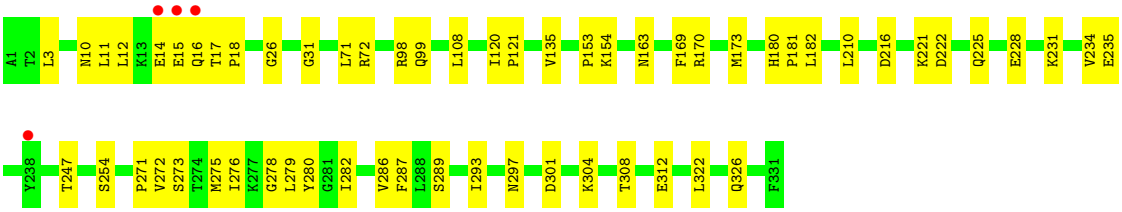
• Molecule 1: L-lactate dehydrogenase A chain

Chain B:



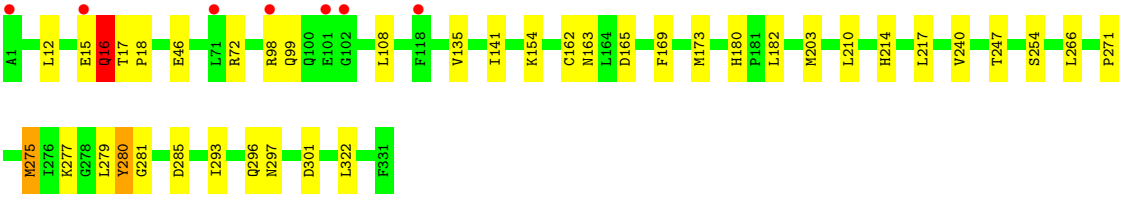
• Molecule 1: L-lactate dehydrogenase A chain

Chain C:



• Molecule 1: L-lactate dehydrogenase A chain

Chain D:


A1
L12
E15
Q16
T17
P18
E46
L71
R72
R98
Q99
Q100
E101
G102
L108
F118
V135
I141
K154
C162
N163
L164
D165
F169
M173
H180
P181
L182
M203
L210
H214
L217
V240
T247
S254
L266
P271
M275
I276
K277
G278
L279
Y280
G281
D285
I293
Q296
N297
D301
L322
F331

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	168.38Å 81.82Å 120.67Å 90.00° 117.65° 90.00°	Depositor
Resolution (Å)	41.74 – 2.05 41.74 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.74-2.05) 99.5 (41.74-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.35 (at 2.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.171 , 0.224 0.169 , (Not available)	Depositor DCC
R_{free} test set	545 reflections (0.60%)	wwPDB-VP
Wilson B-factor (Å^2)	35.2	Xtriage
Anisotropy	0.716	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11255	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: LAC, NAI, 22Y, SO4, EPE

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	0.33	0/2666	0.47	0/3603
1	B	0.37	0/2708	0.51	0/3660
1	C	0.30	0/2670	0.46	0/3608
1	D	0.36	0/2663	0.49	0/3598
All	All	0.34	0/10707	0.48	0/14469

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	2601	0	2702	45	0
1	B	2632	0	2752	50	0
1	C	2605	0	2715	70	0
1	D	2600	0	2712	54	0
2	A	44	0	26	1	0
2	B	44	0	26	3	0
2	C	44	0	26	1	0
2	D	44	0	26	3	0
3	A	15	0	17	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	17	1	0
3	C	15	0	17	6	0
4	A	26	1	16	2	0
4	C	26	1	16	4	0
4	D	26	0	16	0	0
5	A	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	B	6	5	0	1	0
7	A	109	0	0	2	0
7	B	166	0	0	2	0
7	C	76	0	0	0	0
7	D	139	0	0	3	0
All	All	11248	7	11084	195	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 9.

The worst 5 of 195 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:14:GLU:HB3	1:A:15:GLU:CA	1.66	1.24
1:D:154[B]:LYS:CE	1:D:275:MET:HE3	1.76	1.14
1:C:276:ILE:HD11	1:C:286[B]:VAL:HG23	1.19	1.11
1:B:302:LEU:HD13	1:C:11:LEU:HD11	1.34	1.09
1:A:14:GLU:HB3	1:A:15:GLU:HA	1.07	1.06

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	336/331 (102%)	326 (97%)	9 (3%)	1 (0%)	41	32
1	B	339/331 (102%)	325 (96%)	13 (4%)	1 (0%)	41	32
1	C	336/331 (102%)	329 (98%)	6 (2%)	1 (0%)	41	32
1	D	335/331 (101%)	325 (97%)	8 (2%)	2 (1%)	25	15
All	All	1346/1324 (102%)	1305 (97%)	36 (3%)	5 (0%)	34	25

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	280	TYR
1	B	14	GLU
1	D	16	GLN
1	A	14	GLU
1	C	14	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	294/287 (102%)	292 (99%)	2 (1%)	84	84
1	B	297/287 (104%)	296 (100%)	1 (0%)	92	93
1	C	294/287 (102%)	294 (100%)	0	100	100
1	D	293/287 (102%)	290 (99%)	3 (1%)	76	75
All	All	1178/1148 (103%)	1172 (100%)	6 (0%)	88	89

