Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 12:11 PM EDT

PDB ID	:	2O2R
Title	:	Crystal structure of the C-terminal domain of rat 10'formyltetrahydrofolate dehydrogenase in complex with NADPH
Authors	:	Tsybovsky, Y.; Donato, H.; Krupenko, N.I.; Davies, C.; Krupenko, S.A.
Deposited on	:	2006-11-30
Resolution	:	2.20 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:

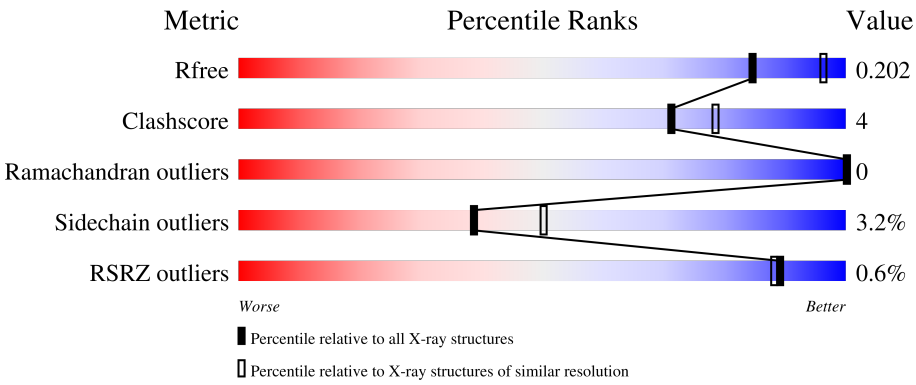
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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% 9% •
1	B	517	% 87% 9% •
1	C	517	% 87% 8% • •
1	D	517	87% 8% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16615 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 Formyltetrahydrofolate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	498	3902	2478	672	731	21	0	15	0
1	B	498	3897	2473	672	731	21	0	16	0
1	C	498	3884	2466	672	725	21	0	13	0
1	D	498	3894	2472	669	732	21	0	15	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	MET	-	initiating methionine	UNP Q5HZB2
A	387	ARG	-	cloning artifact	UNP Q5HZB2
A	388	GLY	-	cloning artifact	UNP Q5HZB2
A	389	SER	-	cloning artifact	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	-	cloning artifact	UNP Q5HZB2
A	396	THR	-	cloning artifact	UNP Q5HZB2
B	386	MET	-	initiating methionine	UNP Q5HZB2
B	387	ARG	-	cloning artifact	UNP Q5HZB2
B	388	GLY	-	cloning artifact	UNP Q5HZB2
B	389	SER	-	cloning artifact	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
B	395	THR	-	cloning artifact	UNP Q5HZB2

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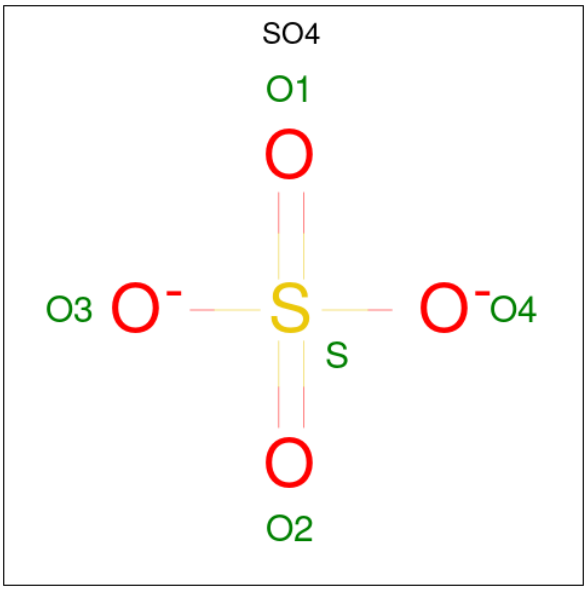
Chain	Residue	Modelled	Actual	Comment	Reference
B	396	THR	-	cloning artifact	UNP Q5HZB2
C	386	MET	-	initiating methionine	UNP Q5HZB2
C	387	ARG	-	cloning artifact	UNP Q5HZB2
C	388	GLY	-	cloning artifact	UNP Q5HZB2
C	389	SER	-	cloning artifact	UNP Q5HZB2
C	390	HIS	-	expression tag	UNP Q5HZB2
C	391	HIS	-	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	-	cloning artifact	UNP Q5HZB2
C	396	THR	-	cloning artifact	UNP Q5HZB2
D	386	MET	-	initiating methionine	UNP Q5HZB2
D	387	ARG	-	cloning artifact	UNP Q5HZB2
D	388	GLY	-	cloning artifact	UNP Q5HZB2
D	389	SER	-	cloning artifact	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	-	cloning artifact	UNP Q5HZB2
D	396	THR	-	cloning artifact	UNP Q5HZB2

