Full wwPDB X-ray Structure Validation Report

Jun 22, 2024 – 11:01 PM EDT

PDB ID	:	6GPL
Title	:	Crystal structure of human GDP-D-mannose 4,6-dehydratase in complex with GDP-4k6d-Man
Authors	:	Pfeiffer, M.; Krojer, T.; Johansson, C.; von Delft, F.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.; Nidetzky, B.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on	:	2018-06-06
Resolution	:	1.76 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 (1)) were used in the production of this report:

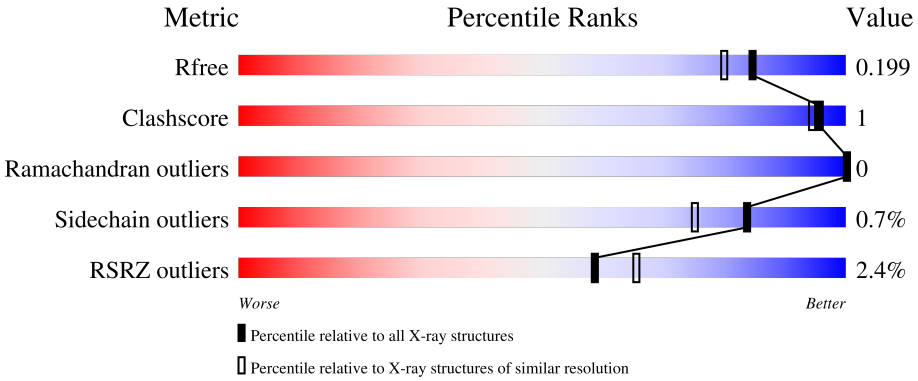
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	B	352	% 93%
1	C	352	% 93%
1	D	352	7% 95%
1	E	352	% 93%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12088 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.

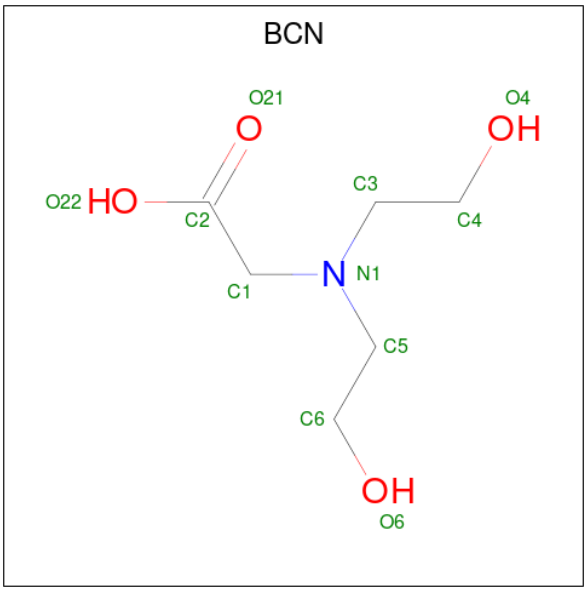
- Molecule 1 is a protein called GDP-mannose 4,6 dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	342	Total	C	N	O	S	0	4	0
			2755	1754	476	515	10			
1	C	341	Total	C	N	O	S	0	1	0
			2706	1726	465	505	10			
1	D	341	Total	C	N	O	S	0	0	0
			2688	1716	462	500	10			
1	E	337	Total	C	N	O	S	0	1	0
			2662	1699	454	498	11			

There are 8 discrepancies between the modelled and reference sequences:

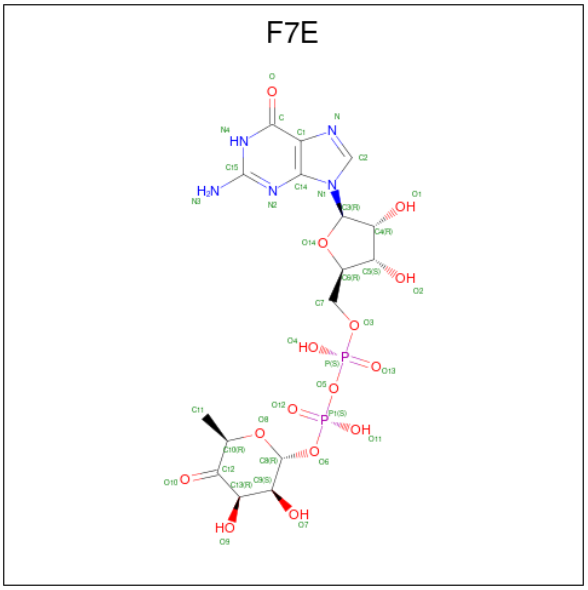
Chain	Residue	Modelled	Actual	Comment	Reference
B	21	SER	-	expression tag	UNP O60547
B	22	MET	-	expression tag	UNP O60547
C	21	SER	-	expression tag	UNP O60547
C	22	MET	-	expression tag	UNP O60547
D	21	SER	-	expression tag	UNP O60547
D	22	MET	-	expression tag	UNP O60547
E	21	SER	-	expression tag	UNP O60547
E	22	MET	-	expression tag	UNP O60547

- Molecule 2 is BICINE (three-letter code: BCN) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 3 is [[(2 {R},3 {S},4 {R},5 {R})-5-(2-azanyl-6-oxidanylidene-1 {H}-purin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2 {R},3 {S},4 {R},6 {R})-6-methyl-3,4-bis(oxidanyl)-5-oxidanylidene-oxan-2-yl] hydrogen phosphate (three-letter code: F7E) (formula: $C_{16}H_{23}N_5O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			38	16	5	15	2		

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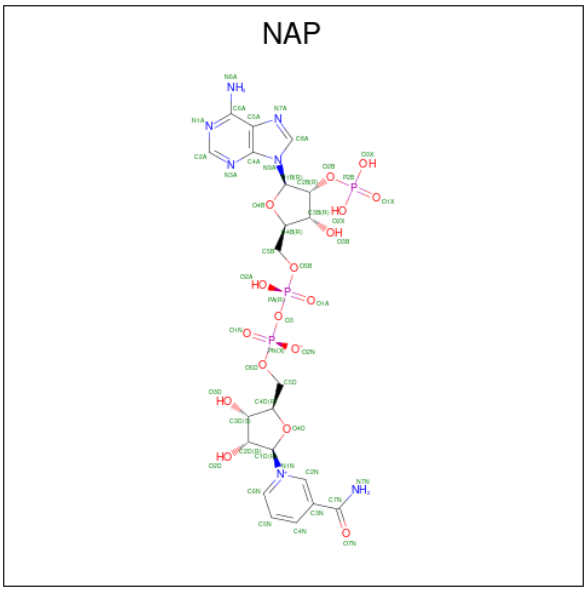
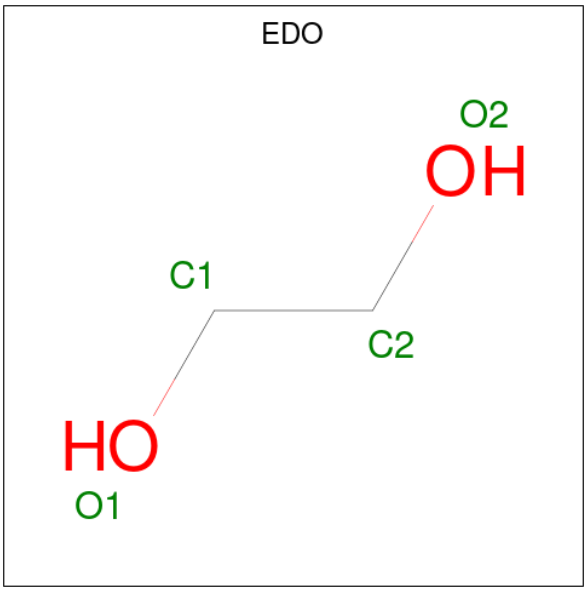
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	D	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	E	1	Total	C	N	O	P	0	0
			38	16	5	15	2		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	247	Total O 247 247	0	0
6	C	234	Total O 234 234	0	0
6	D	187	Total O 187 187	0	0

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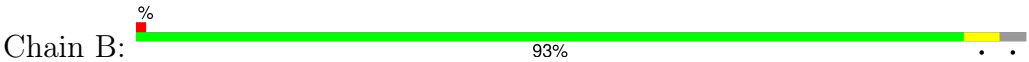
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	218	Total O 218 218	0	0

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.

