Full wwPDB X-ray Structure Validation Report (i)

Sep 14, 2023 – 01:47 pm BST

PDB ID	:	8CEK
Title	:	Succinyl-CoA Reductase from Clostridium kluyveri (SucD) with NADPH
Authors	:	Pfister, P.; Diehl, C.; Erb, T.J.
Deposited on	:	2023-02-02
Resolution	:	2.15 Å(reported)

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

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

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

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

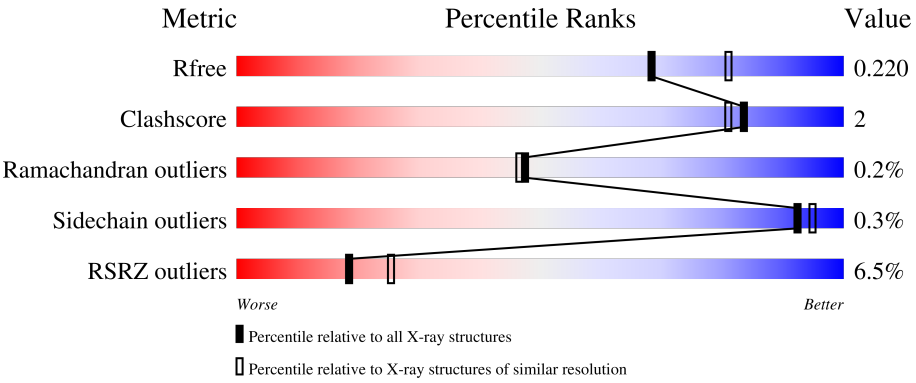
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	453	7% 94% 5%
1	B	453	7% 94% 6%
1	C	453	5% 92% 6%
1	D	453	7% 94% 5%

2 Entry composition

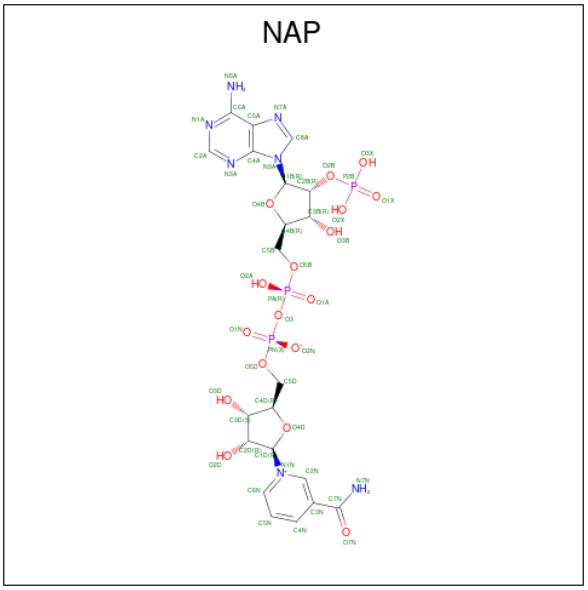
There are 3 unique types of molecules in this entry. The entry contains 14888 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Succinate-semialdehyde dehydrogenase (acetylating).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	1	0
			3416	2163	577	661	15			
1	B	449	Total	C	N	O	S	0	0	0
			3407	2157	575	660	15			
1	C	448	Total	C	N	O	S	0	0	0
			3400	2152	574	659	15			
1	D	449	Total	C	N	O	S	0	0	0
			3407	2157	575	660	15			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	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 water.

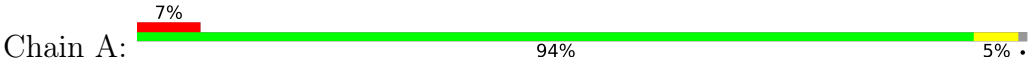
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	271	Total	O	0	0
			271	271		
3	B	283	Total	O	0	0
			283	283		
3	C	211	Total	O	0	0
			211	211		
3	D	301	Total	O	0	0
			301	301		

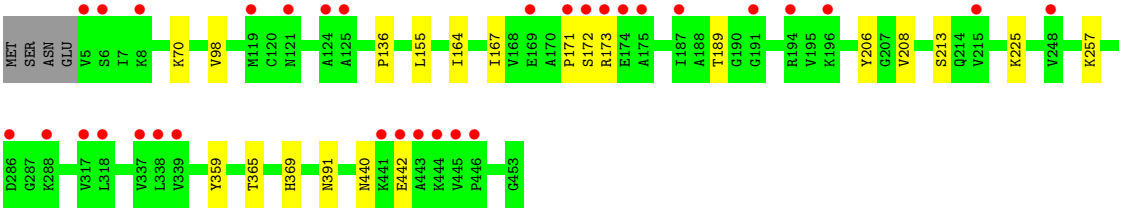
3 Residue-property plots (i)

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: Succinate-semialdehyde dehydrogenase (acetylating)

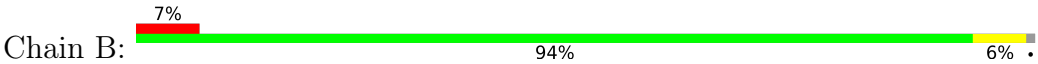
Chain A:

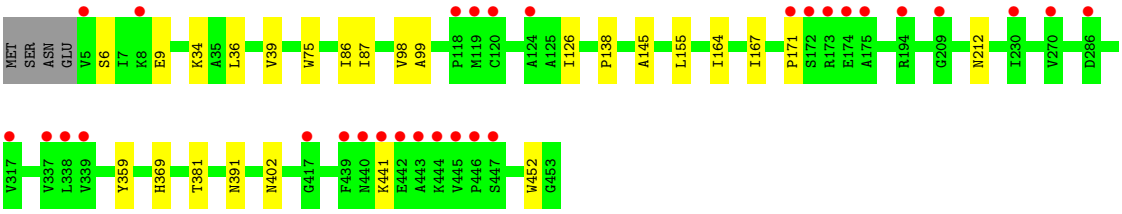




• Molecule 1: Succinate-semialdehyde dehydrogenase (acetylating)

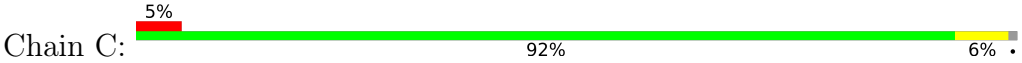
Chain B:

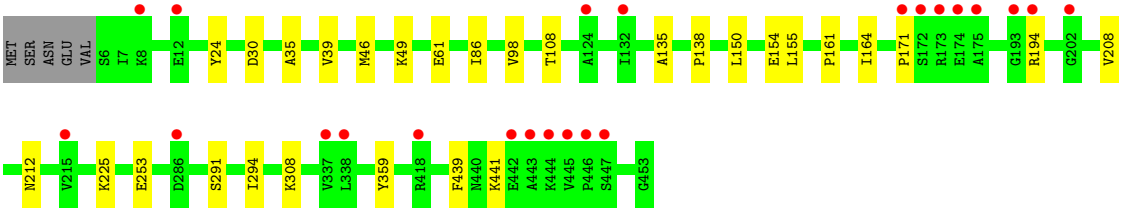




• Molecule 1: Succinate-semialdehyde dehydrogenase (acetylating)