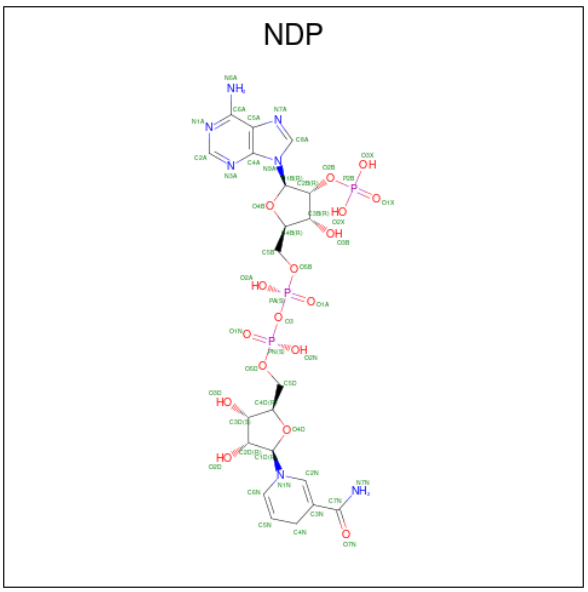
- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

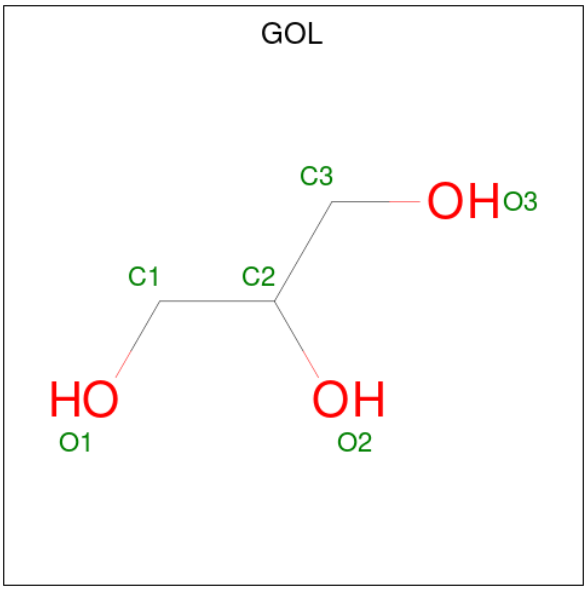
- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
3	B	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
3	C	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
3	D	1	31	10	5	13	3	0	0

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



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

- Molecule 5 is water.

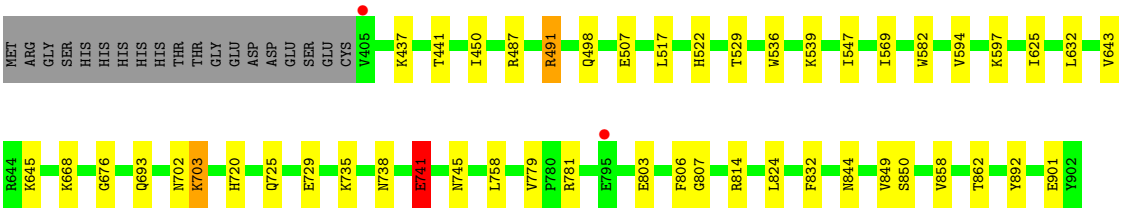
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	173	173	173	0	2
5	B	173	173	173	0	2
5	C	229	229	229	0	4
5	D	210	210	210	0	3

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.

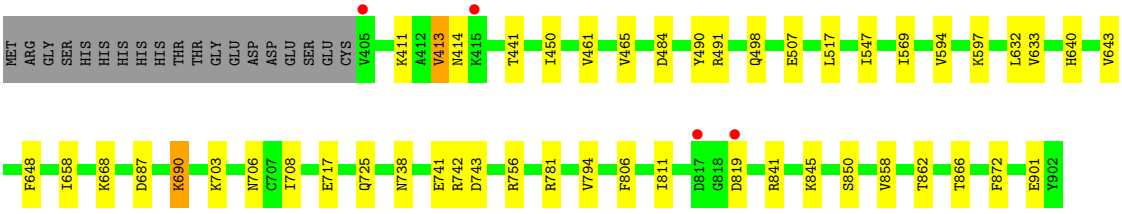
• Molecule 1: Formyltetrahydrofolate dehydrogenase

Chain A:



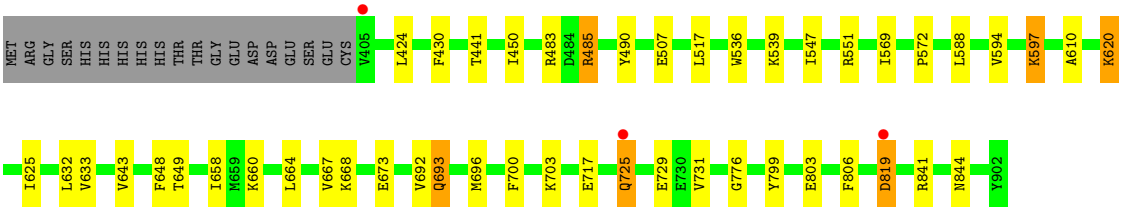
• Molecule 1: Formyltetrahydrofolate dehydrogenase

