Full wwPDB X-ray Structure Validation Report (i)

May 3, 2022 – 02:15 PM EDT

PDB ID	:	6NA4
Title	:	Co crystal structure of ECR with Butryl-CoA
Authors	:	DeMirci, H.
Deposited on	:	2018-12-05
Resolution	:	1.72 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 following versions of software and data (see references (i)) were used in the production of this report:

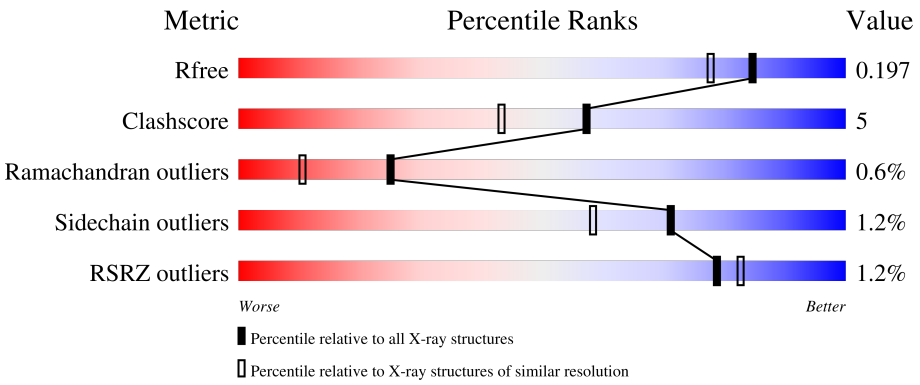
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 1.72 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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	448	.% 92% 8%
1	B	448	94% 5% •
1	C	448	.% 93% 6% •
1	D	448	2% 91% 8% ••

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAP	A	501	X	-	-	-
2	NAP	B	501	X	-	-	-
2	NAP	D	501	X	-	-	-
3	VES	C	502	-	-	X	-
3	VES	D	504	-	-	X	-
6	NDP	C	503	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16338 atoms, of which 25 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.

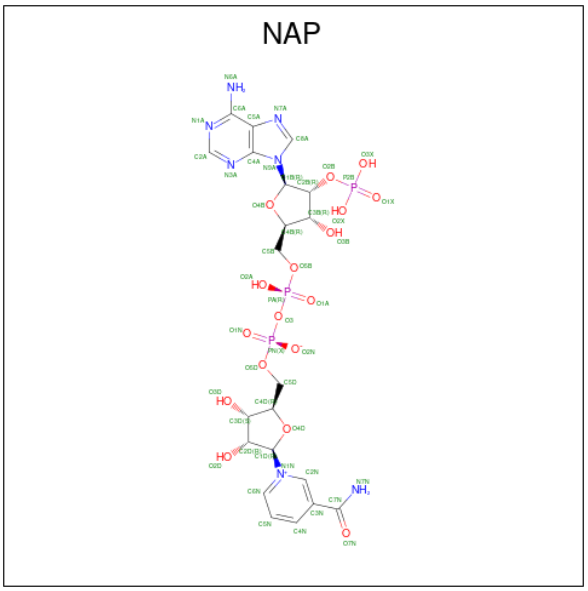
- Molecule 1 is a protein called Putative crotonyl-CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	3525	2212	636	663	14	0	10	0
1	B	448	3546	2225	639	668	14	7	10	0
1	C	447	3519	2209	638	658	14	0	9	0
1	D	445	3477	2186	625	652	14	0	6	0

There are 16 discrepancies between the modelled and reference sequences:

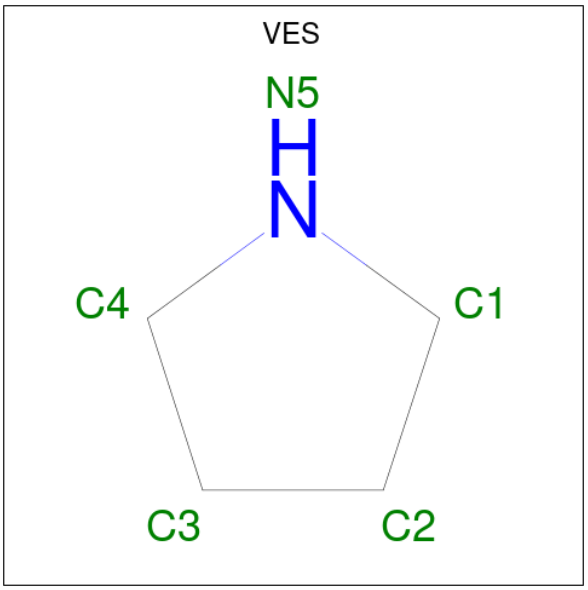
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLU	-	expression tag	UNP E4N096
A	-2	GLY	-	expression tag	UNP E4N096
A	-1	ARG	-	expression tag	UNP E4N096
A	0	HIS	-	expression tag	UNP E4N096
B	-3	GLU	-	expression tag	UNP E4N096
B	-2	GLY	-	expression tag	UNP E4N096
B	-1	ARG	-	expression tag	UNP E4N096
B	0	HIS	-	expression tag	UNP E4N096
C	-3	GLU	-	expression tag	UNP E4N096
C	-2	GLY	-	expression tag	UNP E4N096
C	-1	ARG	-	expression tag	UNP E4N096
C	0	HIS	-	expression tag	UNP E4N096
D	-3	GLU	-	expression tag	UNP E4N096
D	-2	GLY	-	expression tag	UNP E4N096
D	-1	ARG	-	expression tag	UNP E4N096
D	0	HIS	-	expression tag	UNP E4N096

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is Pyrrolidine (three-letter code: VES) (formula: C_4H_9N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			5	4	1		

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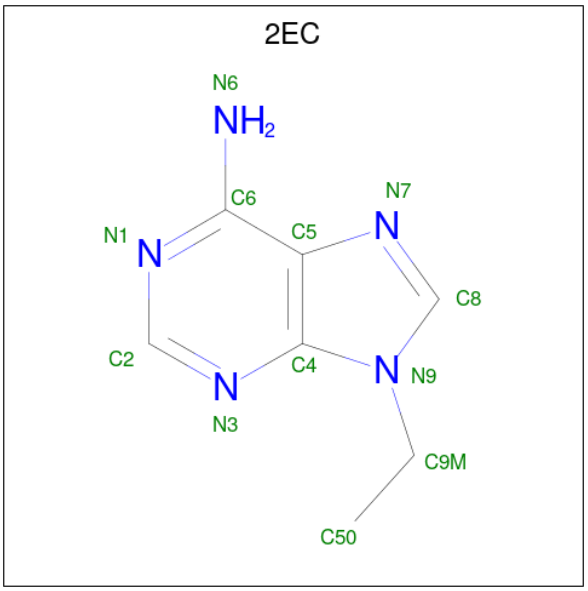
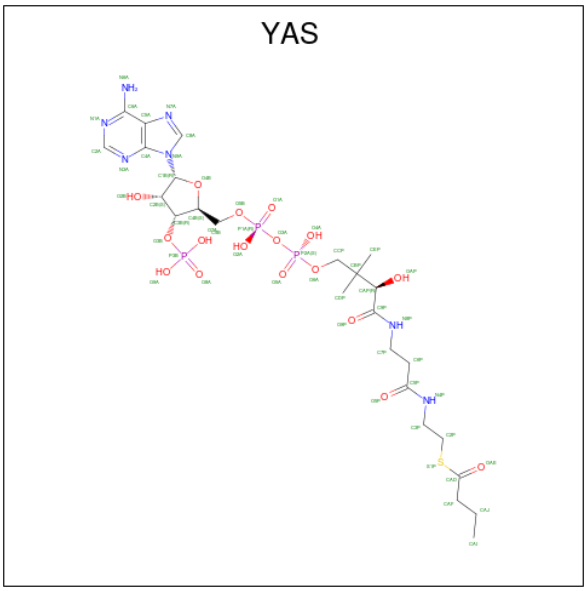
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	B	1	5	4	1	0	0
			Total	C	N		
3	C	1	5	4	1	0	0
			Total	C	N		
3	D	1	5	4	1	0	0
			Total	C	N		
3	D	1	5	4	1	0	0

- Molecule 4 is 9-ETHYL-9H-PURIN-6-YLAMINE (three-letter code: 2EC) (formula: $C_7H_9N_5$) (labeled as "Ligand of Interest" by depositor).



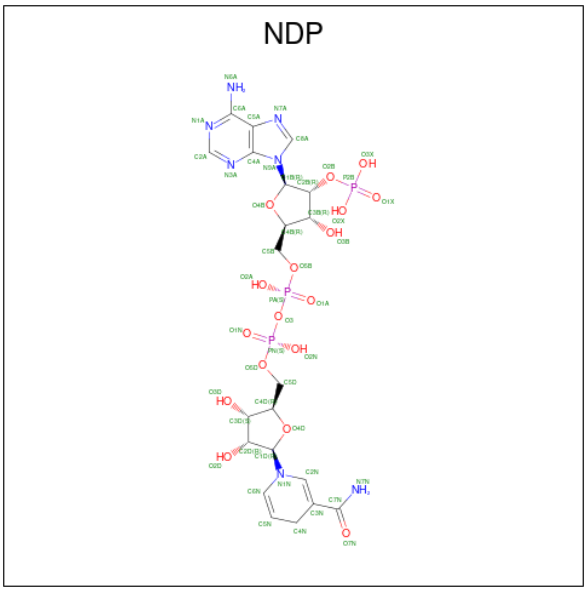
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
4	A	1	11	6	5	0	0
			Total	C	N		
4	B	1	12	7	5	0	0

- Molecule 5 is {S}-[2-[3-[[(2 {R})-4-[[[(2 {S},3 {R},4 {S},5 {R})-5-(6-aminopurin-9-yl)-4-oxidanyl-3-phosphonooxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-3,3-dimethyl-2-oxidanyl-butanoyl]amino]propanoylamino]ethyl] butanethioate (three-letter code: YAS) (formula: $C_{25}H_{42}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
5	C	1	53	25	7	17	3	1	1	0
5	D	1	53	25	7	17	3	1	1	0

- Molecule 6 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
6	C	1	73	21	25	7	17	3	0	0

- Molecule 7 is water.

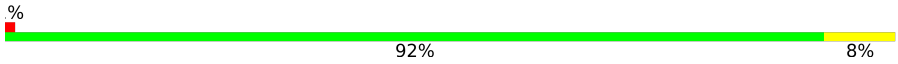
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	444	454	454	0	6
			Total	O		
7	B	496	500	500	0	4
			Total	O		
7	C	484	491	491	0	6
			Total	O		
7	D	448	455	455	0	7

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.