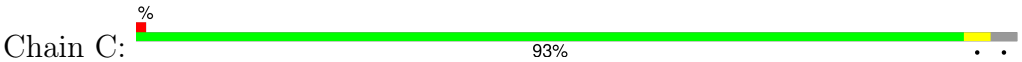
• Molecule 1: GDP-mannose 4,6 dehydratase

Chain B:



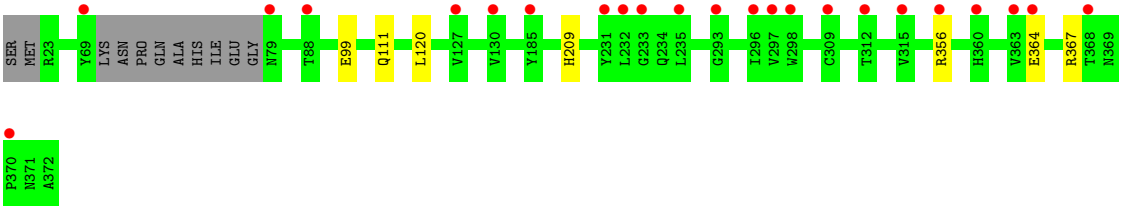
• Molecule 1: GDP-mannose 4,6 dehydratase

Chain C:



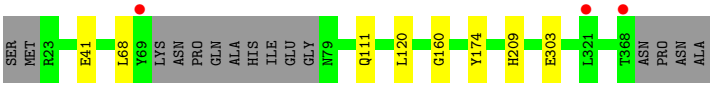
• Molecule 1: GDP-mannose 4,6 dehydratase

Chain D:



• Molecule 1: GDP-mannose 4,6 dehydratase

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.26Å 122.77Å 139.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.09 – 1.76 39.09 – 1.76	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.09-1.76) 100.0 (39.09-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.169 , 0.190 0.178 , 0.199	Depositor DCC
R_{free} test set	7486 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12088	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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: BCN, EDO, F7E, NAP

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	B	0.53	0/2816	0.70	2/3813 (0.1%)
1	C	0.51	0/2766	0.68	1/3748 (0.0%)
1	D	0.51	0/2747	0.67	0/3723
1	E	0.53	0/2720	0.66	0/3689
All	All	0.52	0/11049	0.68	3/14973 (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	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	144	LEU	CB-CG-CD1	8.23	124.99	111.00
1	B	23	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	B	308	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	214	ARG	Sidechain

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	B	2755	0	2677	11	0
1	C	2706	0	2633	5	0
1	D	2688	0	2619	4	0
1	E	2662	0	2576	5	0
2	B	11	0	12	0	0
3	B	38	0	0	0	0
3	C	38	0	0	0	0
3	D	38	0	0	0	0
3	E	38	0	0	0	0
4	B	48	0	25	1	0
4	C	48	0	25	0	0
4	D	48	0	25	1	0
4	E	48	0	25	1	0
5	B	16	0	24	0	0
5	C	8	0	12	0	0
5	D	12	0	18	0	0
6	B	247	0	0	4	0
6	C	234	0	0	2	0
6	D	187	0	0	1	0
6	E	218	0	0	1	0
All	All	12088	0	10671	25	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (25) 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:244:ASP:OD1	1:B:282[A]:ARG:NH1	1.76	1.16
1:B:299[B]:GLU:CD	6:B:502:HOH:O	1.94	1.04
1:D:364:GLU:OE1	1:D:367:ARG:NH2	1.94	0.98
1:B:299[B]:GLU:CG	6:B:502:HOH:O	2.22	0.85
1:C:142:CYS:O	1:C:144:LEU:HD13	1.90	0.70
1:E:303:GLU:OE2	6:E:4101:HOH:O	2.10	0.70
1:B:299[B]:GLU:HG3	6:B:502:HOH:O	1.87	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:PRO:O	1:B:148:VAL:HG12	2.11	0.51
6:C:2182:HOH:O	1:D:120:LEU:HD11	2.10	0.50
1:B:144:LEU:O	1:B:148:VAL:HG22	2.12	0.49
1:B:120:LEU:HG	1:B:123:TYR:HB3	1.95	0.47
1:D:356:ARG:NH1	6:D:3104:HOH:O	2.47	0.47
1:C:120:LEU:HG	1:C:123:TYR:HB3	1.97	0.47
1:B:299[A]:GLU:HG2	1:B:306:VAL:HG22	1.97	0.46
1:D:209:HIS:CE1	4:D:3002:NAP:C4N	2.98	0.46
1:B:144:LEU:HB3	1:B:148:VAL:HG13	1.99	0.44
1:E:41:GLU:HG2	1:E:68:LEU:HD21	1.99	0.44
1:B:209:HIS:CE1	4:B:403:NAP:C4N	3.01	0.43
1:C:41:GLU:HG2	1:C:68:LEU:HD21	2.01	0.42
6:B:595:HOH:O	1:E:120:LEU:HD11	2.19	0.42
1:E:160:GLY:HA3	1:E:174:TYR:O	2.20	0.41
1:B:282[B]:ARG:NH1	1:B:305:GLU:OE2	2.41	0.41
1:C:291:HIS:HE1	6:C:2242:HOH:O	2.03	0.41
1:E:209:HIS:CE1	4:E:4002:NAP:C4N	3.04	0.40
1:C:160:GLY:HA3	1:C:174:TYR:O	2.21	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	B	342/352 (97%)	335 (98%)	7 (2%)	0	100	100
1	C	338/352 (96%)	332 (98%)	6 (2%)	0	100	100
1	D	337/352 (96%)	331 (98%)	6 (2%)	0	100	100
1	E	334/352 (95%)	329 (98%)	5 (2%)	0	100	100
All	All	1351/1408 (96%)	1327 (98%)	24 (2%)	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	B	292/304 (96%)	291 (100%)	1 (0%)	92	89
1	C	286/304 (94%)	282 (99%)	4 (1%)	67	52
1	D	283/304 (93%)	281 (99%)	2 (1%)	84	75
1	E	280/304 (92%)	279 (100%)	1 (0%)	91	87
All	All	1141/1216 (94%)	1133 (99%)	8 (1%)	84	75

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	111	GLN
1	C	111	GLN
1	C	144	LEU
1	C	290	LEU
1	C	346	LYS
1	D	99	GLU
1	D	111	GLN
1	E	111	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	304	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)

18 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	$\#\|Z\| > 2$
4	NAP	C	2002	-	46,52,52	1.21	4 (8%)	61,80,80	1.31	6 (9%)
5	EDO	D	3003	-	3,3,3	0.44	0	2,2,2	0.38	0
4	NAP	D	3002	-	46,52,52	1.12	4 (8%)	61,80,80	1.43	6 (9%)
5	EDO	B	405	-	3,3,3	0.52	0	2,2,2	0.30	0
5	EDO	D	3005	-	3,3,3	0.38	0	2,2,2	0.28	0
5	EDO	D	3004	-	3,3,3	0.21	0	2,2,2	0.46	0
5	EDO	B	404	-	3,3,3	0.47	0	2,2,2	0.31	0
5	EDO	B	406	-	3,3,3	0.51	0	2,2,2	0.10	0
4	NAP	E	4002	-	46,52,52	1.08	2 (4%)	61,80,80	1.37	6 (9%)
3	F7E	E	4001	-	35,41,41	1.02	3 (8%)	40,64,64	0.76	0
2	BCN	B	401	-	10,10,10	0.95	0	11,11,11	0.89	0
4	NAP	B	403	-	46,52,52	1.09	4 (8%)	61,80,80	1.28	5 (8%)
5	EDO	C	2004	-	3,3,3	0.63	0	2,2,2	0.13	0
3	F7E	C	2001	-	35,41,41	1.04	4 (11%)	40,64,64	0.79	1 (2%)
5	EDO	C	2003	-	3,3,3	0.33	0	2,2,2	0.35	0
3	F7E	B	402	-	35,41,41	1.05	3 (8%)	40,64,64	0.87	1 (2%)
3	F7E	D	3001	-	35,41,41	1.30	2 (5%)	40,64,64	0.85	0
5	EDO	B	407	-	3,3,3	0.42	0	2,2,2	0.25	0