Chain B:



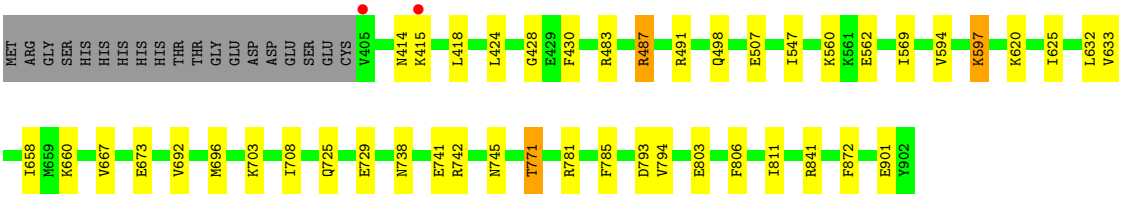
• Molecule 1: Formyltetrahydrofolate dehydrogenase

Chain C:



• Molecule 1: Formyltetrahydrofolate dehydrogenase

Chain D:


MET
ARG
GLY
SER
HIS
HIS
HIS
HIS
HIS
THR
THR
GLY
GLU
ASP
ASP
GLU
SER
GLU
CYS
V405
N414
K415
L418
L424
G428
E429
F430
R483
R487
R491
Q498
E507
I547
K560
K561
E562
I569
V594
K597
K620
I625
L632
V633
I658
M659
K660
V667
E673
V692
M696
K703
I708
Q725
E729
N738
E741
R742
N745
T771
R781
F785
D793
V794
E803
F806
I811
R841
F872
E901
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	258.70Å 194.30Å 97.10Å 90.00° 108.90° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 49.85 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.20) 99.2 (49.85-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.66 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.180 , 0.202 0.179 , 0.202	Depositor DCC
R_{free} test set	11302 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 44.2	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	0.95	EDS
Total number of atoms	16615	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: SO4, NDP, GOL

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	0.59	0/4041	0.65	2/5463 (0.0%)
1	B	0.59	0/4050	0.63	0/5475
1	C	0.65	0/4023	0.67	1/5439 (0.0%)
1	D	0.60	0/4039	0.65	0/5461
All	All	0.61	0/16153	0.65	3/21838 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	741[A]	GLU	OE1-CD-OE2	-5.43	116.78	123.30
1	A	741[B]	GLU	OE1-CD-OE2	-5.43	116.78	123.30
1	C	485	ARG	NE-CZ-NH2	-5.38	117.61	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	741[A]	GLU	Sidechain
1	A	741[B]	GLU	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	3902	0	3927	30	0
1	B	3897	0	3914	29	0
1	C	3884	0	3905	33	0
1	D	3894	0	3906	29	0
2	A	25	0	0	0	0
2	B	25	0	0	0	0
2	C	30	0	0	0	0
2	D	25	0	0	0	0
3	A	31	0	11	0	0
3	B	31	0	11	0	0
3	C	31	0	11	0	0
3	D	31	0	11	1	0
4	A	6	0	8	0	0
4	B	6	0	8	2	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	A	173	0	0	3	0
5	B	173	0	0	3	0
5	C	229	0	0	1	0
5	D	210	0	0	2	0
All	All	16615	0	15728	111	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 4.