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	12	LEU
1	D	16	GLN
1	D	275	MET
1	A	72	ARG
1	A	13	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	A	296	GLN
1	B	326	GLN
1	D	16	GLN
1	D	296	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)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EPE	C	802	-	15,15,15	0.83	1 (6%)	18,20,20	1.93	5 (27%)
2	NAI	B	801	-	42,48,48	1.93	13 (30%)	47,73,73	1.40	7 (14%)
3	EPE	A	802	-	15,15,15	0.80	1 (6%)	18,20,20	1.77	5 (27%)
2	NAI	D	801	-	42,48,48	2.02	13 (30%)	47,73,73	1.52	8 (17%)
2	NAI	A	801	-	42,48,48	2.02	11 (26%)	47,73,73	1.51	8 (17%)
3	EPE	B	802	-	15,15,15	0.88	1 (6%)	18,20,20	2.00	7 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	22Y	A	803	-	28,28,28	0.97	3 (10%)	36,39,39	1.09	2 (5%)
5	SO4	A	804	-	4,4,4	0.16	0	6,6,6	0.25	0
5	SO4	D	803	-	4,4,4	0.20	0	6,6,6	0.12	0
5	SO4	C	804	-	4,4,4	0.16	0	6,6,6	0.21	0
4	22Y	C	803	-	28,28,28	0.92	2 (7%)	36,39,39	1.10	2 (5%)
6	LAC	B	803	-	5,5,5	0.80	0	4,6,6	0.90	0
4	22Y	D	802	-	28,28,28	1.30	4 (14%)	36,39,39	1.13	1 (2%)
2	NAI	C	801	-	42,48,48	2.05	12 (28%)	47,73,73	1.52	7 (14%)

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	EPE	C	802	-	-	4/9/19/19	0/1/1/1
2	NAI	B	801	-	-	5/25/72/72	0/5/5/5
3	EPE	A	802	-	-	3/9/19/19	0/1/1/1
2	NAI	D	801	-	-	4/25/72/72	0/5/5/5
2	NAI	A	801	-	-	3/25/72/72	0/5/5/5
3	EPE	B	802	-	-	2/9/19/19	0/1/1/1
4	22Y	A	803	-	-	0/16/16/16	0/3/3/3
4	22Y	C	803	-	-	0/16/16/16	0/3/3/3
6	LAC	B	803	-	-	4/4/4/4	-
4	22Y	D	802	-	-	0/16/16/16	0/3/3/3
2	NAI	C	801	-	-	6/25/72/72	0/5/5/5

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	NAI	C4N-C3N	-5.30	1.39	1.49
2	B	801	NAI	C6N-C5N	4.79	1.41	1.33
2	C	801	NAI	C4N-C3N	-4.78	1.40	1.49
2	A	801	NAI	C6N-C5N	4.65	1.41	1.33
2	A	801	NAI	C2B-C3B	-4.59	1.40	1.53

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	801	NAI	O4D-C1D-N1N	5.13	118.08	108.06
3	C	802	EPE	C5-N4-C3	4.73	119.47	108.83
2	A	801	NAI	O4D-C1D-N1N	4.71	117.25	108.06
2	C	801	NAI	O4D-C1D-N1N	4.66	117.16	108.06
2	B	801	NAI	N3A-C2A-N1A	-4.42	121.77	128.68

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	801	NAI	C5D-O5D-PN-O3
3	A	802	EPE	C9-C10-S-O1S
3	A	802	EPE	C9-C10-S-O3S
3	B	802	EPE	C8-C7-N4-C3
3	B	802	EPE	S-C10-C9-N1

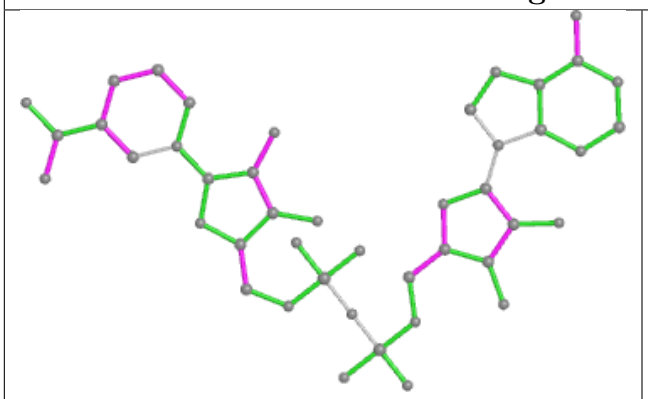
There are no ring outliers.

10 monomers are involved in 23 short contacts:

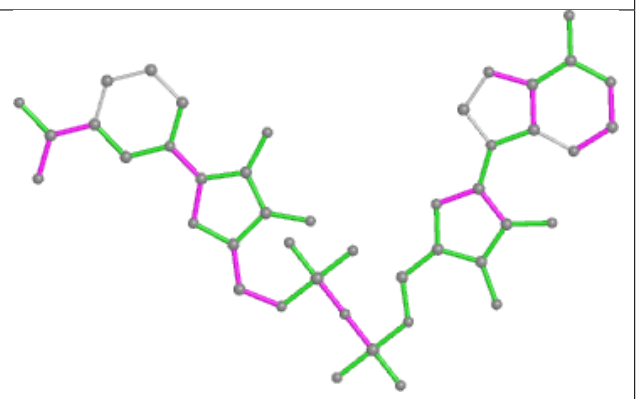
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	802	EPE	6	0
2	B	801	NAI	3	0
3	A	802	EPE	2	0
2	D	801	NAI	3	0
2	A	801	NAI	1	0
3	B	802	EPE	1	0
4	A	803	22Y	2	0
4	C	803	22Y	4	0
6	B	803	LAC	1	0
2	C	801	NAI	1	0

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.