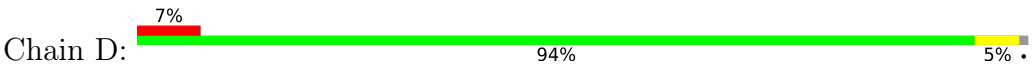
Chain C:

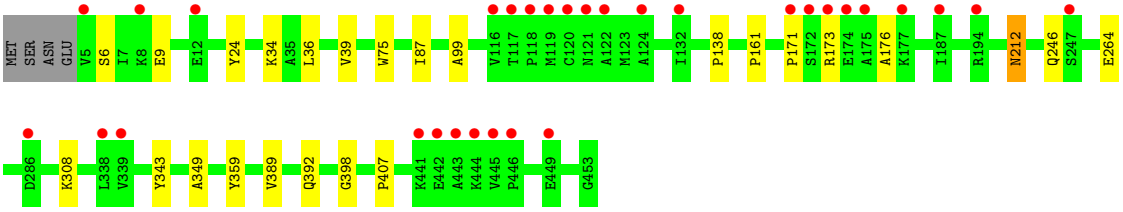




• Molecule 1: Succinate-semialdehyde dehydrogenase (acetylating)

Chain D:




MET
SER
ASN
GLU
V5
S6
I7
K8
E9
E12
Y24
K34
A35
L36
V39
W75
I87
A99
V116
T117
P118
M119
C120
N121
A122
M123
A124
I132
P138
P161
P171
S172
R173
E174
A175
A176
K177
I187
R194
N212
Q246
S247
E264
D286
K308
L338
V339
Y343
A349
Y359
V369
Q392
G398
P407
K441
E442
A443
K444
V445
P446
E449
G453

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	140.05Å 190.83Å 190.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.66 – 2.15 29.66 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.66-2.15) 99.9 (29.66-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.198 , 0.222 0.198 , 0.220	Depositor DCC
R_{free} test set	2004 reflections (1.45%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.047 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14888	wwPDB-VP
Average B, all atoms (Å^2)	47.0	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 41.25 % 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 2.4257e-04. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.28	0/3473	0.47	0/4696
1	B	0.28	0/3464	0.46	0/4685
1	C	0.28	0/3457	0.47	0/4675
1	D	0.29	0/3464	0.46	0/4685
All	All	0.28	0/13858	0.47	0/18741

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

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	3416	0	3467	18	0
1	B	3407	0	3455	13	0
1	C	3400	0	3446	20	0
1	D	3407	0	3455	14	0
2	A	48	0	25	2	0
2	B	48	0	25	2	0
2	C	48	0	25	4	0
2	D	48	0	25	2	0
3	A	271	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	283	0	0	2	0
3	C	211	0	0	6	0
3	D	301	0	0	2	0
All	All	14888	0	13923	67	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LYS:NZ	3:A:602:HOH:O	2.22	0.73
1:C:225:LYS:NZ	3:C:606:HOH:O	2.26	0.68
1:A:70:LYS:NZ	3:A:605:HOH:O	2.27	0.65
1:A:189:THR:HA	1:A:208:VAL:CG2	2.27	0.65
1:A:189:THR:HA	1:A:208:VAL:HG22	1.80	0.63
1:A:136:PRO:HG3	1:A:167:ILE:HD11	1.82	0.61
1:D:36:LEU:O	1:D:39:VAL:HG12	2.02	0.60
2:B:501:NAP:H8A	2:B:501:NAP:H51A	1.87	0.57
1:A:172:SER:OG	1:A:173:ARG:N	2.33	0.57
2:D:501:NAP:O2A	3:D:602:HOH:O	2.18	0.55
1:C:86:ILE:HG12	1:C:98:VAL:HG22	1.90	0.54
1:D:138:PRO:HG3	1:D:171:PRO:HG3	1.89	0.54
1:B:155:LEU:HD13	1:B:164:ILE:HD11	1.90	0.53
1:B:452:TRP:O	3:B:601:HOH:O	2.19	0.52
1:D:173:ARG:NH2	2:D:501:NAP:O2X	2.42	0.52
1:C:439:PHE:HE2	1:C:441:LYS:HD2	1.75	0.52
1:C:155:LEU:HD13	1:C:164:ILE:HD11	1.92	0.51
1:D:87:ILE:HD13	1:D:99:ALA:HB2	1.94	0.50
1:B:87:ILE:HD13	1:B:99:ALA:HB2	1.94	0.49
1:C:138:PRO:HG3	1:C:171:PRO:HG3	1.94	0.49
1:C:291:SER:HA	1:C:294:ILE:HG13	1.95	0.49
1:B:6:SER:HB3	1:B:9:GLU:HG3	1.94	0.49
1:C:24:TYR:OH	1:C:161:PRO:HD3	2.14	0.48
1:A:208:VAL:HB	2:A:501:NAP:N7N	2.29	0.48
1:A:208:VAL:O	1:A:208:VAL:HG23	2.14	0.47
1:D:6:SER:HB3	1:D:9:GLU:HG3	1.95	0.47
1:C:30:ASP:OD2	3:C:603:HOH:O	2.20	0.47
1:D:308:LYS:NZ	3:D:608:HOH:O	2.40	0.46
1:D:24:TYR:OH	1:D:161:PRO:HD3	2.15	0.46
1:C:39:VAL:CG2	1:C:154:GLU:HG3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ASN:OD1	1:A:442:GLU:HG3	2.17	0.45
1:B:34:LYS:HB2	1:B:75:TRP:CH2	2.52	0.45
1:B:86:ILE:HG12	1:B:98:VAL:HG22	1.97	0.45
1:A:172:SER:HG	1:A:173:ARG:H	1.63	0.45
1:A:206:TYR:HB3	3:A:690:HOH:O	2.17	0.45
1:C:308:LYS:HG2	1:D:264:GLU:OE2	2.17	0.45
1:A:189:THR:HA	1:A:208:VAL:HG21	1.98	0.44
1:D:173:ARG:HA	1:D:176:ALA:HB3	1.99	0.44
1:A:257:LYS:HB3	1:A:257:LYS:HE2	1.69	0.44
1:C:108:THR:HG22	1:C:135:ALA:HB3	2.00	0.44
1:A:155:LEU:HD13	1:A:164:ILE:HD11	2.00	0.43
1:B:138:PRO:HG3	1:B:171:PRO:HG3	1.99	0.43
1:C:194:ARG:HH11	2:C:501:NAP:C8A	2.31	0.43
1:B:145:ALA:HA	1:B:167:ILE:HD13	2.01	0.43
2:B:501:NAP:H51A	2:B:501:NAP:C8A	2.47	0.43
1:C:39:VAL:HG22	1:C:154:GLU:HG3	2.00	0.43
1:D:34:LYS:HB2	1:D:75:TRP:CH2	2.54	0.43
1:A:172:SER:HB2	2:A:501:NAP:N6A	2.34	0.42
1:D:212:ASN:HA	1:D:246:GLN:HG3	2.00	0.42
1:A:98:VAL:HG11	1:B:381:THR:HA	2.00	0.42
1:B:402:ASN:HB2	3:B:611:HOH:O	2.19	0.42
1:D:343:TYR:CG	1:D:349:ALA:HB2	2.54	0.42
1:D:398:GLY:O	1:D:407:PRO:HA	2.19	0.42
2:C:501:NAP:H52A	3:C:615:HOH:O	2.20	0.42
1:C:35:ALA:O	1:C:39:VAL:HG23	2.19	0.42
1:C:253:GLU:HG2	3:C:729:HOH:O	2.20	0.42
1:B:36:LEU:HD11	1:B:126:ILE:HD12	2.01	0.42
1:B:36:LEU:O	1:B:39:VAL:HG12	2.20	0.42
1:A:369:HIS:HA	1:A:391:ASN:OD1	2.20	0.42
1:A:213:SER:HA	1:A:365:THR:O	2.20	0.41
1:C:194:ARG:HH12	2:C:501:NAP:P2B	2.43	0.41
1:C:49:LYS:HG3	3:C:748:HOH:O	2.20	0.41
1:C:46:MET:HE1	1:C:150:LEU:HD11	2.02	0.41
1:B:369:HIS:HA	1:B:391:ASN:OD1	2.20	0.41
1:C:61:GLU:OE1	3:C:604:HOH:O	2.22	0.40
1:D:389:VAL:CG1	1:D:392:GLN:HG3	2.51	0.40
1:C:208:VAL:HB	2:C:501:NAP:N7N	2.35	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	448/453 (99%)	439 (98%)	8 (2%)	1 (0%)	47	46
1	B	447/453 (99%)	440 (98%)	6 (1%)	1 (0%)	47	46
1	C	446/453 (98%)	439 (98%)	6 (1%)	1 (0%)	47	46
1	D	447/453 (99%)	437 (98%)	9 (2%)	1 (0%)	47	46
All	All	1788/1812 (99%)	1755 (98%)	29 (2%)	4 (0%)	47	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	PRO
1	C	212	ASN
1	B	212	ASN
1	D	212	ASN