All (111) 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:C:841[B]:ARG:HG2	1:C:841[B]:ARG:HH11	1.14	1.11
1:D:725[A]:GLN:NE2	1:D:729:GLU:OE2	1.84	1.10
1:B:841[B]:ARG:HG2	1:B:841[B]:ARG:HH11	1.02	1.08
1:A:725[A]:GLN:NE2	1:A:729:GLU:OE2	1.88	1.06
1:C:692:VAL:O	1:C:696:MET:HG3	1.64	0.97
1:B:841[B]:ARG:HG2	1:B:841[B]:ARG:NH1	1.82	0.90
1:A:569:ILE:HD12	1:A:594:VAL:HG21	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725[A]:GLN:HE21	1:A:729:GLU:CD	1.82	0.83
1:C:610:ALA:HB2	1:C:625:ILE:HD12	1.67	0.76
1:A:491[B]:ARG:HH12	1:A:498:GLN:HE22	1.32	0.75
1:D:487:ARG:HG2	1:D:487:ARG:HH11	1.49	0.75
1:A:725[A]:GLN:NE2	1:A:729:GLU:CD	2.38	0.74
1:B:569:ILE:HD12	1:B:594:VAL:HG21	1.70	0.74
1:C:725[A]:GLN:OE1	1:C:729:GLU:OE2	2.07	0.73
1:D:428:GLY:HA3	1:D:620:LYS:HD2	1.69	0.72
1:C:799:TYR:CE2	1:C:803[A]:GLU:HG3	2.24	0.71
1:C:841[B]:ARG:HG2	1:C:841[B]:ARG:NH1	1.93	0.71
1:A:738:ASN:HB3	1:A:741[A]:GLU:HG3	1.73	0.70
1:A:491[A]:ARG:NH2	5:A:3169:HOH:O	2.24	0.69
1:C:648:PHE:CD1	1:C:658:ILE:HD12	2.25	0.69
1:D:491[B]:ARG:HH12	1:D:498:GLN:HE22	1.42	0.68
1:D:771:THR:CG2	1:D:793:ASP:OD1	2.42	0.67
1:A:491[B]:ARG:HH12	1:A:498:GLN:NE2	1.92	0.66
1:C:776:GLY:O	5:C:3227:HOH:O	2.14	0.65
1:D:692:VAL:O	1:D:696:MET:HG2	1.97	0.64
1:B:414:ASN:OD1	1:B:742:ARG:NH2	2.33	0.60
1:C:569:ILE:HD12	1:C:594:VAL:HG21	1.84	0.58
1:A:487:ARG:NH1	1:C:490[B]:TYR:OH	2.37	0.58
1:C:696:MET:HE1	1:C:731:VAL:HG23	1.86	0.58
1:C:696:MET:HE3	1:C:700:PHE:HE2	1.70	0.56
1:D:771:THR:HG21	1:D:793:ASP:OD1	2.04	0.56
1:B:687:ASP:HB3	1:B:690:LYS:HD3	1.87	0.55
1:D:771:THR:HG23	1:D:793:ASP:OD1	2.06	0.55
1:D:781[B]:ARG:HD2	1:D:785:PHE:CD2	2.42	0.55
1:D:560[B]:LYS:HE3	1:D:562:GLU:HG2	1.89	0.54
1:C:648:PHE:CD1	1:C:658:ILE:CD1	2.91	0.53
1:C:632:LEU:C	1:C:632:LEU:HD23	2.28	0.53
1:D:658:ILE:HD11	3:D:903:NDP:C2A	2.39	0.53
1:D:794:VAL:HG21	1:D:811:ILE:HG23	1.91	0.53
1:D:901:GLU:OE2	5:D:3206:HOH:O	2.19	0.53
1:A:517:LEU:CD2	1:A:522:HIS:CE1	2.92	0.52
1:D:708:ILE:CG2	1:D:872:PHE:HE1	2.22	0.52
1:A:632:LEU:C	1:A:632:LEU:HD23	2.30	0.52
1:A:539:LYS:HD3	1:C:536:TRP:CE2	2.45	0.51
1:C:819:ASP:C	1:C:819:ASP:OD2	2.48	0.51
1:C:643:VAL:O	1:C:668:LYS:HE3	2.10	0.51
1:A:850:SER:HB3	1:A:858:VAL:HG11	1.92	0.51
1:B:461:VAL:HG22	1:B:633:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:ASN:OD1	1:D:742:ARG:NH2	2.40	0.49
1:D:708:ILE:CG2	1:D:872:PHE:CE1	2.95	0.49
1:A:693[B]:GLN:NE2	5:A:3148:HOH:O	2.46	0.49
1:D:424:LEU:O	1:D:430:PHE:HA	2.12	0.48
5:B:3056:HOH:O	1:D:483:ARG:HD3	2.12	0.48
1:B:491[B]:ARG:HH12	1:B:498:GLN:HE22	1.63	0.47
1:B:738:ASN:HB3	1:B:741[A]:GLU:HG3	1.96	0.47
1:D:569:ILE:HD12	1:D:594:VAL:HG21	1.97	0.47
1:A:720:HIS:CD2	1:A:814:ARG:HG2	2.49	0.47
1:A:702:ASN:O	1:A:703:LYS:HG2	2.15	0.47
1:D:487:ARG:HH11	1:D:487:ARG:CG	2.24	0.47