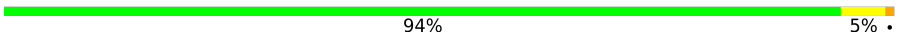
• Molecule 1: Putative crotonyl-CoA reductase

Chain A:



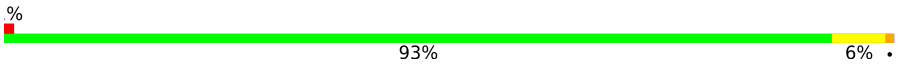
• Molecule 1: Putative crotonyl-CoA reductase

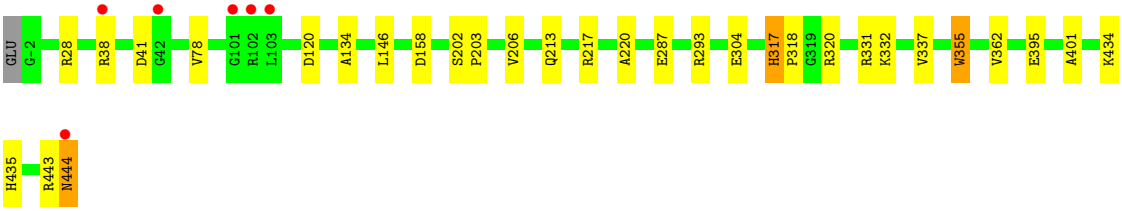
Chain B:



• Molecule 1: Putative crotonyl-CoA reductase

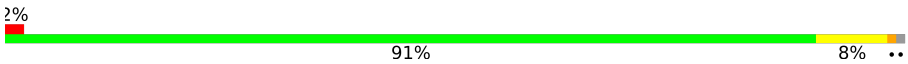
Chain C:

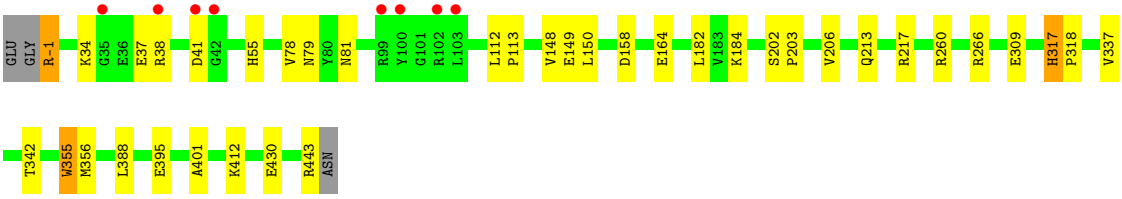




• Molecule 1: Putative crotonyl-CoA reductase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	109.34Å 78.83Å 138.79Å 90.00° 108.06° 90.00°	Depositor
Resolution (Å)	39.41 – 1.72 39.41 – 1.72	Depositor EDS
% Data completeness (in resolution range)	95.8 (39.41-1.72) 87.9 (39.41-1.72)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.05 (at 1.72Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.170 , 0.198 0.169 , 0.197	Depositor DCC
R_{free} test set	1997 reflections (0.88%)	wwPDB-VP
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	16338	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5949e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: YAS, VES, NDP, 2EC, 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	A	0.36	0/3607	0.54	0/4887
1	B	0.38	0/3628	0.56	0/4917
1	C	0.35	0/3601	0.53	0/4881
1	D	0.36	0/3559	0.54	0/4825
All	All	0.36	0/14395	0.54	0/19510

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	3525	0	3448	31	0
1	B	3546	0	3471	22	0
1	C	3519	0	3446	29	0
1	D	3477	0	3406	43	0
2	A	48	0	22	1	0
2	B	48	0	24	6	0
2	D	48	0	23	7	0
3	A	5	0	9	1	0
3	B	5	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5	0	9	5	0
3	D	10	0	18	7	0
4	A	11	0	4	0	0
4	B	12	0	9	0	0
5	C	53	0	0	1	0
5	D	53	0	0	3	0
6	C	48	25	24	3	0
7	A	454	0	0	12	0
7	B	500	0	0	3	0
7	C	491	0	0	7	0
7	D	455	0	0	14	0
All	All	16313	25	13922	139	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 5.

All (139) 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)
2:B:501:NAP:O4D	2:B:501:NAP:C4D	1.66	1.24
2:B:501:NAP:C4B	2:B:501:NAP:O4B	1.65	1.18
5:D:502:YAS:O2A	7:D:601:HOH:O	1.67	1.12
1:A:145:CYS:SG	7:A:1027:HOH:O	2.26	0.94
1:D:395:GLU:OE1	7:D:602:HOH:O	1.89	0.88
1:D:443:ARG:O	7:D:603:HOH:O	1.92	0.86
2:D:501:NAP:H6N	2:D:501:NAP:H4D	1.58	0.85
1:A:205:LEU:HG	7:A:1027:HOH:O	1.74	0.85
1:D:430:GLU:OE2	7:D:604:HOH:O	1.94	0.84
1:D:260:ARG:NH2	7:D:606:HOH:O	2.03	0.83
1:C:120:ASP:OD1	7:C:601:HOH:O	1.98	0.82
1:B:232:GLY:HA2	2:B:501:NAP:H2B	1.62	0.79
1:C:434:LYS:HE3	1:C:435:HIS:NE2	1.99	0.78
1:C:220:ALA:HB2	1:C:337[B]:VAL:HG21	1.66	0.78
1:A:220:ALA:HB2	1:A:337[B]:VAL:HG21	1.65	0.77
1:D:149:GLU:OE1	1:D:184:LYS:NZ	2.20	0.72
1:D:149:GLU:N	7:D:605:HOH:O	2.23	0.72
1:D:150:LEU:N	7:D:605:HOH:O	2.02	0.71
1:A:213:GLN:HG3	1:A:337[B]:VAL:CG1	2.23	0.69
1:D:206:VAL:HG12	3:D:503:VES:H22C	1.75	0.69
1:D:34:LYS:O	1:D:37:GLU:HG2	1.93	0.68
1:C:317:HIS:H	1:C:318:PRO:CD	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:LYS:HD2	7:D:613:HOH:O	1.96	0.66
1:D:266:ARG:HH12	3:D:504:VES:C1	2.09	0.66
1:C:217:ARG:CZ	3:C:502:VES:H11C	2.26	0.65
1:D:164:GLU:OE2	7:D:605:HOH:O	2.14	0.65
2:D:501:NAP:C6N	3:D:503:VES:H31C	2.27	0.65
1:A:320[A]:ARG:NH2	7:A:606:HOH:O	2.29	0.64
1:D:317:HIS:H	1:D:318:PRO:CD	2.10	0.64
1:C:146:LEU:HB3	7:C:970:HOH:O	1.98	0.63
1:D:266:ARG:HH22	3:D:504:VES:H21C	1.64	0.62
1:D:148:VAL:HB	7:D:605:HOH:O	1.98	0.62
1:A:317:HIS:H	1:A:318:PRO:CD	2.13	0.61
1:B:388:LEU:O	1:B:443:ARG:HD2	1.99	0.61
1:D:266:ARG:HH12	3:D:504:VES:C2	2.12	0.61
1:A:381:LYS:HD3	7:A:925:HOH:O	2.01	0.61
1:D:266:ARG:HH12	3:D:504:VES:H21C	1.65	0.60
1:B:357:SER:OG	7:B:603:HOH:O	2.16	0.60
1:C:304:GLU:OE1	7:C:603:HOH:O	2.16	0.60
1:A:25:GLU:O	7:A:602:HOH:O	2.17	0.59
1:C:206[A]:VAL:HG13	7:C:695:HOH:O	2.02	0.59
1:C:217:ARG:NE	3:C:502:VES:H11C	2.18	0.59
1:A:213:GLN:HG3	1:A:337[B]:VAL:HG11	1.85	0.59
6:C:503:NDP:O4B	6:C:503:NDP:C4B	2.37	0.58
1:B:317:HIS:H	1:B:318:PRO:CD	2.17	0.58
1:A:213:GLN:HG3	1:A:337[B]:VAL:HG12	1.85	0.58
1:D:79:ASN:HD21	1:D:412:LYS:NZ	2.01	0.57
1:D:-1:ARG:NH2	7:D:614:HOH:O	2.36	0.57
1:B:296[A]:LYS:HG2	1:B:328:TYR:OH	2.04	0.57
1:B:213:GLN:HG3	1:B:337:VAL:HG22	1.86	0.57
3:C:502:VES:H41C	1:D:217:ARG:CZ	2.34	0.57
1:A:136:LYS:HE2	7:A:675:HOH:O	2.06	0.56
1:A:154:ASP:HB2	1:A:163:PRO:HD3	1.87	0.56
1:D:202[A]:SER:OG	1:D:203:PRO:HD3	2.04	0.56
1:B:81:ASN:HD22	1:B:82:THR:N	2.03	0.55
1:A:184:LYS:NZ	7:A:605:HOH:O	2.26	0.55
1:B:81:ASN:HD22	1:B:82:THR:H	1.55	0.55
1:D:213:GLN:HG3	1:D:337:VAL:CG2	2.37	0.55
2:B:501:NAP:O4B	2:B:501:NAP:C5B	2.50	0.55
1:A:340:ALA:HB1	2:A:501:NAP:H3D	1.89	0.54
2:D:501:NAP:H4D	2:D:501:NAP:C6N	2.35	0.54
1:B:232:GLY:CA	2:B:501:NAP:H2B	2.36	0.54
1:C:38:ARG:HD3	1:C:41:ASP:OD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:ARG:HH12	3:D:504:VES:H12C	1.72	0.54
1:C:293[A]:ARG:HD2	7:C:992:HOH:O	2.08	0.53
6:C:503:NDP:H6N	6:C:503:NDP:H4D	1.88	0.53
1:B:154:ASP:HB2	1:B:163:PRO:HD3	1.91	0.53
1:B:317:HIS:CG	1:B:318:PRO:HD3	2.44	0.53
1:C:434:LYS:HE3	1:C:435:HIS:HE2	1.72	0.52
1:D:317:HIS:H	1:D:318:PRO:HD2	1.75	0.51
1:A:220:ALA:HB2	1:A:337[B]:VAL:CG2	2.39	0.51
1:C:317:HIS:N	1:C:318:PRO:CD	2.74	0.51
1:A:98:GLU:OE1	1:A:102:ARG:NH2	2.44	0.51
1:D:55:HIS:ND1	7:D:610:HOH:O	2.35	0.50
1:A:-1:ARG:NH1	7:A:609[A]:HOH:O	2.44	0.50
1:D:213:GLN:HG3	1:D:337:VAL:HG21	1.93	0.50
1:D:356[B]:MET:SD	5:D:502:YAS:CDP	3.00	0.49
1:C:320[B]:ARG:NH1	7:C:602:HOH:O	2.06	0.49
3:C:502:VES:H12C	1:D:217:ARG:HG2	1.95	0.49
1:D:112:LEU:HB3	1:D:113:PRO:HD2	1.95	0.48
1:D:317:HIS:N	1:D:318:PRO:CD	2.76	0.48
1:C:202[A]:SER:OG	1:C:203:PRO:HD3	2.14	0.48
1:C:213:GLN:HG3	1:C:337[B]:VAL:HG11	1.94	0.48
1:B:296[A]:LYS:HG2	1:B:328:TYR:CZ	2.49	0.48
1:A:287[B]:GLU:H	1:A:287[B]:GLU:CD	2.17	0.47
7:A:1027:HOH:O	5:C:501:YAS:CAI	2.62	0.47
1:C:213:GLN:HG3	1:C:337[B]:VAL:CG1	2.45	0.47
1:C:220:ALA:HB2	1:C:337[B]:VAL:CG2	2.41	0.47
1:C:443:ARG:HA	1:C:444:ASN:HA	1.63	0.47
1:A:320[A]:ARG:NH1	7:A:603:HOH:O	2.21	0.46
1:D:317:HIS:CG	1:D:318:PRO:HD3	2.51	0.46
1:A:317:HIS:N	1:A:318:PRO:CD	2.76	0.46
1:D:260:ARG:HD2	1:D:260:ARG:O	2.15	0.46
1:B:121:LEU:C	1:B:121:LEU:HD12	2.35	0.46
2:D:501:NAP:N7N	7:D:612:HOH:O	2.36	0.46
1:D:38:ARG:HG2	1:D:41:ASP:OD2	2.14	0.46
1:C:337[A]:VAL:HG12	1:C:362:VAL:HB	1.97	0.46
1:A:365:HIS:HB2	1:C:355:TRP:O	2.16	0.46
1:B:136:LYS:HE2	7:B:761:HOH:O	2.15	0.46
1:B:317:HIS:N	1:B:318:PRO:CD	2.79	0.45
2:D:501:NAP:C6N	2:D:501:NAP:C4D	2.94	0.45
1:B:151:GLU:OE2	1:C:134:ALA:N	2.43	0.45
1:A:222:LEU:HD11	1:A:250:ALA:CB	2.47	0.45
1:C:317:HIS:H	1:C:318:PRO:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:503:NDP:O4B	6:C:503:NDP:C5B	2.65	0.44
1:D:79:ASN:ND2	1:D:412:LYS:NZ	2.63	0.44
1:C:146:LEU:HD12	1:C:146:LEU:HA	1.62	0.44
1:A:40:PHE:HB3	1:A:48:LYS:HG2	1.99	0.44
1:A:434[B]:LYS:HE3	7:A:906:HOH:O	2.17	0.44
1:C:395:GLU:H	1:C:395:GLU:CD	2.19	0.44
2:B:501:NAP:O4D	2:B:501:NAP:C5D	2.55	0.43
1:D:79:ASN:ND2	1:D:412:LYS:HZ3	2.16	0.43
1:B:213:GLN:HG3	1:B:337:VAL:CG2	2.48	0.43
1:B:317:HIS:H	1:B:318:PRO:HD2	1.83	0.43
1:D:309:GLU:OE1	7:D:607:HOH:O	2.21	0.43
1:A:121:LEU:HG	1:A:143:ALA:HB3	1.99	0.43
1:B:-3[A]:GLU:O	7:B:604:HOH:O	2.21	0.42
3:C:502:VES:H21C	1:D:217:ARG:HD3	2.00	0.42
1:D:355:TRP:CD1	1:D:355:TRP:C	2.93	0.42
1:C:320[B]:ARG:HD2	7:C:602:HOH:O	2.19	0.42
1:B:157:ASN:O	1:B:158:ASP:CB	2.68	0.42
1:B:202[B]:SER:N	1:B:203:PRO:HD3	2.35	0.41
1:C:287:GLU:O	1:C:320[A]:ARG:NH2	2.53	0.41
1:D:342:THR:OG1	2:D:501:NAP:H3D	2.20	0.41
1:D:356[B]:MET:SD	5:D:502:YAS:C6P	3.09	0.41
1:A:317:HIS:H	1:A:318:PRO:HD2	1.83	0.41
1:C:78:VAL:HG11	1:C:401:ALA:HA	2.02	0.41
1:C:331:ARG:HG2	1:C:332:LYS:N	2.36	0.41
1:A:205:LEU:C	1:A:205:LEU:HD23	2.40	0.41
1:A:353:TYR:O	1:A:357:SER:HB2	2.20	0.41
1:D:78:VAL:HG11	1:D:401:ALA:HA	2.03	0.41
3:A:502:VES:H22C	7:A:666:HOH:O	2.21	0.41
2:D:501:NAP:H6N	2:D:501:NAP:C4D	2.39	0.41
1:A:121:LEU:C	1:A:121:LEU:HD12	2.40	0.40
1:A:31:THR:HA	1:A:115:HIS:O	2.21	0.40
1:A:213:GLN:HG3	1:A:337[A]:VAL:HG22	2.03	0.40
1:D:182:LEU:C	1:D:182:LEU:HD23	2.41	0.40
1:B:202[A]:SER:N	1:B:203:PRO:HD3	2.36	0.40
1:D:79:ASN:HD21	1:D:412:LYS:HZ3	1.67	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	455/448 (102%)	441 (97%)	11 (2%)	3 (1%)	22 8
1	B	457/448 (102%)	442 (97%)	12 (3%)	3 (1%)	22 8
1	C	454/448 (101%)	439 (97%)	13 (3%)	2 (0%)	34 18
1	D	449/448 (100%)	433 (96%)	14 (3%)	2 (0%)	34 18
All	All	1815/1792 (101%)	1755 (97%)	50 (3%)	10 (1%)	25 10