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
4	NAP	C	2002	-	-	4/31/67/67	0/5/5/5
5	EDO	D	3003	-	-	1/1/1/1	-
4	NAP	D	3002	-	-	6/31/67/67	0/5/5/5
5	EDO	B	405	-	-	0/1/1/1	-
5	EDO	D	3005	-	-	1/1/1/1	-
5	EDO	D	3004	-	-	1/1/1/1	-
5	EDO	B	404	-	-	1/1/1/1	-
5	EDO	B	406	-	-	0/1/1/1	-
4	NAP	E	4002	-	-	5/31/67/67	0/5/5/5
3	F7E	E	4001	-	-	2/17/57/57	0/4/4/4
2	BCN	B	401	-	-	2/10/10/10	-
4	NAP	B	403	-	-	6/31/67/67	0/5/5/5
5	EDO	C	2004	-	-	1/1/1/1	-
3	F7E	C	2001	-	-	2/17/57/57	0/4/4/4
5	EDO	C	2003	-	-	0/1/1/1	-
3	F7E	B	402	-	-	2/17/57/57	0/4/4/4
3	F7E	D	3001	-	-	3/17/57/57	0/4/4/4
5	EDO	B	407	-	-	0/1/1/1	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3001	F7E	P1-O6	4.61	1.73	1.59
3	D	3001	F7E	C1-C	-4.43	1.38	1.47
4	C	2002	NAP	O4D-C1D	4.09	1.46	1.40
4	E	4002	NAP	PN-O3	3.64	1.63	1.59
4	C	2002	NAP	PN-O3	3.50	1.63	1.59
3	B	402	F7E	P1-O6	3.42	1.69	1.59
4	B	403	NAP	O4D-C1D	3.41	1.45	1.40
4	B	403	NAP	PN-O3	3.05	1.62	1.59
3	C	2001	F7E	P1-O6	2.98	1.68	1.59
3	E	4001	F7E	P1-O6	2.97	1.68	1.59
4	D	3002	NAP	C2A-N3A	2.95	1.36	1.32
4	E	4002	NAP	C2A-N3A	2.92	1.36	1.32
3	C	2001	F7E	C2-N	-2.84	1.30	1.34
4	D	3002	NAP	PN-O3	2.80	1.62	1.59
3	C	2001	F7E	C1-C	-2.68	1.42	1.47
3	E	4001	F7E	C2-N	-2.62	1.30	1.34
4	D	3002	NAP	O4D-C1D	2.60	1.44	1.40
3	B	402	F7E	C1-C	-2.52	1.42	1.47
4	B	403	NAP	C4N-C3N	2.47	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2001	F7E	C1-C14	-2.35	1.37	1.43
4	C	2002	NAP	C2A-N3A	2.27	1.35	1.32
3	E	4001	F7E	C1-C14	-2.21	1.37	1.43
3	B	402	F7E	C2-N	-2.17	1.31	1.34
4	B	403	NAP	C3N-C7N	2.13	1.53	1.50
4	D	3002	NAP	O4D-C4D	-2.02	1.40	1.45
4	C	2002	NAP	C2N-N1N	2.02	1.37	1.35

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	4002	NAP	N3A-C2A-N1A	-5.10	121.75	128.67
4	B	403	NAP	O4B-C1B-N9A	5.05	115.44	108.75
4	D	3002	NAP	N3A-C2A-N1A	-4.86	122.08	128.67
4	D	3002	NAP	O4B-C1B-N9A	4.60	114.85	108.75
4	C	2002	NAP	N3A-C2A-N1A	-4.49	122.58	128.67
4	C	2002	NAP	O4B-C1B-N9A	4.26	114.39	108.75
4	E	4002	NAP	O4B-C1B-N9A	3.71	113.67	108.75
4	E	4002	NAP	C4B-O4B-C1B	-3.50	106.72	109.92
4	B	403	NAP	N3A-C2A-N1A	-3.17	124.36	128.67
4	D	3002	NAP	N6A-C6A-N1A	2.79	124.29	118.33
4	B	403	NAP	N6A-C6A-N1A	2.77	124.26	118.33
4	D	3002	NAP	C1B-N9A-C4A	-2.45	122.34	126.64
4	E	4002	NAP	N6A-C6A-N1A	2.42	123.50	118.33
4	E	4002	NAP	C6N-N1N-C1D	-2.42	114.98	119.73
4	B	403	NAP	C6N-N1N-C1D	-2.37	115.07	119.73
4	D	3002	NAP	C6N-N1N-C1D	-2.30	115.21	119.73
3	C	2001	F7E	C6-O14-C3	-2.25	107.86	109.92
4	E	4002	NAP	C1B-N9A-C4A	-2.24	122.70	126.64
4	B	403	NAP	O2B-P2B-O1X	-2.24	101.34	109.33
4	C	2002	NAP	N6A-C6A-N1A	2.23	123.10	118.33
3	B	402	F7E	C6-O14-C3	-2.09	108.01	109.92
4	D	3002	NAP	O7N-C7N-C3N	2.08	122.14	119.60
4	C	2002	NAP	C6N-N1N-C1D	-2.06	115.69	119.73
4	C	2002	NAP	O2N-PN-O1N	2.04	121.92	112.44
4	C	2002	NAP	C4A-C5A-N7A	-2.04	107.19	109.34

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	F7E	C8-O6-P1-O5

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Mol	Chain	Res	Type	Atoms
3	C	2001	F7E	C8-O6-P1-O5
3	D	3001	F7E	C8-O6-P1-O5
3	E	4001	F7E	C8-O6-P1-O5
4	B	403	NAP	O4D-C1D-N1N-C2N
4	B	403	NAP	O4D-C1D-N1N-C6N
4	B	403	NAP	C2D-C1D-N1N-C2N
4	B	403	NAP	C2D-C1D-N1N-C6N
4	C	2002	NAP	O4D-C1D-N1N-C2N
4	C	2002	NAP	O4D-C1D-N1N-C6N
4	C	2002	NAP	C2D-C1D-N1N-C2N
4	C	2002	NAP	C2D-C1D-N1N-C6N
4	D	3002	NAP	O4D-C1D-N1N-C2N
4	D	3002	NAP	O4D-C1D-N1N-C6N
4	D	3002	NAP	C2D-C1D-N1N-C2N
4	D	3002	NAP	C2D-C1D-N1N-C6N
4	E	4002	NAP	O4D-C1D-N1N-C2N
4	E	4002	NAP	O4D-C1D-N1N-C6N
4	E	4002	NAP	C2D-C1D-N1N-C2N
4	E	4002	NAP	C2D-C1D-N1N-C6N
2	B	401	BCN	N1-C5-C6-O6
5	D	3003	EDO	O1-C1-C2-O2
5	D	3005	EDO	O1-C1-C2-O2
5	B	404	EDO	O1-C1-C2-O2
3	B	402	F7E	P1-O5-P-O3
3	C	2001	F7E	P1-O5-P-O3
3	D	3001	F7E	P1-O5-P-O3
3	E	4001	F7E	P1-O5-P-O3
4	B	403	NAP	C2B-O2B-P2B-O3X
5	D	3004	EDO	O1-C1-C2-O2
4	B	403	NAP	C2B-O2B-P2B-O1X
4	D	3002	NAP	C2B-O2B-P2B-O1X
2	B	401	BCN	N1-C3-C4-O4
3	D	3001	F7E	C8-O6-P1-O12
4	D	3002	NAP	C2B-O2B-P2B-O3X
4	E	4002	NAP	C2B-O2B-P2B-O2X
5	C	2004	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3002	NAP	1	0