1:B:490[A]:TYR:OH	1:D:487:ARG:NH1	2.48	0.46
1:C:424:LEU:O	1:C:430:PHE:HA	2.16	0.46
1:C:441:THR:HG23	1:C:450:ILE:HB	1.97	0.46
1:D:632:LEU:C	1:D:632:LEU:HD23	2.36	0.46
1:A:529:THR:HG21	1:A:582:TRP:HA	1.97	0.46
1:D:597:LYS:HG2	1:D:633:VAL:HG11	1.98	0.46
1:B:484:ASP:OD2	5:B:3168:HOH:O	2.21	0.45
1:C:660:LYS:HG3	1:D:660:LYS:HG3	1.97	0.45
1:A:844:ASN:HD22	1:D:841[B]:ARG:HH21	1.64	0.45
1:D:620:LYS:HG2	5:D:3126:HOH:O	2.17	0.45
1:A:824:LEU:HD21	1:A:849:VAL:HG13	1.98	0.45
1:B:794:VAL:HG21	1:B:811:ILE:HG23	1.98	0.44
1:A:441:THR:HG23	1:A:450:ILE:HB	1.99	0.44
1:B:841[B]:ARG:HH12	1:C:844:ASN:ND2	2.16	0.44
1:B:411:LYS:HG2	1:B:413:VAL:HG22	2.00	0.44
1:D:597:LYS:HG2	1:D:633:VAL:CG1	2.48	0.44
1:B:706:ASN:HD21	4:B:3002:GOL:H12	1.82	0.43
1:C:692:VAL:O	1:C:696:MET:CG	2.52	0.43
1:A:779:VAL:HG12	1:A:781[B]:ARG:HG2	2.01	0.43
1:C:620:LYS:O	1:C:620:LYS:HG2	2.19	0.43
1:B:648:PHE:CD1	1:B:658:ILE:CD1	3.02	0.43
1:B:465:VAL:HG11	1:B:640:HIS:CE1	2.54	0.43
1:B:648:PHE:CD1	1:B:658:ILE:HD12	2.54	0.43
1:A:536:TRP:CE2	1:C:539:LYS:HD3	2.54	0.43
5:A:3055:HOH:O	1:C:483:ARG:HD3	2.19	0.42
1:B:708:ILE:CG2	1:B:872:PHE:CE1	3.02	0.42
1:D:738:ASN:HB3	1:D:741[A]:GLU:HG3	2.02	0.42
1:B:850:SER:HB3	1:B:858:VAL:HG11	2.01	0.42
1:C:664:LEU:HD21	1:D:660:LYS:HD3	2.01	0.42
1:A:676:GLY:HA2	1:A:832:PHE:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:ARG:HD3	1:C:588:LEU:O	2.19	0.42
1:C:696:MET:CE	1:C:700:PHE:HE2	2.31	0.42
1:B:756[B]:ARG:HD3	5:B:3099:HOH:O	2.20	0.41
1:A:758:LEU:HD21	1:A:807:GLY:HA3	2.02	0.41
1:A:862:THR:HB	1:B:901:GLU:HB2	2.02	0.41
1:B:866:THR:HG21	4:B:3002:GOL:H11	2.02	0.41
1:A:758:LEU:CD2	1:A:807:GLY:HA3	2.51	0.41
1:B:441:THR:HG23	1:B:450:ILE:HB	2.03	0.41
1:C:572:PRO:HG3	1:C:649:THR:HG22	2.03	0.41
1:C:693[A]:GLN:HE21	1:C:693[A]:GLN:HB3	1.65	0.41
1:C:696:MET:CE	1:C:700:PHE:CE2	3.04	0.41
1:A:569:ILE:CD1	1:A:594:VAL:HG21	2.38	0.40
1:A:645:LYS:HE3	1:A:892:TYR:CE1	2.56	0.40
1:B:632:LEU:C	1:B:632:LEU:HD23	2.42	0.40
1:C:597:LYS:HG2	1:C:633:VAL:HG11	2.03	0.40
1:A:901:GLU:HB2	1:B:862:THR:HB	2.04	0.40
1:B:643:VAL:O	1:B:668:LYS:HE3	2.21	0.40
1:A:643:VAL:O	1:A:668:LYS:HE3	2.22	0.40
1:B:491[B]:ARG:NH1	1:B:498:GLN:HE22	2.19	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	511/517 (99%)	498 (98%)	13 (2%)	0	100	100
1	B	512/517 (99%)	495 (97%)	17 (3%)	0	100	100
1	C	509/517 (98%)	493 (97%)	16 (3%)	0	100	100
1	D	511/517 (99%)	496 (97%)	15 (3%)	0	100	100
All	All	2043/2068 (99%)	1982 (97%)	61 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	424/426 (100%)	411 (97%)	13 (3%)	40	51
1	B	425/426 (100%)	408 (96%)	17 (4%)	31	40
1	C	422/426 (99%)	406 (96%)	16 (4%)	33	42
1	D	424/426 (100%)	409 (96%)	15 (4%)	36	46
All	All	1695/1704 (100%)	1634 (96%)	61 (4%)	39	45