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ASP
1	A	317	HIS
1	B	158	ASP
1	B	317	HIS
1	C	158	ASP
1	C	317	HIS
1	D	158	ASP
1	D	317	HIS
1	B	366	PHE
1	A	366	PHE

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	369/359 (103%)	366 (99%)	3 (1%)	81 73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	371/359 (103%)	363 (98%)	8 (2%)	52	33
1	C	367/359 (102%)	364 (99%)	3 (1%)	81	73
1	D	363/359 (101%)	359 (99%)	4 (1%)	73	62
All	All	1470/1436 (102%)	1452 (99%)	18 (1%)	71	58

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	TYR
1	A	355	TRP
1	A	369	TYR
1	B	-3[A]	GLU
1	B	-3[B]	GLU
1	B	28	ARG
1	B	80	TYR
1	B	81	ASN
1	B	355	TRP
1	B	369	TYR
1	B	421	ARG
1	C	28	ARG
1	C	355	TRP
1	C	444	ASN
1	D	-1	ARG
1	D	81	ASN
1	D	355	TRP
1	D	388	LEU

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

Mol	Chain	Res	Type
1	B	81	ASN
1	D	79	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)

13 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	VES	D	503	-	5,5,5	0.30	0	5,5,5	1.62	1 (20%)
3	VES	A	502	-	5,5,5	0.30	0	5,5,5	1.64	1 (20%)
2	NAP	D	501	-	45,52,52	3.94	16 (35%)	56,80,80	1.68	14 (25%)
5	YAS	C	501	-	47,55,55	3.31	15 (31%)	58,81,81	1.77	9 (15%)
3	VES	C	502	-	5,5,5	0.26	0	5,5,5	1.60	1 (20%)
5	YAS	D	502	-	47,55,55	3.28	22 (46%)	58,81,81	2.20	15 (25%)
2	NAP	A	501	-	45,52,52	4.71	26 (57%)	56,80,80	2.27	12 (21%)
2	NAP	B	501	-	45,52,52	3.50	15 (33%)	56,80,80	1.56	10 (17%)
4	2EC	B	503	-	11,13,13	1.69	2 (18%)	8,18,18	2.08	3 (37%)
6	NDP	C	503	-	45,52,52	7.81	25 (55%)	53,80,80	3.59	18 (33%)
3	VES	B	502	-	5,5,5	0.28	0	5,5,5	1.60	1 (20%)
3	VES	D	504	-	5,5,5	0.41	0	5,5,5	1.70	1 (20%)
4	2EC	A	503	-	10,12,13	1.63	2 (20%)	8,17,18	2.07	2 (25%)

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	VES	D	503	-	-	-	0/1/1/1
3	VES	A	502	-	-	-	0/1/1/1
2	NAP	D	501	-	6/6/12/12	6/31/67/67	0/5/5/5
5	YAS	C	501	-	-	16/50/70/70	0/3/3/3
3	VES	C	502	-	-	-	0/1/1/1
5	YAS	D	502	-	-	7/50/70/70	0/3/3/3
2	NAP	A	501	-	3/3/12/12	5/31/67/67	0/5/5/5
2	NAP	B	501	-	1/1/12/12	8/31/67/67	0/5/5/5
4	2EC	B	503	-	-	0/2/2/2	0/2/2/2
6	NDP	C	503	-	2/2/17/17	12/30/77/77	0/5/5/5
3	VES	B	502	-	-	-	0/1/1/1
3	VES	D	504	-	-	-	0/1/1/1
4	2EC	A	503	-	-	-	0/2/2/2

