Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2024 – 09:51 PM EST

PDB ID	:	1DQA
Title	:	COMPLEX OF THE CATALYTIC PORTION OF HUMAN HMG-COA REDUCTASE WITH HMG, COA, AND NADP+
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Deposited on	:	1999-12-30
Resolution	:	2.00 Å(reported)

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

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

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

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

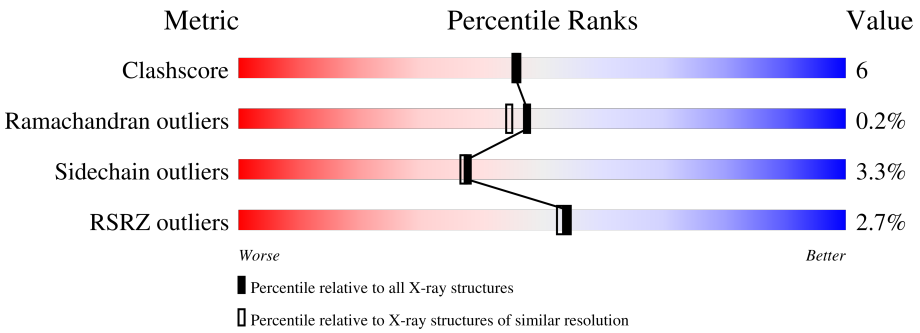
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	467	4% 73% 15% 12%
1	B	467	2% 76% 10% • 13%
1	C	467	2% 77% 8% • 13%
1	D	467	% 75% 9% • 15%

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	COA	A	101	X	-	-	-
2	COA	B	102	X	-	-	-
2	COA	C	103	X	-	-	-
2	COA	D	104	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12909 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.

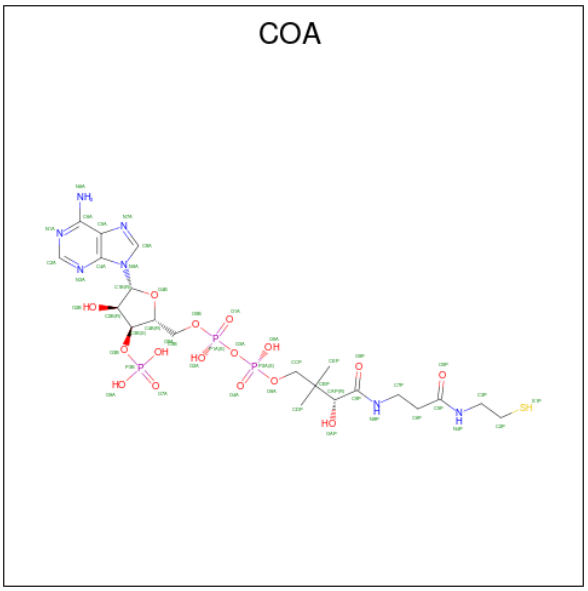
- Molecule 1 is a protein called PROTEIN (HMG-COA REDUCTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	409	3044	1897	537	580	30	0	0	0
1	B	405	3010	1876	530	575	29	0	0	0
1	C	404	3011	1876	535	570	30	0	0	0
1	D	396	2945	1832	522	561	30	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

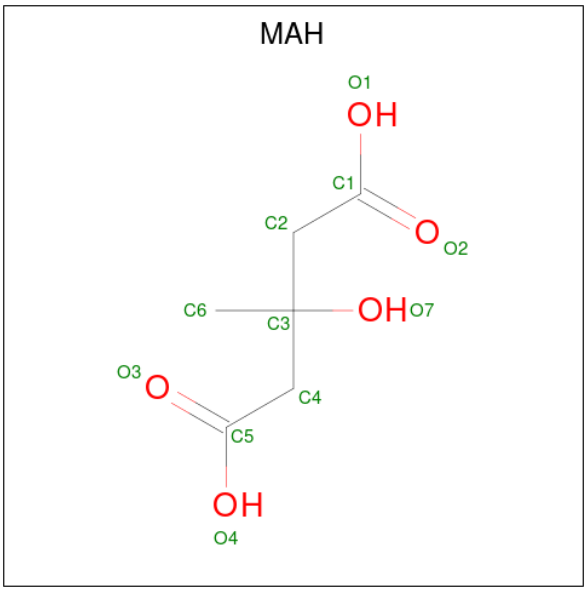
Chain	Residue	Modelled	Actual	Comment	Reference
A	485	ILE	MET	engineered mutation	UNP P04035
B	485	ILE	MET	engineered mutation	UNP P04035
C	485	ILE	MET	engineered mutation	UNP P04035
D	485	ILE	MET	engineered mutation	UNP P04035

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



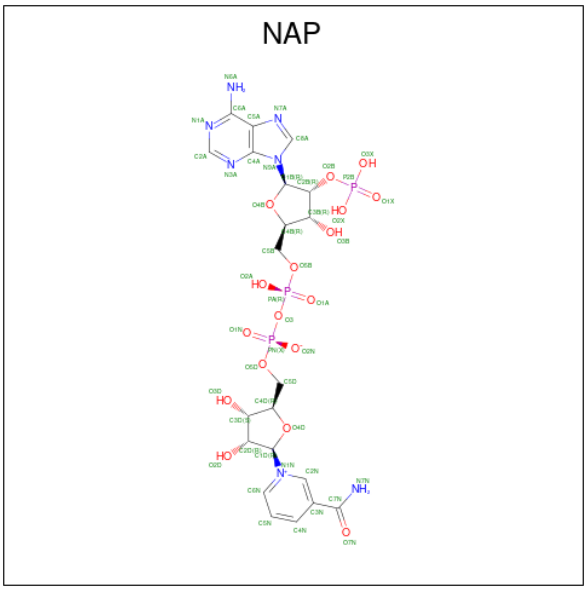
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	48	21	7	16	3	1	0	0
2	B	1	48	21	7	16	3	1	0	0
2	C	1	48	21	7	16	3	1	0	0
2	D	1	48	21	7	16	3	1	0	0

- Molecule 3 is 3-HYDROXY-3-METHYL-GLUTARIC ACID (three-letter code: MAH) (formula: $C_6H_{10}O_5$).



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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	121	121	121	0	0

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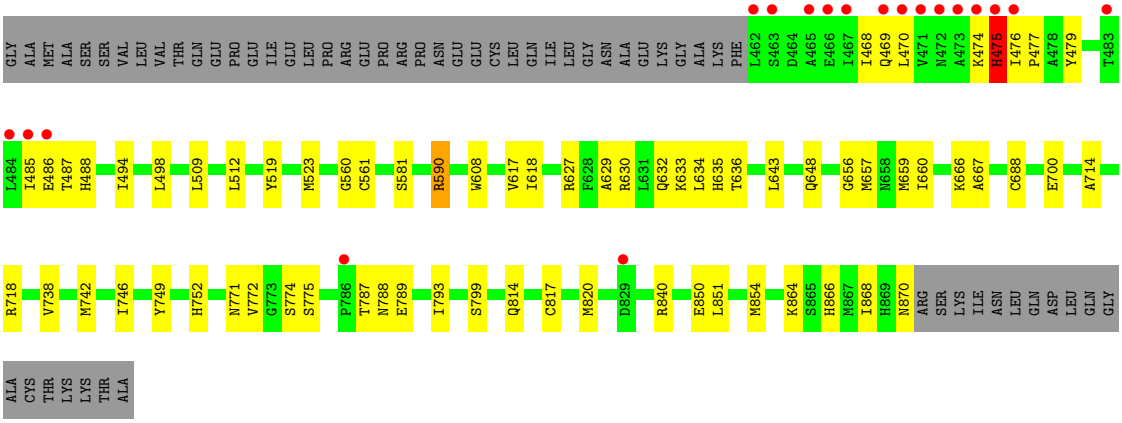
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	119	119	119	0	0
			Total	O		
5	C	106	106	106	0	0
			Total	O		
5	D	125	125	125	0	0

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.

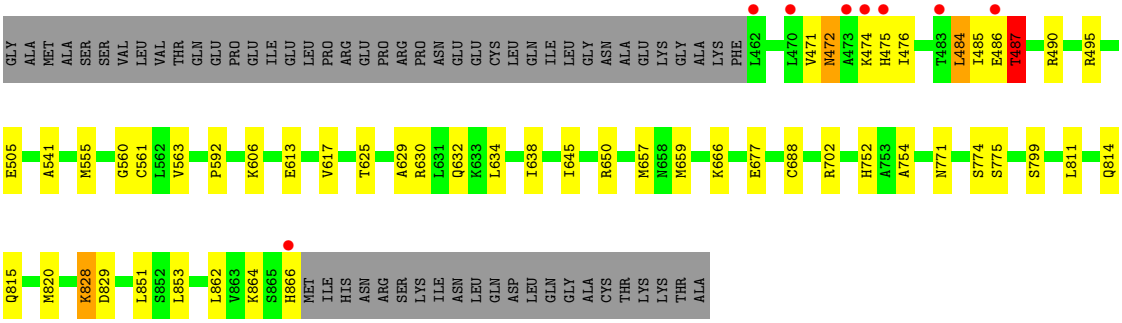
• Molecule 1: PROTEIN (HMG-COA REDUCTASE)

Chain A:



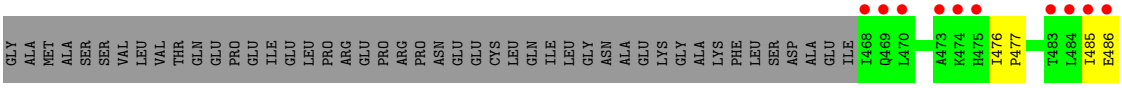
• Molecule 1: PROTEIN (HMG-COA REDUCTASE)

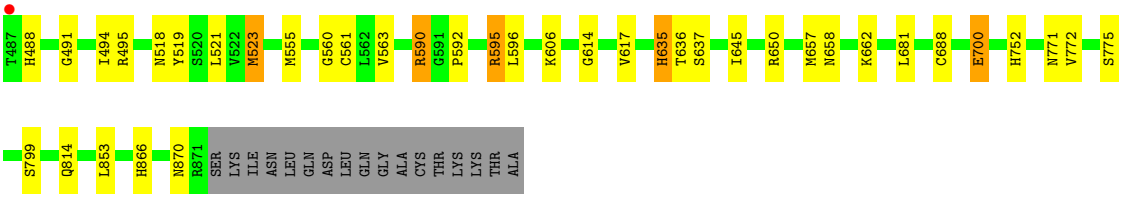
Chain B:



• Molecule 1: PROTEIN (HMG-COA REDUCTASE)