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	437	LYS
1	A	491[A]	ARG
1	A	491[B]	ARG
1	A	507	GLU
1	A	547	ILE
1	A	597	LYS
1	A	625	ILE
1	A	703	LYS
1	A	735	LYS
1	A	745	ASN
1	A	803[A]	GLU
1	A	803[B]	GLU
1	A	806	PHE
1	B	413	VAL
1	B	507	GLU
1	B	517	LEU
1	B	547	ILE
1	B	597	LYS
1	B	690	LYS
1	B	703	LYS
1	B	717	GLU
1	B	725[A]	GLN

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Mol	Chain	Res	Type
1	B	725[B]	GLN
1	B	743[A]	ASP
1	B	743[B]	ASP
1	B	781[A]	ARG
1	B	781[B]	ARG
1	B	806	PHE
1	B	819	ASP
1	B	845	LYS
1	C	507	GLU
1	C	517	LEU
1	C	547	ILE
1	C	551	ARG
1	C	597	LYS
1	C	620	LYS
1	C	667	VAL
1	C	673	GLU
1	C	693[A]	GLN
1	C	693[B]	GLN
1	C	703	LYS
1	C	717	GLU
1	C	725[A]	GLN
1	C	725[B]	GLN
1	C	806	PHE
1	C	819	ASP
1	D	415	LYS
1	D	418	LEU
1	D	487	ARG
1	D	507	GLU
1	D	547	ILE
1	D	597	LYS
1	D	625	ILE
1	D	667	VAL
1	D	673	GLU
1	D	703	LYS
1	D	745	ASN
1	D	771	THR
1	D	803[A]	GLU
1	D	803[B]	GLU
1	D	806	PHE

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	498	GLN
1	A	706	ASN
1	A	745	ASN
1	A	750	ASN
1	B	498	GLN
1	B	706	ASN
1	B	750	ASN
1	C	498	GLN
1	C	541	GLN
1	C	706	ASN
1	C	797	HIS
1	D	498	GLN
1	D	706	ASN
1	D	745	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)

29 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	A	3001	-	5,5,5	0.36	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	2009	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	C	2010	-	4,4,4	0.15	0	6,6,6	0.10	0
4	GOL	D	3004	-	5,5,5	0.37	0	5,5,5	0.37	0
2	SO4	B	2003	-	4,4,4	0.19	0	6,6,6	0.21	0
2	SO4	A	2006	-	4,4,4	0.16	0	6,6,6	0.44	0
2	SO4	A	2011	-	4,4,4	0.12	0	6,6,6	0.15	0
2	SO4	B	2005	-	4,4,4	0.12	0	6,6,6	0.24	0
3	NDP	C	903	-	27,33,52	1.24	3 (11%)	35,52,80	1.42	5 (14%)
2	SO4	D	2004	-	4,4,4	0.12	0	6,6,6	0.15	0
4	GOL	B	3002	-	5,5,5	0.39	0	5,5,5	0.38	0
2	SO4	B	2020	-	4,4,4	0.18	0	6,6,6	0.18	0
2	SO4	C	2001	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	D	2016	-	4,4,4	0.20	0	6,6,6	0.61	0
3	NDP	D	903	-	27,33,52	1.18	2 (7%)	35,52,80	1.49	5 (14%)
2	SO4	C	2007	-	4,4,4	0.16	0	6,6,6	0.45	0
3	NDP	B	903	-	27,33,52	1.24	2 (7%)	35,52,80	1.39	3 (8%)
2	SO4	A	2019	-	4,4,4	0.16	0	6,6,6	0.12	0
2	SO4	A	2015	-	4,4,4	0.19	0	6,6,6	0.56	0
2	SO4	C	2013	-	4,4,4	0.22	0	6,6,6	0.53	0
2	SO4	A	2002	-	4,4,4	0.14	0	6,6,6	0.15	0
2	SO4	D	2008	-	4,4,4	0.20	0	6,6,6	0.43	0
2	SO4	B	2014	-	4,4,4	0.22	0	6,6,6	0.55	0
2	SO4	D	2021	-	4,4,4	0.19	0	6,6,6	0.16	0
4	GOL	C	3003	-	5,5,5	0.39	0	5,5,5	0.33	0
2	SO4	C	2018	-	4,4,4	0.14	0	6,6,6	0.24	0
2	SO4	D	2012	-	4,4,4	0.15	0	6,6,6	0.12	0
3	NDP	A	903	-	27,33,52	1.27	4 (14%)	35,52,80	1.38	5 (14%)
2	SO4	C	2017	-	4,4,4	0.22	0	6,6,6	0.32	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
3	NDP	B	903	-	-	4/17/37/77	0/3/3/5
4	GOL	A	3001	-	-	4/4/4/4	-
3	NDP	C	903	-	-	3/17/37/77	0/3/3/5
4	GOL	C	3003	-	-	0/4/4/4	-
4	GOL	D	3004	-	-	0/4/4/4	-
4	GOL	B	3002	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	A	903	-	-	2/17/37/77	0/3/3/5
3	NDP	D	903	-	-	3/17/37/77	0/3/3/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903	NDP	C2A-N3A	3.90	1.38	1.32
3	B	903	NDP	C2A-N3A	3.85	1.38	1.32
3	C	903	NDP	C2A-N3A	3.72	1.38	1.32
3	D	903	NDP	C2A-N3A	3.34	1.37	1.32
3	A	903	NDP	C2A-N1A	2.50	1.38	1.33
3	B	903	NDP	C2A-N1A	2.48	1.38	1.33
3	C	903	NDP	C2A-N1A	2.24	1.38	1.33
3	C	903	NDP	PN-O5D	2.16	1.63	1.54
3	A	903	NDP	P2B-O2B	2.15	1.63	1.59
3	A	903	NDP	PN-O5D	2.13	1.63	1.54
3	D	903	NDP	PN-O5D	2.13	1.63	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	903	NDP	N3A-C2A-N1A	-5.71	119.76	128.68
3	B	903	NDP	N3A-C2A-N1A	-5.30	120.39	128.68
3	A	903	NDP	N3A-C2A-N1A	-5.13	120.66	128.68
3	C	903	NDP	N3A-C2A-N1A	-4.73	121.29	128.68
3	B	903	NDP	O2N-PN-O1N	3.37	123.89	110.68
3	D	903	NDP	O5D-PN-O3	-2.86	95.04	104.64
3	A	903	NDP	O2N-PN-O1N	2.75	121.46	110.68
3	A	903	NDP	O4B-C1B-C2B	-2.73	101.86	106.59
3	C	903	NDP	O4B-C1B-C2B	-2.65	101.98	106.59
3	C	903	NDP	PA-O3-PN	-2.65	123.74	132.83
3	C	903	NDP	O5D-PN-O3	-2.60	95.93	104.64
3	D	903	NDP	PA-O3-PN	-2.59	123.95	132.83
3	A	903	NDP	PA-O3-PN	-2.55	124.07	132.83
3	D	903	NDP	O4B-C1B-C2B	-2.43	102.37	106.59
3	A	903	NDP	C4A-C5A-N7A	-2.37	106.93	109.40
3	B	903	NDP	PA-O3-PN	-2.18	125.34	132.83
3	C	903	NDP	C4A-C5A-N7A	-2.16	107.15	109.40
3	D	903	NDP	C1B-N9A-C4A	-2.11	122.93	126.64