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	363/366 (99%)	362 (100%)	1 (0%)	92	95
1	B	362/366 (99%)	360 (99%)	2 (1%)	86	90
1	C	361/366 (99%)	360 (100%)	1 (0%)	92	95
1	D	362/366 (99%)	361 (100%)	1 (0%)	92	95
All	All	1448/1464 (99%)	1443 (100%)	5 (0%)	92	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	359	TYR
1	B	359	TYR
1	B	441	LYS
1	C	359	TYR
1	D	359	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAP	C	501	-	45,52,52	2.15	7 (15%)	56,80,80	1.62	14 (25%)
2	NAP	B	501	-	45,52,52	2.18	8 (17%)	56,80,80	1.61	13 (23%)
2	NAP	D	501	-	45,52,52	2.21	6 (13%)	56,80,80	1.65	16 (28%)
2	NAP	A	501	-	45,52,52	2.17	6 (13%)	56,80,80	1.64	16 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	C	501	-	-	9/31/67/67	0/5/5/5
2	NAP	B	501	-	-	5/31/67/67	0/5/5/5
2	NAP	D	501	-	-	7/31/67/67	0/5/5/5
2	NAP	A	501	-	-	5/31/67/67	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	NAP	P2B-O2B	11.05	1.80	1.59
2	A	501	NAP	P2B-O2B	10.92	1.79	1.59
2	B	501	NAP	P2B-O2B	10.62	1.79	1.59
2	C	501	NAP	P2B-O2B	10.55	1.79	1.59
2	A	501	NAP	PN-O5D	5.09	1.79	1.59
2	B	501	NAP	PN-O5D	5.07	1.79	1.59
2	C	501	NAP	PN-O5D	4.87	1.79	1.59
2	D	501	NAP	PN-O5D	4.87	1.79	1.59
2	D	501	NAP	C7N-N7N	2.86	1.38	1.33
2	B	501	NAP	C7N-N7N	2.82	1.38	1.33
2	C	501	NAP	C7N-N7N	2.79	1.38	1.33
2	A	501	NAP	C7N-N7N	2.78	1.38	1.33
2	D	501	NAP	C2N-N1N	2.61	1.38	1.35
2	B	501	NAP	C2A-N1A	2.54	1.38	1.33
2	C	501	NAP	C2A-N1A	2.48	1.38	1.33
2	A	501	NAP	C2A-N1A	2.42	1.38	1.33
2	A	501	NAP	C2N-N1N	2.35	1.37	1.35
2	A	501	NAP	O2B-C2B	-2.31	1.35	1.44
2	D	501	NAP	C2A-N1A	2.31	1.38	1.33
2	C	501	NAP	O2B-C2B	-2.30	1.35	1.44
2	B	501	NAP	O2B-C2B	-2.29	1.35	1.44
2	C	501	NAP	C2N-N1N	2.26	1.37	1.35
2	D	501	NAP	O2B-C2B	-2.23	1.36	1.44
2	B	501	NAP	C2D-C1D	2.21	1.57	1.53
2	C	501	NAP	C4A-N3A	2.10	1.38	1.35
2	B	501	NAP	C2N-N1N	2.01	1.37	1.35
2	B	501	NAP	C4A-N3A	2.01	1.38	1.35