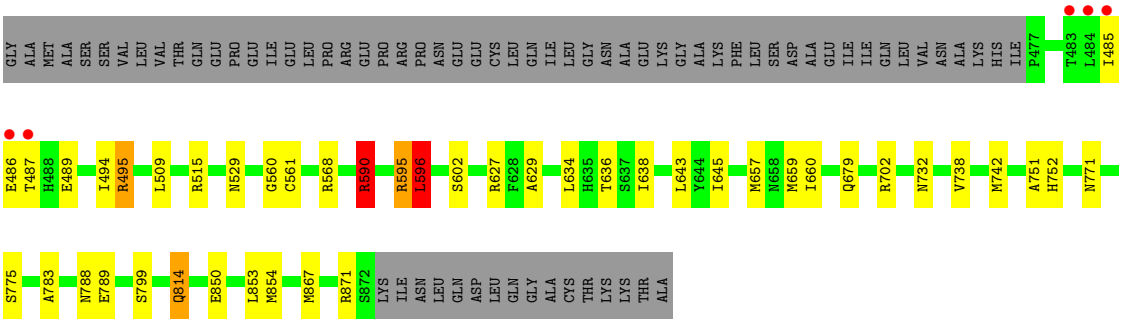
Chain C:





• Molecule 1: PROTEIN (HMG-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	73.92Å 172.63Å 73.99Å 90.00° 117.50° 90.00°	Depositor
Resolution (Å)	44.00 – 2.00 38.37 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.00-2.00) 49.9 (38.37-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	6.65 (at 2.00Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.168 , 0.197 0.166 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	17.4	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 59.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.053 for h,-k,-h-l 0.069 for -h-l,-k,l 0.046 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12909	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: COA, NAP, MAH

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	0.55	0/3089	0.72	1/4177 (0.0%)
1	B	0.54	0/3054	0.73	2/4130 (0.0%)
1	C	0.54	0/3056	0.74	4/4131 (0.1%)
1	D	0.57	0/2989	0.77	6/4039 (0.1%)
All	All	0.55	0/12188	0.74	13/16477 (0.1%)

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	A	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	590	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	B	495	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	D	568	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	C	590	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	D	495	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	D	590	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	495	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	D	596	LEU	CA-CB-CG	-6.02	101.45	115.30
1	C	495	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	D	590	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	C	596	LEU	CA-CB-CG	-5.71	102.18	115.30
1	A	475	HIS	CA-CB-CG	-5.25	104.67	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	814	GLN	CA-CB-CG	5.16	124.74	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	749	TYR	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	A	3044	0	3085	45	0
1	B	3010	0	3052	49	0
1	C	3011	0	3056	38	0
1	D	2945	0	2981	26	0
2	A	48	0	32	2	0
2	B	48	0	32	4	0
2	C	48	0	32	6	0
2	D	48	0	32	1	0
3	A	11	0	8	2	0
3	B	11	0	8	1	0
3	C	11	0	8	0	0
3	D	11	0	8	0	0
4	A	48	0	25	7	0
4	B	48	0	25	5	0
4	C	48	0	25	0	0
4	D	48	0	25	4	0
5	A	121	0	0	4	0
5	B	119	0	0	1	0
5	C	106	0	0	2	0
5	D	125	0	0	0	0
All	All	12909	0	12434	160	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 6.

All (160) 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:657:MET:HG2	4:A:1:NAP:C4N	1.93	0.99
1:B:657:MET:HG2	4:B:2:NAP:C4N	1.93	0.99
1:A:866:HIS:HE1	2:A:101:COA:HN4	1.19	0.86
1:B:625:THR:HG22	1:B:666:LYS:HD2	1.58	0.84
1:A:475:HIS:ND1	1:A:475:HIS:O	2.12	0.81
1:D:627:ARG:HD3	4:D:4:NAP:O3X	1.83	0.78
1:B:555:MET:HE3	1:B:563:VAL:HG22	1.66	0.78
1:C:650:ARG:HH11	1:C:650:ARG:HG2	1.49	0.78
1:A:657:MET:HG2	4:A:1:NAP:C3N	2.13	0.76
1:A:523:MET:HE3	1:A:523:MET:HA	1.68	0.74
1:C:866:HIS:HD2	1:C:870:ASN:HD22	1.38	0.72
1:A:789:GLU:HG2	5:A:2311:HOH:O	1.90	0.71
1:A:474:LYS:O	1:A:475:HIS:C	2.27	0.71
1:A:581:SER:OG	1:A:840:ARG:HD2	1.94	0.68
1:D:595:ARG:HD2	1:D:679:GLN:OE1	1.95	0.66
1:D:638:ILE:HG22	1:D:643:LEU:HD13	1.78	0.65
1:B:657:MET:HG2	4:B:2:NAP:C3N	2.27	0.64
1:C:866:HIS:HE1	2:C:103:COA:H31	1.61	0.64
1:C:866:HIS:CE1	2:C:103:COA:H31	2.32	0.64
1:A:468:ILE:HG12	1:A:498:LEU:HD11	1.80	0.63
1:B:561:CYS:SG	1:B:866:HIS:HB3	2.38	0.63
1:A:636:THR:CG2	1:A:643:LEU:HD11	2.28	0.63
1:D:487:THR:HG22	1:D:489:GLU:H	1.63	0.62
1:C:650:ARG:HG2	1:C:650:ARG:NH1	2.14	0.62
1:B:632:GLN:HE21	1:B:650:ARG:N	1.99	0.61
1:A:475:HIS:O	1:A:475:HIS:CG	2.54	0.60
1:B:629:ALA:O	1:B:630:ARG:HD3	2.02	0.60
1:A:866:HIS:CE1	2:A:101:COA:HN4	2.10	0.60
1:B:629:ALA:HB2	1:B:659:MET:HG2	1.83	0.59
1:C:518:ASN:ND2	1:C:521:LEU:HD13	2.17	0.59
1:C:560:GLY:O	1:C:561:CYS:HB2	2.03	0.58
1:B:472:ASN:C	1:B:474:LYS:H	2.05	0.58
1:C:523:MET:HE1	5:C:2103:HOH:O	2.03	0.58
1:C:606:LYS:HG3	1:C:636:THR:OG1	2.04	0.58
1:C:555:MET:HE3	1:C:563:VAL:HG22	1.83	0.58
1:D:853:LEU:HD13	2:D:104:COA:H32	1.85	0.58
1:C:662:LYS:HD2	1:D:867:MET:SD	2.45	0.57
1:B:771:ASN:OD1	1:B:775:SER:OG	2.23	0.57
1:C:870:ASN:HD21	4:D:4:NAP:H1D	1.68	0.57
1:A:636:THR:HG22	1:A:643:LEU:HD11	1.87	0.56
1:D:560:GLY:O	1:D:561:CYS:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:TYR:O	1:A:523:MET:HG2	2.07	0.55
1:A:477:PRO:HB3	1:A:479:TYR:CE2	2.41	0.55
1:A:633:LYS:HE2	1:A:648:GLN:OE1	2.07	0.55
1:C:555:MET:CE	1:C:563:VAL:HA	2.36	0.55
1:B:866:HIS:NE2	2:B:102:COA:H31	2.22	0.54
1:B:629:ALA:HB2	1:B:659:MET:SD	2.48	0.54
1:C:771:ASN:OD1	1:C:775:SER:OG	2.26	0.53
1:A:817:CYS:HA	1:A:820:MET:HE3	1.91	0.53
1:D:485:ILE:HG22	1:D:486:GLU:N	2.23	0.53
1:D:629:ALA:HB2	1:D:659:MET:HG2	1.90	0.53
4:A:1:NAP:H71N	1:B:866:HIS:CD2	2.27	0.53
1:C:866:HIS:HD2	1:C:870:ASN:ND2	2.03	0.53
1:A:494:ILE:O	1:A:498:LEU:HD13	2.09	0.53
1:A:560:GLY:O	1:A:561:CYS:HB2	2.09	0.52
1:C:853:LEU:HD13	2:C:103:COA:H32	1.91	0.52
1:C:799:SER:HB2	5:C:2219:HOH:O	2.10	0.52
1:A:590:ARG:NH2	4:A:1:NAP:O7N	2.43	0.52
1:A:627:ARG:HD3	4:A:1:NAP:O3X	2.09	0.52
1:C:595:ARG:HD2	1:C:681:LEU:HG	1.91	0.52
1:D:485:ILE:HG22	1:D:486:GLU:H	1.76	0.51
1:C:866:HIS:HE1	2:C:103:COA:C3P	2.22	0.51
1:D:771:ASN:OD1	1:D:775:SER:OG	2.28	0.51
1:A:474:LYS:O	1:A:476:ILE:N	2.44	0.51
1:A:468:ILE:HG12	1:A:498:LEU:CD1	2.40	0.51
1:C:555:MET:HE3	1:C:563:VAL:HA	1.93	0.51
1:A:629:ALA:HB2	1:A:659:MET:HG2	1.93	0.50
1:B:487:THR:HG23	1:B:490:ARG:HB3	1.93	0.50
1:D:590:ARG:HB2	1:D:660:ILE:HG22	1.93	0.50
1:A:629:ALA:O	1:A:630:ARG:HD2	2.11	0.50
1:B:629:ALA:HB2	1:B:659:MET:CG	2.41	0.50
3:A:201:MAH:C1	4:B:2:NAP:C4N	2.89	0.50
1:A:738:VAL:O	1:A:742:MET:HG2	2.12	0.49
1:B:862:LEU:HD12	1:B:866:HIS:CE1	2.47	0.49
1:A:488:HIS:CD2	1:A:523:MET:HG3	2.46	0.49
1:A:632:GLN:HG3	5:A:2297:HOH:O	2.11	0.49
1:D:485:ILE:HD13	1:D:494:ILE:HD12	1.95	0.49
1:D:590:ARG:NH2	4:D:4:NAP:O7N	2.45	0.49
4:A:1:NAP:N7N	1:B:866:HIS:CD2	2.81	0.49
1:B:476:ILE:HD13	1:B:484:LEU:HD21	1.93	0.49
1:B:560:GLY:O	1:B:561:CYS:HB2	2.13	0.49
1:C:485:ILE:HD11	1:C:494:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:658:ASN:O	1:C:662:LYS:HG3	2.13	0.48
1:A:635:HIS:CD2	1:A:700:GLU:OE2	2.67	0.48
1:B:862:LEU:HD12	1:B:866:HIS:HE1	1.79	0.48
1:B:475:HIS:C	1:B:476:ILE:HG13	2.33	0.48
1:B:561:CYS:HB2	1:B:866:HIS:HB3	1.94	0.48
1:C:662:LYS:NZ	1:C:662:LYS:HB3	2.29	0.48
1:C:772:VAL:HG23	1:D:771:ASN:ND2	2.28	0.47
2:B:102:COA:O9P	2:B:102:COA:H62	2.14	0.47
1:A:485:ILE:HG22	1:A:486:GLU:N	2.29	0.47
1:C:485:ILE:HG22	1:C:486:GLU:N	2.29	0.47
1:D:495:ARG:HD2	1:D:529:ASN:OD1	2.14	0.47
1:B:541:ALA:HB2	1:B:555:MET:HE1	1.96	0.47
1:C:866:HIS:CD2	1:C:870:ASN:HD22	2.26	0.47
1:C:614:GLY:O	1:C:617:VAL:HG22	2.15	0.47
1:C:555:MET:CE	1:C:563:VAL:HG22	2.44	0.47
1:B:853:LEU:HD13	2:B:102:COA:H32	1.97	0.47
1:B:592:PRO:HD2	1:B:645:ILE:O	2.15	0.46
1:B:799:SER:HB2	5:B:2458:HOH:O	2.16	0.46
1:D:487:THR:HG22	1:D:489:GLU:N	2.31	0.46
1:A:608:TRP:CH2	1:A:617:VAL:HG21	2.51	0.46
1:A:771:ASN:OD1	1:A:775:SER:OG	2.34	0.46
1:C:635:HIS:HD2	1:C:700:GLU:OE2	1.98	0.46
1:A:774:SER:HA	1:A:799:SER:O	2.16	0.46
1:A:793:ILE:HD13	1:A:851:LEU:HG	1.98	0.46
1:B:606:LYS:HD2	1:B:638:ILE:HD12	1.98	0.46
1:C:485:ILE:HD12	1:C:491:GLY:HA2	1.98	0.46
1:B:862:LEU:CD1	1:B:866:HIS:CE1	2.99	0.45
1:A:866:HIS:HD2	1:A:870:ASN:OD1	1.99	0.45
1:B:541:ALA:HB2	1:B:555:MET:CE	2.47	0.45
1:D:636:THR:HG22	1:D:645:ILE:HG23	1.97	0.45
1:C:662:LYS:HB3	1:C:662:LYS:HZ2	1.82	0.45
1:B:485:ILE:HG21	1:B:490:ARG:HD3	1.99	0.45
1:B:828:LYS:H	1:B:828:LYS:HG3	1.56	0.45
2:C:103:COA:H62	2:C:103:COA:O9P	2.17	0.45
1:D:850:GLU:O	1:D:854:MET:HG2	2.17	0.45
1:B:811:LEU:O	1:B:815:GLN:HG3	2.18	0.44
1:C:590:ARG:HA	1:C:590:ARG:HD3	1.59	0.44
1:B:754:ALA:HA	1:B:775:SER:OG	2.18	0.44
1:A:656:GLY:O	1:A:660:ILE:HG12	2.18	0.44
1:B:677:GLU:H	1:B:677:GLU:CD	2.22	0.43
1:B:657:MET:HG2	4:B:2:NAP:C5N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:738:VAL:O	1:D:742:MET:HG2	2.17	0.43
1:B:828:LYS:HD2	1:B:829:ASP:H	1.83	0.43
1:A:850:GLU:O	1:A:854:MET:HG2	2.19	0.43
1:A:746:ILE:HD13	5:A:2455:HOH:O	2.18	0.43
1:A:714:ALA:O	1:A:718:ARG:HG3	2.18	0.43
1:A:590:ARG:HD3	1:A:590:ARG:HA	1.54	0.43
4:A:1:NAP:C4N	3:B:202:MAH:C1	2.96	0.43
1:C:870:ASN:HD21	4:D:4:NAP:C1D	2.31	0.43
1:B:474:LYS:HD3	1:B:474:LYS:HA	1.86	0.43
1:D:590:ARG:HD3	1:D:590:ARG:HA	1.57	0.43
1:D:596:LEU:HD13	1:D:602:SER:HA	2.00	0.43
1:B:828:LYS:HD2	1:B:829:ASP:OD1	2.18	0.42
1:B:613:GLU:H	1:B:613:GLU:CD	2.22	0.42
1:A:772:VAL:HG23	1:B:771:ASN:ND2	2.35	0.42
3:A:201:MAH:O2	4:B:2:NAP:C4N	2.67	0.42
1:C:590:ARG:HD3	1:C:688:CYS:SG	2.59	0.42
1:B:866:HIS:ND1	1:B:866:HIS:N	2.65	0.42
1:B:471:VAL:HG22	1:B:476:ILE:HB	2.01	0.42
1:D:751:ALA:HB1	1:D:853:LEU:HD23	2.01	0.42
1:B:702:ARG:O	1:B:799:SER:HA	2.19	0.42
1:C:866:HIS:HE1	2:C:103:COA:N4P	2.17	0.42
1:D:702:ARG:O	1:D:799:SER:HA	2.19	0.42
1:B:484:LEU:HD12	1:B:484:LEU:HA	1.93	0.41
1:A:864:LYS:HG2	5:A:2089:HOH:O	2.21	0.41
1:A:629:ALA:C	1:A:630:ARG:HD2	2.41	0.41
1:D:732:ASN:HA	1:D:854:MET:HE1	2.03	0.41
1:C:476:ILE:HA	1:C:477:PRO:HD3	1.85	0.41
1:C:592:PRO:HD2	1:C:645:ILE:O	2.20	0.41
1:A:618:ILE:HG23	1:A:667:ALA:HB1	2.03	0.41
1:C:488:HIS:HB3	1:C:519:TYR:HB2	2.03	0.41
1:B:866:HIS:HE2	2:B:102:COA:H31	1.85	0.40
1:B:774:SER:HA	1:B:799:SER:O	2.22	0.40
1:D:783:ALA:HB1	1:D:788:ASN:HB3	2.03	0.40
1:A:470:LEU:O	1:A:470:LEU:HD13	2.22	0.40
1:B:561:CYS:CB	1:B:866:HIS:HB3	2.51	0.40
1:B:613:GLU:O	1:B:617:VAL:HG23	2.22	0.40
1:B:820:MET:HE2	1:B:820:MET:HB2	1.94	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	407/467 (87%)	391 (96%)	15 (4%)	1 (0%)	47	44
1	B	403/467 (86%)	381 (94%)	19 (5%)	3 (1%)	22	16
1	C	402/467 (86%)	388 (96%)	14 (4%)	0	100	100
1	D	394/467 (84%)	378 (96%)	16 (4%)	0	100	100
All	All	1606/1868 (86%)	1538 (96%)	64 (4%)	4 (0%)	47	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	475	HIS
1	B	484	LEU
1	B	864	LYS
1	B	487	THR

