Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2023 – 05:44 PM EDT

PDB ID	:	3RHQ
Title	:	Crystal structure of the C707A mutant of C-Terminal domain of 10'FORMY LTETRAHYDROFOLATE DEHYDROGENASE in complex with NADP
Authors	:	Tsybovsky, Y.
Deposited on	:	2011-04-12
Resolution	:	2.10 Å(reported)

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

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

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

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

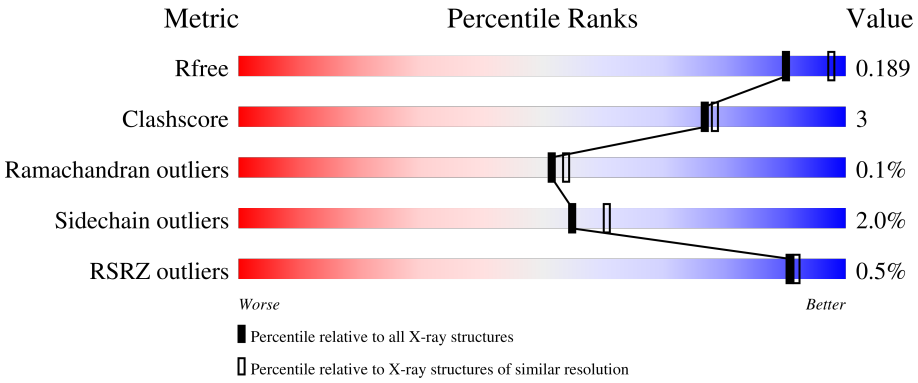
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	517	87% 8% .
1	B	517	% 89% 8% .
1	C	517	88% 8% .
1	D	517	% 90% 6% .

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17942 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 Aldehyde dehydrogenase 1 family, member L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	19	0
			3915	2486	673	737	19			
1	B	498	Total	C	N	O	S	0	18	0
			3905	2479	673	734	19			
1	C	498	Total	C	N	O	S	0	16	0
			3893	2472	674	728	19			
1	D	498	Total	C	N	O	S	0	18	0
			3902	2477	670	736	19			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	MET	-	expression tag	UNP Q5HZB2
A	387	ARG	-	expression tag	UNP Q5HZB2
A	388	GLY	-	expression tag	UNP Q5HZB2
A	389	SER	-	expression tag	UNP Q5HZB2
A	390	HIS	-	expression tag	UNP Q5HZB2
A	391	HIS	-	expression tag	UNP Q5HZB2
A	392	HIS	-	expression tag	UNP Q5HZB2
A	393	HIS	-	expression tag	UNP Q5HZB2
A	394	HIS	-	expression tag	UNP Q5HZB2
A	395	THR	-	expression tag	UNP Q5HZB2
A	396	THR	-	expression tag	UNP Q5HZB2
A	707	ALA	CYS	engineered mutation	UNP Q5HZB2
B	386	MET	-	expression tag	UNP Q5HZB2
B	387	ARG	-	expression tag	UNP Q5HZB2
B	388	GLY	-	expression tag	UNP Q5HZB2
B	389	SER	-	expression tag	UNP Q5HZB2
B	390	HIS	-	expression tag	UNP Q5HZB2
B	391	HIS	-	expression tag	UNP Q5HZB2
B	392	HIS	-	expression tag	UNP Q5HZB2
B	393	HIS	-	expression tag	UNP Q5HZB2
B	394	HIS	-	expression tag	UNP Q5HZB2

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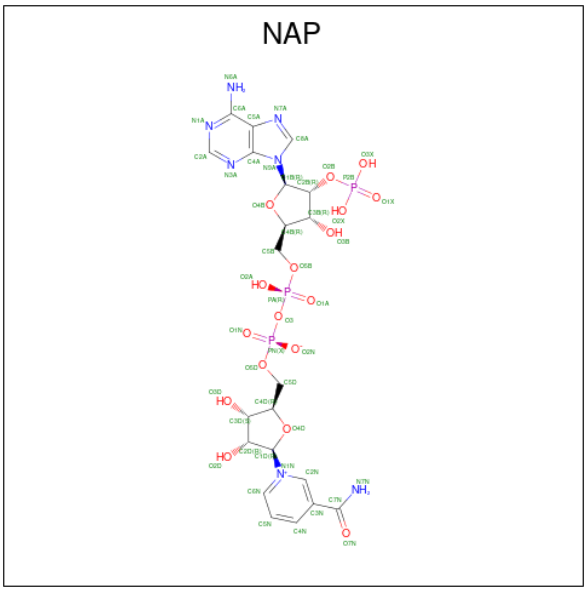
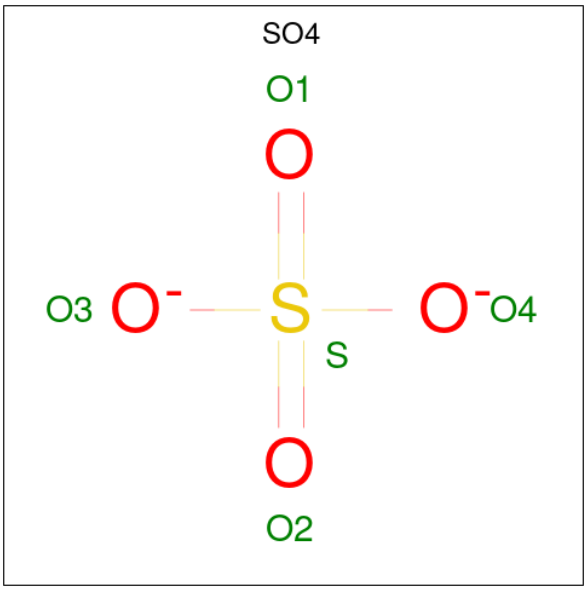
Chain	Residue	Modelled	Actual	Comment	Reference
B	395	THR	-	expression tag	UNP Q5HZB2
B	396	THR	-	expression tag	UNP Q5HZB2
B	707	ALA	CYS	engineered mutation	UNP Q5HZB2
C	386	MET	-	expression tag	UNP Q5HZB2
C	387	ARG	-	expression tag	UNP Q5HZB2
C	388	GLY	-	expression tag	UNP Q5HZB2
C	389	SER	-	expression tag	UNP Q5HZB2
C	390	HIS	-	expression tag	UNP Q5HZB2
C	391	HIS	-	expression tag	UNP Q5HZB2
C	392	HIS	-	expression tag	UNP Q5HZB2
C	393	HIS	-	expression tag	UNP Q5HZB2
C	394	HIS	-	expression tag	UNP Q5HZB2
C	395	THR	-	expression tag	UNP Q5HZB2
C	396	THR	-	expression tag	UNP Q5HZB2
C	707	ALA	CYS	engineered mutation	UNP Q5HZB2
D	386	MET	-	expression tag	UNP Q5HZB2
D	387	ARG	-	expression tag	UNP Q5HZB2
D	388	GLY	-	expression tag	UNP Q5HZB2
D	389	SER	-	expression tag	UNP Q5HZB2
D	390	HIS	-	expression tag	UNP Q5HZB2
D	391	HIS	-	expression tag	UNP Q5HZB2
D	392	HIS	-	expression tag	UNP Q5HZB2
D	393	HIS	-	expression tag	UNP Q5HZB2
D	394	HIS	-	expression tag	UNP Q5HZB2
D	395	THR	-	expression tag	UNP Q5HZB2
D	396	THR	-	expression tag	UNP Q5HZB2
D	707	ALA	CYS	engineered mutation	UNP Q5HZB2