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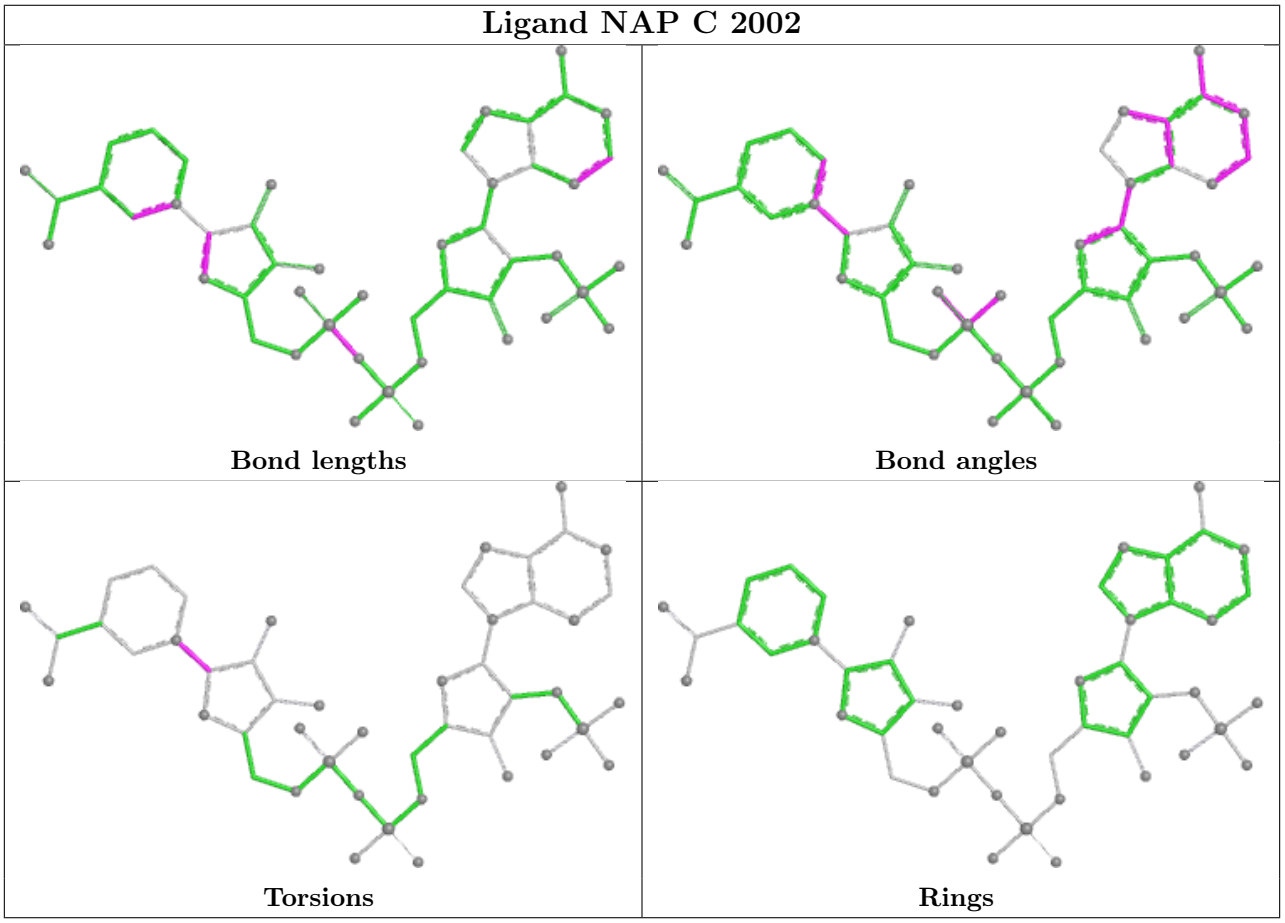
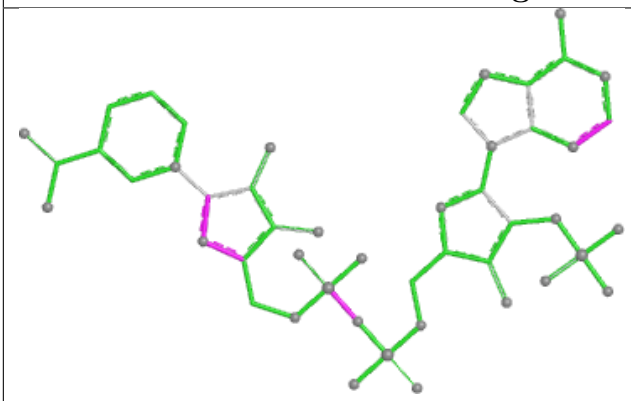
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	4002	NAP	1	0
4	B	403	NAP	1	0

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.