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	327/375 (87%)	314 (96%)	13 (4%)	31	29
1	B	323/375 (86%)	313 (97%)	10 (3%)	40	40
1	C	323/375 (86%)	315 (98%)	8 (2%)	47	49
1	D	316/375 (84%)	305 (96%)	11 (4%)	36	35
All	All	1289/1500 (86%)	1247 (97%)	42 (3%)	38	37

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	469	GLN
1	A	487	THR
1	A	509	LEU
1	A	512	LEU
1	A	590	ARG
1	A	634	LEU
1	A	666	LYS
1	A	688	CYS
1	A	752	HIS
1	A	787	THR
1	A	788	ASN
1	A	814	GLN
1	A	868	ILE
1	B	472	ASN
1	B	486	GLU
1	B	487	THR
1	B	505	GLU
1	B	634	LEU
1	B	688	CYS
1	B	752	HIS
1	B	814	GLN
1	B	828	LYS
1	B	851	LEU
1	C	523	MET
1	C	595	ARG
1	C	635	HIS
1	C	637	SER
1	C	657	MET
1	C	700	GLU
1	C	752	HIS
1	C	814	GLN
1	D	509	LEU
1	D	515	ARG
1	D	590	ARG
1	D	595	ARG
1	D	596	LEU
1	D	634	LEU
1	D	657	MET
1	D	752	HIS
1	D	789	GLU
1	D	814	GLN
1	D	871	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	488	HIS
1	A	635	HIS
1	A	788	ASN
1	A	866	HIS
1	B	469	GLN
1	B	472	ASN
1	B	475	HIS
1	B	632	GLN
1	B	819	GLN
1	C	472	ASN
1	C	635	HIS
1	C	861	HIS
1	C	866	HIS
1	C	870	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)

12 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	COA	B	102	-	41,50,50	1.79	7 (17%)	52,75,75	1.26	7 (13%)
3	MAH	B	202	-	10,10,10	1.48	2 (20%)	9,14,14	0.98	0
3	MAH	C	204	-	10,10,10	1.29	1 (10%)	9,14,14	1.05	0
2	COA	D	104	-	41,50,50	1.80	5 (12%)	52,75,75	1.42	7 (13%)
4	NAP	C	3	-	45,52,52	1.73	3 (6%)	56,80,80	1.47	7 (12%)
4	NAP	B	2	-	45,52,52	1.75	6 (13%)	56,80,80	1.53	9 (16%)
2	COA	C	103	-	41,50,50	1.83	6 (14%)	52,75,75	1.25	9 (17%)
2	COA	A	101	-	41,50,50	1.69	6 (14%)	52,75,75	1.21	7 (13%)
3	MAH	D	203	-	10,10,10	1.30	1 (10%)	9,14,14	1.02	0
4	NAP	D	4	-	45,52,52	1.83	5 (11%)	56,80,80	1.52	7 (12%)
3	MAH	A	201	-	10,10,10	1.66	1 (10%)	9,14,14	1.10	0
4	NAP	A	1	-	45,52,52	1.79	7 (15%)	56,80,80	1.54	7 (12%)

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	COA	B	102	-	1/1/11/13	7/44/64/64	0/3/3/3
3	MAH	B	202	-	-	0/10/10/10	-
3	MAH	C	204	-	-	0/10/10/10	-
2	COA	D	104	-	1/1/11/13	9/44/64/64	0/3/3/3
4	NAP	C	3	-	-	11/31/67/67	0/5/5/5
4	NAP	B	2	-	-	9/31/67/67	0/5/5/5
2	COA	C	103	-	1/1/11/13	6/44/64/64	0/3/3/3
2	COA	A	101	-	1/1/11/13	1/44/64/64	0/3/3/3
3	MAH	D	203	-	-	0/10/10/10	-
4	NAP	D	4	-	-	12/31/67/67	0/5/5/5
3	MAH	A	201	-	-	0/10/10/10	-
4	NAP	A	1	-	-	8/31/67/67	0/5/5/5