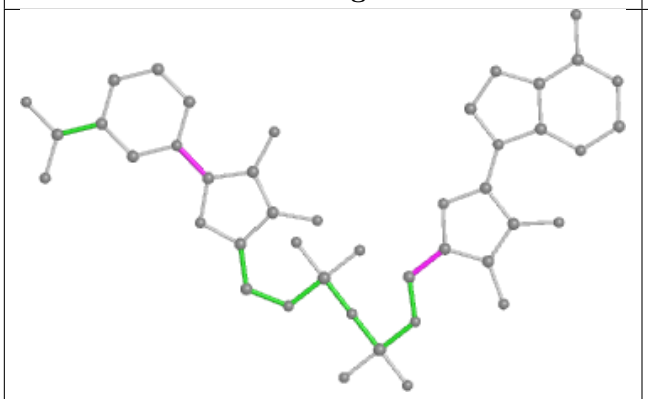
Ligand NAI B 801



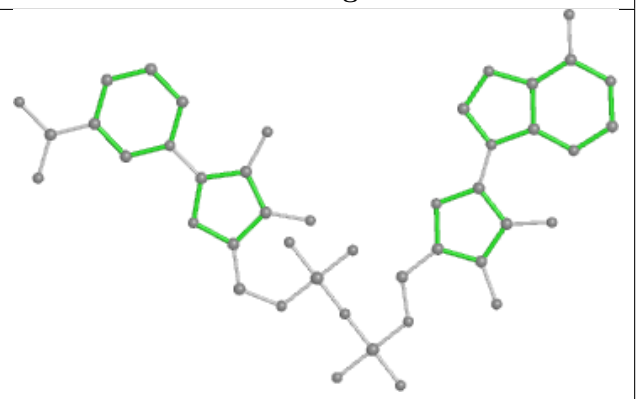
Bond lengths



Bond angles

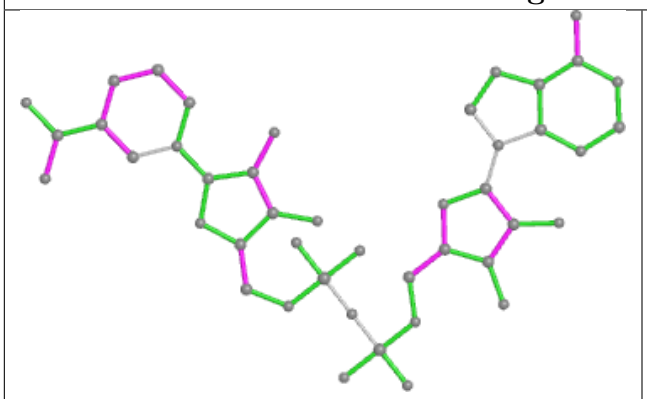


Torsions

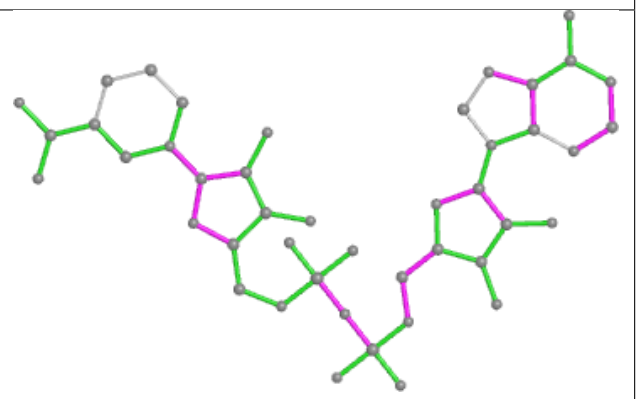


Rings

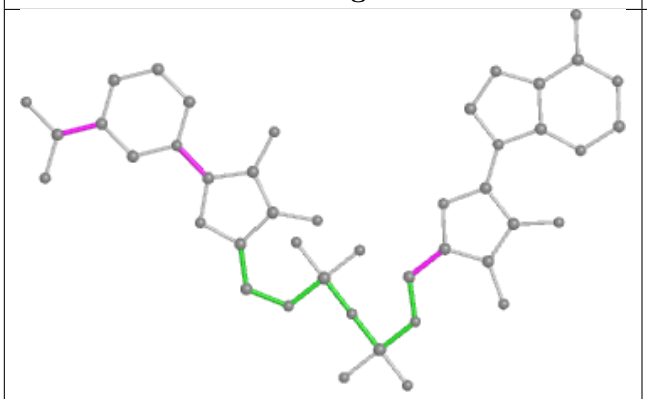
Ligand NAI D 801



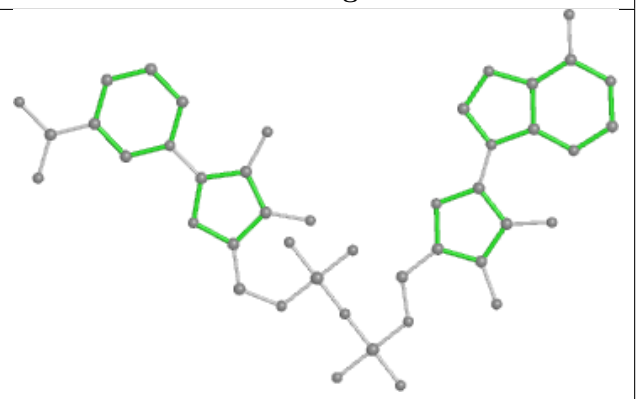
Bond lengths



Bond angles

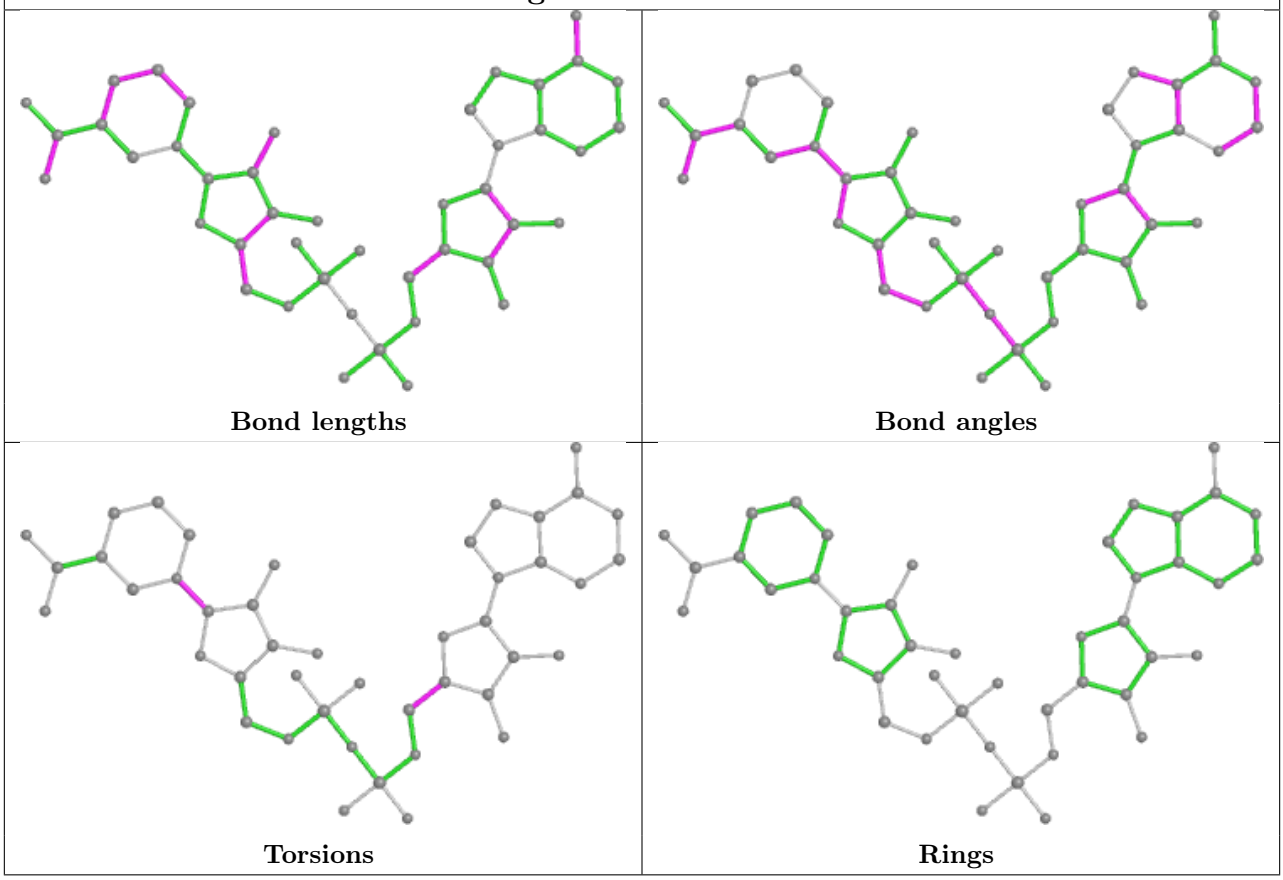


Torsions

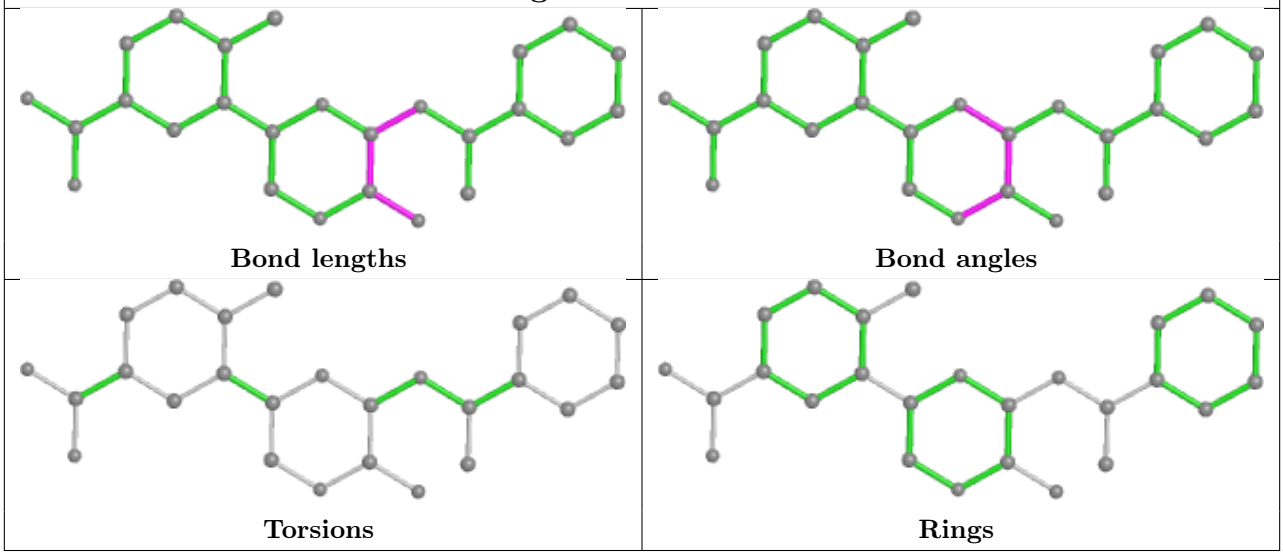


Rings

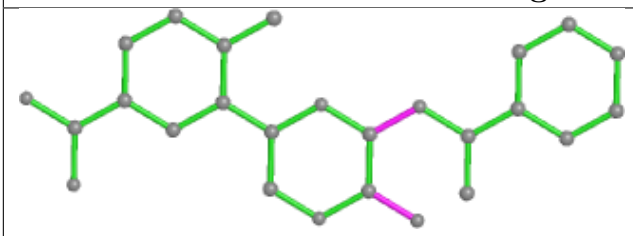
Ligand NAI A 801



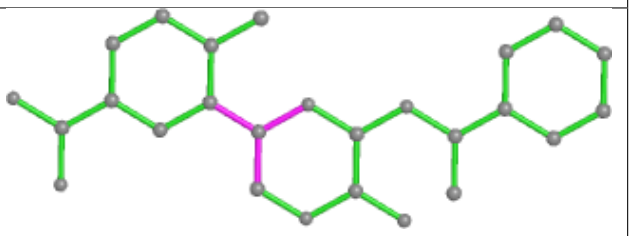