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	NAP	PN-O3-PA	-5.60	113.59	132.83
2	A	501	NAP	PN-O3-PA	-5.57	113.72	132.83
2	B	501	NAP	PN-O3-PA	-5.56	113.75	132.83
2	C	501	NAP	PN-O3-PA	-5.54	113.82	132.83
2	A	501	NAP	O3X-P2B-O2X	3.14	119.62	107.64
2	C	501	NAP	O3X-P2B-O2X	3.08	119.40	107.64
2	D	501	NAP	O3X-P2B-O2X	3.04	119.27	107.64
2	B	501	NAP	O3X-P2B-O2X	3.02	119.17	107.64
2	B	501	NAP	O2B-P2B-O1X	-2.91	98.14	109.39
2	C	501	NAP	O2B-P2B-O1X	-2.86	98.36	109.39
2	B	501	NAP	PA-O5B-C5B	-2.83	105.08	121.68
2	D	501	NAP	O2B-P2B-O1X	-2.82	98.52	109.39
2	A	501	NAP	O2B-P2B-O1X	-2.81	98.54	109.39
2	B	501	NAP	O7N-C7N-C3N	2.79	122.97	119.63
2	D	501	NAP	O2A-PA-O1A	2.78	126.00	112.24
2	B	501	NAP	O2A-PA-O1A	2.78	125.97	112.24
2	A	501	NAP	PA-O5B-C5B	-2.76	105.49	121.68
2	A	501	NAP	O2A-PA-O1A	2.74	125.80	112.24
2	C	501	NAP	PA-O5B-C5B	-2.74	105.64	121.68
2	C	501	NAP	O2A-PA-O1A	2.73	125.76	112.24
2	D	501	NAP	PA-O5B-C5B	-2.72	105.71	121.68
2	C	501	NAP	O7N-C7N-C3N	2.68	122.83	119.63
2	B	501	NAP	PN-O5D-C5D	-2.66	106.06	121.68
2	A	501	NAP	O7N-C7N-C3N	2.64	122.80	119.63
2	C	501	NAP	PN-O5D-C5D	-2.64	106.22	121.68
2	D	501	NAP	O7N-C7N-C3N	2.60	122.74	119.63
2	D	501	NAP	PN-O5D-C5D	-2.58	106.56	121.68
2	A	501	NAP	PN-O5D-C5D	-2.48	107.15	121.68
2	C	501	NAP	O4B-C4B-C3B	2.43	109.93	105.11
2	D	501	NAP	O5D-PN-O1N	-2.40	99.71	109.07
2	D	501	NAP	O2N-PN-O1N	2.38	124.00	112.24
2	A	501	NAP	O5D-PN-O1N	-2.36	99.83	109.07
2	C	501	NAP	O5D-PN-O1N	-2.36	99.85	109.07
2	B	501	NAP	O5D-PN-O1N	-2.35	99.90	109.07
2	B	501	NAP	O2N-PN-O1N	2.33	123.76	112.24
2	C	501	NAP	O2N-PN-O1N	2.33	123.75	112.24
2	A	501	NAP	O2N-PN-O1N	2.32	123.73	112.24
2	D	501	NAP	C5B-C4B-C3B	-2.31	106.54	115.18
2	C	501	NAP	C5B-C4B-C3B	-2.27	106.69	115.18
2	D	501	NAP	O2N-PN-O5D	-2.26	97.24	107.75
2	C	501	NAP	O2N-PN-O5D	-2.25	97.32	107.75
2	B	501	NAP	O2N-PN-O5D	-2.23	97.41	107.75
2	A	501	NAP	O2N-PN-O5D	-2.18	97.62	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	NAP	C5B-C4B-C3B	-2.18	107.02	115.18
2	D	501	NAP	O7N-C7N-N7N	-2.17	119.49	122.58
2	A	501	NAP	C3B-C2B-C1B	-2.17	98.80	102.89
2	A	501	NAP	O7N-C7N-N7N	-2.17	119.50	122.58
2	B	501	NAP	O7N-C7N-N7N	-2.14	119.53	122.58
2	C	501	NAP	O7N-C7N-N7N	-2.14	119.54	122.58
2	D	501	NAP	O4B-C4B-C3B	2.10	109.27	105.11
2	D	501	NAP	C2A-N1A-C6A	-2.10	115.17	118.75
2	B	501	NAP	O2X-P2B-O1X	2.09	118.85	110.68
2	D	501	NAP	C3B-C2B-C1B	-2.08	98.98	102.89
2	A	501	NAP	O4B-C4B-C3B	2.07	109.21	105.11
2	A	501	NAP	C2A-N1A-C6A	-2.07	115.21	118.75
2	D	501	NAP	O2X-P2B-O1X	2.06	118.75	110.68
2	C	501	NAP	O2X-P2B-O1X	2.06	118.75	110.68
2	B	501	NAP	C5B-C4B-C3B	-2.03	107.58	115.18
2	A	501	NAP	O2X-P2B-O1X	2.03	118.61	110.68

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	NAP	C5B-O5B-PA-O1A
2	D	501	NAP	C5B-O5B-PA-O3
2	B	501	NAP	O4B-C4B-C5B-O5B
2	C	501	NAP	C3D-C4D-C5D-O5D
2	D	501	NAP	C3D-C4D-C5D-O5D
2	C	501	NAP	O4B-C4B-C5B-O5B
2	C	501	NAP	O4D-C4D-C5D-O5D
2	A	501	NAP	PA-O3-PN-O5D
2	B	501	NAP	PA-O3-PN-O5D
2	C	501	NAP	PA-O3-PN-O5D
2	D	501	NAP	PA-O3-PN-O5D
2	B	501	NAP	C2B-O2B-P2B-O1X
2	D	501	NAP	C2B-O2B-P2B-O1X
2	D	501	NAP	O4D-C4D-C5D-O5D
2	D	501	NAP	C5B-O5B-PA-O2A
2	A	501	NAP	C3D-C4D-C5D-O5D
2	C	501	NAP	C3B-C4B-C5B-O5B
2	C	501	NAP	C3B-C2B-O2B-P2B
2	C	501	NAP	C1B-C2B-O2B-P2B
2	A	501	NAP	C2B-O2B-P2B-O1X
2	B	501	NAP	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
2	C	501	NAP	C2B-O2B-P2B-O2X
2	A	501	NAP	O4D-C4D-C5D-O5D
2	C	501	NAP	PN-O3-PA-O1A
2	A	501	NAP	C5D-O5D-PN-O1N
2	B	501	NAP	C5D-O5D-PN-O1N

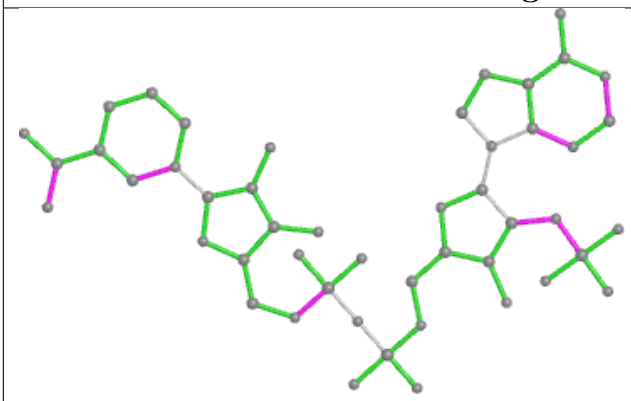
There are no ring outliers.

4 monomers are involved in 10 short contacts:

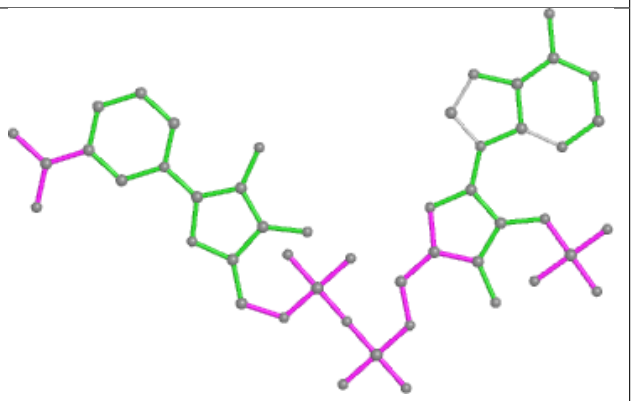
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	NAP	4	0
2	B	501	NAP	2	0
2	D	501	NAP	2	0
2	A	501	NAP	2	0