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	503	NDP	O4B-C4B	41.56	2.37	1.45
2	A	501	NAP	C2D-C1D	-15.45	1.30	1.53
6	C	503	NDP	O4B-C1B	-15.15	1.19	1.41
6	C	503	NDP	C3B-C4B	-13.88	1.17	1.53
5	C	501	YAS	C2B-C3B	-12.63	1.24	1.52
5	D	502	YAS	C2B-C3B	-11.50	1.27	1.52
2	D	501	NAP	C3B-C4B	-10.99	1.24	1.53
2	A	501	NAP	O4D-C1D	10.83	1.56	1.41
2	D	501	NAP	C2D-C3D	-10.28	1.25	1.53
5	D	502	YAS	O4B-C4B	-10.23	1.22	1.45
2	A	501	NAP	O4B-C1B	-10.12	1.27	1.41
2	A	501	NAP	C3B-C4B	-9.51	1.28	1.53
2	B	501	NAP	O4D-C4D	9.38	1.66	1.45
2	B	501	NAP	C3B-C4B	-9.14	1.29	1.53
2	B	501	NAP	O4B-C4B	9.13	1.65	1.45
6	C	503	NDP	O4D-C1D	9.00	1.63	1.42
6	C	503	NDP	C8A-N7A	-8.99	1.18	1.34
6	C	503	NDP	C4A-N3A	-8.71	1.23	1.35
2	A	501	NAP	O4D-C4D	-8.45	1.26	1.45
2	B	501	NAP	C3D-C4D	-8.44	1.31	1.53
5	C	501	YAS	O4B-C1B	8.24	1.52	1.41
5	C	501	YAS	O4B-C4B	-8.12	1.26	1.45
2	D	501	NAP	O4D-C1D	8.08	1.52	1.41
2	D	501	NAP	O4D-C4D	-8.01	1.27	1.45
2	D	501	NAP	O4B-C1B	7.70	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAP	O4B-C4B	7.69	1.62	1.45
6	C	503	NDP	O4D-C4D	7.55	1.61	1.45
2	D	501	NAP	C3B-C2B	7.39	1.69	1.52
2	D	501	NAP	C7N-N7N	7.25	1.46	1.33
5	C	501	YAS	C5P-N4P	6.70	1.48	1.33
2	A	501	NAP	O3D-C3D	-6.66	1.27	1.43
2	B	501	NAP	O4D-C1D	-6.66	1.31	1.41
2	D	501	NAP	O4B-C4B	6.60	1.59	1.45
2	B	501	NAP	O4B-C1B	-6.60	1.31	1.41
6	C	503	NDP	C5A-C4A	6.59	1.58	1.40
5	C	501	YAS	C9P-N8P	6.52	1.47	1.33
2	B	501	NAP	C7N-N7N	6.12	1.44	1.33
2	A	501	NAP	O7N-C7N	-6.01	1.12	1.24
5	D	502	YAS	O4B-C1B	5.34	1.48	1.41
5	D	502	YAS	C9P-N8P	5.28	1.45	1.33
2	A	501	NAP	C7N-N7N	5.21	1.42	1.33
6	C	503	NDP	C2D-C3D	-5.13	1.39	1.53
6	C	503	NDP	C7N-N7N	5.07	1.46	1.33
5	D	502	YAS	O9P-C9P	-5.07	1.13	1.23
5	C	501	YAS	C3B-C4B	4.84	1.65	1.52
2	D	501	NAP	C3D-C4D	4.75	1.65	1.53
2	A	501	NAP	C3N-C7N	4.73	1.57	1.50
5	D	502	YAS	C5P-N4P	4.59	1.43	1.33
2	D	501	NAP	P2B-O2B	4.38	1.67	1.59
5	D	502	YAS	OAE-CAD	-4.37	1.13	1.21
6	C	503	NDP	O3D-C3D	4.30	1.53	1.43
6	C	503	NDP	C6N-N1N	4.25	1.47	1.37
2	A	501	NAP	O2B-C2B	-4.20	1.28	1.44
5	D	502	YAS	O5P-C5P	-4.17	1.14	1.23
5	C	501	YAS	C2B-C1B	4.16	1.60	1.53
2	D	501	NAP	O2D-C2D	4.09	1.52	1.43
6	C	503	NDP	C6N-C5N	4.05	1.40	1.33
2	B	501	NAP	O2B-C2B	-4.05	1.29	1.44
6	C	503	NDP	O2D-C2D	3.98	1.52	1.43
6	C	503	NDP	C2A-N3A	-3.94	1.25	1.32
2	D	501	NAP	C2D-C1D	3.93	1.59	1.53
2	A	501	NAP	P2B-O2X	-3.85	1.40	1.54
2	A	501	NAP	C2N-N1N	-3.82	1.30	1.35
5	D	502	YAS	C3B-C4B	3.79	1.63	1.52
5	C	501	YAS	O2B-C2B	3.71	1.51	1.43
6	C	503	NDP	P2B-O2B	3.68	1.66	1.59
6	C	503	NDP	C3D-C4D	-3.67	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAP	PN-O2N	-3.46	1.39	1.55
2	B	501	NAP	O2D-C2D	-3.43	1.34	1.43
2	D	501	NAP	C6A-N6A	3.41	1.46	1.34
2	A	501	NAP	C4A-N3A	-3.35	1.31	1.35
2	B	501	NAP	P2B-O2B	3.30	1.65	1.59
6	C	503	NDP	C6A-N6A	3.30	1.46	1.34
2	A	501	NAP	PN-O1N	-3.29	1.39	1.50
2	A	501	NAP	P2B-O1X	-3.29	1.39	1.50
5	D	502	YAS	P3B-O9A	-3.24	1.42	1.54
5	D	502	YAS	C2B-C1B	3.22	1.58	1.53
5	C	501	YAS	CAF-CAD	3.22	1.54	1.50
5	C	501	YAS	P3B-O3B	3.17	1.65	1.59
6	C	503	NDP	C2N-C3N	3.13	1.43	1.34
2	A	501	NAP	C3B-C2B	3.12	1.59	1.52
6	C	503	NDP	O3B-C3B	-3.10	1.35	1.43
2	A	501	NAP	PA-O2A	-3.09	1.40	1.55
2	A	501	NAP	P2B-O3X	-3.08	1.43	1.54
5	C	501	YAS	C6A-N6A	3.07	1.45	1.34
2	D	501	NAP	C3N-C7N	3.05	1.55	1.50
2	B	501	NAP	C6A-N6A	3.00	1.45	1.34
5	C	501	YAS	CAD-S1P	2.97	1.83	1.76
2	D	501	NAP	O3D-C3D	2.94	1.49	1.43
6	C	503	NDP	C7N-C3N	2.93	1.55	1.48
5	D	502	YAS	OAP-CAP	-2.92	1.36	1.42
2	A	501	NAP	C8A-N7A	-2.81	1.29	1.34
2	A	501	NAP	C6N-N1N	-2.80	1.28	1.35
4	B	503	2EC	C6-N6	2.72	1.43	1.34
2	B	501	NAP	O3D-C3D	2.68	1.49	1.43
5	D	502	YAS	O2B-C2B	2.63	1.49	1.43
5	D	502	YAS	P3B-O8A	-2.63	1.42	1.50
4	B	503	2EC	C9M-N9	-2.60	1.47	1.49
4	A	503	2EC	C2-N1	-2.53	1.29	1.33
2	A	501	NAP	O5B-C5B	-2.53	1.35	1.44
5	C	501	YAS	P1A-O5B	2.48	1.69	1.59
5	D	502	YAS	P3B-O7A	-2.46	1.45	1.54
2	D	501	NAP	PA-O5B	2.45	1.69	1.59
2	A	501	NAP	C2A-N1A	-2.42	1.29	1.33
2	A	501	NAP	PA-O1A	-2.42	1.42	1.50
2	B	501	NAP	O3B-C3B	2.37	1.48	1.43
5	D	502	YAS	P2A-O4A	-2.34	1.44	1.55
5	D	502	YAS	O6A-CCP	-2.33	1.36	1.43
5	D	502	YAS	C6A-N6A	2.31	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	502	YAS	P1A-O1A	-2.30	1.42	1.50
5	C	501	YAS	O9P-C9P	-2.29	1.18	1.23
2	B	501	NAP	O7N-C7N	-2.28	1.19	1.24
5	C	501	YAS	C6P-C5P	2.24	1.55	1.51
6	C	503	NDP	C2D-C1D	-2.23	1.46	1.53
5	D	502	YAS	C8A-N7A	-2.23	1.30	1.34
2	B	501	NAP	C3B-C2B	2.22	1.57	1.52
5	D	502	YAS	C4A-N3A	-2.18	1.32	1.35
6	C	503	NDP	C5D-C4D	-2.15	1.44	1.51
6	C	503	NDP	C5A-N7A	2.14	1.47	1.39
2	A	501	NAP	P2B-O2B	2.13	1.63	1.59
6	C	503	NDP	O7N-C7N	-2.09	1.19	1.24
5	D	502	YAS	CAF-CAD	2.05	1.53	1.50
4	A	503	2EC	C6-N6	2.03	1.41	1.34

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	503	NDP	O4B-C4B-C3B	-13.65	78.10	105.11
6	C	503	NDP	O3B-C3B-C4B	-8.91	85.27	111.05
2	A	501	NAP	C2D-C3D-C4D	-8.38	86.36	102.64
6	C	503	NDP	O4B-C4B-C5B	-8.31	82.02	109.37
6	C	503	NDP	C3N-C2N-N1N	-7.90	111.83	123.10
6	C	503	NDP	C4D-O4D-C1D	-7.89	92.07	109.47
2	A	501	NAP	O3D-C3D-C4D	7.15	131.72	111.05
5	D	502	YAS	P2A-O3A-P1A	-5.61	113.59	132.83
2	A	501	NAP	C5D-C4D-C3D	5.56	136.01	115.18
5	C	501	YAS	CAF-CAD-S1P	5.55	119.92	113.46
6	C	503	NDP	C1D-N1N-C2N	-5.34	112.21	121.11
6	C	503	NDP	C1B-N9A-C4A	-5.26	117.40	126.64
5	D	502	YAS	O6A-CCP-CBP	-5.01	102.50	110.55
2	A	501	NAP	O5D-C5D-C4D	-4.95	91.97	108.99
6	C	503	NDP	C2B-C3B-C4B	4.85	112.53	101.99
5	D	502	YAS	C2B-C3B-C4B	-4.77	94.77	103.22
5	C	501	YAS	N3A-C2A-N1A	-4.75	121.26	128.68
2	B	501	NAP	N3A-C2A-N1A	-4.70	121.33	128.68
2	A	501	NAP	O2D-C2D-C1D	4.67	128.09	110.85
6	C	503	NDP	C2D-C3D-C4D	4.63	111.64	102.64
4	A	503	2EC	N3-C2-N1	-4.58	121.52	128.68
5	D	502	YAS	C1B-N9A-C4A	-4.50	118.74	126.64
5	D	502	YAS	O3B-C3B-C4B	4.47	126.24	110.08
6	C	503	NDP	O5D-C5D-C4D	-4.46	93.64	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	NAP	N3A-C2A-N1A	-4.37	121.86	128.68
5	D	502	YAS	N3A-C2A-N1A	-4.37	121.86	128.68
2	A	501	NAP	N3A-C2A-N1A	-4.28	121.99	128.68
5	C	501	YAS	P2A-O3A-P1A	-4.26	118.22	132.83
6	C	503	NDP	O3D-C3D-C4D	4.17	123.11	111.05
5	C	501	YAS	O6A-CCP-CBP	-4.08	103.99	110.55
5	C	501	YAS	OAE-CAD-CAF	-4.07	119.18	123.99
6	C	503	NDP	O3D-C3D-C2D	4.05	124.92	111.82
2	B	501	NAP	O2B-P2B-O1X	-4.03	93.85	109.39
5	D	502	YAS	C4A-C5A-N7A	-4.00	105.23	109.40
5	D	502	YAS	O3B-P3B-O8A	-3.99	93.99	109.39
4	B	503	2EC	N3-C2-N1	-3.90	122.59	128.68
2	D	501	NAP	O2B-P2B-O1X	-3.57	95.60	109.39
2	D	501	NAP	O5D-C5D-C4D	-3.57	96.70	108.99
2	B	501	NAP	O2B-C2B-C1B	3.56	122.92	110.10
2	D	501	NAP	O2B-C2B-C1B	3.46	122.56	110.10
2	B	501	NAP	O4B-C1B-C2B	-3.46	100.59	106.59
2	B	501	NAP	C1B-N9A-C4A	-3.39	120.68	126.64
2	D	501	NAP	C4A-C5A-N7A	-3.36	105.90	109.40
6	C	503	NDP	PN-O3-PA	-3.32	121.43	132.83
2	D	501	NAP	O4B-C1B-C2B	-3.32	100.83	106.59
3	D	503	VES	C1-N5-C4	3.28	112.28	104.96
2	A	501	NAP	O4D-C4D-C3D	-3.27	98.64	105.11
6	C	503	NDP	O4B-C1B-C2B	3.27	112.25	106.59
5	D	502	YAS	OAE-CAD-S1P	-3.20	118.46	122.61
5	D	502	YAS	O2B-C2B-C3B	3.18	120.18	111.17
4	B	503	2EC	C50-C9M-N9	3.17	117.79	112.55
3	B	502	VES	C1-N5-C4	3.16	112.02	104.96
3	C	502	VES	C1-N5-C4	3.16	112.01	104.96
3	A	502	VES	C1-N5-C4	3.14	111.97	104.96
5	D	502	YAS	C5B-C4B-C3B	3.04	124.49	114.40
5	C	501	YAS	C2B-C3B-C4B	-2.93	98.03	103.22
6	C	503	NDP	N3A-C2A-N1A	-2.86	124.21	128.68
5	C	501	YAS	C1B-N9A-C4A	-2.85	121.63	126.64
2	B	501	NAP	C4A-C5A-N7A	-2.85	106.43	109.40
3	D	504	VES	C1-N5-C4	2.81	111.24	104.96
2	D	501	NAP	C3N-C2N-N1N	2.77	123.14	120.43
5	D	502	YAS	OAE-CAD-CAF	2.74	127.23	123.99
2	A	501	NAP	C2N-N1N-C1D	-2.72	113.07	119.14
5	C	501	YAS	C4A-C5A-N7A	-2.64	106.65	109.40
5	D	502	YAS	O4B-C1B-C2B	-2.63	103.09	106.93
2	A	501	NAP	C4A-C5A-N7A	-2.58	106.71	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	NAP	C3B-C2B-C1B	2.57	107.72	102.89
2	B	501	NAP	O3X-P2B-O2B	2.55	117.40	105.99
2	D	501	NAP	C3D-C2D-C1D	2.53	104.78	100.98
2	B	501	NAP	C2D-C3D-C4D	2.48	107.47	102.64
2	B	501	NAP	C2B-C3B-C4B	-2.48	96.61	101.99
2	D	501	NAP	O3X-P2B-O2B	2.39	116.70	105.99
2	D	501	NAP	PN-O3-PA	-2.39	124.63	132.83
4	A	503	2EC	C4-C5-N7	-2.37	106.92	109.40
2	A	501	NAP	PN-O3-PA	-2.34	124.80	132.83
2	D	501	NAP	C1B-N9A-C4A	-2.33	122.54	126.64
2	A	501	NAP	O2D-C2D-C3D	2.33	119.35	111.82
5	D	502	YAS	C7P-N8P-C9P	-2.30	118.49	122.59
6	C	503	NDP	C3D-C2D-C1D	2.29	105.78	101.43
2	B	501	NAP	O3B-C3B-C2B	-2.22	104.87	111.17
2	D	501	NAP	C6N-N1N-C2N	-2.21	119.96	121.97
5	D	502	YAS	CAJ-CAF-CAD	2.15	118.04	112.72
6	C	503	NDP	O3B-C3B-C2B	2.12	117.18	111.17
2	A	501	NAP	C2B-C3B-C4B	2.09	106.54	101.99
2	D	501	NAP	O2B-C2B-C3B	-2.08	104.14	111.68
6	C	503	NDP	O4D-C1D-C2D	2.04	111.07	106.64
4	B	503	2EC	C4-C5-N7	-2.03	107.28	109.40
5	C	501	YAS	CEP-CBP-CAP	2.01	112.31	108.82