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4	NAP	C4A-N3A	9.44	1.48	1.35
4	C	3	NAP	C4A-N3A	8.77	1.47	1.35
4	A	1	NAP	C4A-N3A	8.59	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2	NAP	C4A-N3A	8.43	1.47	1.35
2	C	103	COA	C4A-N3A	8.20	1.47	1.35
2	D	104	COA	C4A-N3A	8.05	1.46	1.35
2	B	102	COA	C4A-N3A	7.97	1.46	1.35
2	A	101	COA	C4A-N3A	7.88	1.46	1.35
2	D	104	COA	P3B-O7A	3.79	1.62	1.50
3	A	201	MAH	C6-C3	3.63	1.56	1.52
4	B	2	NAP	P2B-O1X	3.36	1.61	1.50
4	C	3	NAP	P2B-O1X	3.27	1.61	1.50
2	B	102	COA	P3B-O7A	3.25	1.61	1.50
2	C	103	COA	P3B-O7A	3.20	1.60	1.50
4	A	1	NAP	PA-O1A	3.09	1.61	1.50
2	C	103	COA	P2A-O4A	3.09	1.61	1.50
2	B	102	COA	P2A-O4A	3.05	1.61	1.50
3	B	202	MAH	C6-C3	3.03	1.56	1.52
2	C	103	COA	P1A-O1A	2.96	1.61	1.50
4	A	1	NAP	P2B-O1X	2.94	1.60	1.50
2	A	101	COA	P3B-O7A	2.90	1.59	1.50
4	D	4	NAP	P2B-O1X	2.85	1.59	1.50
2	D	104	COA	P1A-O1A	2.84	1.61	1.50
4	B	2	NAP	C4N-C3N	2.78	1.44	1.39
2	B	102	COA	P1A-O1A	2.75	1.60	1.50
4	B	2	NAP	PA-O1A	2.67	1.60	1.50
4	D	4	NAP	C4N-C3N	2.64	1.43	1.39
4	A	1	NAP	O4B-C1B	2.50	1.44	1.41
2	A	101	COA	P2A-O4A	2.48	1.59	1.50
2	A	101	COA	P1A-O1A	2.41	1.59	1.50
2	D	104	COA	P2A-O4A	2.41	1.59	1.50
2	B	102	COA	P3B-O3B	2.40	1.63	1.59
3	C	204	MAH	C6-C3	2.39	1.55	1.52
4	D	4	NAP	PA-O1A	2.35	1.59	1.50
4	A	1	NAP	C4N-C3N	2.33	1.43	1.39
2	C	103	COA	C5A-C4A	2.29	1.47	1.40
2	D	104	COA	C5A-C4A	2.23	1.46	1.40
4	B	2	NAP	PN-O1N	2.23	1.58	1.50
4	D	4	NAP	O4B-C1B	2.22	1.44	1.41
3	B	202	MAH	O1-C1	-2.17	1.23	1.30
4	B	2	NAP	O4B-C1B	2.17	1.44	1.41
2	C	103	COA	P3B-O3B	2.16	1.63	1.59
2	A	101	COA	CDP-CBP	2.16	1.58	1.53
4	A	1	NAP	PN-O1N	2.15	1.58	1.50
3	D	203	MAH	C6-C3	2.15	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	COA	C5A-C4A	2.13	1.46	1.40
2	B	102	COA	C5A-C4A	2.11	1.46	1.40
4	C	3	NAP	C2N-N1N	-2.05	1.32	1.35
4	A	1	NAP	C2N-N1N	-2.01	1.32	1.35
2	B	102	COA	P3B-O9A	2.01	1.62	1.54

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2	NAP	O7N-C7N-N7N	-6.12	113.89	122.58
4	D	4	NAP	O7N-C7N-N7N	-6.11	113.89	122.58
4	A	1	NAP	O7N-C7N-N7N	-6.10	113.91	122.58
4	C	3	NAP	O7N-C7N-N7N	-5.94	114.14	122.58
2	D	104	COA	O5P-C5P-C6P	-4.16	114.40	122.02
4	A	1	NAP	O7N-C7N-C3N	4.05	124.48	119.63
4	D	4	NAP	O7N-C7N-C3N	4.01	124.43	119.63
4	C	3	NAP	O7N-C7N-C3N	3.95	124.36	119.63
4	B	2	NAP	O7N-C7N-C3N	3.92	124.33	119.63
4	A	1	NAP	PN-O3-PA	-3.68	120.20	132.83
4	D	4	NAP	C3N-C2N-N1N	3.64	123.99	120.43
2	C	103	COA	O5P-C5P-C6P	-3.61	115.41	122.02
4	A	1	NAP	C3N-C2N-N1N	3.52	123.86	120.43
2	D	104	COA	C6P-C7P-N8P	-3.44	104.95	111.90
4	B	2	NAP	C5A-C6A-N6A	3.43	125.57	120.35
4	B	2	NAP	C3N-C7N-N7N	3.36	121.78	117.75
2	C	103	COA	C6P-C7P-N8P	-3.35	105.13	111.90
4	C	3	NAP	C3N-C2N-N1N	3.34	123.69	120.43
4	D	4	NAP	C3N-C7N-N7N	3.26	121.66	117.75
4	A	1	NAP	C5A-C6A-N6A	3.25	125.29	120.35
4	D	4	NAP	O4D-C1D-C2D	-3.22	102.22	106.93
4	B	2	NAP	PN-O3-PA	-3.21	121.80	132.83
4	A	1	NAP	C3N-C7N-N7N	3.20	121.60	117.75
4	C	3	NAP	C3N-C7N-N7N	3.12	121.50	117.75
2	B	102	COA	O5P-C5P-C6P	-3.04	116.45	122.02
4	C	3	NAP	PN-O3-PA	-3.03	122.43	132.83
4	D	4	NAP	PN-O3-PA	-2.98	122.59	132.83
2	D	104	COA	C6P-C5P-N4P	2.95	121.38	116.42
2	A	101	COA	C7P-N8P-C9P	-2.94	117.34	122.59
4	B	2	NAP	C3N-C2N-N1N	2.85	123.21	120.43
4	C	3	NAP	C5A-C6A-N6A	2.82	124.63	120.35
2	B	102	COA	C6P-C7P-N8P	-2.74	106.37	111.90
2	D	104	COA	C3B-C2B-C1B	2.67	105.80	99.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	101	COA	C7P-C6P-C5P	-2.65	107.94	112.36
2	A	101	COA	O5P-C5P-C6P	-2.57	117.32	122.02
2	B	102	COA	C3B-C2B-C1B	2.54	105.51	99.89
2	C	103	COA	C4A-C5A-N7A	2.53	112.03	109.40
2	C	103	COA	C3B-C2B-C1B	2.50	105.42	99.89
2	D	104	COA	C7P-C6P-C5P	2.49	116.50	112.36
4	D	4	NAP	C5A-C6A-N6A	2.49	124.13	120.35
2	B	102	COA	C4A-C5A-N7A	2.48	111.98	109.40
4	B	2	NAP	O4D-C1D-C2D	-2.43	103.38	106.93
2	D	104	COA	C7P-N8P-C9P	-2.40	118.32	122.59
2	A	101	COA	CEP-CBP-CAP	2.35	112.90	108.82
2	B	102	COA	O3B-C3B-C4B	2.34	118.54	110.08
4	C	3	NAP	O4D-C1D-C2D	-2.33	103.52	106.93
2	B	102	COA	C7P-C6P-C5P	2.32	116.22	112.36
2	A	101	COA	C4A-C5A-N7A	2.31	111.81	109.40
2	A	101	COA	C3B-C2B-C1B	2.29	104.96	99.89
4	B	2	NAP	N6A-C6A-N1A	-2.24	113.92	118.57
2	A	101	COA	C3P-N4P-C5P	-2.24	118.67	122.84
4	A	1	NAP	N6A-C6A-N1A	-2.21	113.99	118.57
2	D	104	COA	O3B-C3B-C4B	2.19	118.01	110.08
2	C	103	COA	CDP-CBP-CAP	2.16	112.57	108.82
2	C	103	COA	CEP-CBP-CAP	2.15	112.55	108.82
2	B	102	COA	CDP-CBP-CAP	2.13	112.52	108.82
2	C	103	COA	C7P-N8P-C9P	-2.05	118.94	122.59
2	C	103	COA	C6P-C5P-N4P	2.04	119.86	116.42
2	C	103	COA	C7P-C6P-C5P	2.01	115.71	112.36
4	B	2	NAP	C2N-C3N-C4N	-2.01	115.98	118.26

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	101	COA	C3B
2	B	102	COA	C3B
2	C	103	COA	C3B
2	D	104	COA	C3B

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	102	COA	CAP-C9P-N8P-C7P
2	C	103	COA	CAP-C9P-N8P-C7P
2	D	104	COA	C2B-C3B-O3B-P3B

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Mol	Chain	Res	Type	Atoms
2	D	104	COA	CAP-C9P-N8P-C7P
2	D	104	COA	S1P-C2P-C3P-N4P
4	A	1	NAP	C2B-O2B-P2B-O2X
4	A	1	NAP	O4D-C1D-N1N-C2N
4	A	1	NAP	C2D-C1D-N1N-C2N
4	B	2	NAP	O4D-C1D-N1N-C2N
4	B	2	NAP	C2D-C1D-N1N-C2N
4	C	3	NAP	O4D-C1D-N1N-C2N
4	C	3	NAP	C2D-C1D-N1N-C2N
4	D	4	NAP	O4D-C1D-N1N-C2N
4	D	4	NAP	C2D-C1D-N1N-C2N
2	D	104	COA	C6P-C5P-N4P-C3P
2	D	104	COA	O5P-C5P-N4P-C3P
2	C	103	COA	O5P-C5P-N4P-C3P
4	A	1	NAP	C3B-C2B-O2B-P2B
4	B	2	NAP	C3B-C2B-O2B-P2B
4	C	3	NAP	C3B-C2B-O2B-P2B
4	D	4	NAP	C3B-C2B-O2B-P2B
2	C	103	COA	C6P-C5P-N4P-C3P
2	C	103	COA	O9P-C9P-N8P-C7P
2	D	104	COA	O9P-C9P-N8P-C7P
2	B	102	COA	C2B-C3B-O3B-P3B
2	D	104	COA	C4B-C3B-O3B-P3B
2	B	102	COA	O9P-C9P-N8P-C7P
4	C	3	NAP	C4N-C3N-C7N-O7N
4	C	3	NAP	C2N-C3N-C7N-O7N
4	C	3	NAP	C4N-C3N-C7N-N7N
4	C	3	NAP	C2N-C3N-C7N-N7N
4	B	2	NAP	C2B-O2B-P2B-O2X
4	C	3	NAP	C2B-O2B-P2B-O2X
4	D	4	NAP	C2B-O2B-P2B-O2X
2	C	103	COA	P1A-O3A-P2A-O4A
4	A	1	NAP	C4B-C5B-O5B-PA
4	B	2	NAP	C4B-C5B-O5B-PA
4	D	4	NAP	C3D-C4D-C5D-O5D
2	A	101	COA	P1A-O3A-P2A-O4A
4	D	4	NAP	PN-O3-PA-O1A
4	C	3	NAP	C4B-C5B-O5B-PA
4	D	4	NAP	C4B-C5B-O5B-PA
4	A	1	NAP	O4B-C4B-C5B-O5B
2	B	102	COA	P1A-O3A-P2A-O4A
2	D	104	COA	P1A-O3A-P2A-O4A

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Mol	Chain	Res	Type	Atoms
2	B	102	COA	O5P-C5P-N4P-C3P
4	B	2	NAP	C1B-C2B-O2B-P2B
4	D	4	NAP	O4D-C4D-C5D-O5D
4	A	1	NAP	C2B-O2B-P2B-O3X
4	A	1	NAP	C2D-C1D-N1N-C6N
4	B	2	NAP	C2B-O2B-P2B-O3X
4	B	2	NAP	C2D-C1D-N1N-C6N
4	C	3	NAP	C2D-C1D-N1N-C6N
4	D	4	NAP	C2B-O2B-P2B-O3X
4	D	4	NAP	C2D-C1D-N1N-C6N
4	B	2	NAP	O4B-C4B-C5B-O5B
4	C	3	NAP	O4B-C4B-C5B-O5B
4	D	4	NAP	O4B-C4B-C5B-O5B
4	D	4	NAP	C4N-C3N-C7N-O7N
2	B	102	COA	O5P-C5P-C6P-C7P
2	C	103	COA	O5P-C5P-C6P-C7P
2	B	102	COA	N4P-C5P-C6P-C7P
2	D	104	COA	N4P-C5P-C6P-C7P

There are no ring outliers.