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

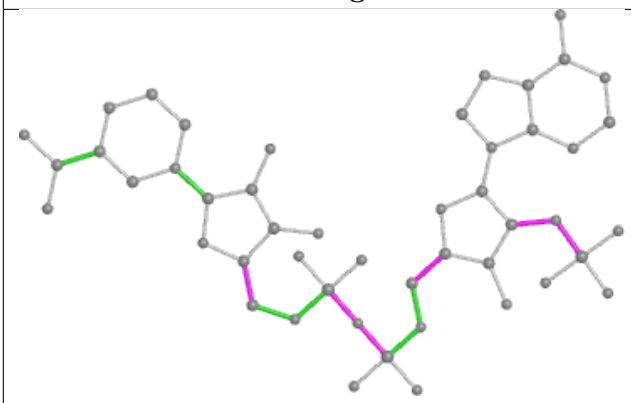
Ligand NAP C 501



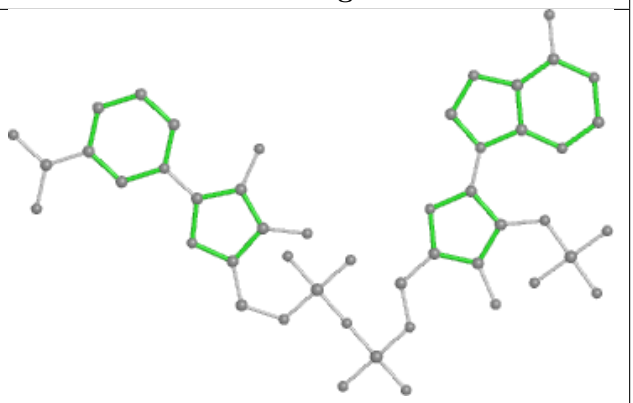
Bond lengths



Bond angles

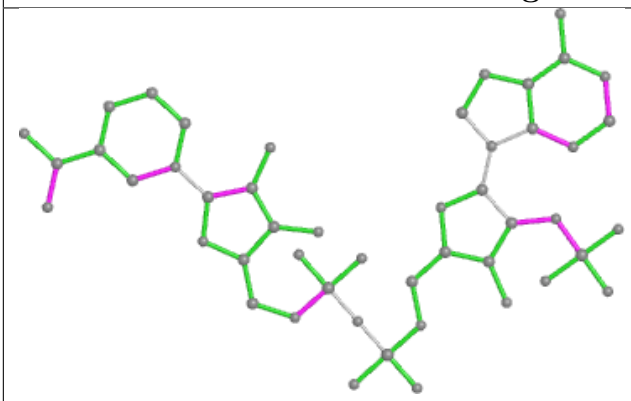


Torsions

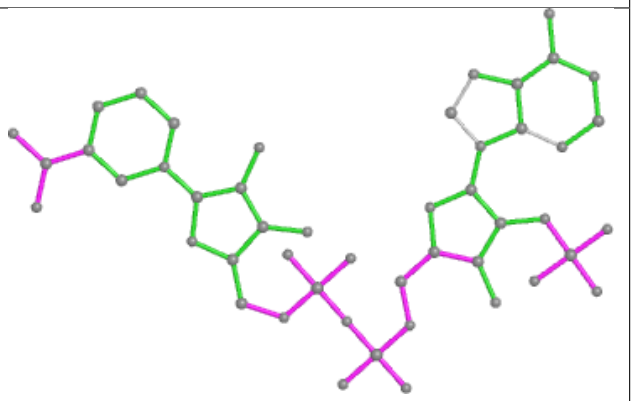


Rings

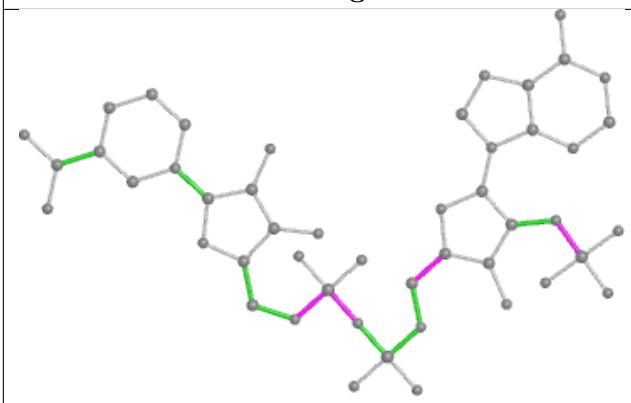
Ligand NAP B 501



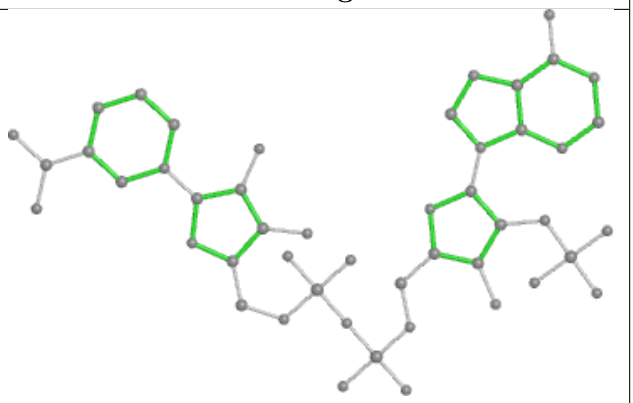
Bond lengths



Bond angles

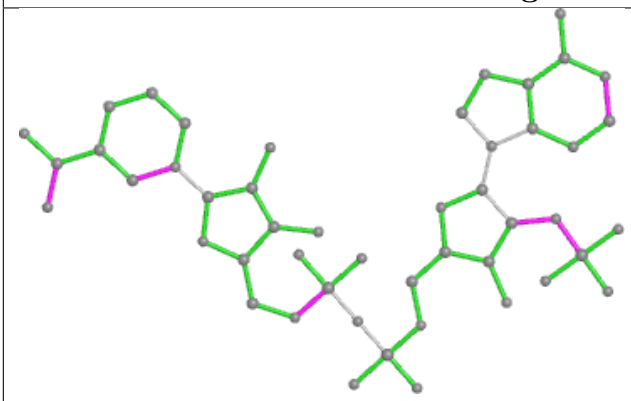


Torsions

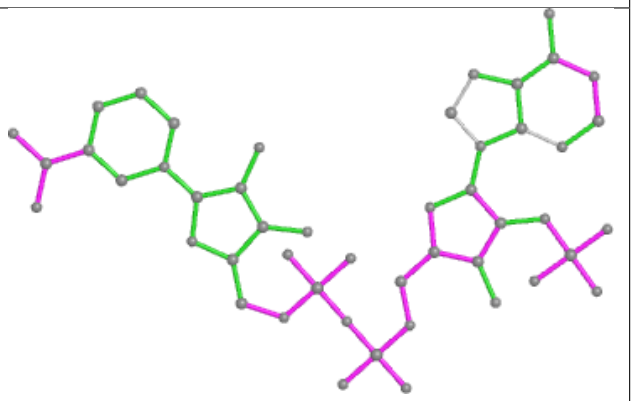


Rings

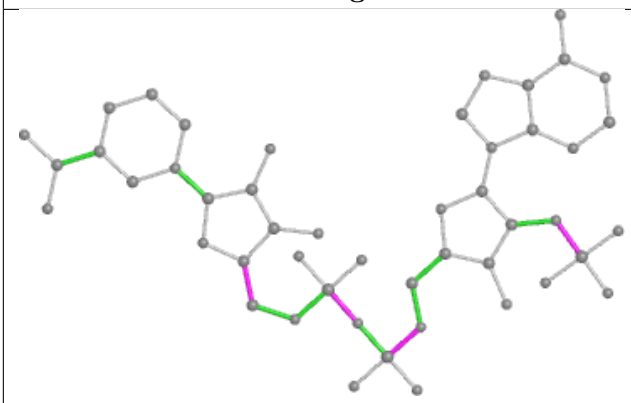
Ligand NAP D 501



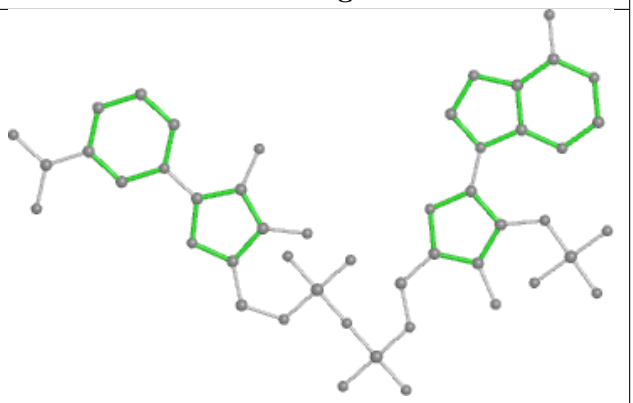
Bond lengths



Bond angles

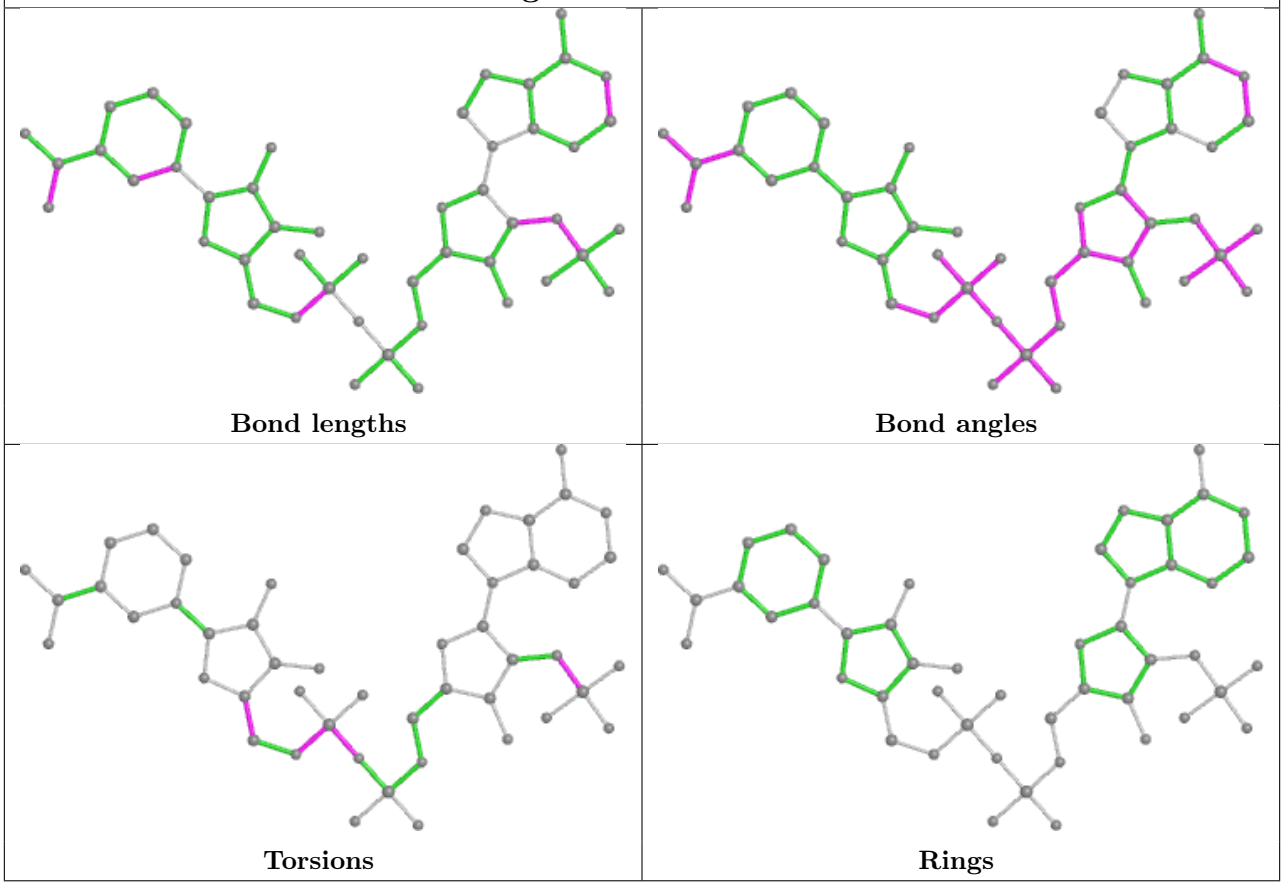


Torsions



Rings

Ligand NAP A 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	449/453 (99%)	0.23	32 (7%)	16	22	32, 43, 70, 112	0
1	B	449/453 (99%)	0.23	30 (6%)	17	24	27, 42, 72, 112	0
1	C	448/453 (98%)	0.24	23 (5%)	28	36	29, 47, 77, 124	0
1	D	449/453 (99%)	0.17	31 (6%)	16	23	27, 41, 71, 121	0
All	All	1795/1812 (99%)	0.22	116 (6%)	18	25	27, 43, 74, 124	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	445	VAL	7.1
1	B	445	VAL	6.4
1	C	174	GLU	6.3