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



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

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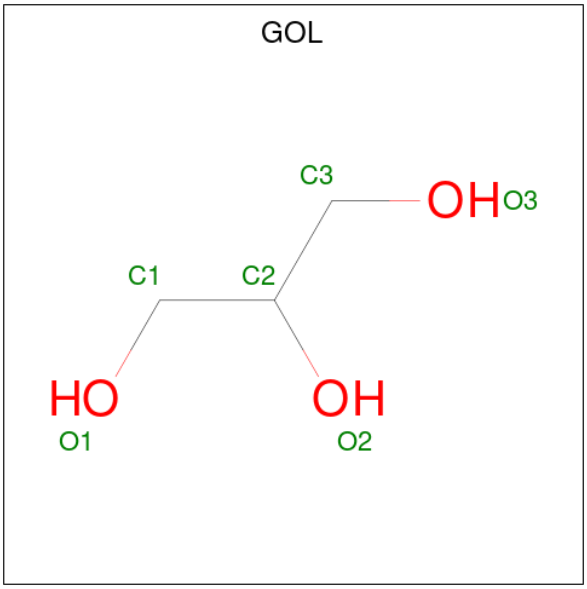
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

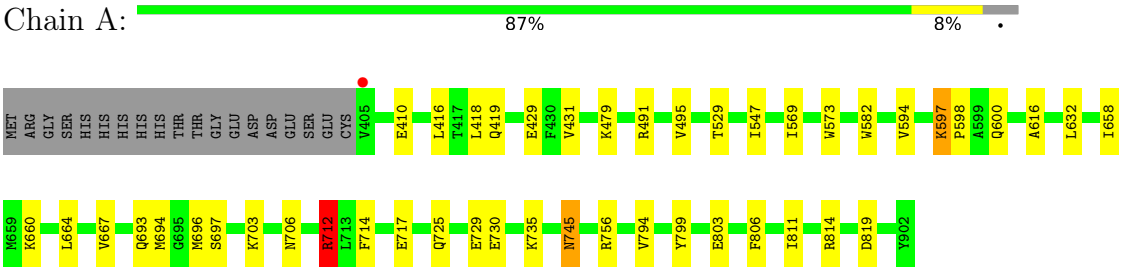
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	495	Total O 495 495	0	1
5	B	469	Total O 469 469	0	2
5	C	512	Total O 512 512	0	3
5	D	495	Total O 495 495	0	2

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.

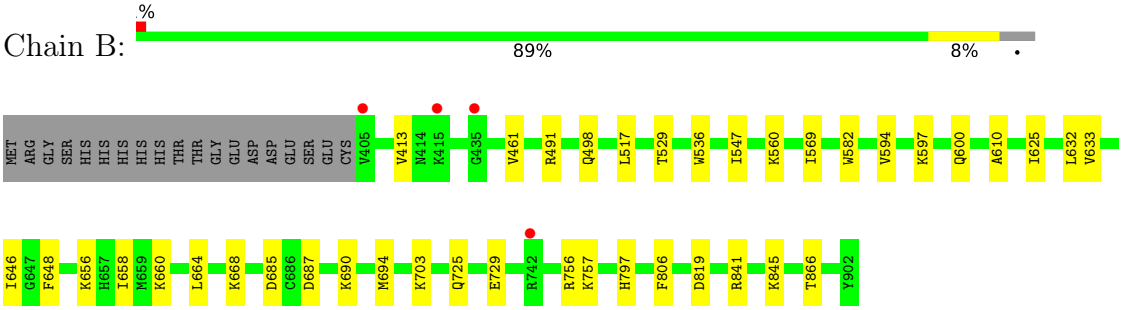
• Molecule 1: Aldehyde dehydrogenase 1 family, member L1

Chain A:



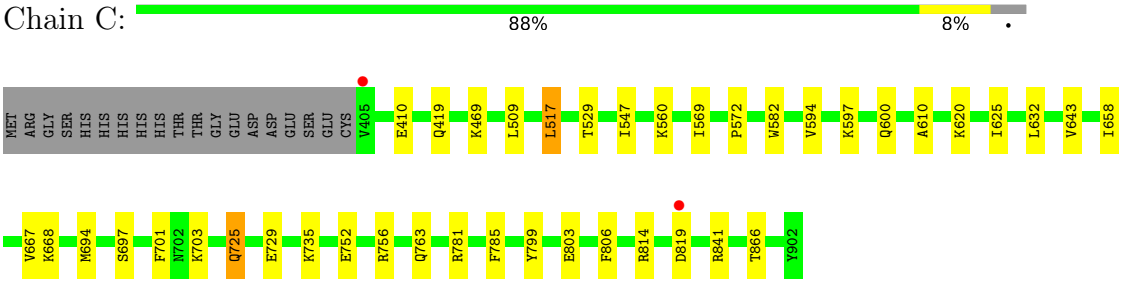
• Molecule 1: Aldehyde dehydrogenase 1 family, member L1

Chain B:



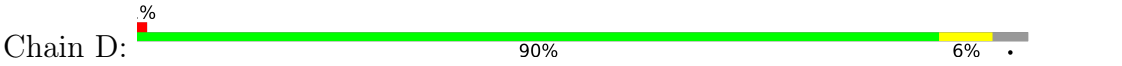
• Molecule 1: Aldehyde dehydrogenase 1 family, member L1

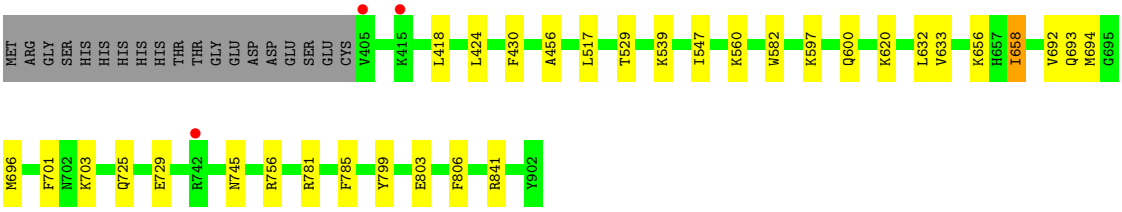
Chain C:



• Molecule 1: Aldehyde dehydrogenase 1 family, member L1

Chain D:




MET
ARG
GLY
SER
HIS
HIS
HIS
HIS
THR
THR
GLY
GLU
ASP
ASP
GLU
SER
GLU
CYS
V405
K415
L418
L424
F430
A456
L517
T529
K539
I547
K560
W582
K597
Q600
K620
L632
V633
K656
H657
I658
V692
Q693
M694
G695
M696
F701
N702
K703
Q725
E729
R742
N745
R756
R781
F785
Y799
E803
F806
R841
Y902

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	258.56Å 194.27Å 97.18Å 90.00° 108.80° 90.00°	Depositor
Resolution (Å)	48.85 – 2.10 48.74 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.6 (48.85-2.10) 95.6 (48.74-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.166 , 0.187 0.167 , 0.189	Depositor DCC
R_{free} test set	12640 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 54.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17942	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, 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	0.49	0/4070	0.57	1/5501 (0.0%)
1	B	0.48	0/4064	0.56	0/5493
1	C	4.47	2/4044 (0.0%)	0.78	2/5466 (0.0%)
1	D	2.86	2/4059 (0.0%)	0.59	4/5487 (0.1%)
All	All	2.67	4/16237 (0.0%)	0.63	7/21947 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	620[A]	LYS	CE-NZ	199.69	6.48	1.49
1	C	620[B]	LYS	CE-NZ	199.69	6.48	1.49
1	D	620[A]	LYS	CD-CE	127.12	4.69	1.51
1	D	620[B]	LYS	CD-CE	127.12	4.69	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	620[A]	LYS	CD-CE-NZ	-26.39	50.99	111.70
1	C	620[B]	LYS	CD-CE-NZ	-26.39	50.99	111.70
1	D	620[A]	LYS	CG-CD-CE	-5.79	94.52	111.90
1	D	620[B]	LYS	CG-CD-CE	-5.79	94.52	111.90
1	A	712	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	D	620[A]	LYS	CD-CE-NZ	-5.01	100.18	111.70
1	D	620[B]	LYS	CD-CE-NZ	-5.01	100.18	111.70

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	3915	0	3938	29	0
1	B	3905	0	3924	24	0
1	C	3893	0	3916	26	0
1	D	3902	0	3915	20	0
2	A	48	0	25	2	0
2	B	48	0	25	2	0
2	C	48	0	25	1	0
2	D	48	0	25	2	0
3	A	40	0	0	0	0
3	B	40	0	0	0	0
3	C	35	0	0	0	0
3	D	25	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	1	0
4	C	6	0	8	1	0
4	D	6	0	8	0	0
5	A	495	0	0	6	0
5	B	469	0	0	9	0
5	C	512	0	0	6	0
5	D	495	0	0	7	0
All	All	17942	0	15825	95	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 3.