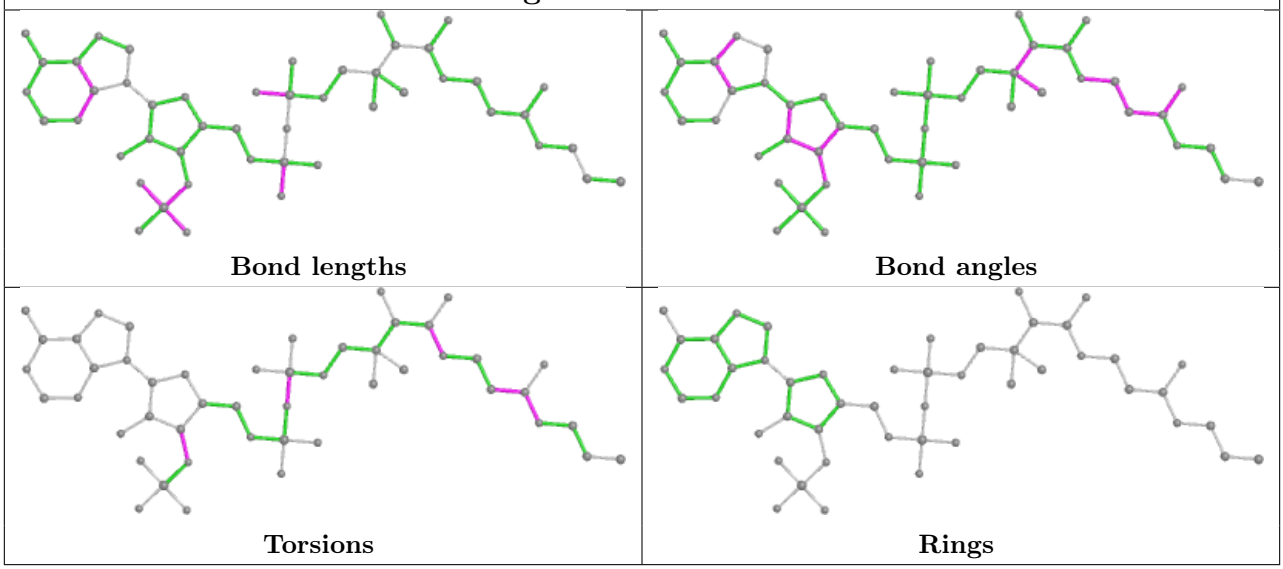
9 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	102	COA	4	0
3	B	202	MAH	1	0
2	D	104	COA	1	0
4	B	2	NAP	5	0
2	C	103	COA	6	0
2	A	101	COA	2	0
4	D	4	NAP	4	0
3	A	201	MAH	2	0
4	A	1	NAP	7	0

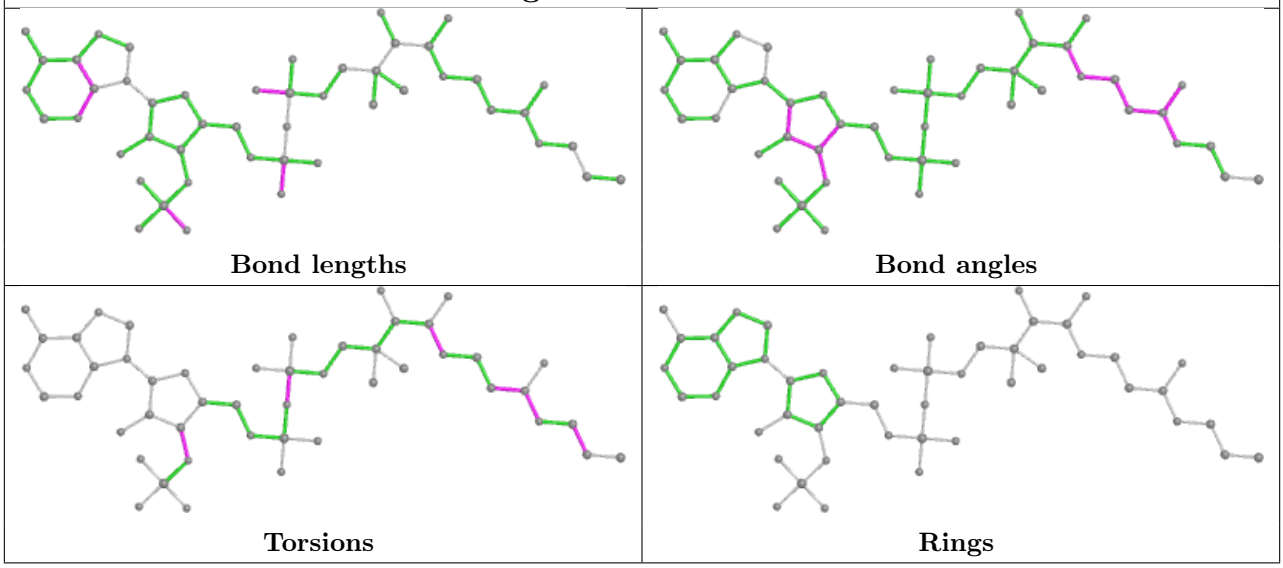
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