1	C	443	ALA	5.7
1	B	171	PRO	5.7
1	D	175	ALA	5.6
1	C	445	VAL	5.5
1	D	445	VAL	5.4
1	C	175	ALA	5.3
1	B	446	PRO	5.2
1	A	194	ARG	5.2
1	B	175	ALA	5.2
1	C	444	LYS	5.2
1	C	172	SER	4.9
1	B	441	LYS	4.8
1	C	171	PRO	4.8
1	B	444	LYS	4.8
1	D	174	GLU	4.7
1	A	173	ARG	4.7
1	A	171	PRO	4.6
1	B	5	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	171	PRO	4.4
1	C	442	GLU	4.0
1	D	443	ALA	4.0
1	D	173	ARG	3.9
1	B	442	GLU	3.9
1	D	444	LYS	3.8
1	A	174	GLU	3.7
1	C	446	PRO	3.7
1	B	174	GLU	3.7
1	D	442	GLU	3.5
1	A	5	VAL	3.5
1	A	339	VAL	3.5
1	A	443	ALA	3.4
1	B	439	PHE	3.4
1	A	317	VAL	3.3
1	B	8	LYS	3.3
1	C	132	ILE	3.3
1	D	441	LYS	3.2
1	C	8	LYS	3.2
1	A	6	SER	3.2
1	D	194	ARG	3.2
1	A	338	LEU	3.2
1	C	194	ARG	3.2
1	A	215	VAL	3.2
1	C	173	ARG	3.1
1	A	444	LYS	3.1
1	A	196	LYS	3.0
1	D	122	ALA	3.0
1	A	187	ILE	3.0
1	B	443	ALA	3.0
1	C	418	ARG	2.9
1	D	286	ASP	2.9
1	D	172	SER	2.9
1	B	124	ALA	2.9
1	D	120	CYS	2.9
1	D	338	LEU	2.9
1	D	446	PRO	2.8
1	A	446	PRO	2.8
1	C	12	GLU	2.8
1	A	8	LYS	2.7
1	B	172	SER	2.7
1	A	442	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	118	PRO	2.7
1	A	125	ALA	2.7
1	C	193	GLY	2.7
1	A	248	VAL	2.7
1	B	317	VAL	2.7
1	D	132	ILE	2.7
1	B	286	ASP	2.6