All (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:MET:HG3	5:B:1165:HOH:O	1.23	1.31
1:A:694:MET:HG3	5:A:1138:HOH:O	1.31	1.24
1:C:694:MET:HG3	5:C:1850:HOH:O	1.12	1.24
1:D:694:MET:HG3	5:D:1265:HOH:O	1.41	1.20
1:C:841[B]:ARG:HG2	1:C:841[B]:ARG:HH11	1.08	1.16
1:A:819:ASP:HB3	5:A:1899:HOH:O	1.65	0.94
1:C:841[B]:ARG:HG2	1:C:841[B]:ARG:NH1	1.88	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:799:TYR:CE2	1:C:803[A]:GLU:HG3	2.16	0.80
1:A:725[A]:GLN:NE2	1:A:729:GLU:OE2	2.15	0.79
1:D:725[A]:GLN:NE2	1:D:729:GLU:OE2	2.20	0.74
1:B:725[A]:GLN:NE2	1:B:729:GLU:OE2	2.21	0.74
1:D:799:TYR:CE2	1:D:803[A]:GLU:HG3	2.22	0.74
1:C:725[A]:GLN:OE1	1:C:729:GLU:OE2	2.09	0.71
1:C:814:ARG:NH1	5:C:1072:HOH:O	2.27	0.67
1:A:410:GLU:OE1	1:A:419[B]:GLN:NE2	2.29	0.65
1:B:756[A]:ARG:NH2	5:B:1856:HOH:O	2.29	0.65
1:A:660:LYS:HD3	1:B:664:LEU:HD21	1.80	0.62
1:B:610:ALA:HB2	1:B:625:ILE:HD12	1.81	0.62
1:B:806:PHE:CE1	2:B:903:NAP:H2D	2.33	0.62
1:D:756:ARG:NH2	5:D:1019:HOH:O	2.33	0.61
1:A:569:ILE:HD12	1:A:594:VAL:HG21	1.81	0.60
1:D:692:VAL:O	1:D:696:MET:HG2	2.02	0.60
1:D:694:MET:CG	5:D:1265:HOH:O	2.21	0.59
1:B:687:ASP:HB2	5:B:1969:HOH:O	2.03	0.58
1:A:600:GLN:NE2	5:A:992:HOH:O	2.38	0.57
1:A:491[B]:ARG:HD2	1:A:495:VAL:HG23	1.86	0.56
1:D:806:PHE:CE1	2:D:903:NAP:H2D	2.41	0.55
1:A:756[A]:ARG:NH2	5:A:1860:HOH:O	2.38	0.55
1:B:648:PHE:CD1	1:B:658:ILE:HD12	2.42	0.55
1:D:781[B]:ARG:HD2	1:D:785:PHE:CD2	2.42	0.54
1:C:866:THR:OG1	4:C:31:GOL:H11	2.07	0.54
1:A:799:TYR:CE2	1:A:803[A]:GLU:HG3	2.43	0.54
1:A:717:GLU:OE2	1:A:814:ARG:HD3	2.08	0.53
1:B:491[B]:ARG:HH12	1:B:498:GLN:HE22	1.57	0.53
2:B:903:NAP:H8A	5:B:1186:HOH:O	2.10	0.52
1:B:600:GLN:NE2	5:B:977:HOH:O	2.42	0.52
1:C:610:ALA:HB2	1:C:625:ILE:HD12	1.92	0.51
1:A:529:THR:HG21	1:A:582:TRP:HA	1.92	0.51
1:C:569:ILE:HD12	1:C:594:VAL:HG21	1.93	0.50
1:C:600:GLN:NE2	5:C:936:HOH:O	2.41	0.50
1:C:410:GLU:OE2	1:C:419[B]:GLN:NE2	2.40	0.50
1:A:416:LEU:CD1	1:A:418:LEU:HD23	2.42	0.50
1:B:866:THR:OG1	4:B:30:GOL:H11	2.12	0.50
1:B:529:THR:HG21	1:B:582:TRP:HA	1.95	0.49
1:C:643:VAL:O	1:C:668:LYS:HE3	2.13	0.48
1:C:529:THR:HG21	1:C:582:TRP:HA	1.95	0.48
1:B:841[B]:ARG:NH1	5:B:1969:HOH:O	2.46	0.47
1:D:600:GLN:NE2	5:D:369:HOH:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:ILE:HD12	1:B:594:VAL:HG21	1.96	0.47
1:D:658:ILE:HD11	2:D:903:NAP:C2A	2.44	0.47
1:D:517:LEU:HD11	1:D:701:PHE:CZ	2.50	0.47
1:A:806:PHE:CE1	2:A:903:NAP:H2D	2.49	0.47
1:B:797:HIS:HD2	5:B:1047:HOH:O	1.97	0.47
1:A:491[A]:ARG:NH2	5:A:1211:HOH:O	2.48	0.46
1:A:725[A]:GLN:HE21	1:A:729:GLU:CD	2.17	0.46
1:A:735:LYS:H	1:A:745:ASN:HD21	1.63	0.46
1:D:456:ALA:HB3	1:D:633:VAL:HG21	1.96	0.46
1:A:664:LEU:HD21	1:B:660:LYS:HD2	1.99	0.45
1:A:429:GLU:HG3	1:A:431:VAL:HG13	1.99	0.45
1:A:479:LYS:NZ	5:A:1749:HOH:O	2.45	0.45
1:B:461:VAL:HG22	1:B:633:VAL:HG13	1.98	0.45
1:C:560[A]:LYS:HD2	5:D:1697:HOH:O	2.18	0.44
1:D:841[B]:ARG:NH2	5:D:1527:HOH:O	2.50	0.44
1:C:469:LYS:HE3	5:C:1034:HOH:O	2.18	0.44
1:D:632:LEU:C	1:D:632:LEU:HD23	2.38	0.44
1:D:529:THR:HG21	1:D:582:TRP:HA	2.00	0.43
1:C:799:TYR:CD2	1:C:803[A]:GLU:HG3	2.54	0.43
1:C:752:GLU:OE2	1:C:756[B]:ARG:NH2	2.49	0.43
1:C:763[A]:GLN:NE2	5:C:1870:HOH:O	2.45	0.43
1:D:799:TYR:CD2	1:D:803[A]:GLU:HG3	2.54	0.43
1:A:694:MET:HE3	1:A:697:SER:HB3	1.99	0.43
1:A:712:ARG:HG2	1:A:714:PHE:CE1	2.54	0.43
1:A:597:LYS:HD2	1:A:598:PRO:O	2.19	0.43
1:A:794:VAL:HG21	1:A:811:ILE:HG23	2.01	0.43
1:C:667:VAL:HG13	1:D:656:LYS:HG2	2.00	0.42
1:C:560[A]:LYS:CD	5:D:1697:HOH:O	2.67	0.42
5:C:1823:HOH:O	1:D:560[A]:LYS:HE2	2.18	0.42
1:B:560[B]:LYS:HE3	5:B:1960:HOH:O	2.18	0.42
1:C:694:MET:HE3	1:C:694:MET:HA	2.01	0.42
1:C:632:LEU:C	1:C:632:LEU:HD23	2.40	0.42
1:A:667:VAL:HG13	1:B:656:LYS:HG2	2.02	0.42
1:B:694:MET:CG	5:B:1165:HOH:O	2.10	0.41
1:B:646:ILE:HG12	1:B:668:LYS:HD3	2.02	0.41
1:B:536:TRP:CE2	1:D:539:LYS:HD3	2.56	0.41
1:C:806:PHE:CE1	2:C:903:NAP:H2D	2.56	0.41
1:A:491[A]:ARG:HD2	1:A:616:ALA:O	2.21	0.41
1:A:632:LEU:HD23	1:A:632:LEU:C	2.41	0.41
1:A:573:TRP:NE1	2:A:903:NAP:O2N	2.53	0.41
1:D:424:LEU:O	1:D:430:PHE:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:MET:SD	1:A:730:GLU:HB2	2.61	0.40
1:B:685:ASP:OD2	1:B:845:LYS:NZ	2.50	0.40
1:C:517:LEU:HD21	1:C:701:PHE:CZ	2.57	0.40
1:B:632:LEU:HD23	1:B:632:LEU:C	2.42	0.40
1:C:781[B]:ARG:HD2	1:C:785:PHE:CE2	2.57	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	515/517 (100%)	500 (97%)	15 (3%)	0	100	100
1	B	514/517 (99%)	499 (97%)	15 (3%)	0	100	100
1	C	512/517 (99%)	495 (97%)	16 (3%)	1 (0%)	47	49
1	D	514/517 (99%)	495 (96%)	19 (4%)	0	100	100
All	All	2055/2068 (99%)	1989 (97%)	65 (3%)	1 (0%)	51	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	572	PRO