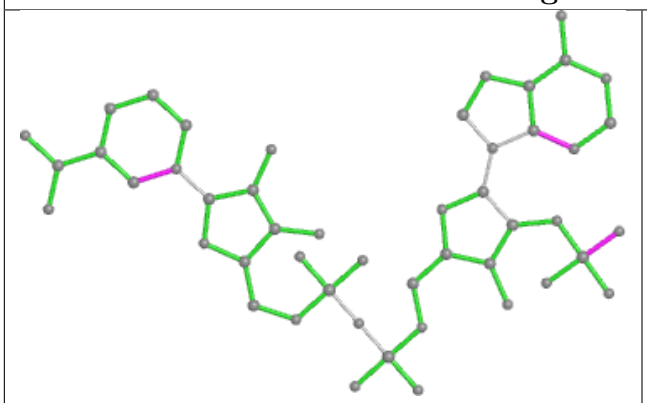
Ligand COA B 102



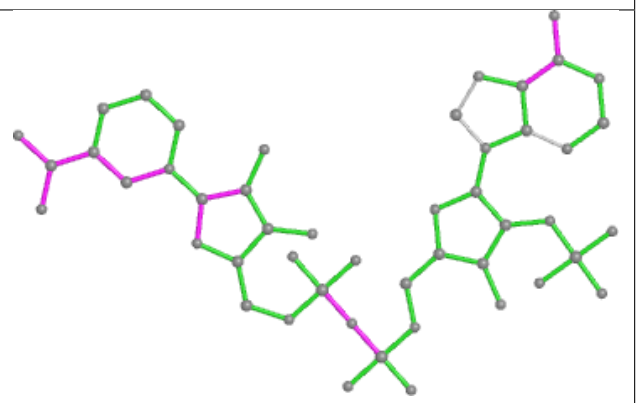
Ligand COA D 104



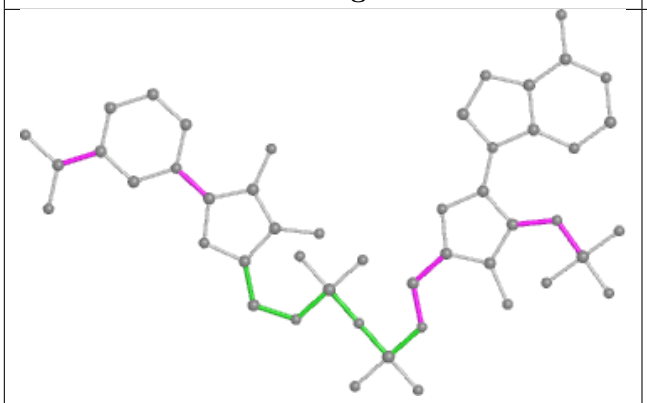
Ligand NAP C 3



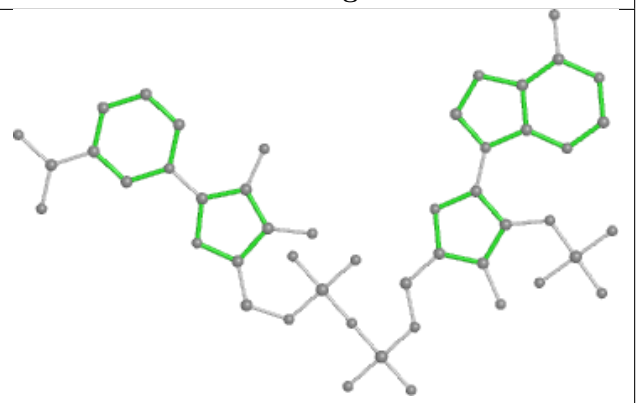
Bond lengths



Bond angles

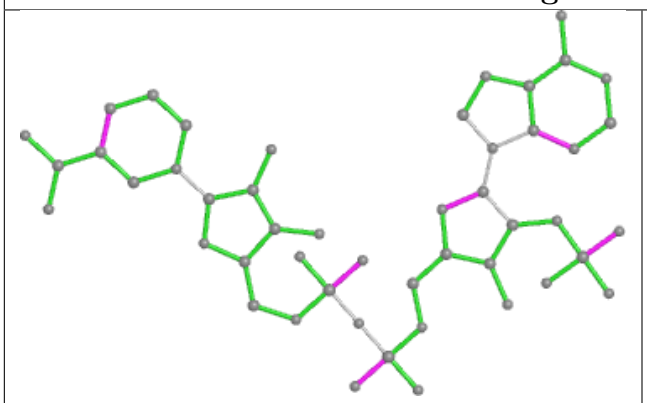


Torsions

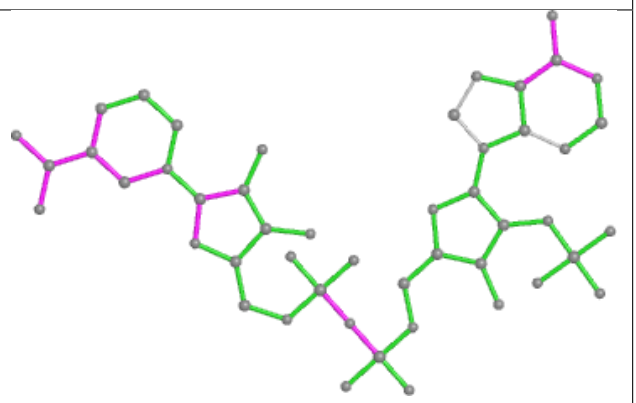


Rings

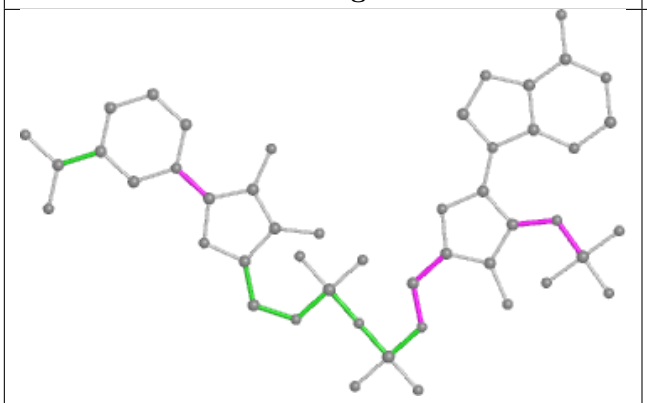
Ligand NAP B 2



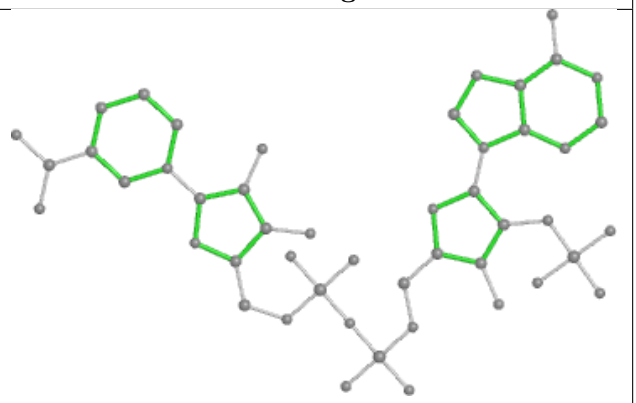
Bond lengths



Bond angles

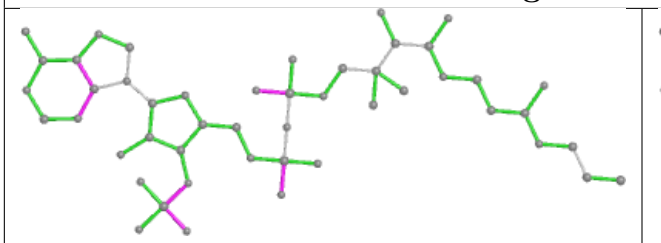


Torsions

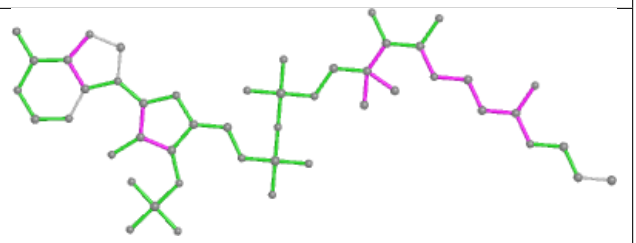


Rings

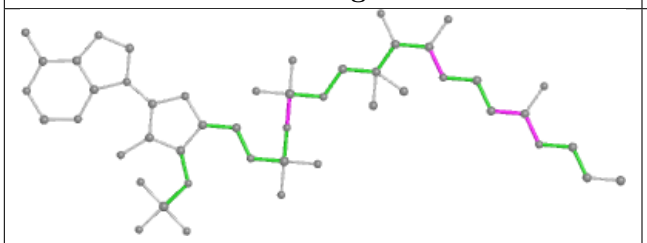
Ligand COA C 103



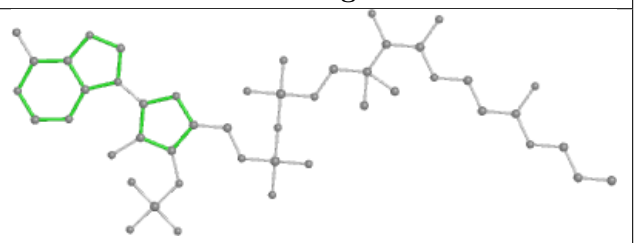
Bond lengths



Bond angles

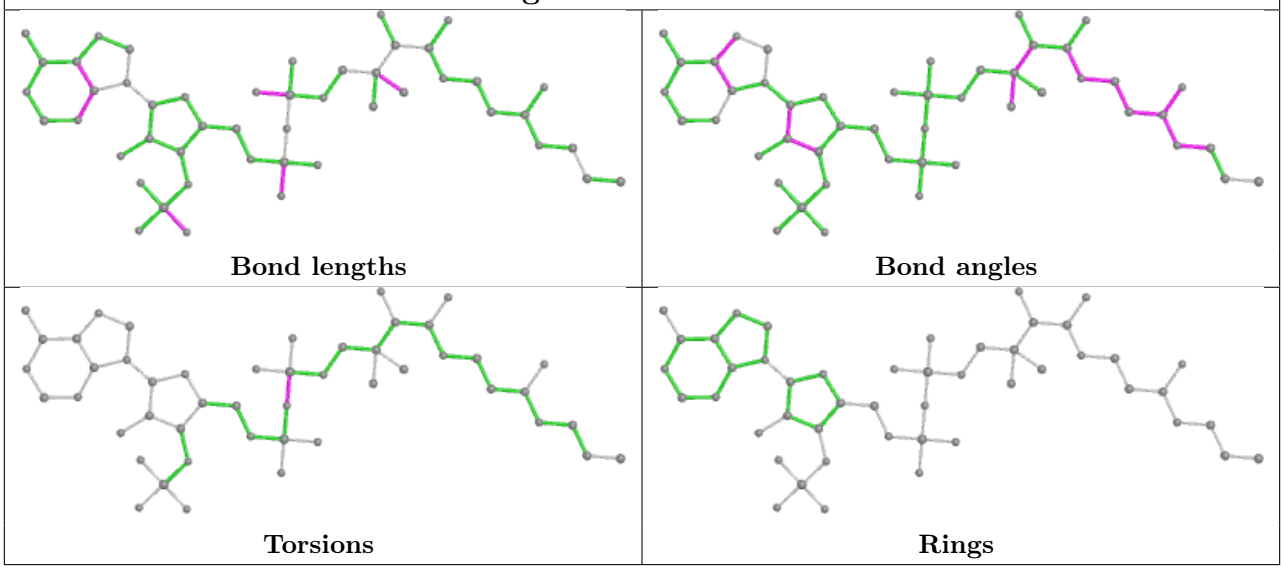


Torsions

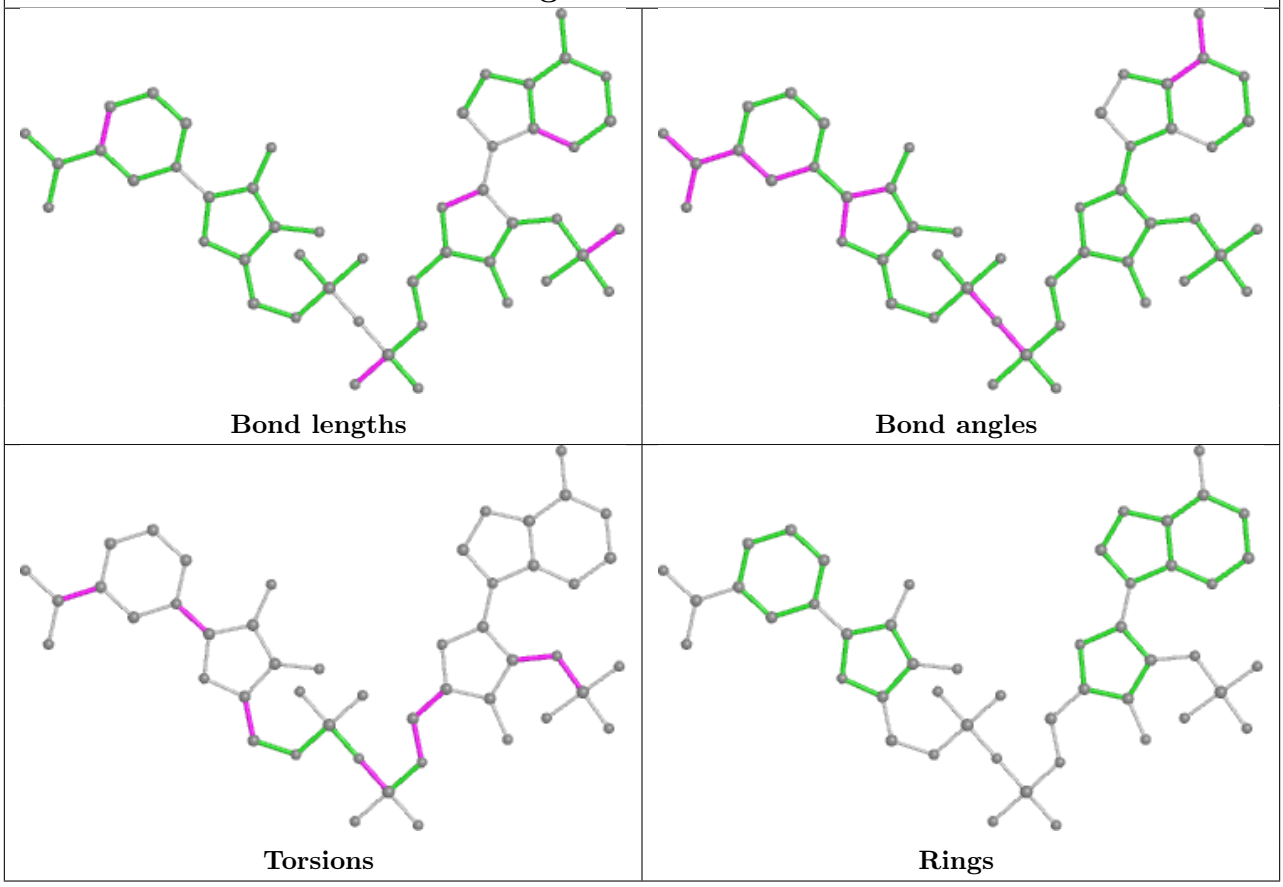


Rings

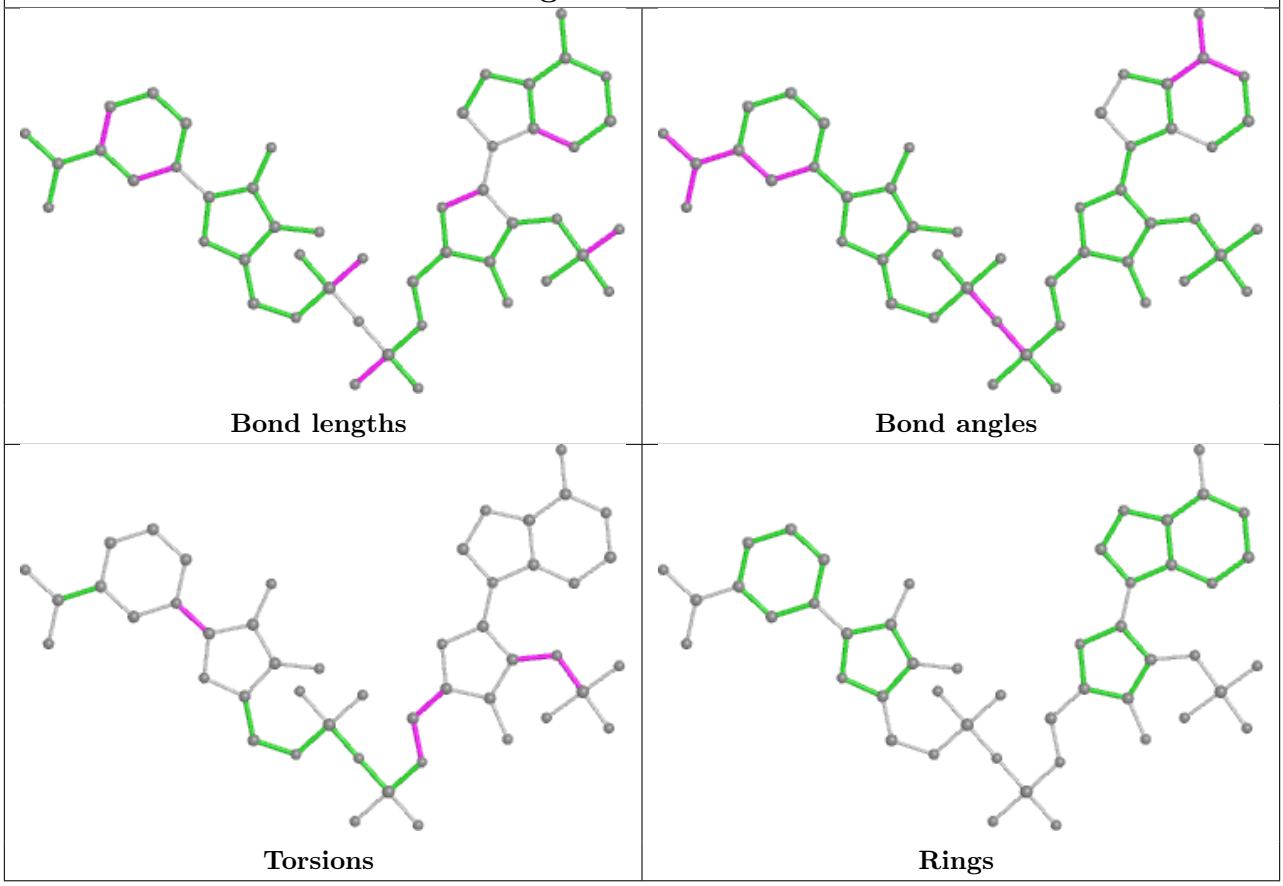
Ligand COA A 101



Ligand NAP D 4



Ligand NAP A 1



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	409/467 (87%)	-0.31	19 (4%)	32	31	8, 17, 45, 68	0
1	B	405/467 (86%)	-0.50	8 (1%)	65	63	9, 17, 42, 74	0
1	C	404/467 (86%)	-0.40	11 (2%)	54	53	8, 16, 43, 71	0
1	D	396/467 (84%)	-0.62	5 (1%)	77	76	8, 15, 32, 62	0
All	All	1614/1868 (86%)	-0.46	43 (2%)	54	53	8, 16, 42, 74	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	LEU	6.0
1	D	484	LEU	5.6
1	C	484	LEU	5.4
1	C	485	ILE	5.3
1	A	476	ILE	5.1
1	A	475	HIS	5.1
1	D	486	GLU	4.7
1	A	473	ALA	4.7
1	A	470	LEU	4.2
1	C	470	LEU	4.2
1	A	471	VAL	4.1
1	D	483	THR	4.1
1	A	474	LYS	4.1
1	C	486	GLU	4.1