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	NAP	C4D
2	A	501	NAP	C2D
2	A	501	NAP	C3D
2	B	501	NAP	C2B
2	D	501	NAP	C4D
2	D	501	NAP	C4B
2	D	501	NAP	C3B
2	D	501	NAP	C2D
2	D	501	NAP	C2B
2	D	501	NAP	C3D
6	C	503	NDP	C4D
6	C	503	NDP	C3D

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAP	C3D-C4D-C5D-O5D
2	B	501	NAP	C2B-O2B-P2B-O1X
2	B	501	NAP	O4D-C1D-N1N-C2N
2	B	501	NAP	O4D-C1D-N1N-C6N
2	B	501	NAP	C2D-C1D-N1N-C2N
2	D	501	NAP	C5B-O5B-PA-O3
2	D	501	NAP	C2B-O2B-P2B-O1X
5	C	501	YAS	C3B-C4B-C5B-O5B
5	C	501	YAS	C4B-C5B-O5B-P1A
5	C	501	YAS	C5B-O5B-P1A-O1A
5	C	501	YAS	C5B-O5B-P1A-O2A
5	C	501	YAS	C5B-O5B-P1A-O3A
5	C	501	YAS	CCP-O6A-P2A-O3A
5	C	501	YAS	CCP-O6A-P2A-O4A
5	C	501	YAS	CCP-O6A-P2A-O5A
5	D	502	YAS	C3B-C4B-C5B-O5B
6	C	503	NDP	O4B-C4B-C5B-O5B
6	C	503	NDP	C3B-C4B-C5B-O5B
6	C	503	NDP	C2B-O2B-P2B-O1X
6	C	503	NDP	C5D-O5D-PN-O3
6	C	503	NDP	C5D-O5D-PN-O2N
6	C	503	NDP	C3D-C4D-C5D-O5D
2	D	501	NAP	O4B-C4B-C5B-O5B
2	D	501	NAP	C3D-C4D-C5D-O5D
5	D	502	YAS	O4B-C4B-C5B-O5B
5	C	501	YAS	O4B-C4B-C5B-O5B
6	C	503	NDP	O4D-C4D-C5D-O5D
5	D	502	YAS	C4B-C5B-O5B-P1A
5	C	501	YAS	OAE-CAD-S1P-C2P
2	A	501	NAP	PN-O3-PA-O5B
2	B	501	NAP	PN-O3-PA-O5B
5	C	501	YAS	CAF-CAD-S1P-C2P
2	D	501	NAP	O4D-C4D-C5D-O5D
5	C	501	YAS	CAP-CBP-CCP-O6A
2	A	501	NAP	O4D-C4D-C5D-O5D
5	C	501	YAS	CEP-CBP-CCP-O6A
6	C	503	NDP	C4D-C5D-O5D-PN
5	D	502	YAS	P2A-O3A-P1A-O1A
6	C	503	NDP	O4D-C1D-N1N-C2N
2	B	501	NAP	C1B-C2B-O2B-P2B
5	D	502	YAS	P1A-O3A-P2A-O5A
2	A	501	NAP	C2B-O2B-P2B-O1X
5	C	501	YAS	CDP-CBP-CCP-O6A

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Mol	Chain	Res	Type	Atoms
2	B	501	NAP	O4B-C4B-C5B-O5B
2	D	501	NAP	C3B-C4B-C5B-O5B
2	B	501	NAP	C2B-O2B-P2B-O3X
5	C	501	YAS	C3B-O3B-P3B-O9A
6	C	503	NDP	C2B-O2B-P2B-O3X
2	A	501	NAP	O4B-C4B-C5B-O5B
5	D	502	YAS	P2A-O3A-P1A-O2A
5	C	501	YAS	O5P-C5P-C6P-C7P
5	D	502	YAS	CCP-O6A-P2A-O5A
6	C	503	NDP	C5D-O5D-PN-O1N
6	C	503	NDP	C2N-C3N-C7N-N7N

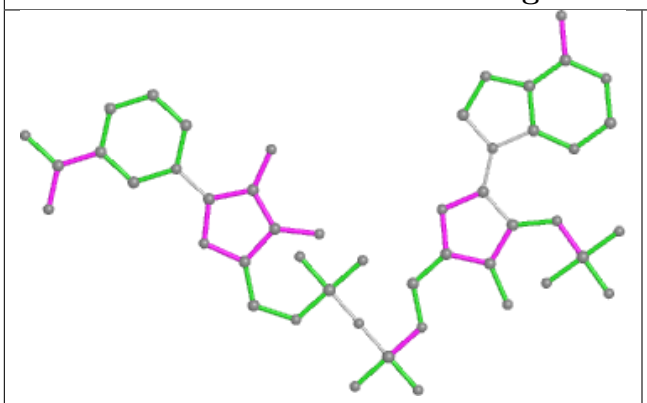
There are no ring outliers.

10 monomers are involved in 33 short contacts:

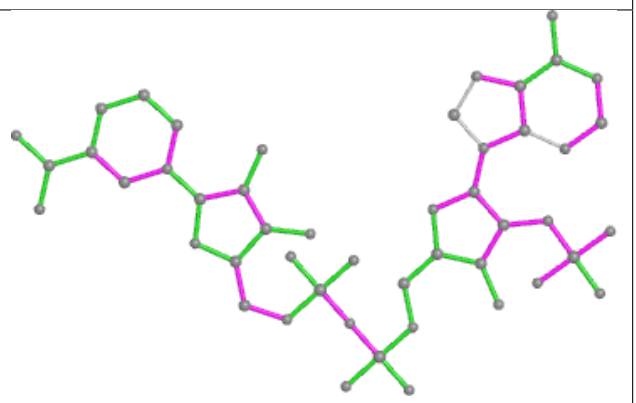
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	503	VES	2	0
3	A	502	VES	1	0
2	D	501	NAP	7	0
5	C	501	YAS	1	0
3	C	502	VES	5	0
5	D	502	YAS	3	0
2	A	501	NAP	1	0
2	B	501	NAP	6	0
6	C	503	NDP	3	0
3	D	504	VES	5	0

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.

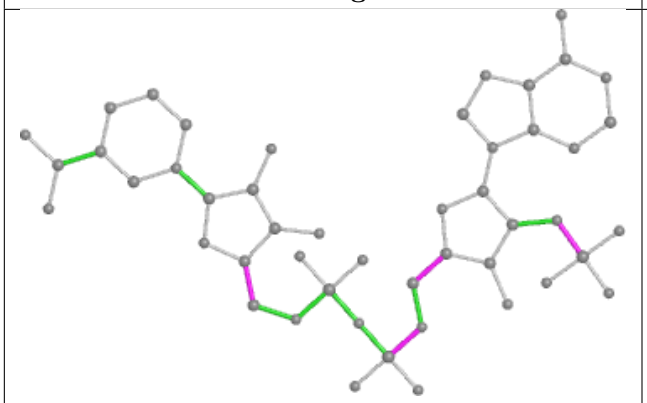
Ligand NAP D 501



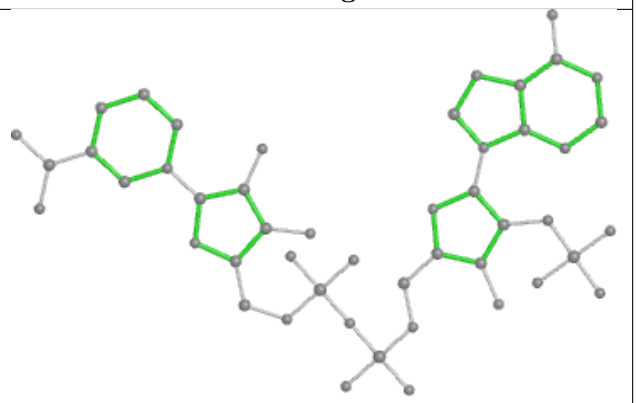
Bond lengths



Bond angles

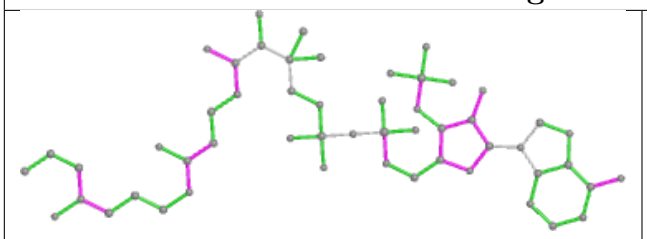


Torsions

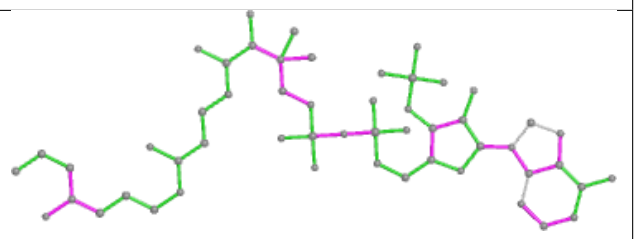


Rings

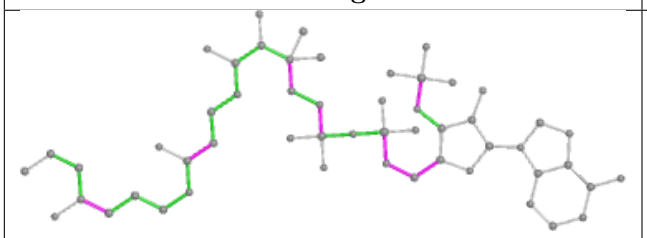
Ligand YAS C 501



Bond lengths



Bond angles



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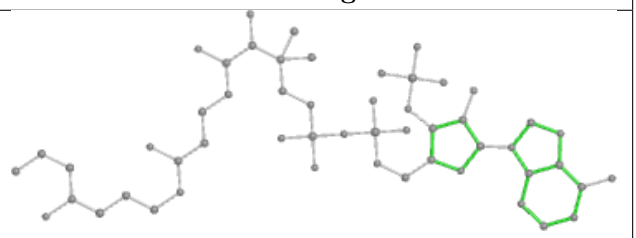
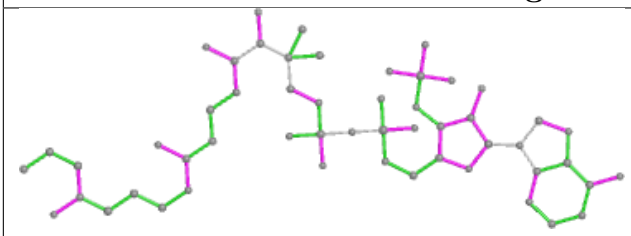


Rings

Ligand YAS D 502



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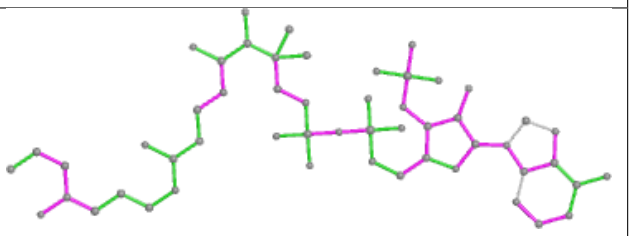
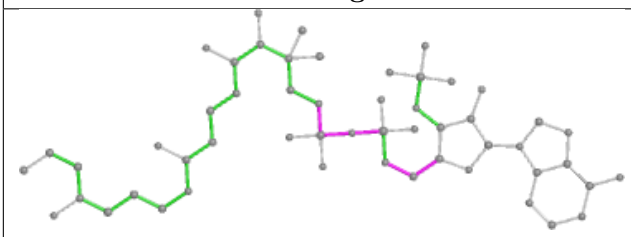