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	427/425 (100%)	418 (98%)	9 (2%)	53 59
1	B	426/425 (100%)	418 (98%)	8 (2%)	57 63
1	C	424/425 (100%)	413 (97%)	11 (3%)	46 50
1	D	426/425 (100%)	418 (98%)	8 (2%)	57 63
All	All	1703/1700 (100%)	1667 (98%)	36 (2%)	55 59

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	547	ILE
1	A	597	LYS
1	A	658	ILE
1	A	693[A]	GLN
1	A	693[B]	GLN
1	A	703	LYS
1	A	706	ASN
1	A	712	ARG
1	A	745	ASN
1	B	413	VAL
1	B	517	LEU
1	B	547	ILE
1	B	597	LYS
1	B	690	LYS
1	B	703	LYS
1	B	757	LYS
1	B	819	ASP
1	C	509	LEU
1	C	517	LEU
1	C	547	ILE
1	C	597	LYS
1	C	658	ILE
1	C	697	SER
1	C	703	LYS
1	C	725[A]	GLN
1	C	725[B]	GLN
1	C	735	LYS
1	C	819	ASP
1	D	418	LEU
1	D	547	ILE
1	D	597	LYS
1	D	658	ILE
1	D	693[A]	GLN

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Mol	Chain	Res	Type
1	D	693[B]	GLN
1	D	703	LYS
1	D	745	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	600	GLN
1	A	706	ASN
1	A	745	ASN
1	B	457	GLN
1	B	600	GLN
1	B	706	ASN
1	B	797	HIS
1	C	600	GLN
1	C	706	ASN
1	C	797	HIS
1	D	407	ASN
1	D	600	GLN
1	D	706	ASN
1	D	745	ASN
1	D	750	ASN
1	D	797	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

36 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	D	903	-	45,52,52	1.60	3 (6%)	56,80,80	1.26	8 (14%)
3	SO4	A	18	-	4,4,4	0.17	0	6,6,6	0.05	0
4	GOL	C	31	-	5,5,5	0.27	0	5,5,5	0.51	0
4	GOL	D	32	-	5,5,5	0.31	0	5,5,5	0.74	0
3	SO4	B	3	-	4,4,4	0.19	0	6,6,6	0.09	0
3	SO4	A	1	-	4,4,4	0.14	0	6,6,6	0.13	0
3	SO4	A	11	-	4,4,4	0.16	0	6,6,6	0.10	0
3	SO4	B	25	-	4,4,4	0.16	0	6,6,6	0.13	0
3	SO4	D	27	-	4,4,4	0.15	0	6,6,6	0.14	0
3	SO4	A	15	-	4,4,4	0.15	0	6,6,6	0.34	0
3	SO4	B	14	-	4,4,4	0.17	0	6,6,6	0.24	0
4	GOL	B	30	-	5,5,5	0.24	0	5,5,5	0.58	0
3	SO4	D	12	-	4,4,4	0.14	0	6,6,6	0.11	0
3	SO4	B	22	-	4,4,4	0.17	0	6,6,6	0.18	0
3	SO4	A	21	-	4,4,4	0.16	0	6,6,6	0.15	0
3	SO4	C	23	-	4,4,4	0.15	0	6,6,6	0.14	0
3	SO4	A	24	-	4,4,4	0.17	0	6,6,6	0.15	0
3	SO4	D	16	-	4,4,4	0.20	0	6,6,6	0.45	0
4	GOL	A	29	-	5,5,5	0.29	0	5,5,5	0.60	0
3	SO4	A	6	-	4,4,4	0.17	0	6,6,6	0.31	0
3	SO4	C	10	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	B	9	-	4,4,4	0.15	0	6,6,6	0.07	0
2	NAP	A	903	-	45,52,52	1.71	4 (8%)	56,80,80	1.21	4 (7%)
2	NAP	B	903	-	45,52,52	1.64	3 (6%)	56,80,80	1.16	4 (7%)
3	SO4	D	8	-	4,4,4	0.15	0	6,6,6	0.20	0
3	SO4	C	13	-	4,4,4	0.14	0	6,6,6	0.43	0
3	SO4	B	4	-	4,4,4	0.12	0	6,6,6	0.13	0
2	NAP	C	903	-	45,52,52	1.62	4 (8%)	56,80,80	1.27	6 (10%)
3	SO4	C	17	-	4,4,4	0.13	0	6,6,6	0.17	0
3	SO4	C	7	-	4,4,4	0.12	0	6,6,6	0.41	0
3	SO4	C	26	-	4,4,4	0.13	0	6,6,6	0.26	0
3	SO4	B	19	-	4,4,4	0.18	0	6,6,6	0.21	0
3	SO4	C	28	-	4,4,4	0.21	0	6,6,6	0.33	0
3	SO4	D	20	-	4,4,4	0.16	0	6,6,6	0.15	0
3	SO4	B	5	-	4,4,4	0.16	0	6,6,6	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	A	2	-	4,4,4	0.15	0	6,6,6	0.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	D	903	-	-	6/31/67/67	0/5/5/5
4	GOL	B	30	-	-	2/4/4/4	-
4	GOL	C	31	-	-	2/4/4/4	-
4	GOL	D	32	-	-	1/4/4/4	-
2	NAP	C	903	-	-	7/31/67/67	0/5/5/5
4	GOL	A	29	-	-	3/4/4/4	-
2	NAP	A	903	-	-	5/31/67/67	0/5/5/5
2	NAP	B	903	-	-	7/31/67/67	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	903	NAP	O7N-C7N	8.84	1.41	1.24
2	B	903	NAP	O7N-C7N	8.71	1.40	1.24
2	C	903	NAP	O7N-C7N	8.52	1.40	1.24
2	D	903	NAP	O7N-C7N	8.52	1.40	1.24
2	A	903	NAP	C2A-N3A	3.99	1.38	1.32
2	B	903	NAP	C2A-N3A	3.71	1.38	1.32
2	C	903	NAP	C2A-N3A	3.59	1.37	1.32
2	D	903	NAP	C2A-N3A	3.43	1.37	1.32
2	A	903	NAP	C2A-N1A	2.60	1.38	1.33
2	B	903	NAP	C2A-N1A	2.38	1.38	1.33
2	D	903	NAP	C2A-N1A	2.19	1.38	1.33
2	A	903	NAP	C2N-N1N	2.17	1.37	1.35
2	C	903	NAP	C2A-N1A	2.17	1.37	1.33
2	C	903	NAP	P2B-O2B	2.02	1.63	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	903	NAP	N3A-C2A-N1A	-5.40	120.25	128.68
2	C	903	NAP	N3A-C2A-N1A	-5.36	120.29	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	903	NAP	N3A-C2A-N1A	-5.27	120.44	128.68
2	D	903	NAP	N3A-C2A-N1A	-5.20	120.54	128.68
2	D	903	NAP	O4D-C1D-C2D	-2.99	102.56	106.93
2	C	903	NAP	O4D-C1D-C2D	-2.94	102.63	106.93
2	A	903	NAP	O4D-C1D-C2D	-2.89	102.71	106.93
2	D	903	NAP	C6N-N1N-C2N	-2.64	119.57	121.97
2	C	903	NAP	C2N-C3N-C4N	2.62	121.23	118.26
2	C	903	NAP	C6N-N1N-C2N	-2.45	119.74	121.97
2	A	903	NAP	C4A-C5A-N7A	-2.35	106.95	109.40
2	D	903	NAP	C5N-C4N-C3N	-2.35	117.57	120.34
2	D	903	NAP	C4A-C5A-N7A	-2.32	106.98	109.40
2	D	903	NAP	O4B-C1B-C2B	-2.25	102.68	106.59
2	C	903	NAP	C5N-C4N-C3N	-2.22	117.71	120.34
2	A	903	NAP	C6N-N1N-C2N	-2.16	120.01	121.97
2	B	903	NAP	O4D-C1D-C2D	-2.11	103.84	106.93
2	D	903	NAP	C5A-C6A-N6A	2.08	123.52	120.35
2	D	903	NAP	C2N-C3N-C4N	2.06	120.60	118.26
2	B	903	NAP	C2N-C3N-C4N	2.05	120.58	118.26
2	C	903	NAP	O4B-C1B-C2B	-2.03	103.07	106.59
2	B	903	NAP	C5N-C4N-C3N	-2.02	117.95	120.34