1	A	469	GLN	3.9
1	B	475	HIS	3.8
1	D	485	ILE	3.8
1	A	483	THR	3.7
1	A	462	LEU	3.6
1	B	473	ALA	3.6
1	A	486	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	483	THR	3.5
1	B	474	LYS	3.5
1	C	487	THR	3.4
1	C	468	ILE	3.3
1	A	485	ILE	3.0
1	B	486	GLU	3.0
1	D	487	THR	2.9
1	B	866	HIS	2.8
1	C	469	GLN	2.7
1	A	466	GLU	2.6
1	A	465	ALA	2.5
1	C	474	LYS	2.5
1	B	470	LEU	2.4
1	A	786	PRO	2.4
1	A	472	ASN	2.4
1	B	462	LEU	2.4
1	C	473	ALA	2.4
1	A	463	SER	2.3
1	C	475	HIS	2.3
1	A	829	ASP	2.2
1	A	467	ILE	2.0
1	B	483	THR	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, 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	NAP	A	1	48/48	0.94	0.10	23,32,40,41	0

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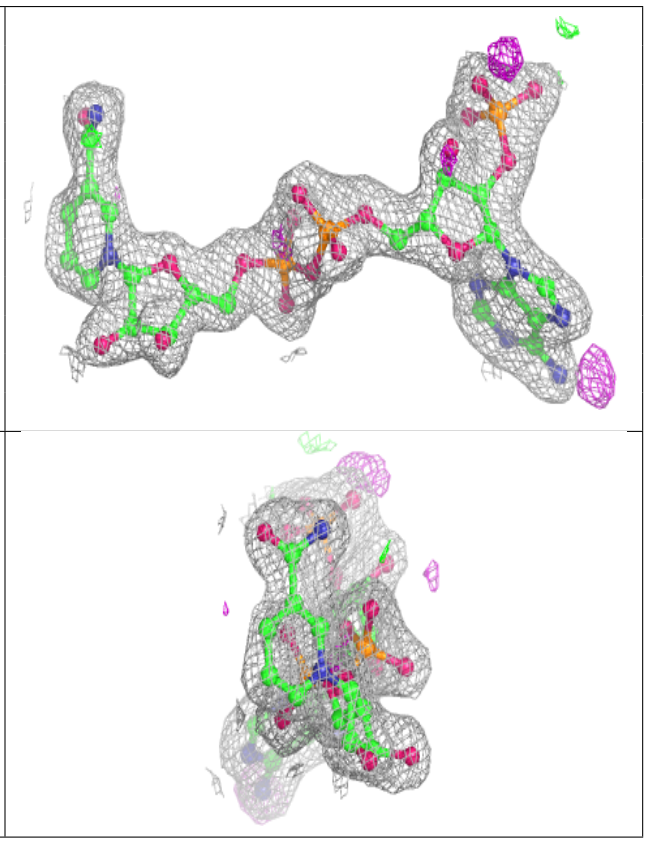
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	COA	C	103	48/48	0.96	0.08	17,23,41,43	0
2	COA	B	102	48/48	0.96	0.08	18,24,35,38	0
4	NAP	B	2	48/48	0.96	0.09	18,28,36,38	0
2	COA	D	104	48/48	0.97	0.08	14,18,30,34	0
4	NAP	C	3	48/48	0.97	0.07	14,18,22,26	0
3	MAH	C	204	11/11	0.98	0.10	12,13,16,17	0
3	MAH	D	203	11/11	0.98	0.08	13,14,18,19	0
2	COA	A	101	48/48	0.98	0.07	11,16,32,37	0
3	MAH	A	201	11/11	0.98	0.08	10,13,19,21	0
3	MAH	B	202	11/11	0.98	0.09	16,18,21,23	0
4	NAP	D	4	48/48	0.98	0.07	14,19,26,29	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.

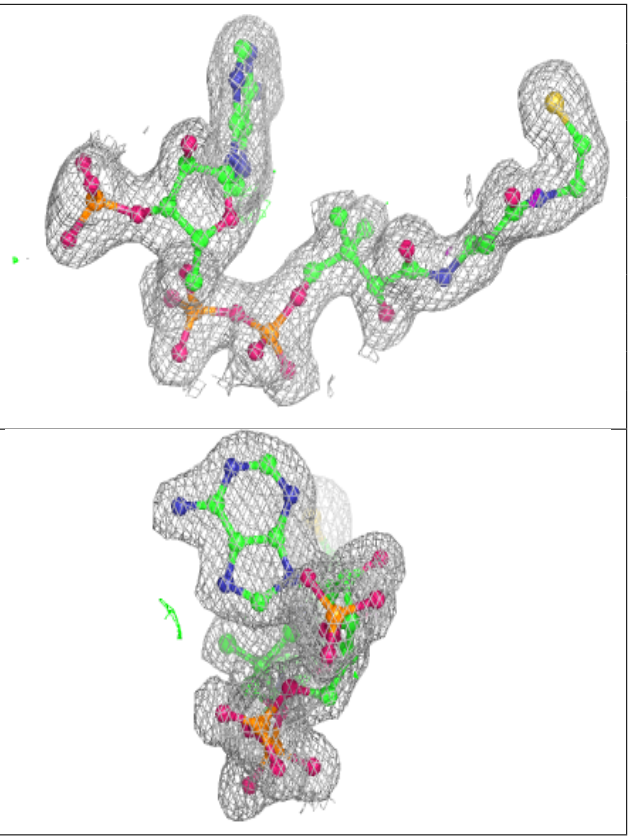
Electron density around NAP A 1:

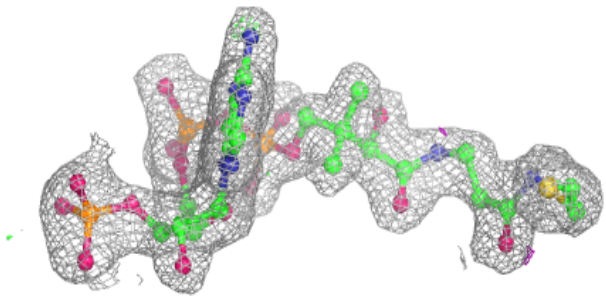
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around COA C 103:

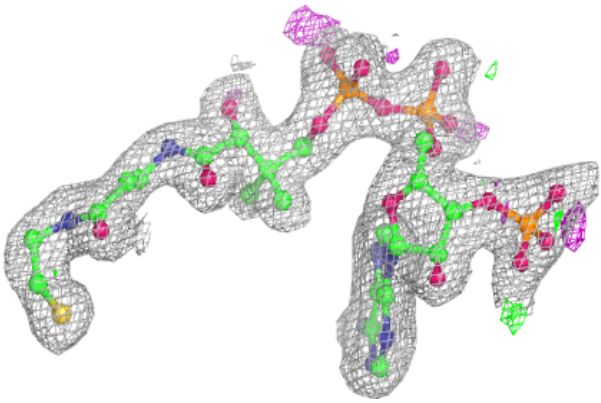
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

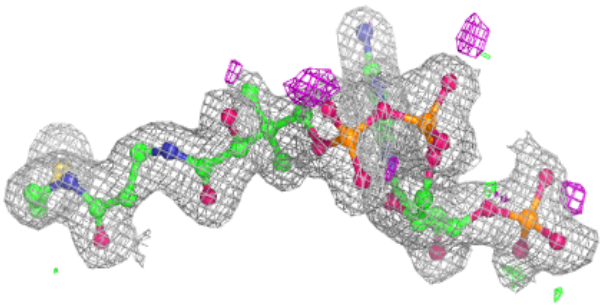


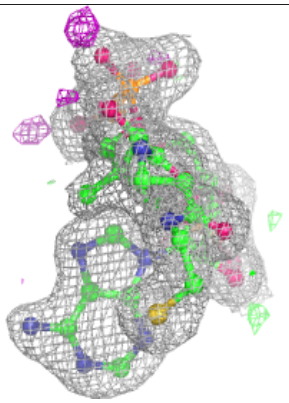


Electron density around COA B 102:

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

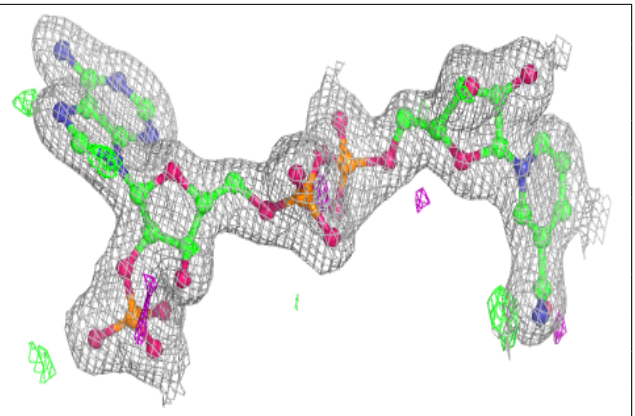


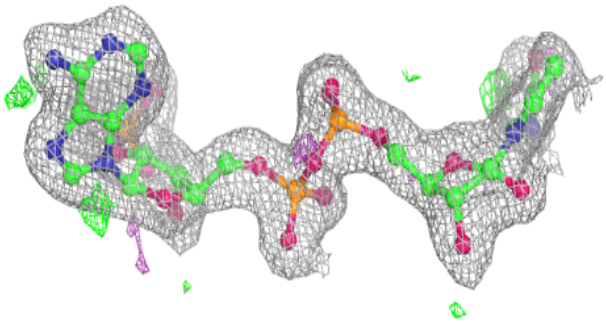


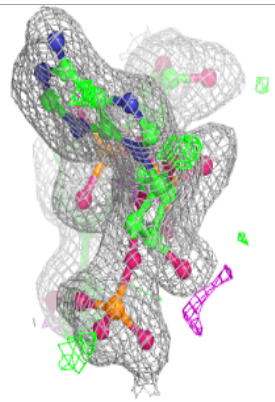


Electron density around NAP B 2:

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

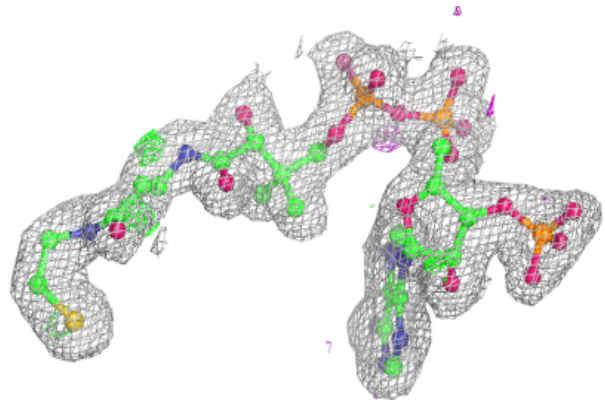


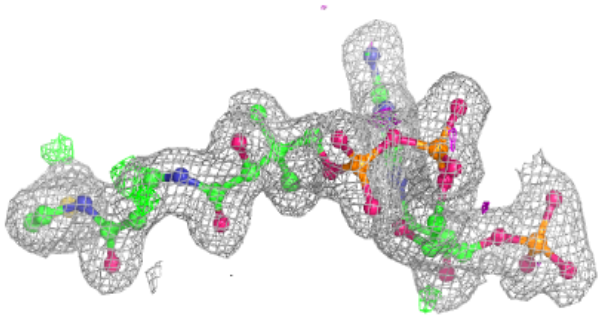


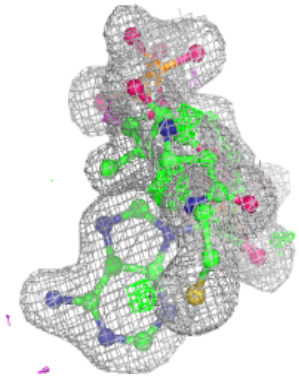


Electron density around COA D 104:

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

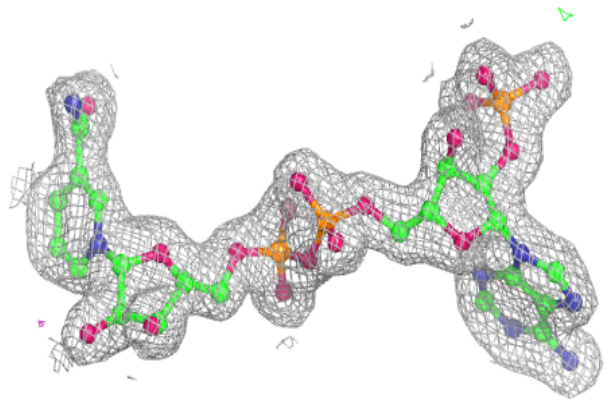


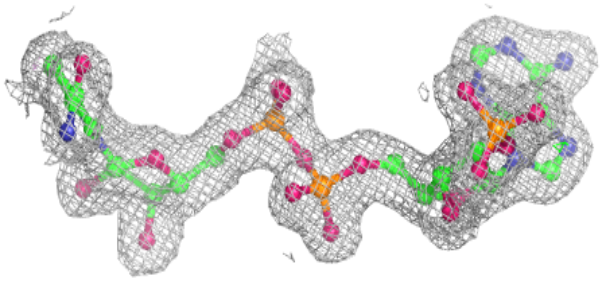


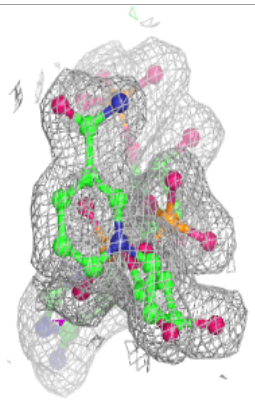


Electron density around NAP C 3:

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

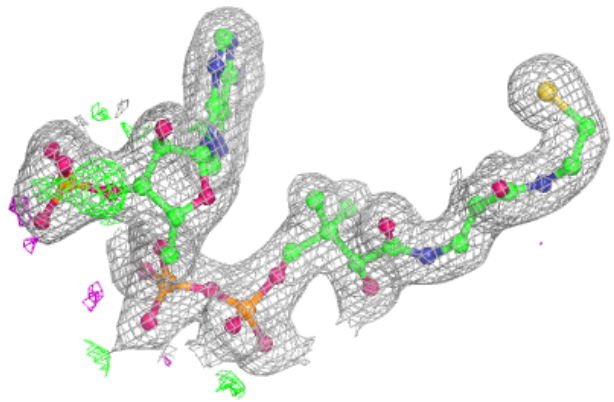


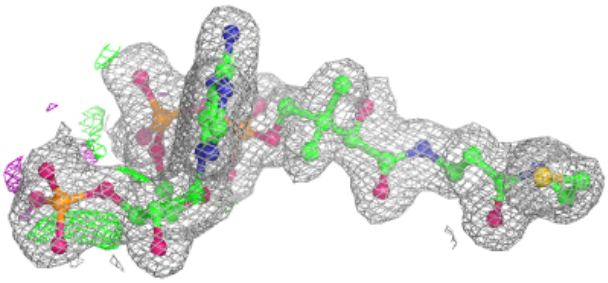


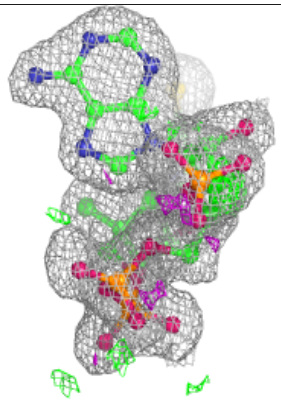


Electron density around COA A 101:

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

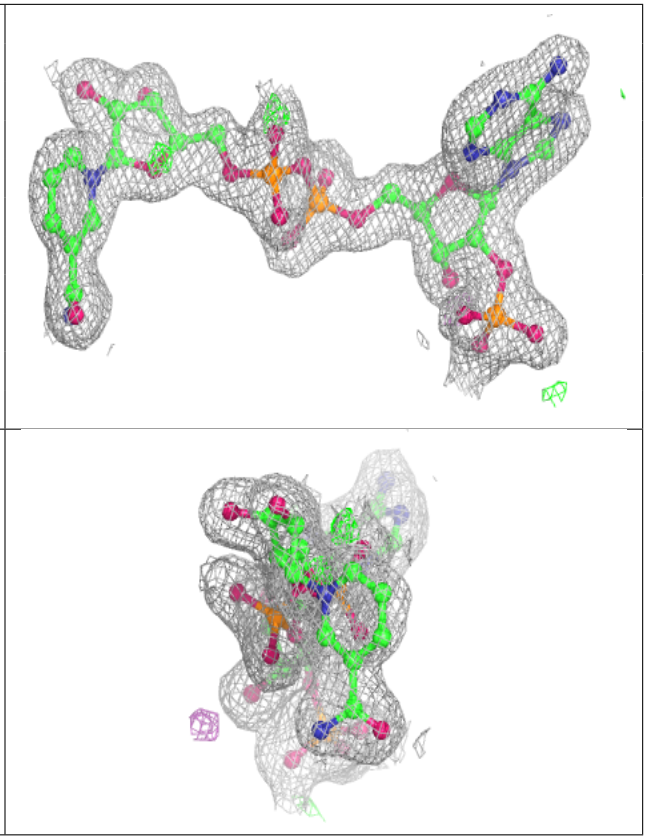






Electron density around NAP D 4:

$2mF_o$-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.