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3001	GOL	O1-C1-C2-C3
4	A	3001	GOL	C1-C2-C3-O3
4	A	3001	GOL	O2-C2-C3-O3
4	B	3002	GOL	C1-C2-C3-O3
3	D	903	NDP	PN-O3-PA-O1A
4	A	3001	GOL	O1-C1-C2-O2
4	B	3002	GOL	O2-C2-C3-O3
3	B	903	NDP	PN-O3-PA-O1A
3	C	903	NDP	PN-O3-PA-O2A
3	B	903	NDP	PN-O3-PA-O2A
3	A	903	NDP	C2B-O2B-P2B-O1X
3	B	903	NDP	C2B-O2B-P2B-O1X
3	C	903	NDP	C2B-O2B-P2B-O1X
3	C	903	NDP	PN-O3-PA-O1A
3	D	903	NDP	PN-O3-PA-O2A
3	B	903	NDP	C1B-C2B-O2B-P2B
3	A	903	NDP	C3B-C2B-O2B-P2B
3	D	903	NDP	C3B-C2B-O2B-P2B

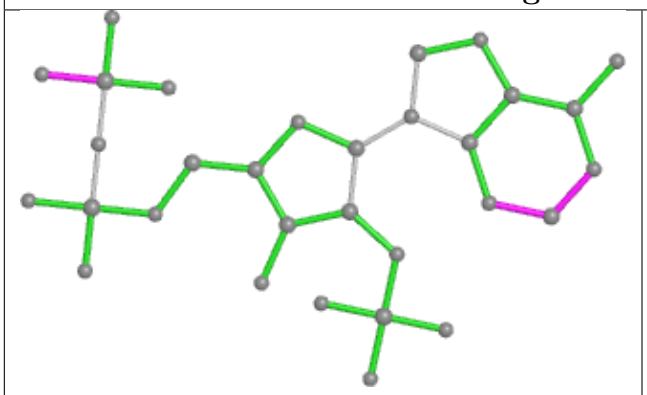
There are no ring outliers.

2 monomers are involved in 3 short contacts:

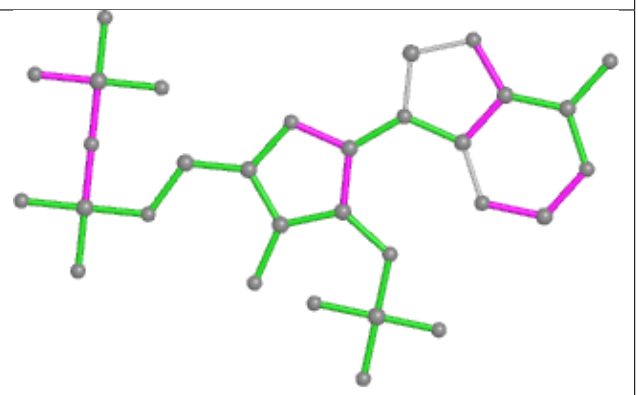
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	3002	GOL	2	0
3	D	903	NDP	1	0

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.