Bond angles



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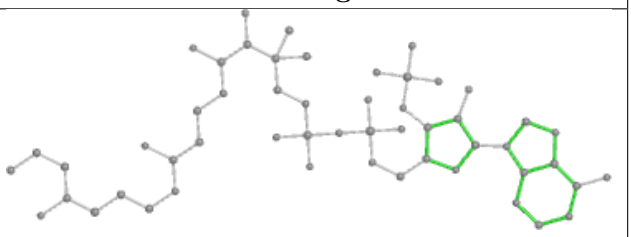
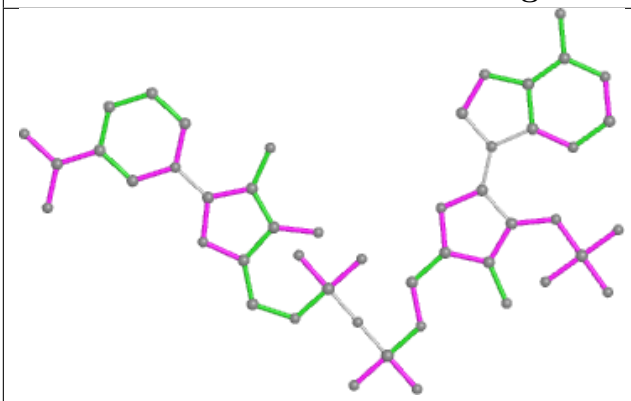
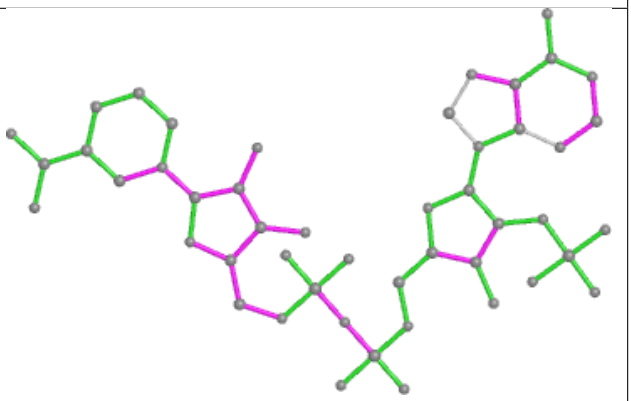