1	A	318	LEU	2.6
1	B	447	SER	2.5
1	B	173	ARG	2.5
1	D	124	ALA	2.5
1	B	194	ARG	2.5
1	C	286	ASP	2.5
1	C	124	ALA	2.5
1	D	8	LYS	2.5
1	A	286	ASP	2.5
1	B	338	LEU	2.5
1	C	215	VAL	2.5
1	B	120	CYS	2.5
1	A	175	ALA	2.4
1	B	118	PRO	2.4
1	A	337	VAL	2.4
1	B	417	GLY	2.4
1	A	172	SER	2.4
1	A	441	LYS	2.4
1	C	337	VAL	2.4
1	D	187	ILE	2.4
1	B	337	VAL	2.3
1	D	247	SER	2.3
1	D	117	THR	2.3
1	A	191	GLY	2.3
1	C	338	LEU	2.2
1	D	119	MET	2.2
1	B	230	ILE	2.2
1	B	209	GLY	2.2
1	D	116	VAL	2.2
1	A	121	ASN	2.2
1	A	288[A]	LYS	2.1
1	A	124	ALA	2.1
1	D	12	GLU	2.1
1	B	119	MET	2.1
1	B	440	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	5	VAL	2.1
1	B	339	VAL	2.1
1	D	121	ASN	2.1
1	D	339	VAL	2.1
1	D	177	LYS	2.1
1	C	447	SER	2.0
1	A	119	MET	2.0
1	A	169	GLU	2.0
1	C	202	GLY	2.0
1	D	449	GLU	2.0
1	B	270	VAL	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)

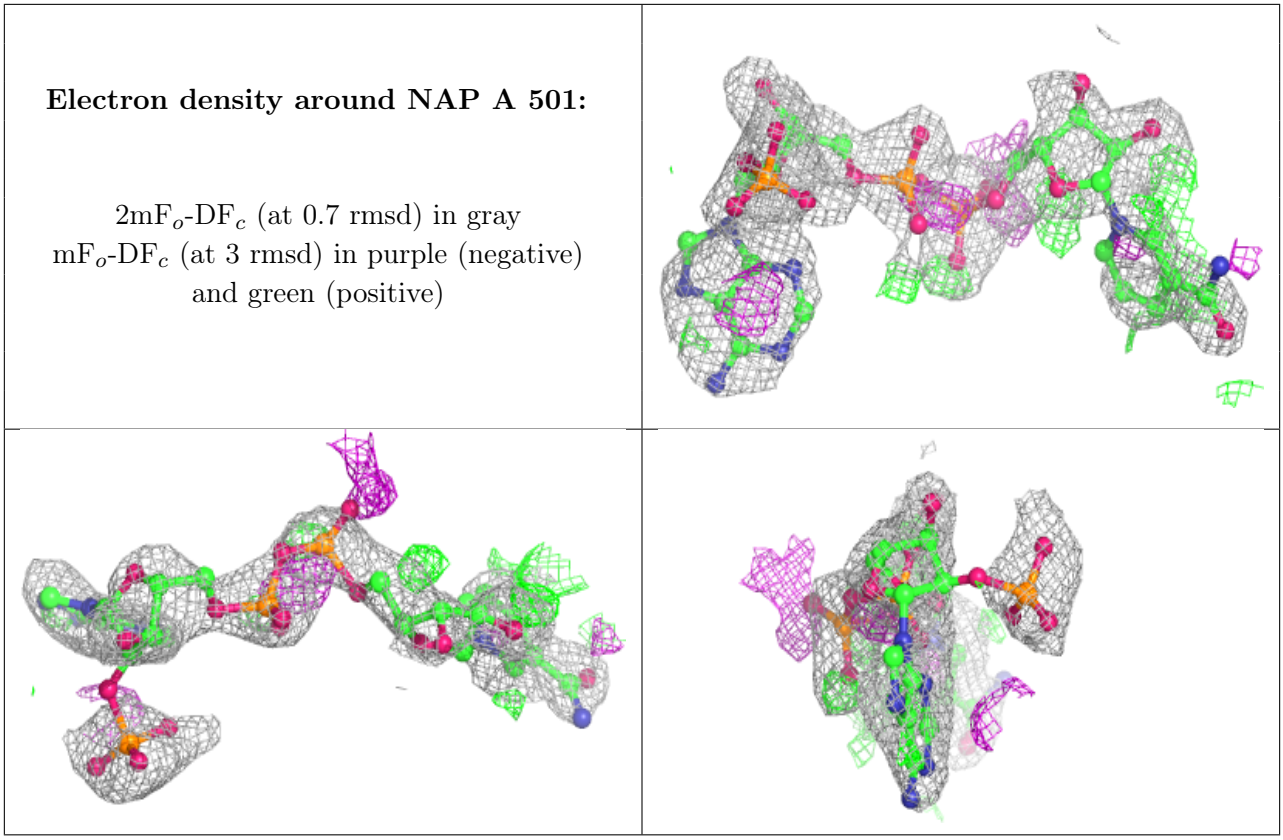
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	NAP	A	501	48/48	0.63	0.32	52,71,84,85	48
2	NAP	D	501	48/48	0.64	0.30	40,64,75,78	48
2	NAP	C	501	48/48	0.65	0.32	50,68,86,91	48
2	NAP	B	501	48/48	0.65	0.31	51,66,79,81	48

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.