Ligand 22Y A 803



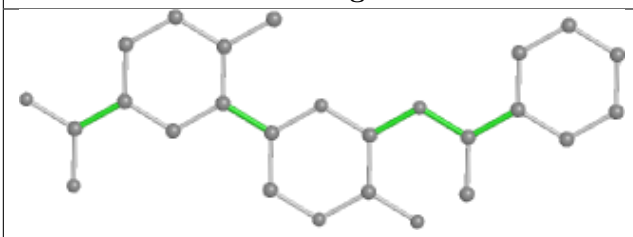
Ligand 22Y C 803



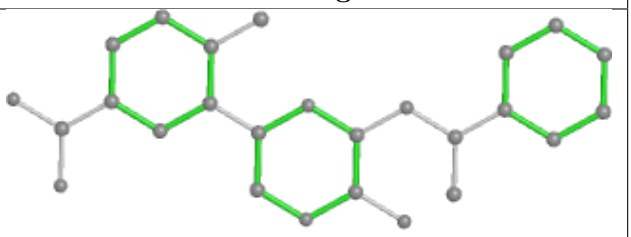
Bond lengths



Bond angles

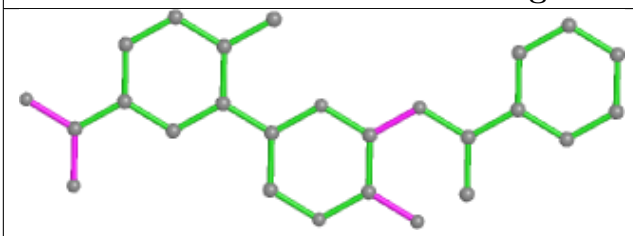


Torsions

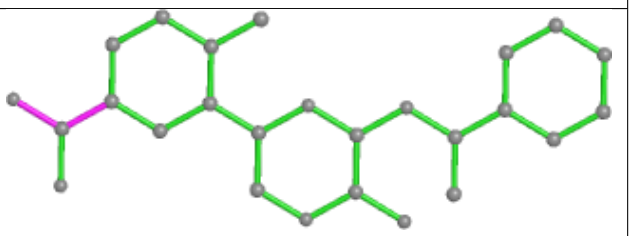


Rings

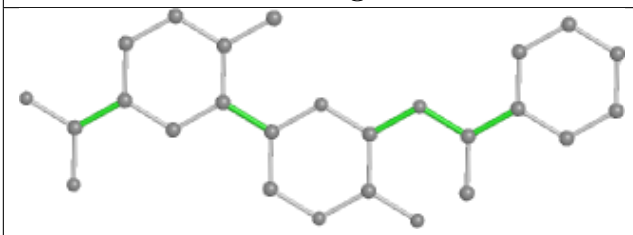
Ligand 22Y D 802



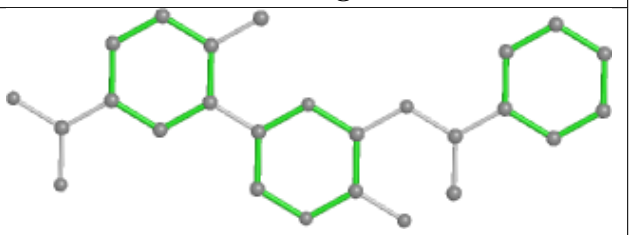
Bond lengths



Bond angles

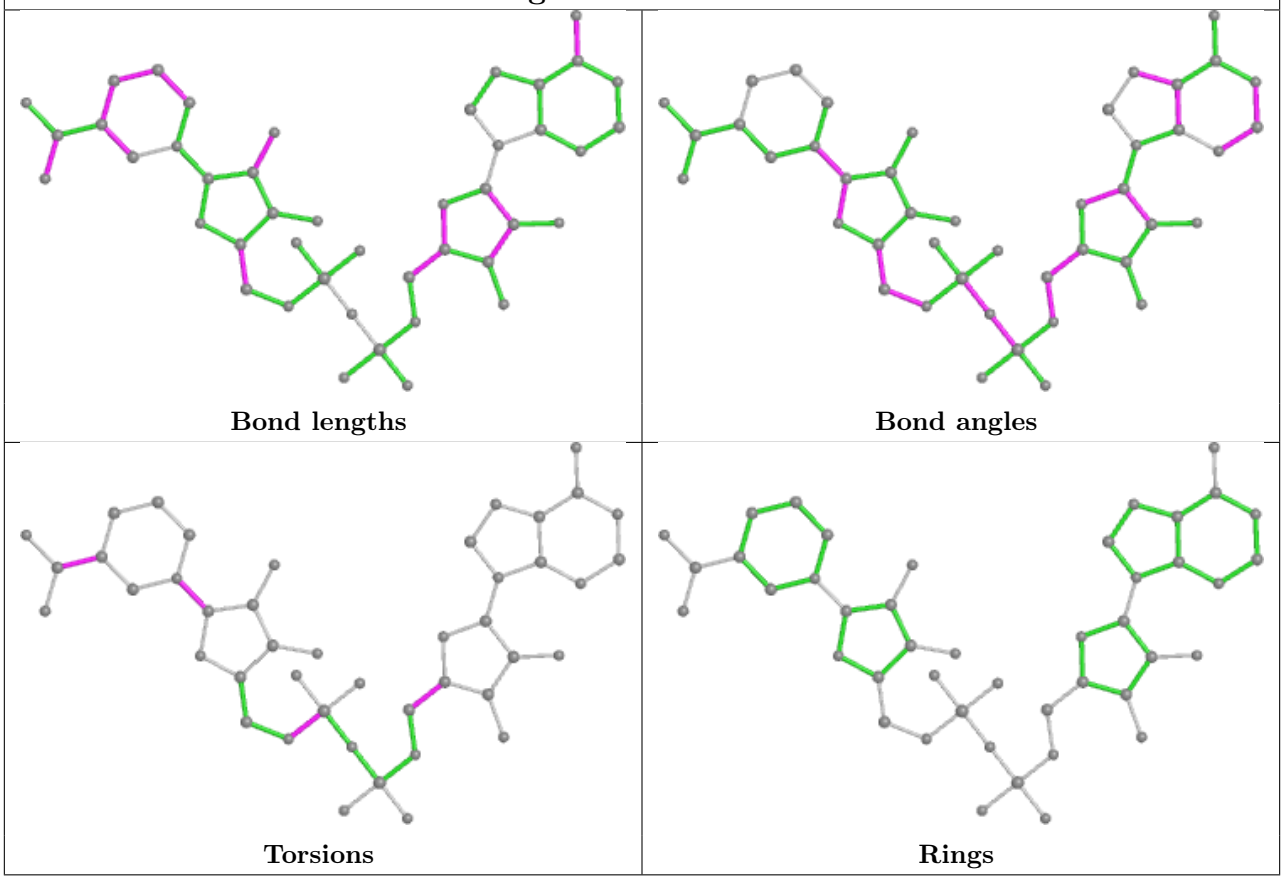


Torsions



Rings

Ligand NAI C 801



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	331/331 (100%)	-0.50	5 (1%)	73	75	29, 46, 81, 126	0