Rings

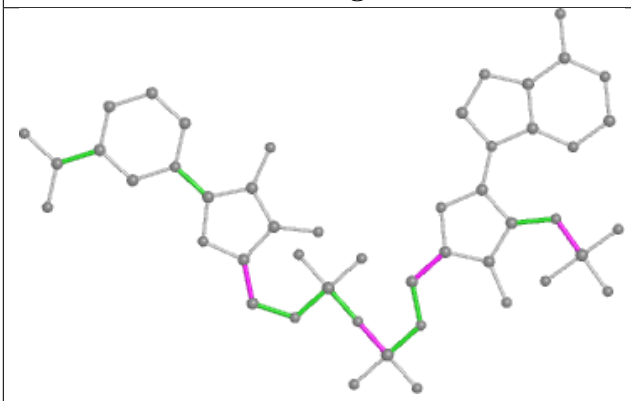
Ligand NAP A 501



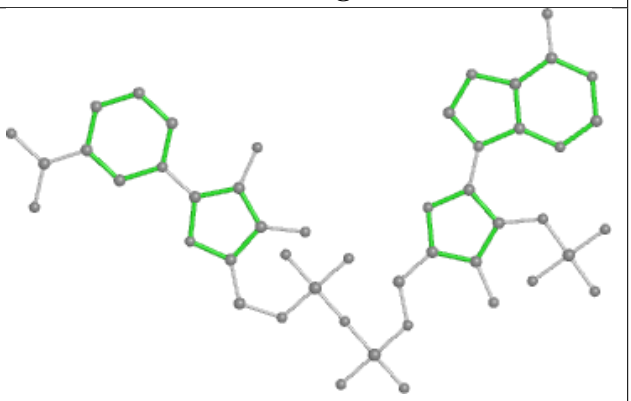
Bond lengths



Bond angles

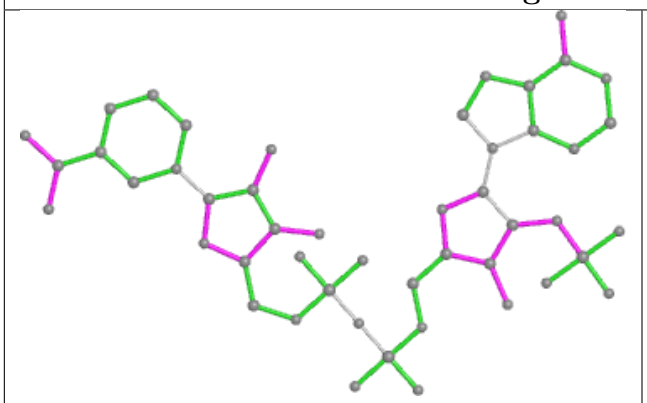


Torsions

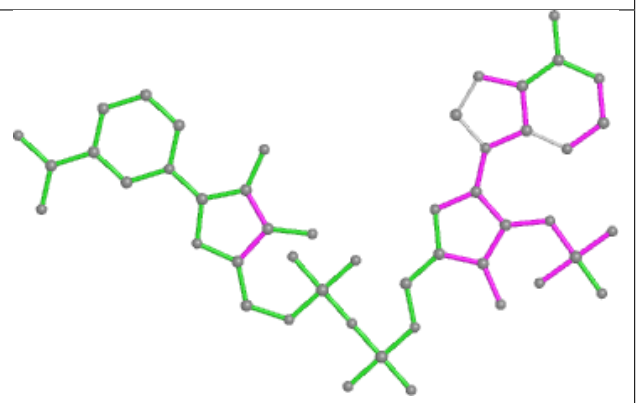


Rings

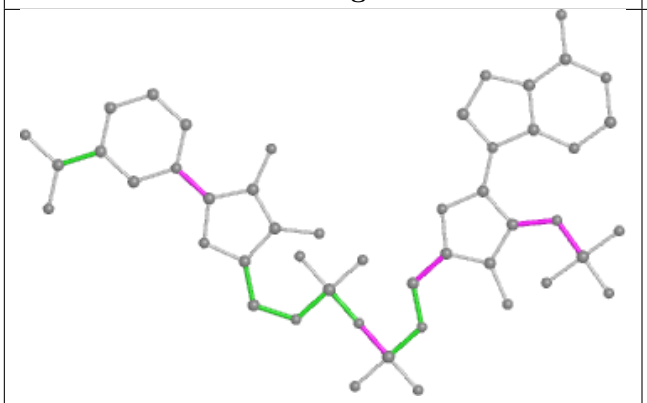
Ligand NAP B 501



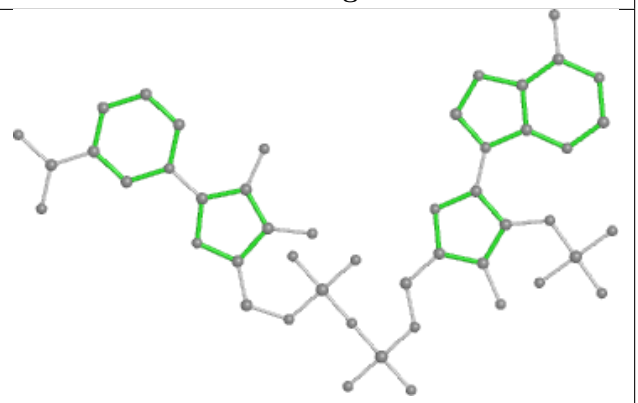
Bond lengths



Bond angles

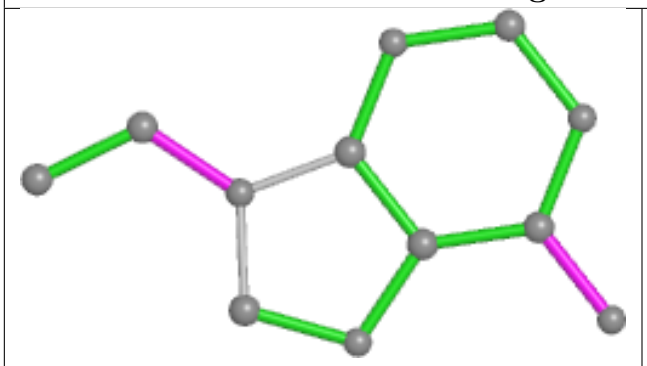


Torsions

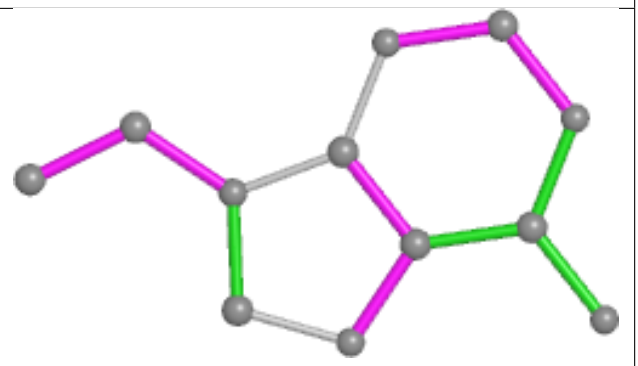


Rings

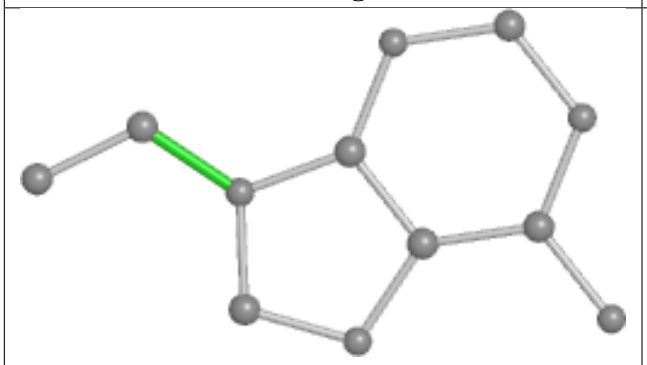
Ligand 2EC B 503



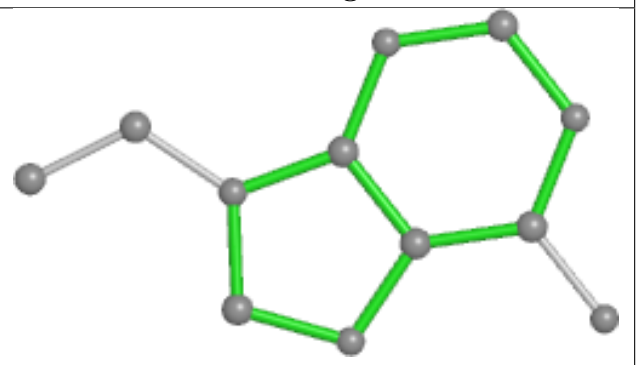
Bond lengths



Bond angles

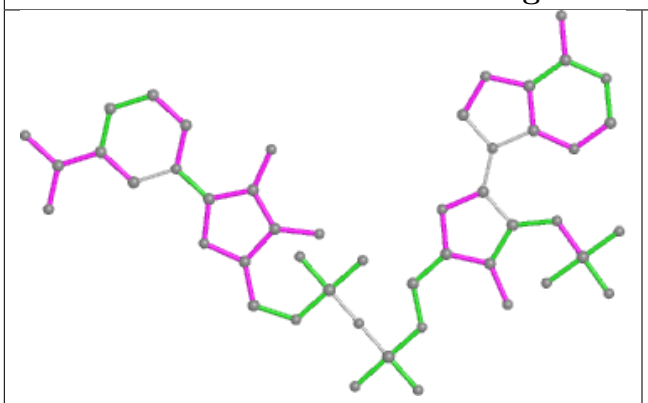


Torsions

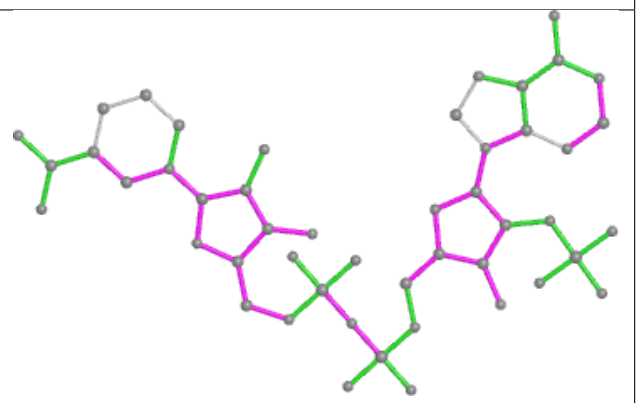


Rings

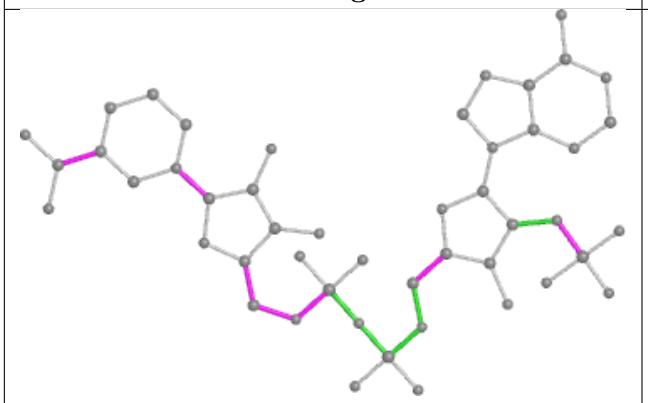
Ligand NDP C 503



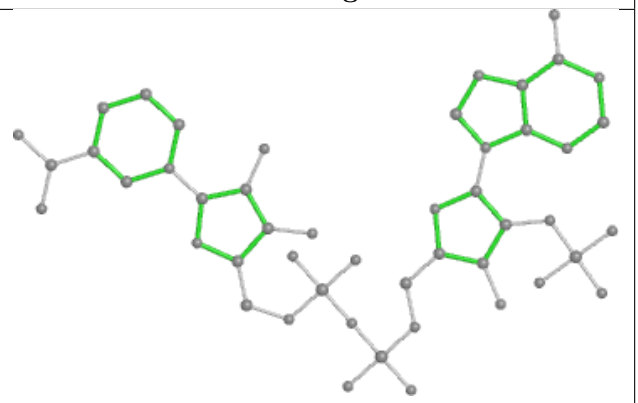
Bond lengths



Bond angles

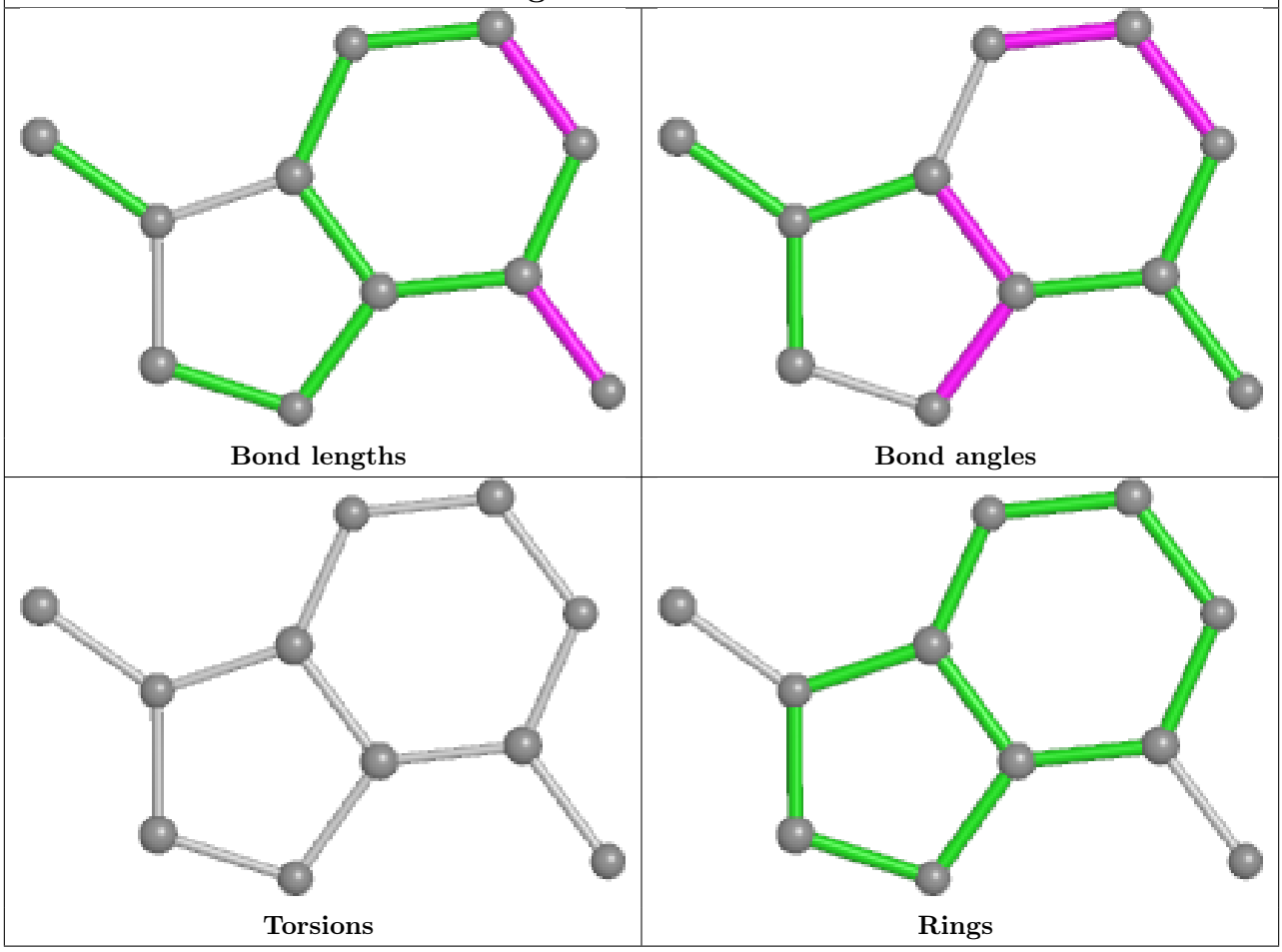


Torsions



Rings

Ligand 2EC A 503



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	446/448 (99%)	-0.32	5 (1%)	80	84	16, 24, 39, 56	0
1	B	448/448 (100%)	-0.42	2 (0%)	92	93	15, 22, 35, 53	0
1	C	447/448 (99%)	-0.32	6 (1%)	77	81	16, 23, 40, 59	0
1	D	445/448 (99%)	-0.27	8 (1%)	68	72	15, 25, 43, 58	0
All	All	1786/1792 (99%)	-0.33	21 (1%)	79	83	15, 23, 40, 59	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	444	ASN	5.6
1	D	42	GLY	4.0
1	D	38	ARG	3.3
1	C	101	GLY	3.2
1	D	103	LEU	3.1
1	C	102	ARG	3.1
1	D	35	GLY	3.1
1	B	-3[A]	GLU	3.0
1	C	42	GLY	3.0
1	A	20	ALA	2.9
1	D	102	ARG	2.7
1	A	38	ARG	2.5
1	D	41	ASP	2.5
1	A	21	LEU	2.3
1	A	13	ALA	2.3
1	B	12	ASP	2.3
1	C	103	LEU	2.3
1	D	100	TYR	2.3
1	A	293	ARG	2.2
1	C	38	ARG	2.2
1	D	99	ARG	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)

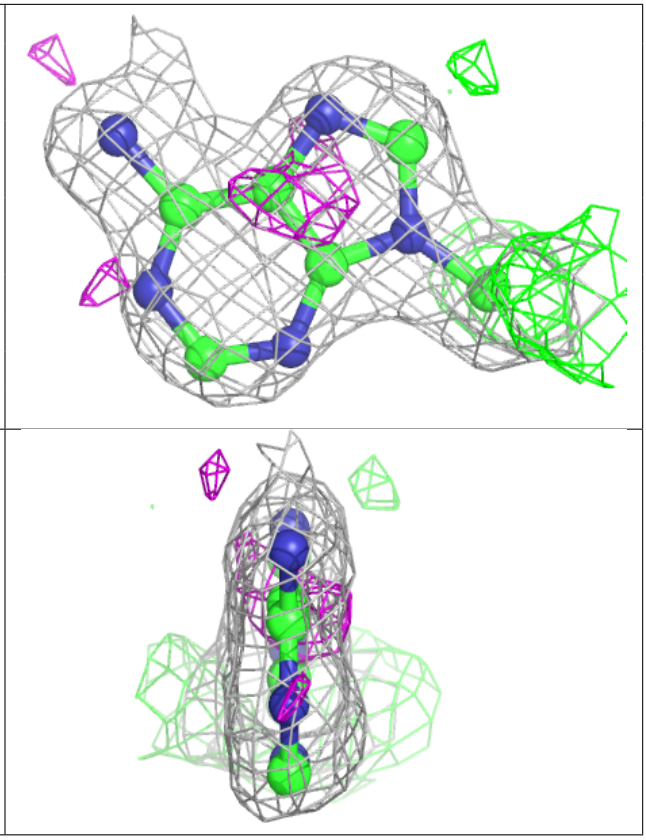
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	2EC	A	503	11/12	0.65	0.26	28,44,51,53	0
4	2EC	B	503	12/12	0.68	0.25	31,46,54,54	0
3	VES	D	504	5/5	0.71	0.38	44,44,49,50	0
5	YAS	C	501	53/53	0.81	0.13	24,33,58,65	1
3	VES	D	503	5/5	0.82	0.19	32,39,42,42	0
5	YAS	D	502	53/53	0.86	0.11	20,28,54,73	1
3	VES	B	502	5/5	0.87	0.19	29,36,38,42	0
3	VES	A	502	5/5	0.88	0.25	30,33,36,41	0
3	VES	C	502	5/5	0.89	0.17	34,42,43,52	0
2	NAP	D	501	48/48	0.95	0.11	22,33,49,61	0
2	NAP	A	501	48/48	0.96	0.09	17,21,33,46	0
2	NAP	B	501	48/48	0.96	0.10	15,19,24,32	0
6	NDP	C	503	48/48	0.96	0.11	20,39,59,64	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.