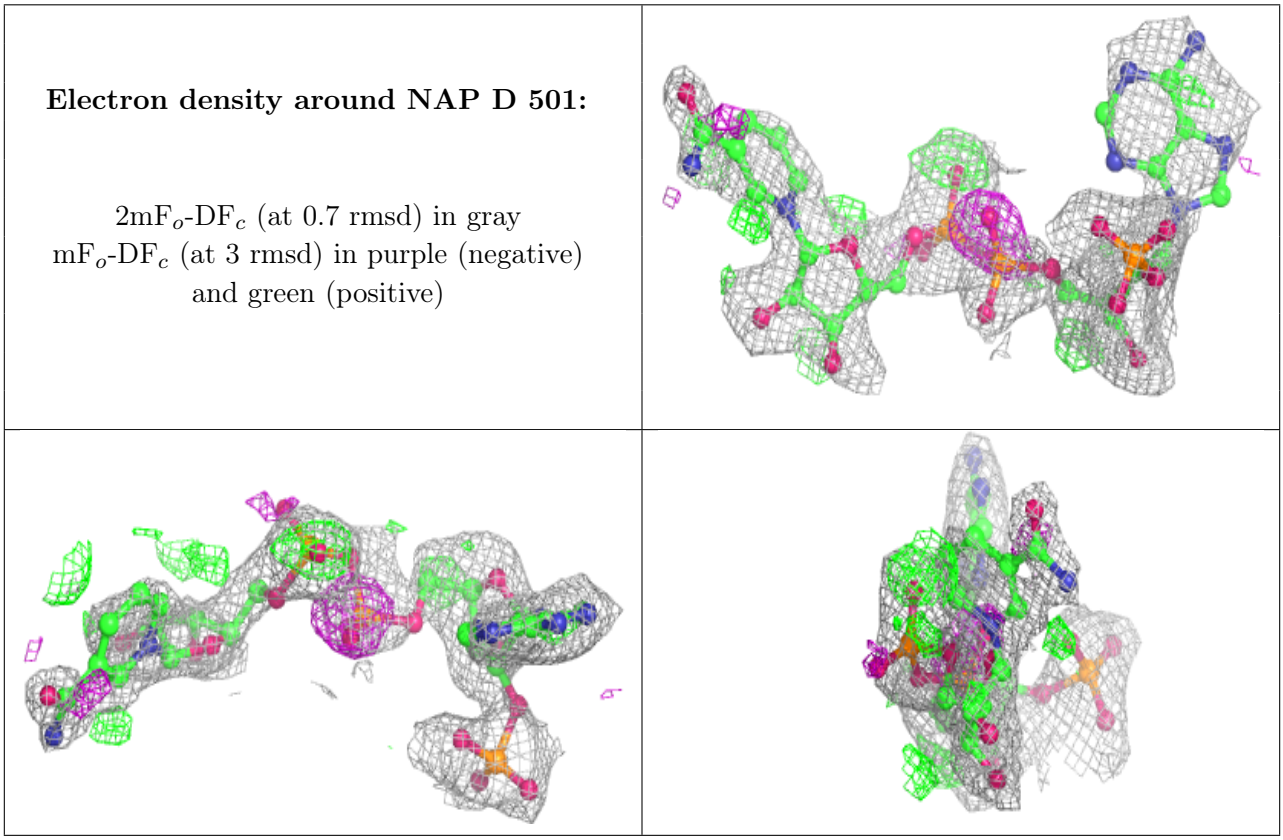
Electron density around NAP A 501:

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



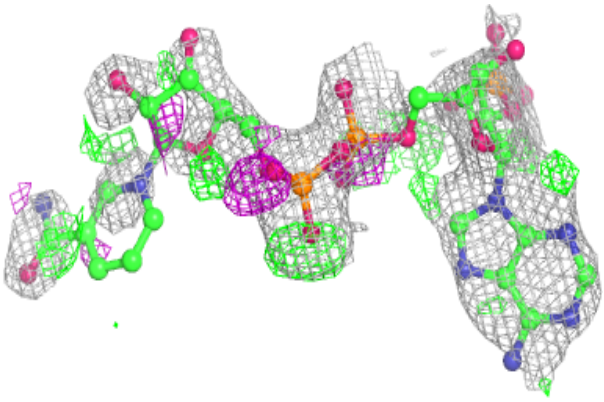
Electron density around NAP D 501:

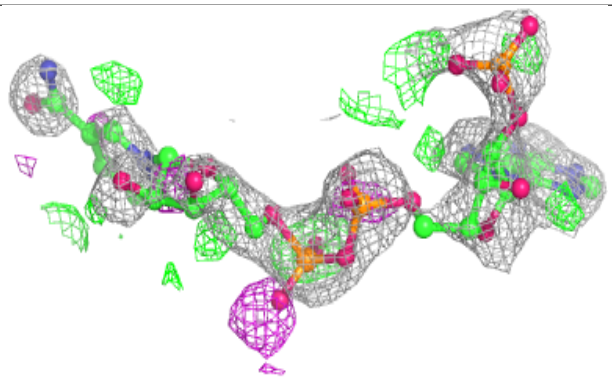
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

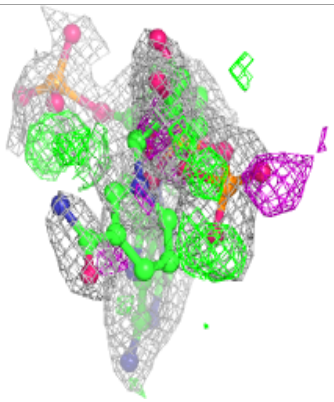


Electron density around NAP C 501:

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

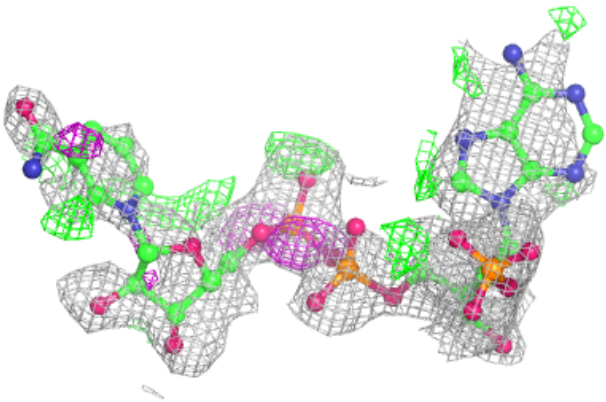


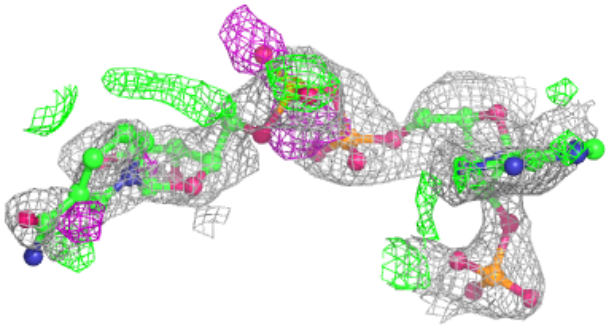


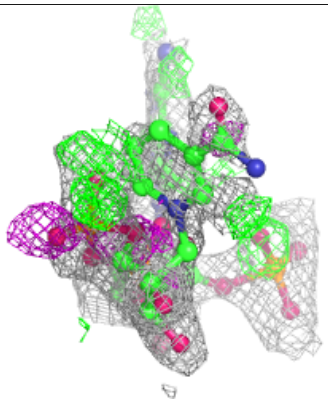


Electron density around NAP B 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.