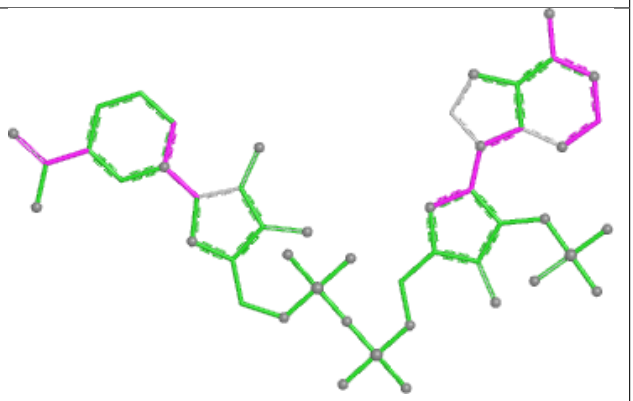
Ligand NAP C 2002



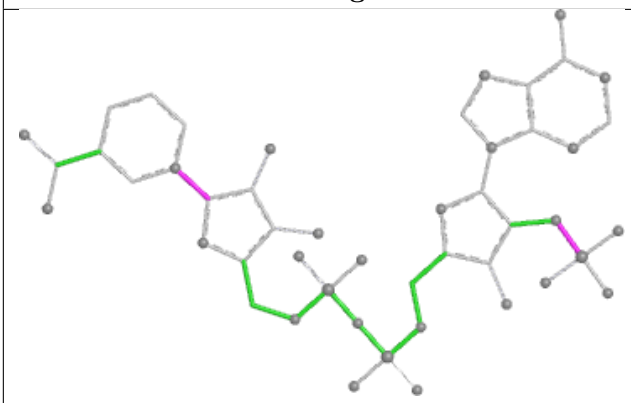
Ligand NAP D 3002



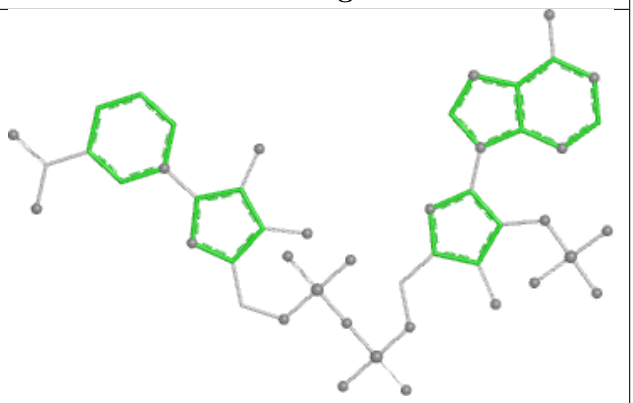
Bond lengths



Bond angles

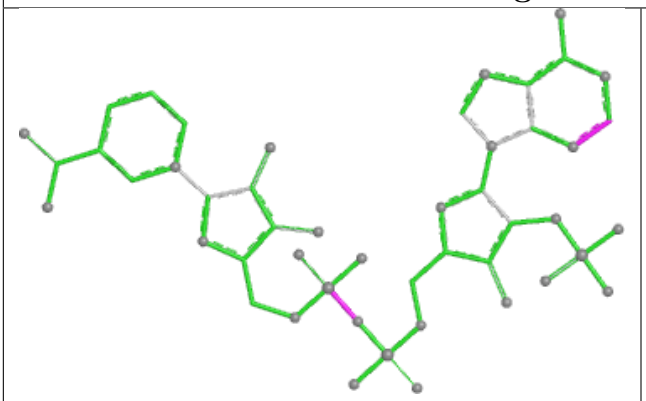


Torsions

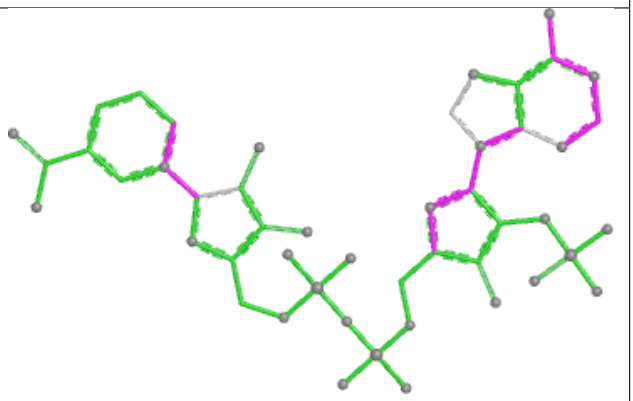


Rings

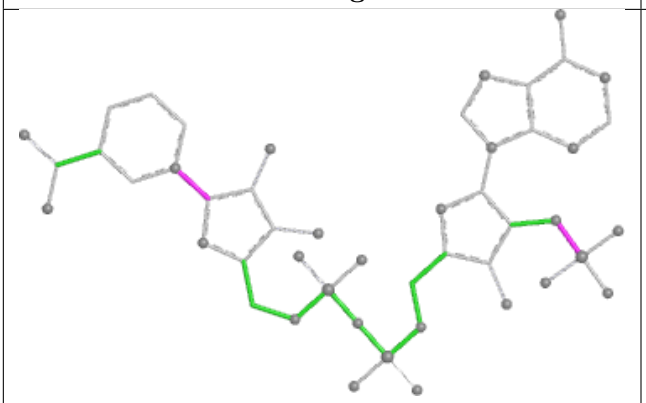
Ligand NAP E 4002



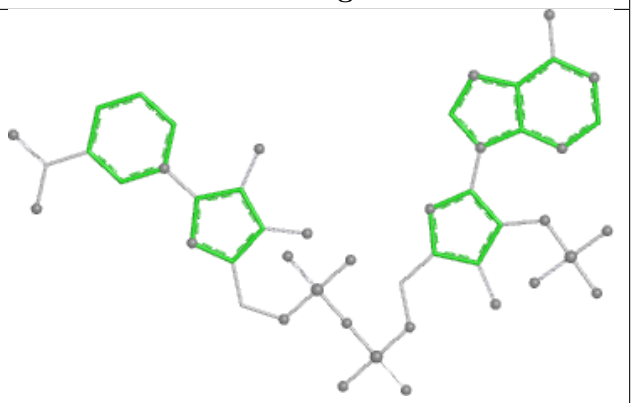
Bond lengths



Bond angles

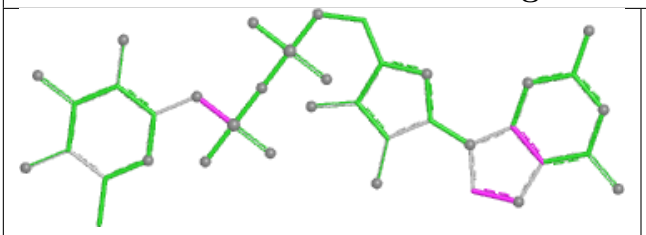


Torsions

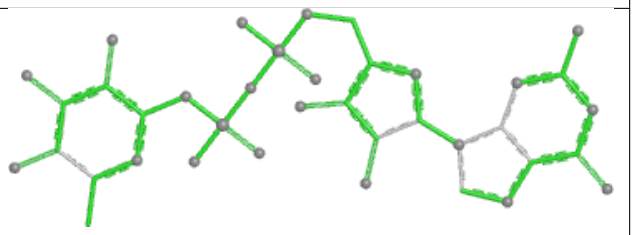


Rings

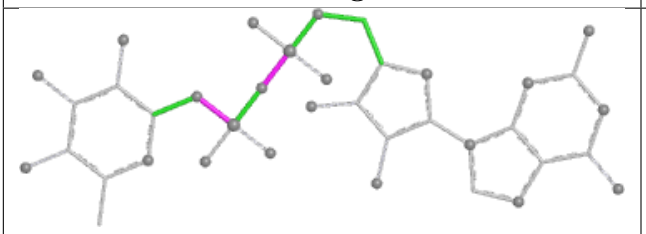
Ligand F7E E 4001



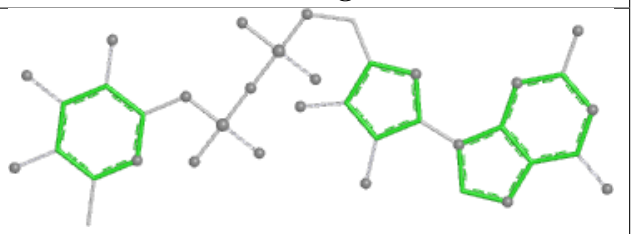
Bond lengths



Bond angles

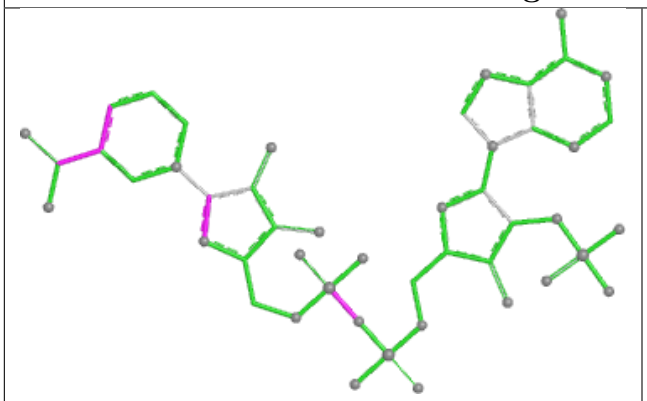


Torsions

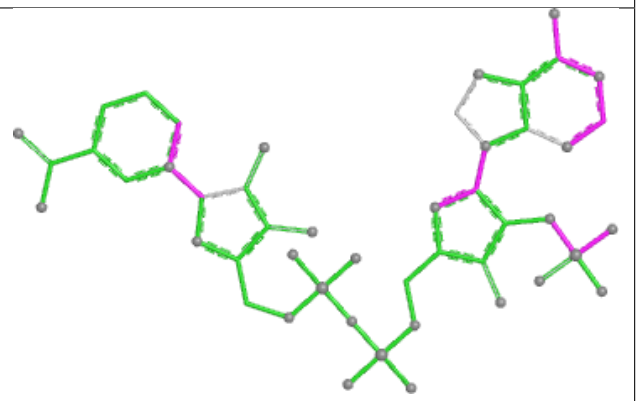


Rings

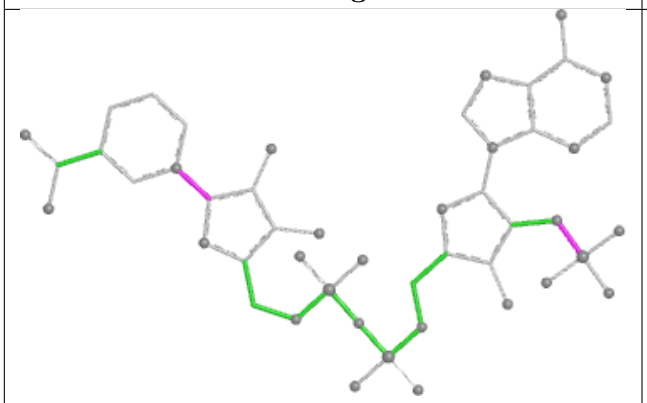
Ligand NAP B 403



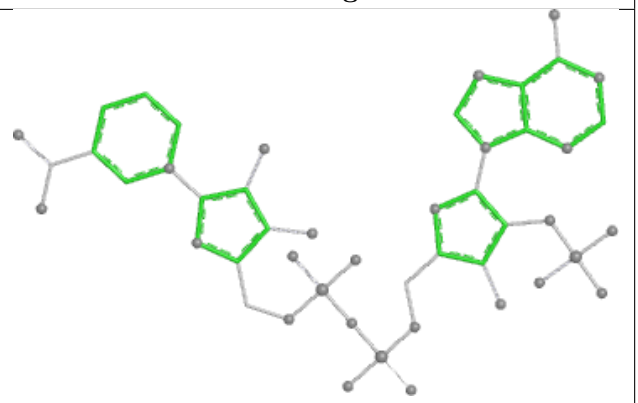
Bond lengths



Bond angles

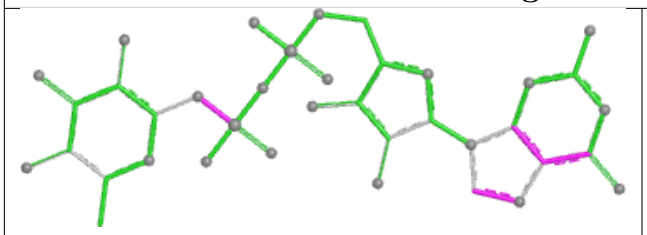


Torsions

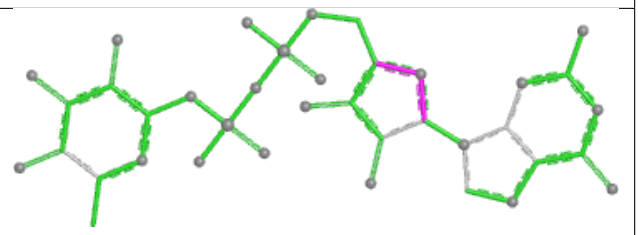


Rings

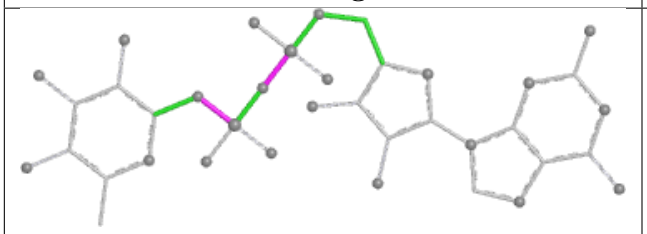
Ligand F7E C 2001



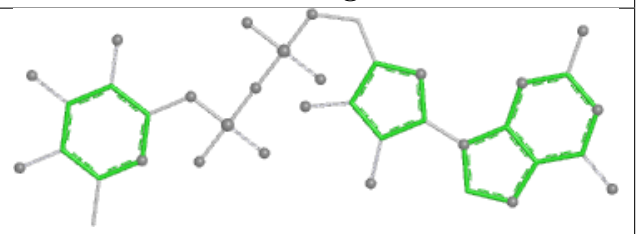
Bond lengths



Bond angles

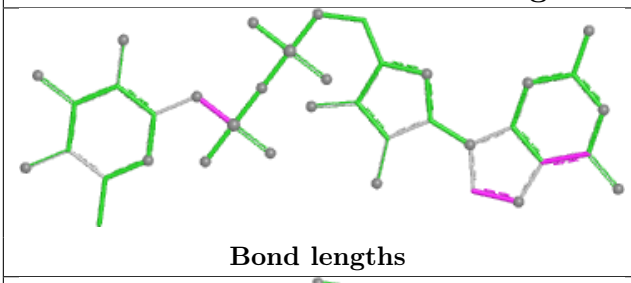


Torsions

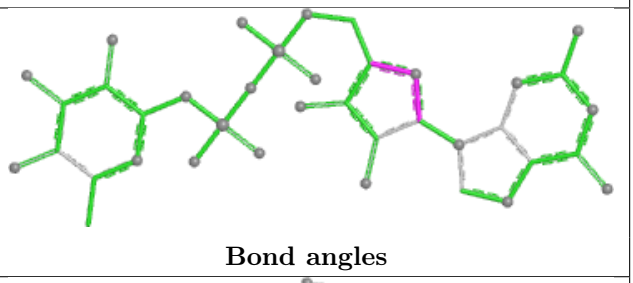


Rings

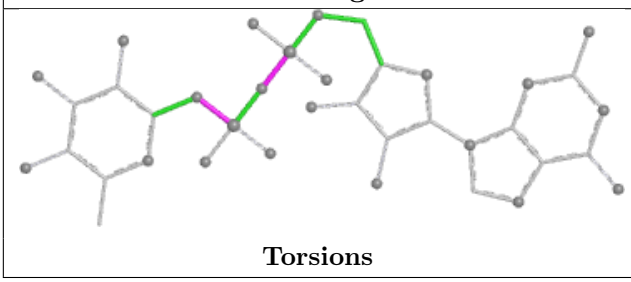
Ligand F7E B 402



Bond lengths



Bond angles



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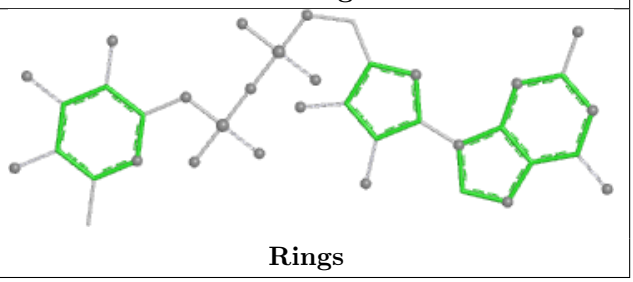
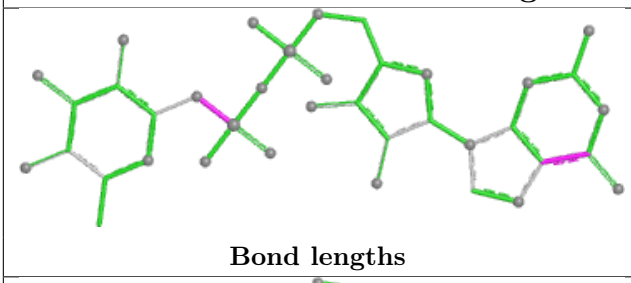
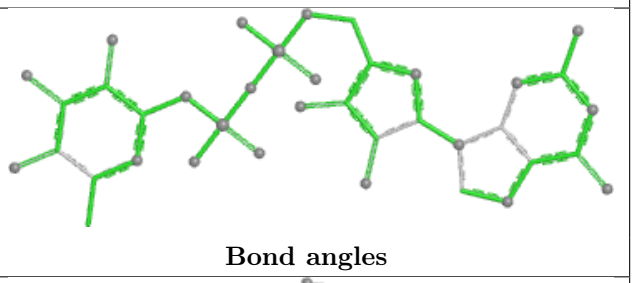


Rings

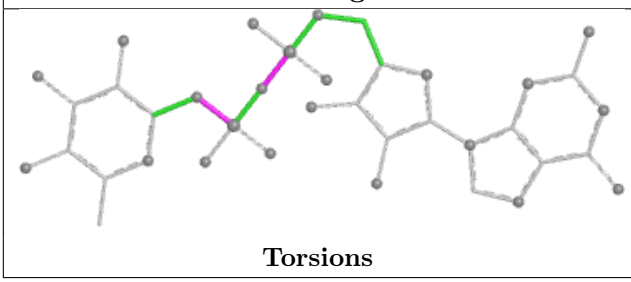