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	903	NAP	C5D-O5D-PN-O1N
2	B	903	NAP	C5D-O5D-PN-O1N
2	C	903	NAP	C5D-O5D-PN-O1N
2	D	903	NAP	C5D-O5D-PN-O1N
4	A	29	GOL	C1-C2-C3-O3
4	A	29	GOL	O2-C2-C3-O3
4	B	30	GOL	C1-C2-C3-O3
4	C	31	GOL	C1-C2-C3-O3
4	B	30	GOL	O2-C2-C3-O3
2	B	903	NAP	PN-O3-PA-O1A
2	C	903	NAP	PN-O3-PA-O1A
2	D	903	NAP	PN-O3-PA-O1A
2	A	903	NAP	C4D-C5D-O5D-PN
2	B	903	NAP	C4D-C5D-O5D-PN
2	C	903	NAP	C4D-C5D-O5D-PN
4	C	31	GOL	O2-C2-C3-O3
4	D	32	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	D	903	NAP	C4D-C5D-O5D-PN
2	A	903	NAP	C5D-O5D-PN-O3
2	B	903	NAP	C5D-O5D-PN-O3
2	C	903	NAP	C5D-O5D-PN-O3
2	D	903	NAP	C5D-O5D-PN-O3
2	A	903	NAP	C5D-O5D-PN-O2N
2	B	903	NAP	C5D-O5D-PN-O2N
2	C	903	NAP	C5D-O5D-PN-O2N
2	D	903	NAP	C5D-O5D-PN-O2N
2	D	903	NAP	PN-O3-PA-O2A
2	A	903	NAP	C2B-O2B-P2B-O1X
2	B	903	NAP	C2B-O2B-P2B-O1X
2	C	903	NAP	C2B-O2B-P2B-O1X
2	C	903	NAP	C3B-C2B-O2B-P2B
2	B	903	NAP	PN-O3-PA-O2A
4	A	29	GOL	O1-C1-C2-O2

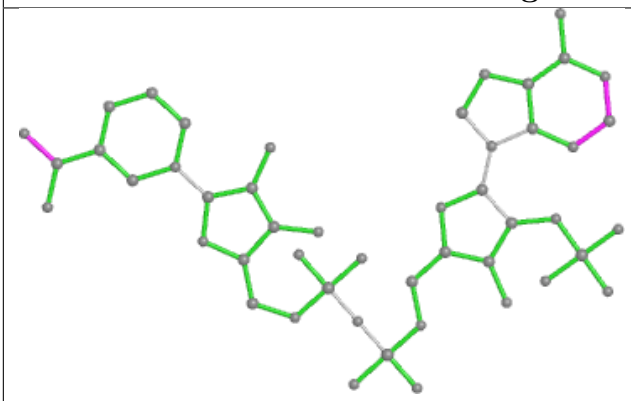
There are no ring outliers.

6 monomers are involved in 9 short contacts:

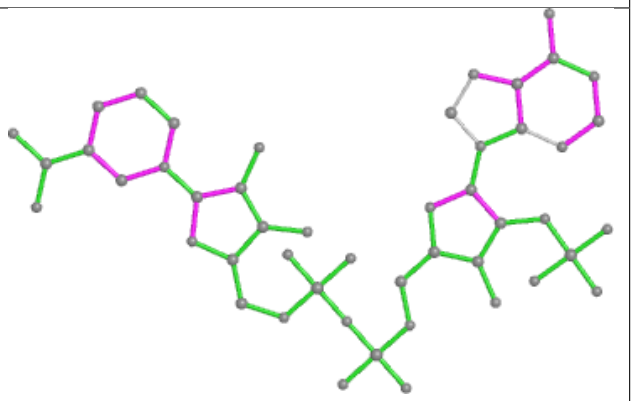
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	903	NAP	2	0
4	C	31	GOL	1	0
4	B	30	GOL	1	0
2	A	903	NAP	2	0
2	B	903	NAP	2	0
2	C	903	NAP	1	0