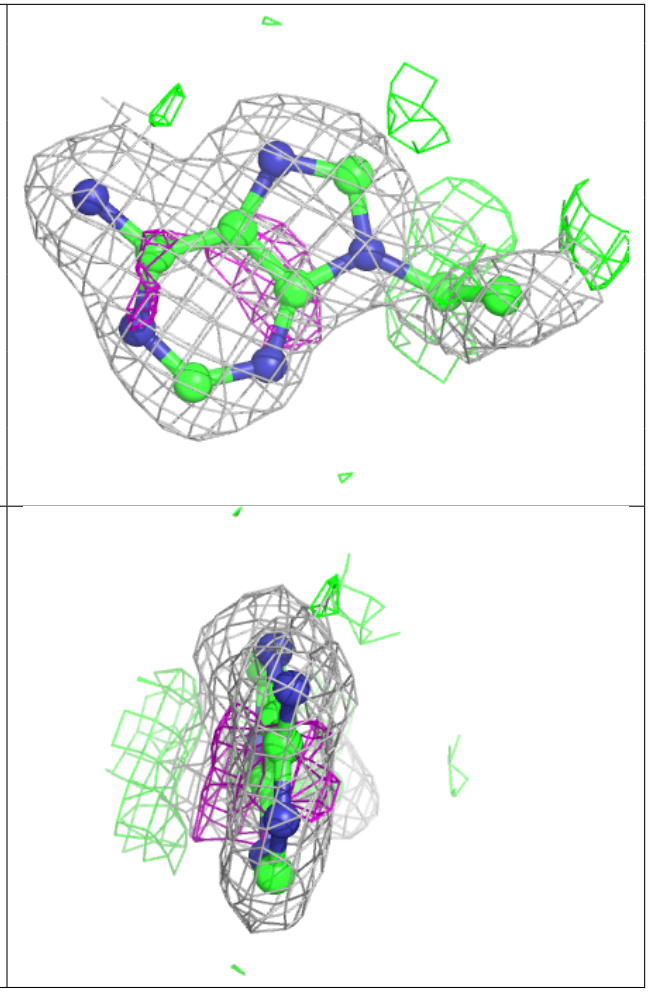
Electron density around 2EC A 503:

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



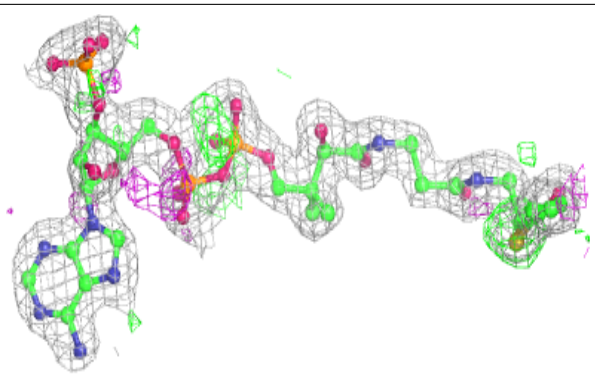
Electron density around 2EC B 503:

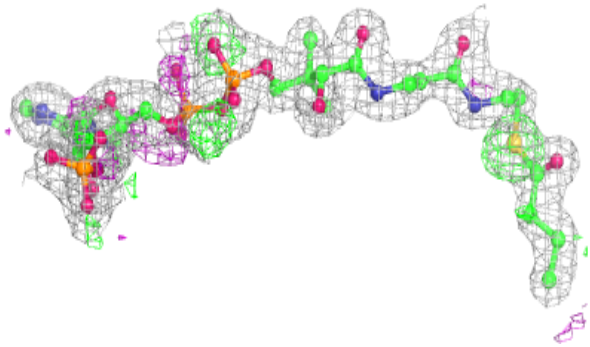
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

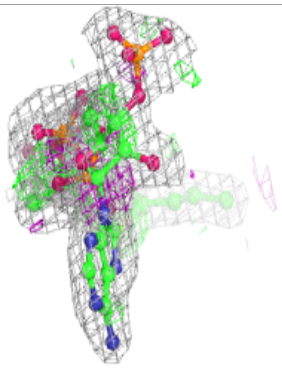


Electron density around YAS C 501:

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







Electron density around YAS D 502:

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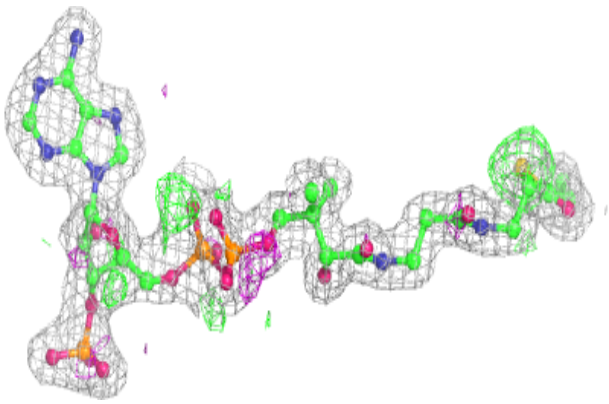
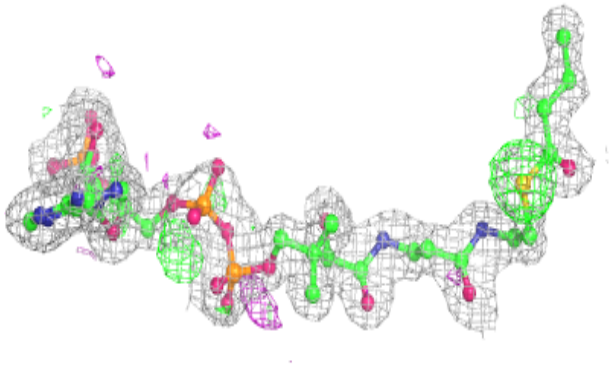
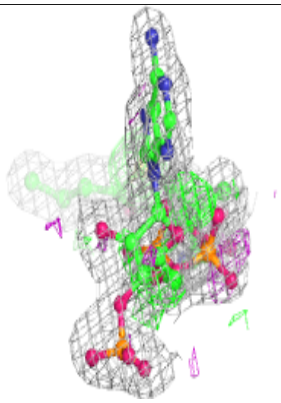
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around NAP D 501:

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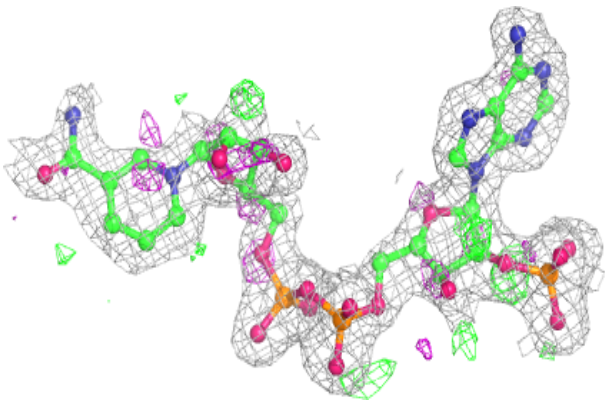
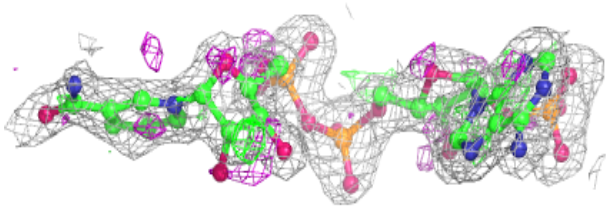
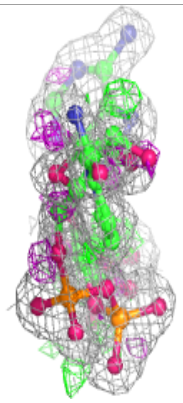
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around NAP A 501:

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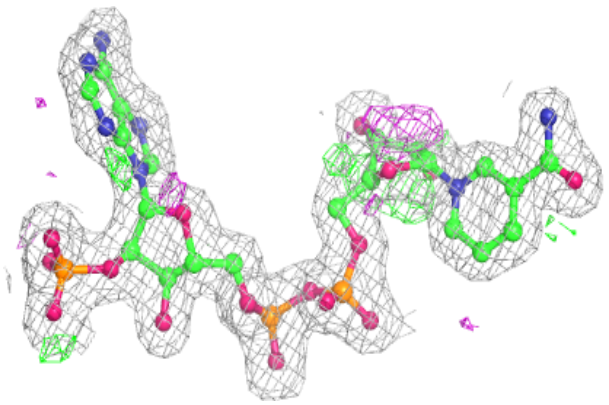
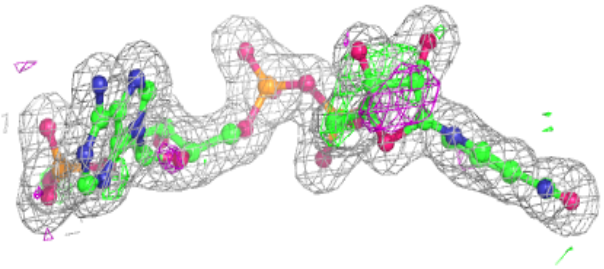
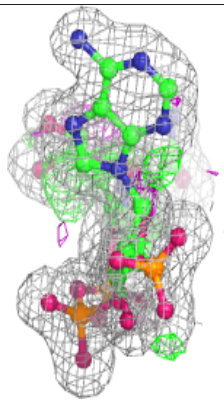
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

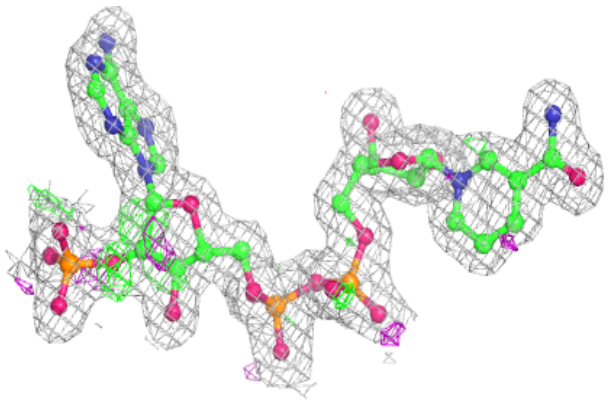


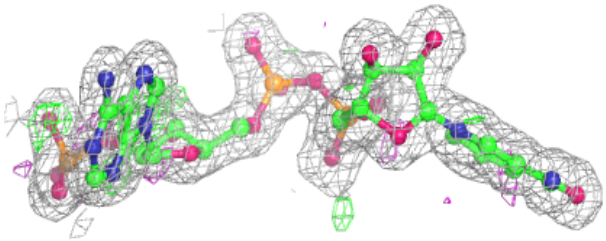


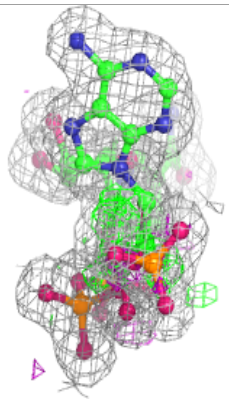


Electron density around NAP B 501:

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







Electron density around NDP C 503:

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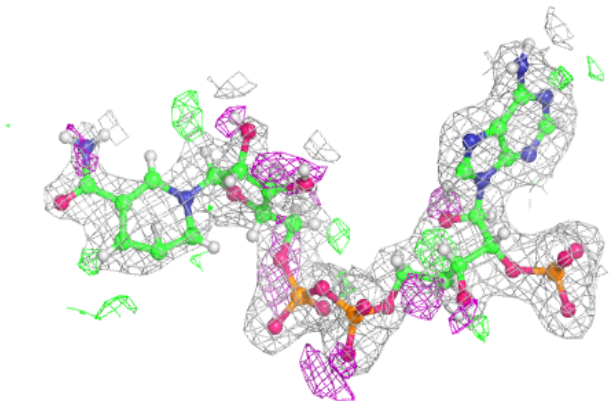
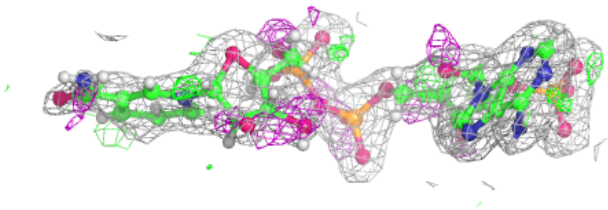
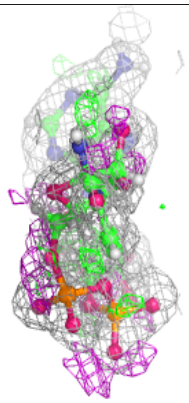
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.