Ligand F7E D 3001



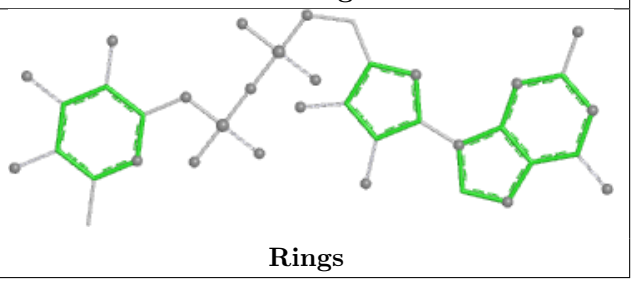
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	B	342/352 (97%)	-0.13	3 (0%)	84	89	17, 24, 44, 67	0
1	C	341/352 (96%)	-0.15	3 (0%)	84	89	17, 26, 43, 72	0
1	D	341/352 (96%)	0.27	23 (6%)	17	23	19, 29, 48, 67	0
1	E	337/352 (95%)	-0.06	3 (0%)	84	89	18, 27, 41, 62	0
All	All	1361/1408 (96%)	-0.02	32 (2%)	59	65	17, 26, 45, 72	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	78	GLY	7.1
1	D	368	THR	5.4
1	C	368	THR	4.1
1	B	69	TYR	3.6
1	D	370	PRO	3.4
1	D	231	TYR	3.4
1	D	312	THR	3.3
1	D	69	TYR	3.2
1	D	360	HIS	3.2
1	D	297	VAL	3.1
1	D	315	VAL	2.8
1	D	309	CYS	2.8
1	D	127	VAL	2.7
1	E	321	LEU	2.7
1	D	79	ASN	2.6
1	B	60[A]	PHE	2.6
1	E	69	TYR	2.5
1	D	356	ARG	2.5
1	D	293	GLY	2.4
1	D	296	ILE	2.4
1	D	232	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	372	ALA	2.2
1	E	368	THR	2.2
1	D	298	TRP	2.2
1	D	88	THR	2.2
1	D	185	TYR	2.1
1	D	364	GLU	2.1
1	D	233	GLY	2.1
1	D	363	VAL	2.1
1	D	235	LEU	2.1
1	D	130	VAL	2.0
1	C	369	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
5	EDO	B	404	4/4	0.65	0.25	53,56,57,59	0
2	BCN	B	401	11/11	0.82	0.17	33,45,52,56	0
5	EDO	D	3003	4/4	0.90	0.19	33,36,37,38	0
5	EDO	D	3005	4/4	0.90	0.09	35,37,39,42	0
5	EDO	B	407	4/4	0.94	0.10	34,36,37,40	0
5	EDO	C	2004	4/4	0.94	0.13	31,37,37,37	0
5	EDO	B	406	4/4	0.95	0.14	32,33,36,36	0
5	EDO	C	2003	4/4	0.96	0.09	35,37,38,41	0
5	EDO	D	3004	4/4	0.96	0.10	37,40,40,43	0
5	EDO	B	405	4/4	0.96	0.10	28,33,35,36	0
4	NAP	C	2002	48/48	0.97	0.11	18,20,33,37	0
4	NAP	D	3002	48/48	0.97	0.12	18,21,36,39	0