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

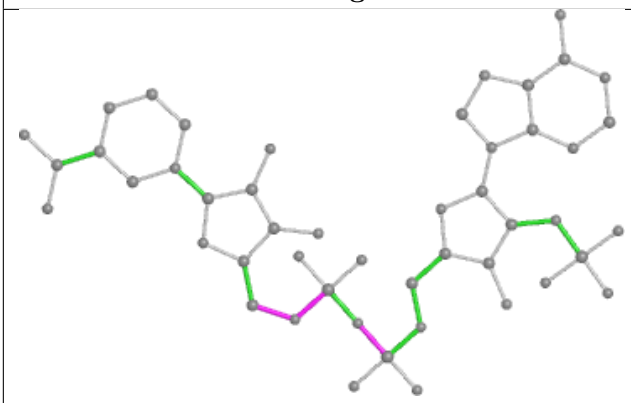
Ligand NAP D 903



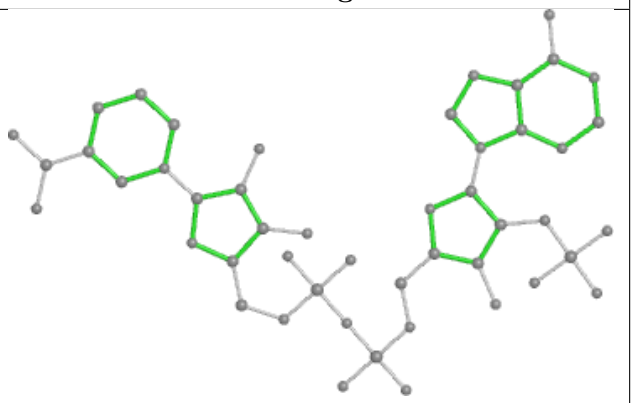
Bond lengths



Bond angles

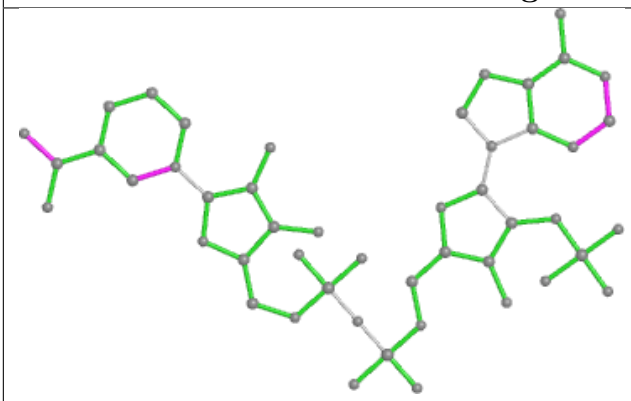


Torsions

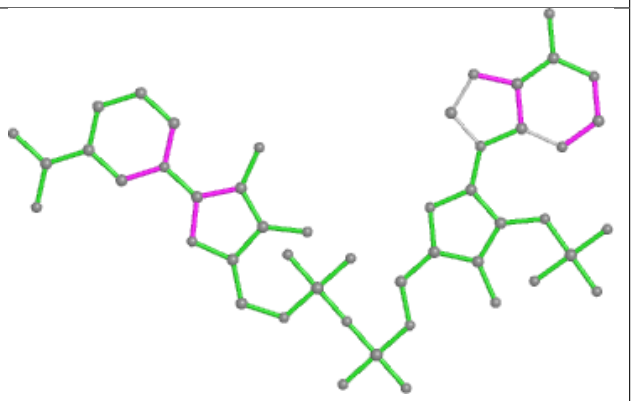


Rings

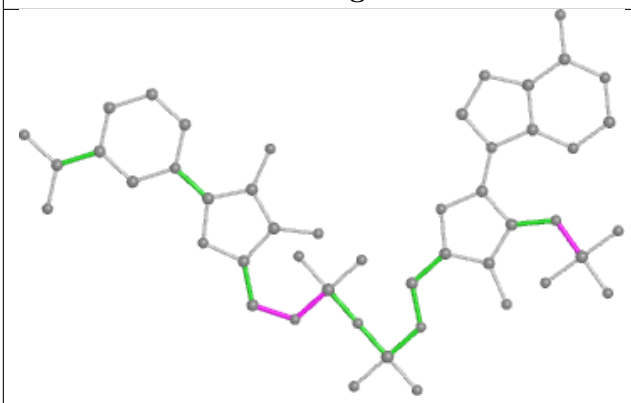
Ligand NAP A 903



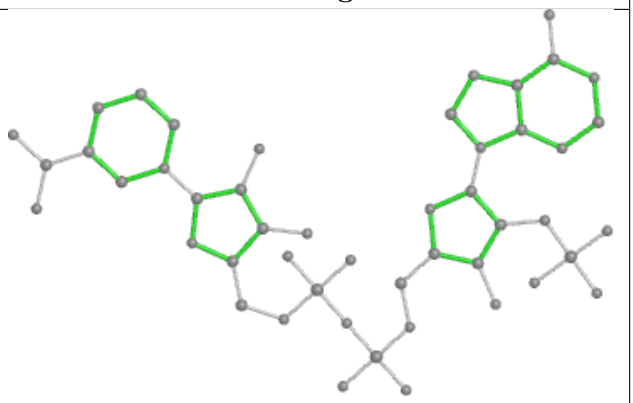
Bond lengths



Bond angles

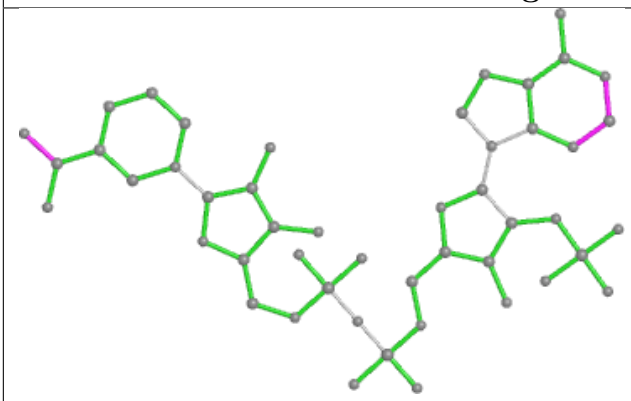


Torsions

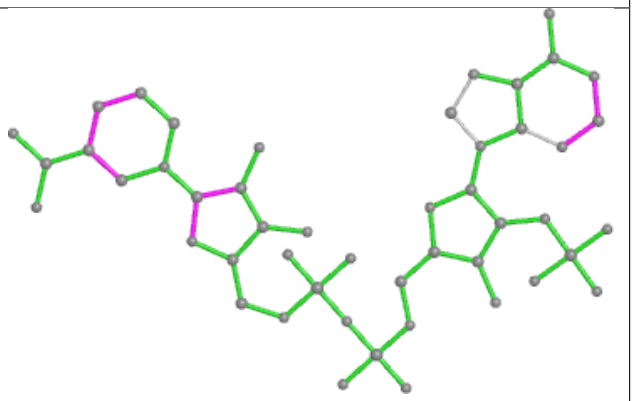


Rings

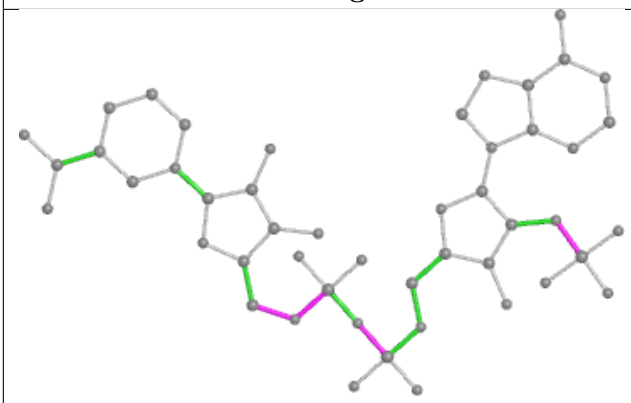
Ligand NAP B 903



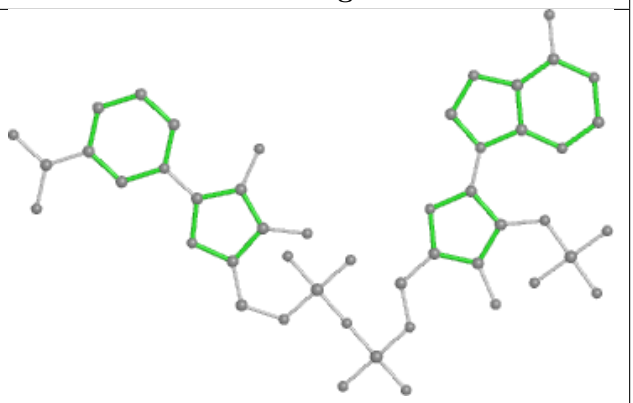
Bond lengths



Bond angles

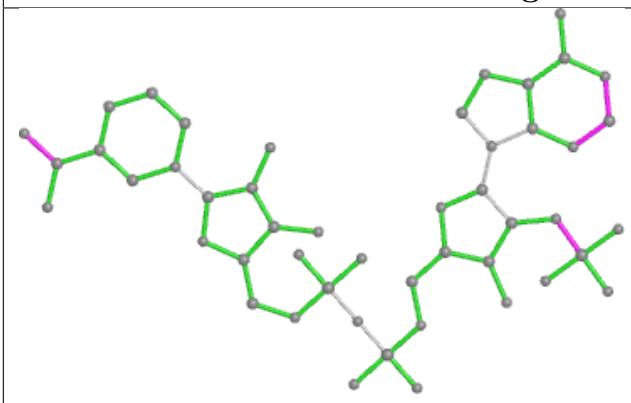


Torsions

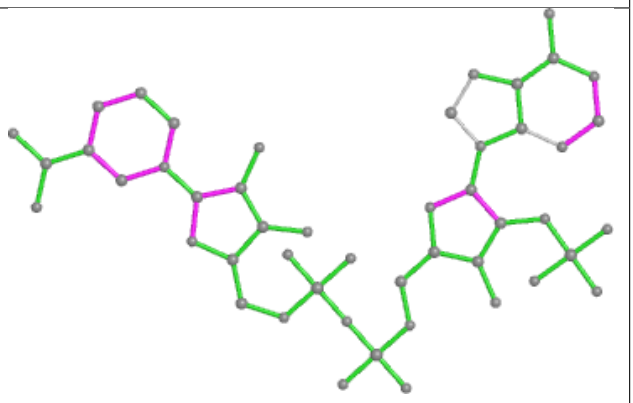


Rings

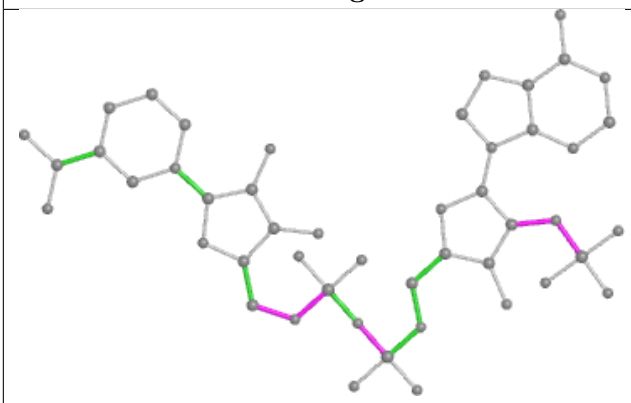
Ligand NAP C 903



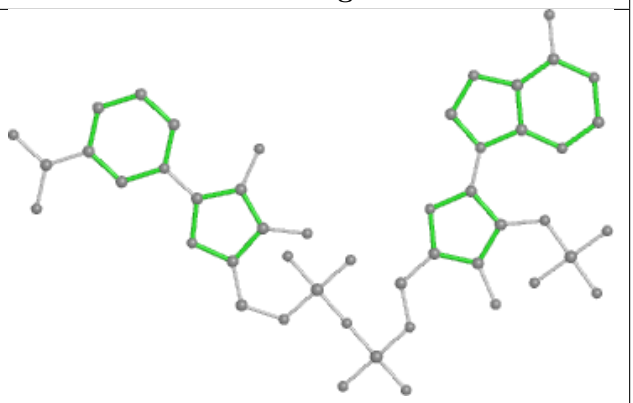
Bond lengths



Bond angles



Torsions



Rings

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	498/517 (96%)	-0.48	1 (0%)	95	95	12, 21, 31, 39	12 (2%)
1	B	498/517 (96%)	-0.43	4 (0%)	86	88	14, 22, 32, 46	11 (2%)
1	C	498/517 (96%)	-0.60	2 (0%)	92	93	12, 18, 27, 41	11 (2%)
1	D	498/517 (96%)	-0.58	3 (0%)	89	91	12, 21, 32, 41	13 (2%)
All	All	1992/2068 (96%)	-0.52	10 (0%)	91	92	12, 21, 31, 46	47 (2%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	405	VAL	5.0
1	B	405	VAL	5.0
1	C	405	VAL	4.5
1	D	405	VAL	4.3
1	B	742	ARG	2.7
1	C	819	ASP	2.7
1	B	415	LYS	2.4
1	D	742	ARG	2.4
1	D	415	LYS	2.3
1	B	435	GLY	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