1	B	331/331 (100%)	-0.64	3 (0%)	84	85	28, 40, 65, 122	0
1	C	331/331 (100%)	-0.29	4 (1%)	79	80	32, 51, 85, 117	0
1	D	331/331 (100%)	-0.46	7 (2%)	63	65	30, 40, 74, 134	0
All	All	1324/1324 (100%)	-0.47	19 (1%)	75	76	28, 44, 80, 134	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	ARG	5.7
1	D	101	GLU	4.9
1	D	1	ALA	3.5
1	B	14	GLU	3.1
1	C	14	GLU	3.1

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)

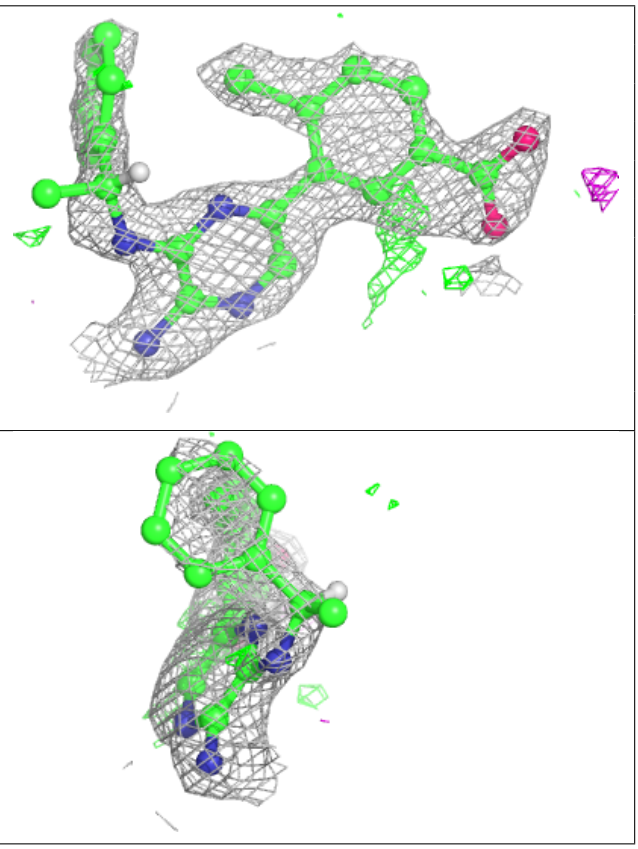
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	22Y	A	803	26/26	0.80	0.25	30,54,63,65	27
3	EPE	C	802	15/15	0.88	0.16	93,96,118,118	0
4	22Y	C	803	26/26	0.89	0.13	47,58,69,74	27
5	SO4	A	804	5/5	0.90	0.21	44,47,57,58	5
5	SO4	C	804	5/5	0.91	0.20	35,41,51,52	5
3	EPE	A	802	15/15	0.92	0.16	82,93,98,98	0
3	EPE	B	802	15/15	0.94	0.16	81,118,125,126	0
4	22Y	D	802	26/26	0.94	0.11	28,44,51,51	26
2	NAI	C	801	44/44	0.95	0.10	42,59,71,77	0
6	LAC	B	803	6/6	0.95	0.12	30,36,50,51	0
2	NAI	D	801	44/44	0.96	0.09	39,50,63,67	0
2	NAI	A	801	44/44	0.96	0.09	41,55,61,66	0
5	SO4	D	803	5/5	0.97	0.16	29,36,44,45	5
2	NAI	B	801	44/44	0.97	0.07	27,36,40,43	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.