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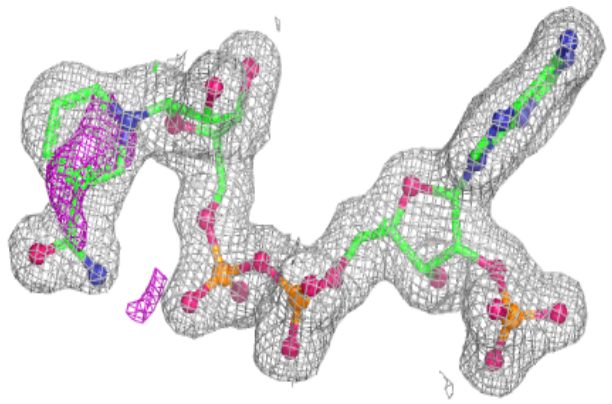
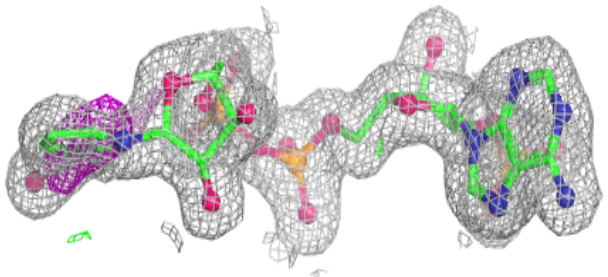
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAP	E	4002	48/48	0.97	0.10	17,19,31,34	0
4	NAP	B	403	48/48	0.97	0.11	16,19,32,33	0
3	F7E	D	3001	38/38	0.98	0.08	22,25,27,28	0
3	F7E	E	4001	38/38	0.98	0.06	19,22,24,24	0
3	F7E	B	402	38/38	0.98	0.06	19,21,23,24	0
3	F7E	C	2001	38/38	0.99	0.08	19,21,23,24	0

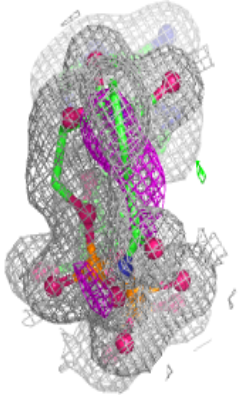
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAP C 2002:

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

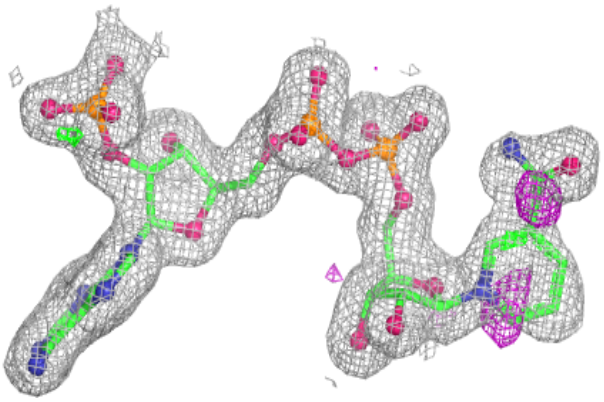


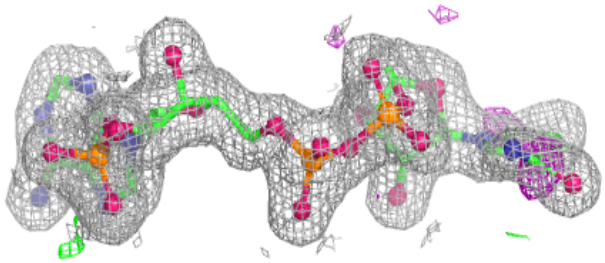


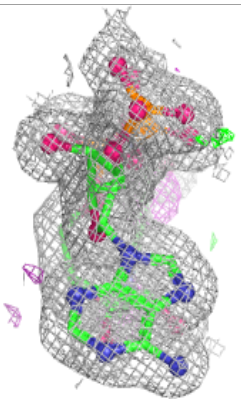


Electron density around NAP D 3002:

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

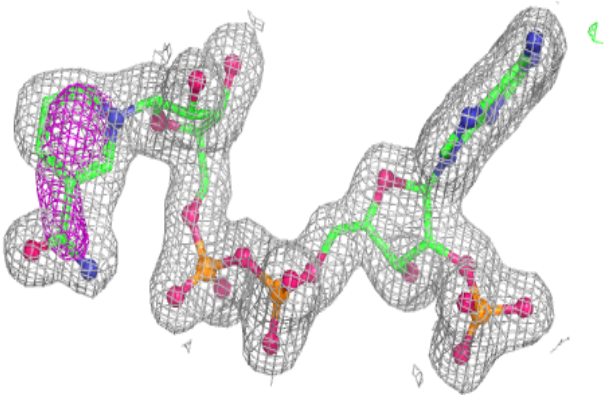


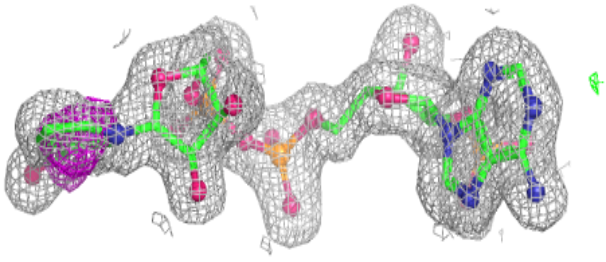


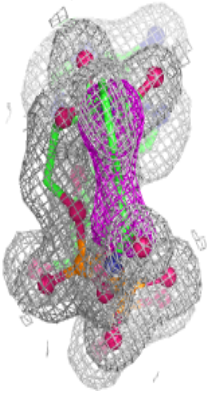


Electron density around NAP E 4002:

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

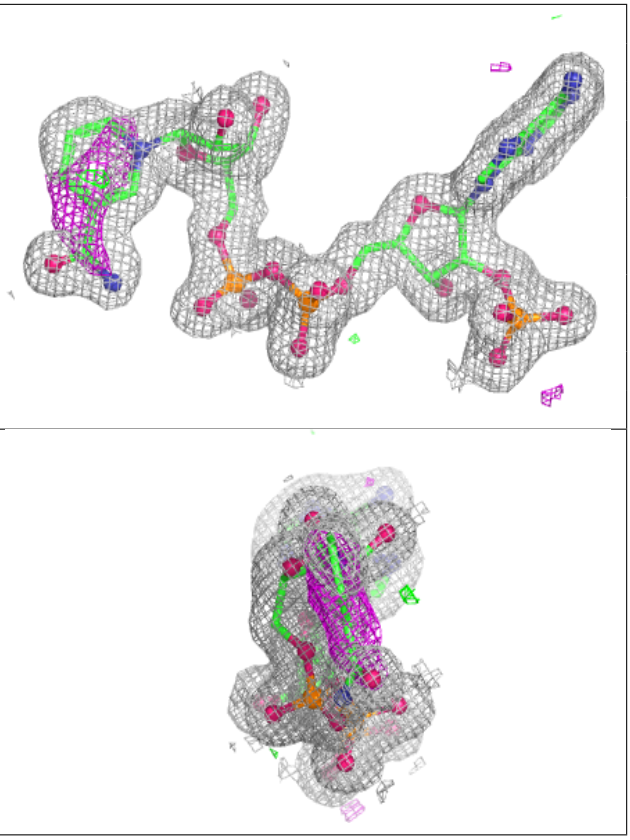






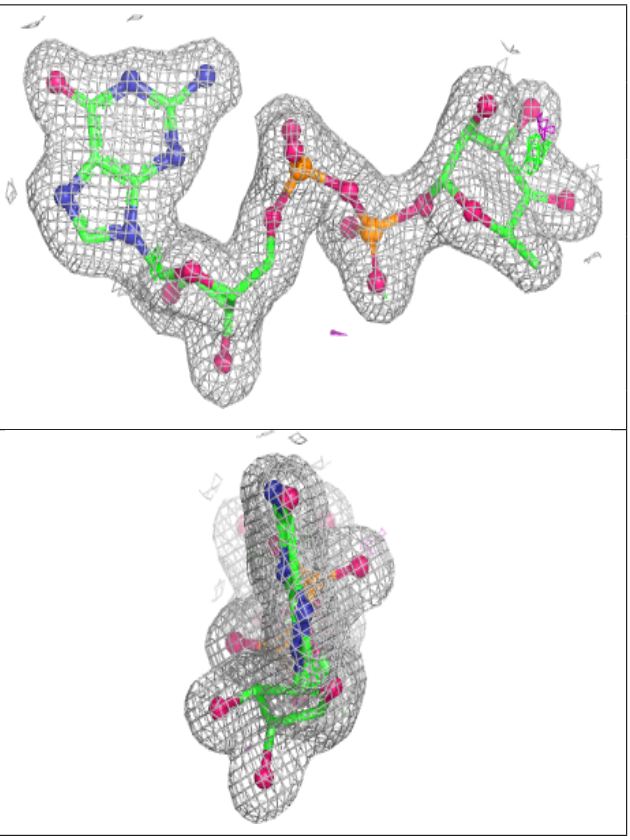
Electron density around NAP B 403:

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



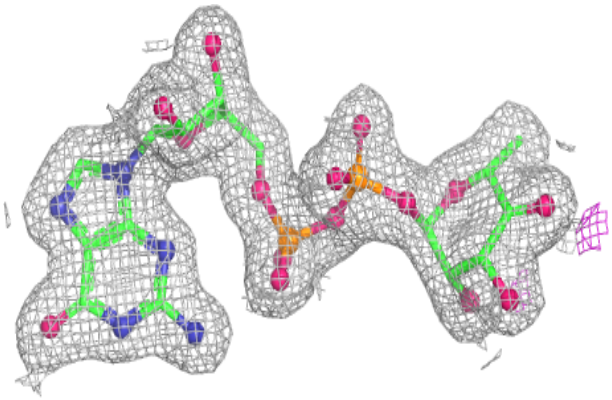
Electron density around F7E D 3001:

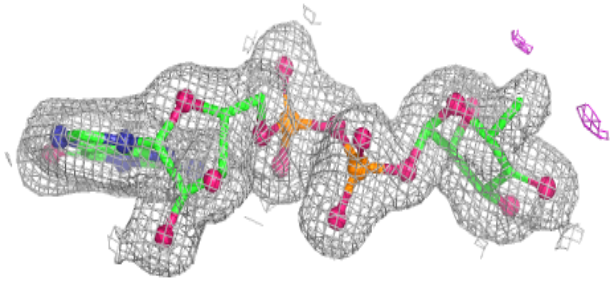
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

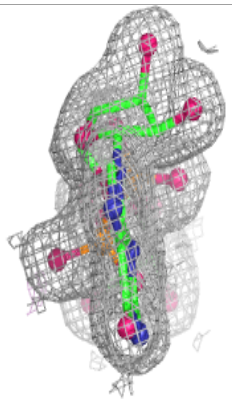


Electron density around F7E E 4001:

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

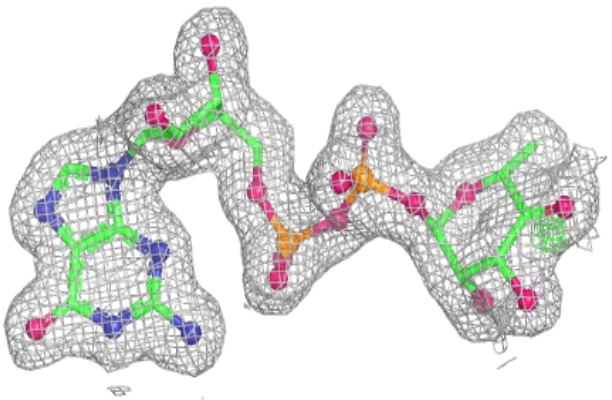


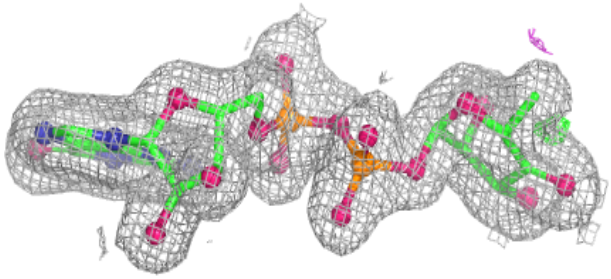


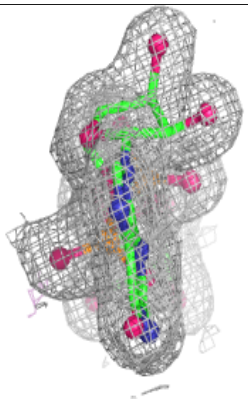


Electron density around F7E B 402:

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

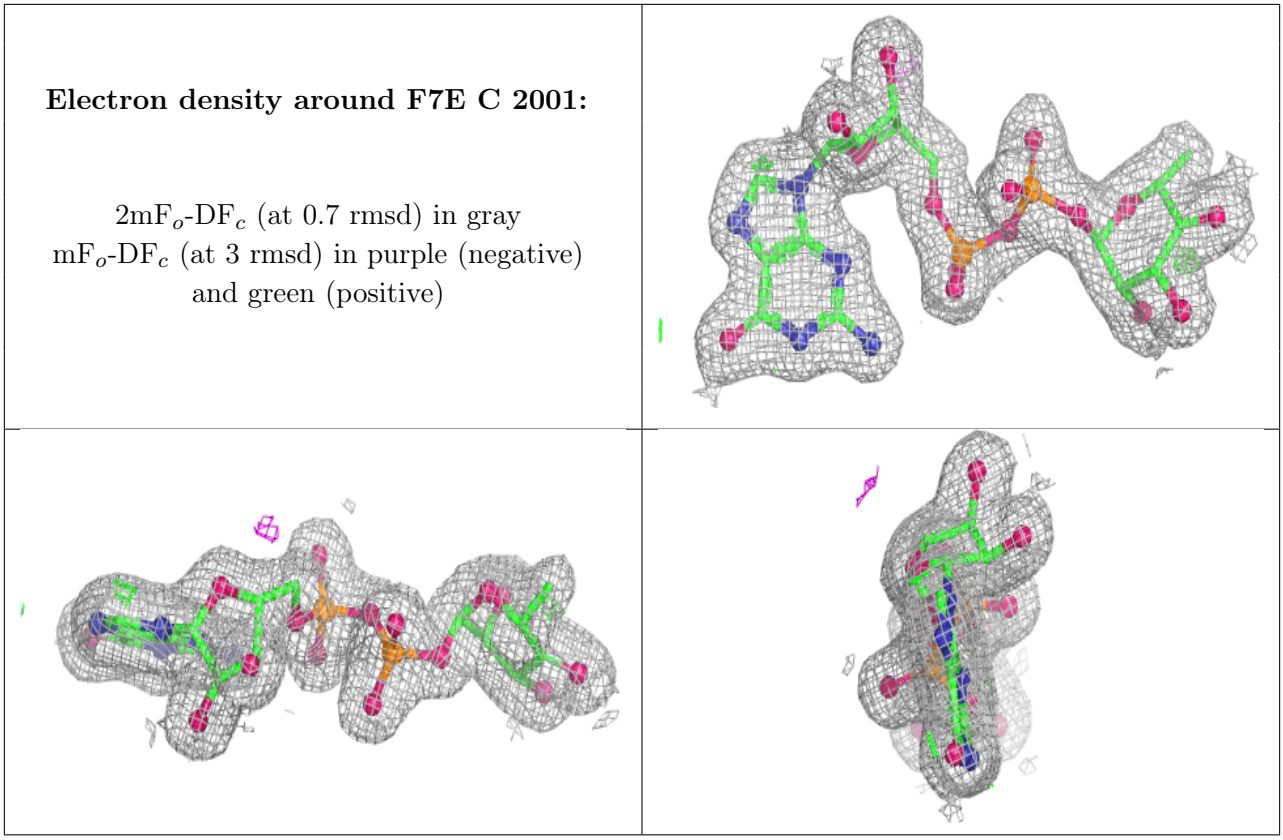






Electron density around F7E C 2001:

$2mF_o$-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.