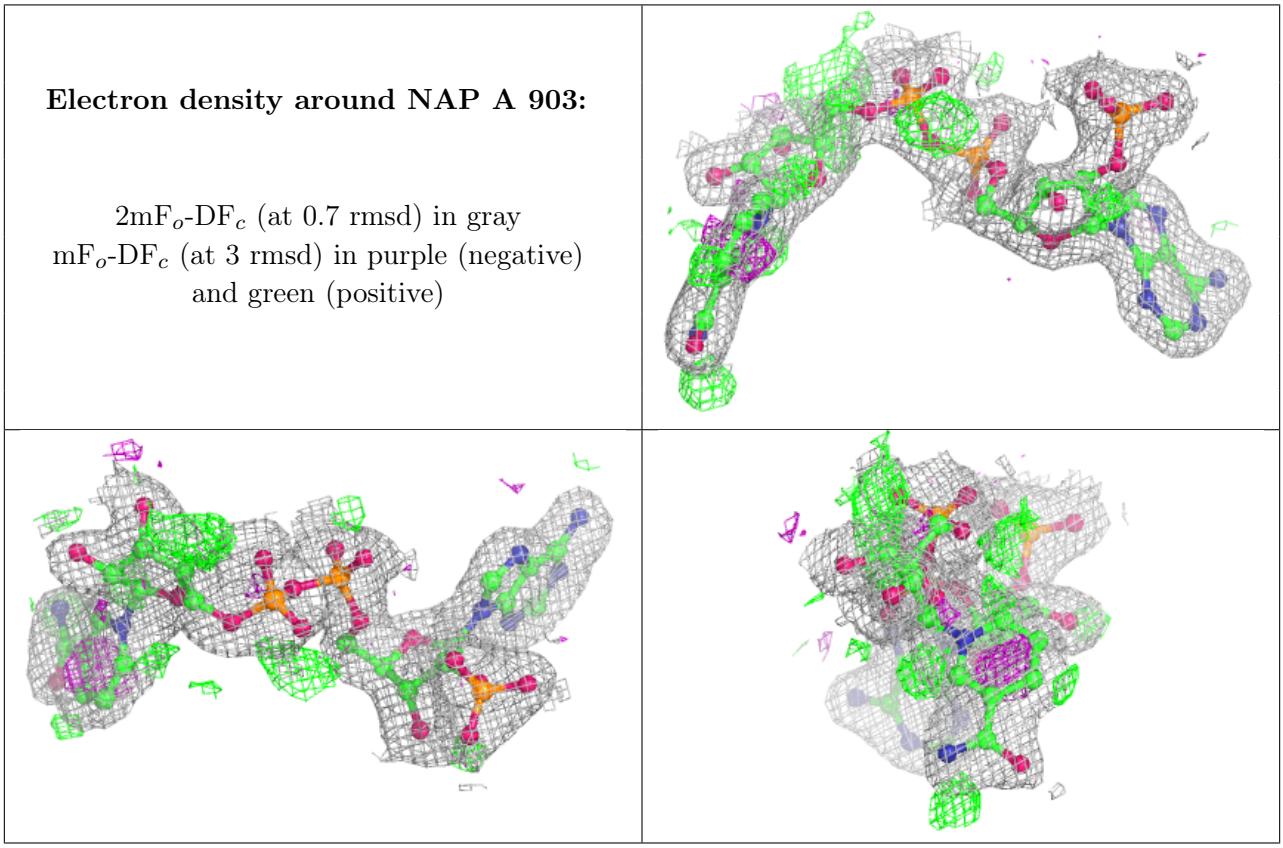
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	SO4	A	11	5/5	0.79	0.27	52,52,53,53	5
4	GOL	A	29	6/6	0.79	0.24	49,50,52,54	0
4	GOL	C	31	6/6	0.82	0.23	43,45,46,47	0
4	GOL	B	30	6/6	0.84	0.24	46,46,47,50	0
3	SO4	D	12	5/5	0.85	0.20	48,48,48,49	5
3	SO4	C	10	5/5	0.85	0.18	46,46,47,47	5
4	GOL	D	32	6/6	0.85	0.20	51,53,54,56	0
3	SO4	A	21	5/5	0.86	0.26	39,40,41,41	5
3	SO4	A	24	5/5	0.88	0.22	37,38,39,39	5
3	SO4	B	9	5/5	0.88	0.14	47,47,48,48	5
3	SO4	D	20	5/5	0.90	0.14	42,42,42,43	5
3	SO4	B	22	5/5	0.92	0.22	41,42,42,42	5
3	SO4	C	23	5/5	0.93	0.16	41,42,43,43	5
3	SO4	D	27	5/5	0.93	0.14	36,36,36,37	5
3	SO4	C	28	5/5	0.94	0.13	34,36,38,38	5
3	SO4	B	19	5/5	0.94	0.15	37,38,39,39	5
3	SO4	C	17	5/5	0.94	0.16	42,42,42,42	5
3	SO4	B	5	5/5	0.94	0.14	34,35,36,37	5
3	SO4	A	6	5/5	0.95	0.12	28,30,32,33	5
3	SO4	A	18	5/5	0.95	0.12	41,41,42,42	5
3	SO4	C	7	5/5	0.95	0.11	32,33,34,34	5
3	SO4	C	26	5/5	0.95	0.14	34,35,35,36	5
3	SO4	B	25	5/5	0.96	0.10	37,37,37,38	5
3	SO4	A	1	5/5	0.96	0.11	44,44,45,46	5
3	SO4	B	3	5/5	0.96	0.15	21,21,21,21	5
2	NAP	A	903	48/48	0.96	0.10	19,26,34,36	0
2	NAP	B	903	48/48	0.96	0.09	22,28,34,35	0
2	NAP	C	903	48/48	0.96	0.10	17,22,28,31	0
2	NAP	D	903	48/48	0.96	0.10	22,25,32,35	0
3	SO4	A	2	5/5	0.97	0.10	31,32,33,34	5
3	SO4	D	16	5/5	0.97	0.11	25,30,32,32	0
3	SO4	B	4	5/5	0.97	0.10	26,28,28,29	5
3	SO4	B	14	5/5	0.97	0.17	34,38,39,39	0
3	SO4	D	8	5/5	0.98	0.10	29,30,31,32	5
3	SO4	A	15	5/5	0.98	0.12	27,31,33,33	0
3	SO4	C	13	5/5	0.98	0.12	27,31,33,33	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.