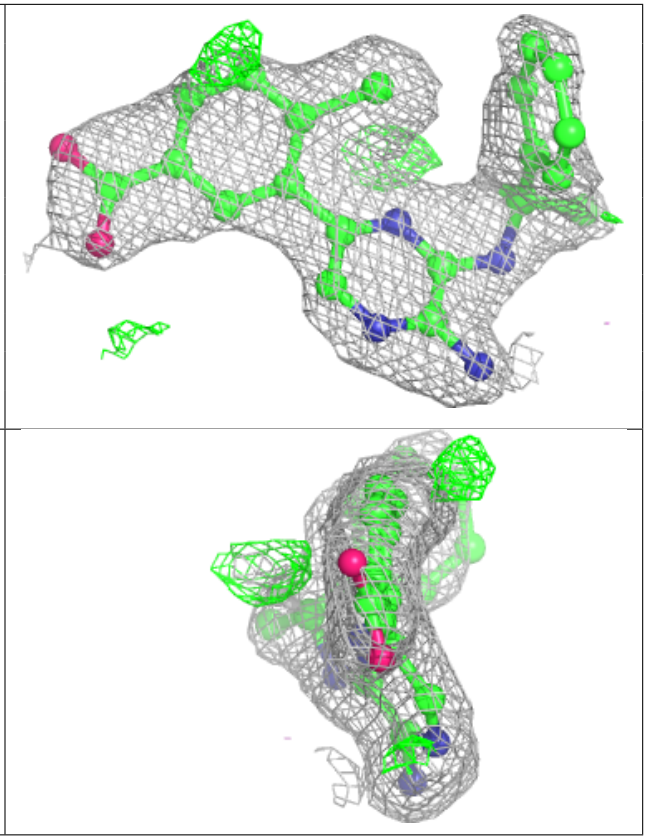
Electron density around 22Y A 803:

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



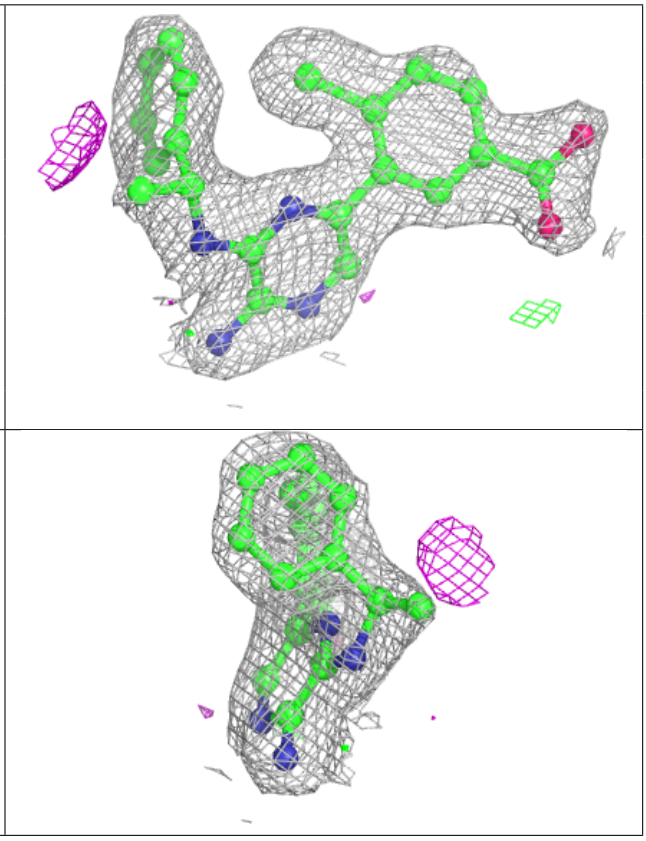
Electron density around 22Y C 803:

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



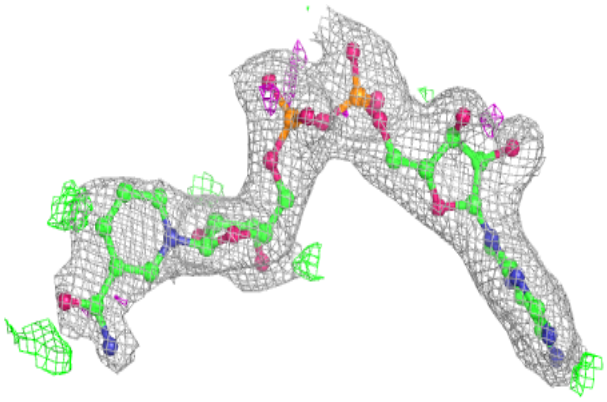
Electron density around 22Y D 802:

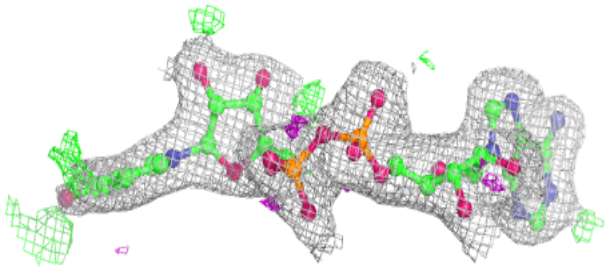
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