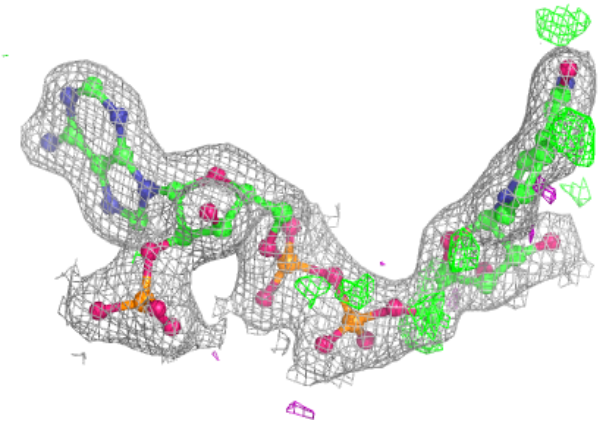
Electron density around NAP A 903:

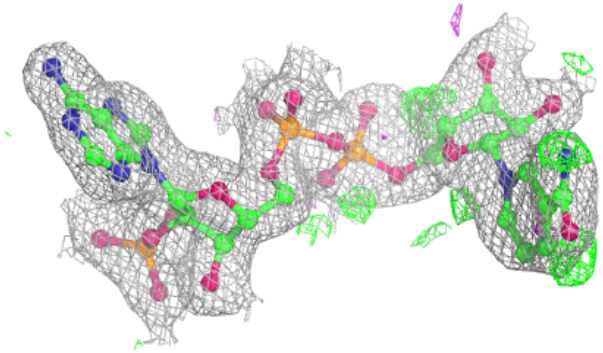
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

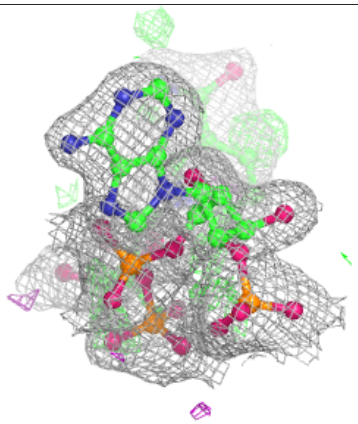


Electron density around NAP B 903:

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

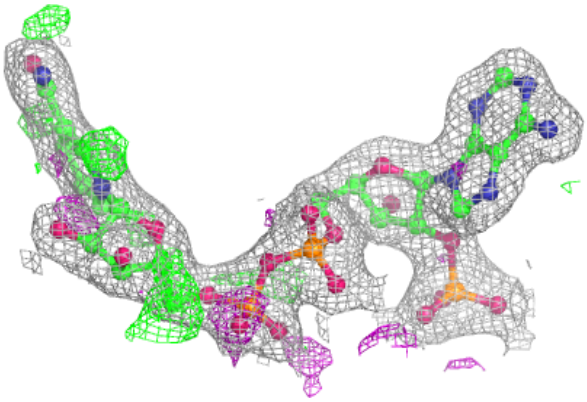


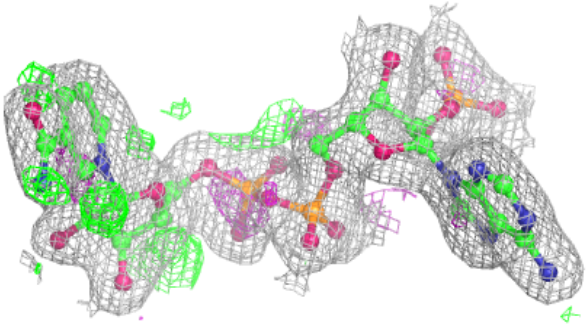


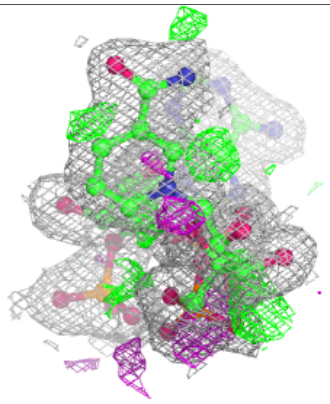


Electron density around NAP C 903:

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

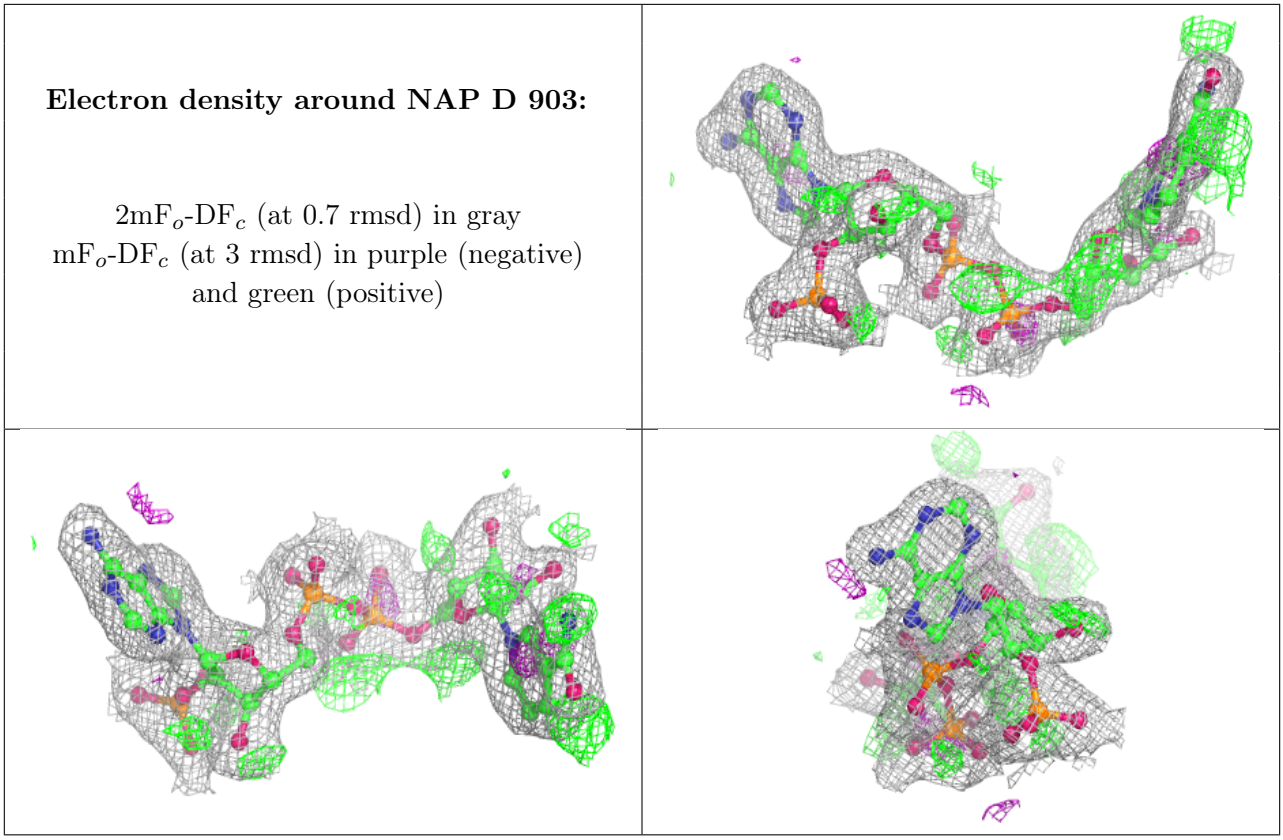






Electron density around NAP D 903:

$2mF_o$-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.