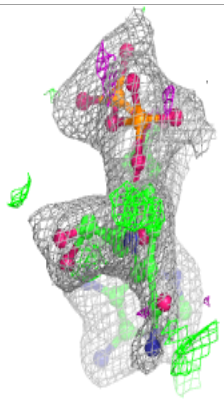


Electron density around NAI C 801:

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







Electron density around NAI D 801:

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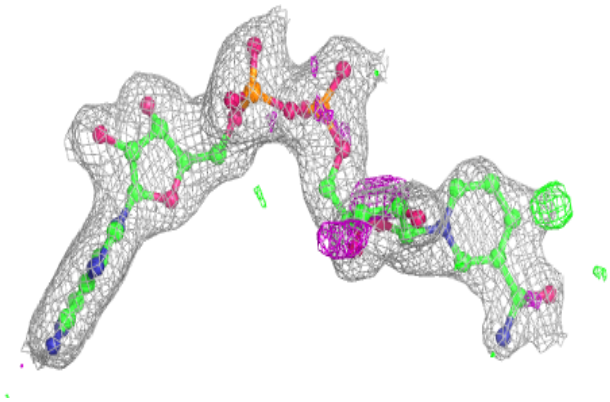
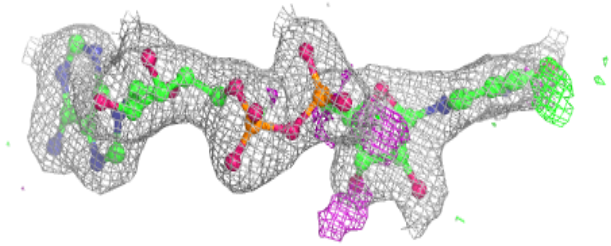
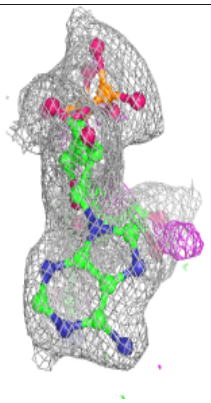
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

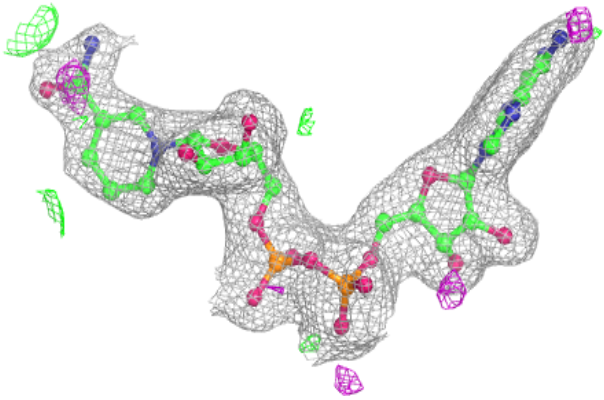


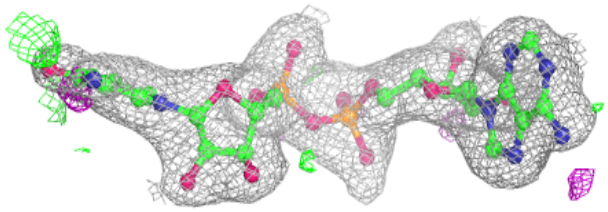


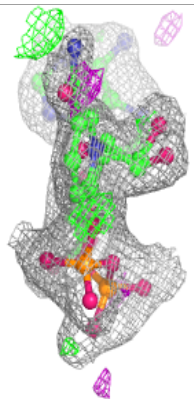


Electron density around NAI A 801:

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

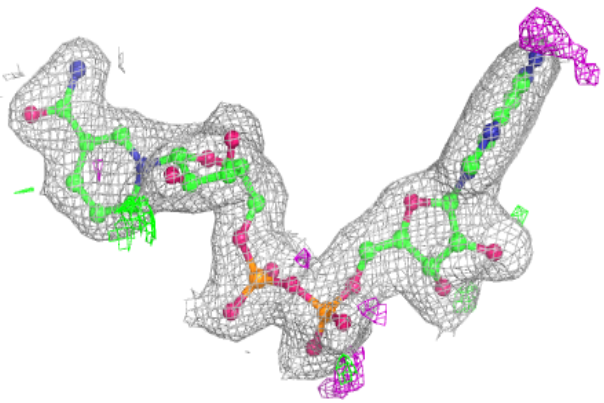


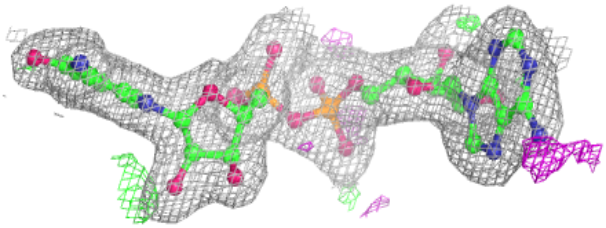


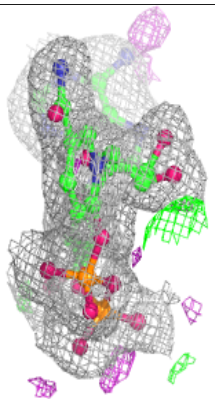


Electron density around NAI B 801:

$2mF_o$-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.