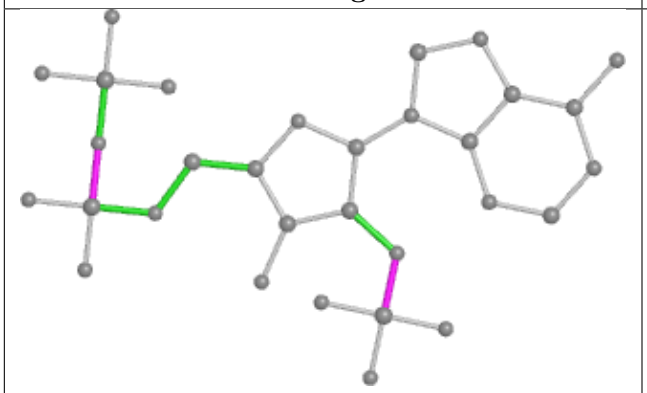
Ligand NDP C 903



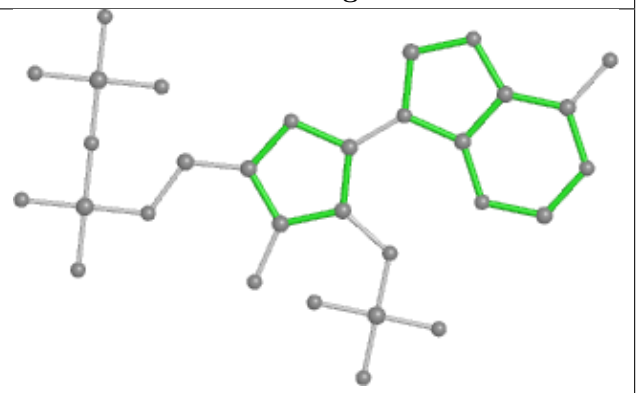
Bond lengths



Bond angles

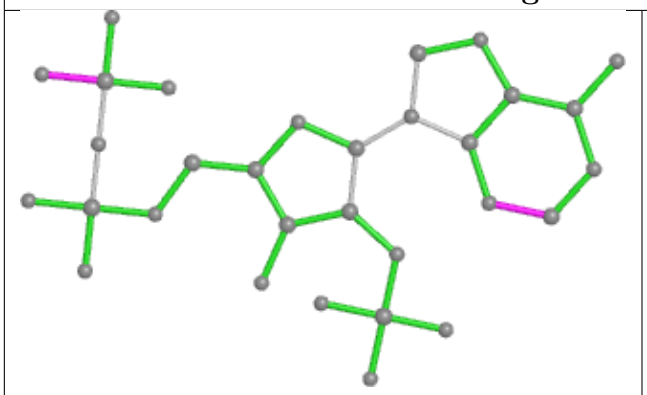


Torsions

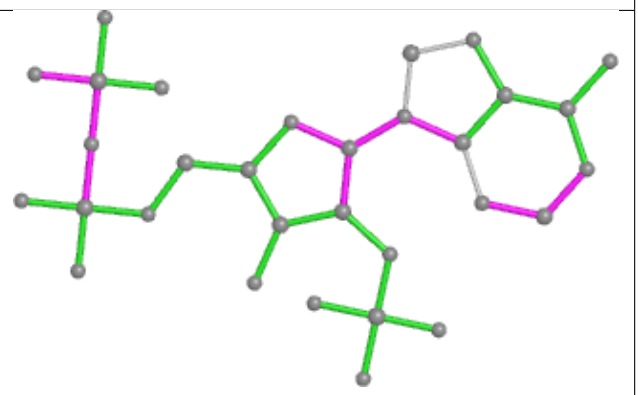


Rings

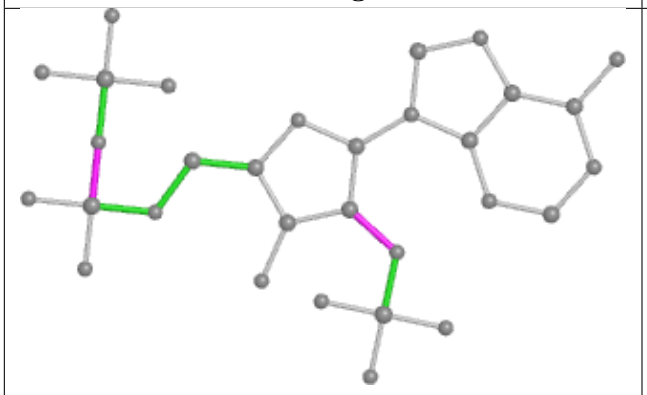
Ligand NDP D 903



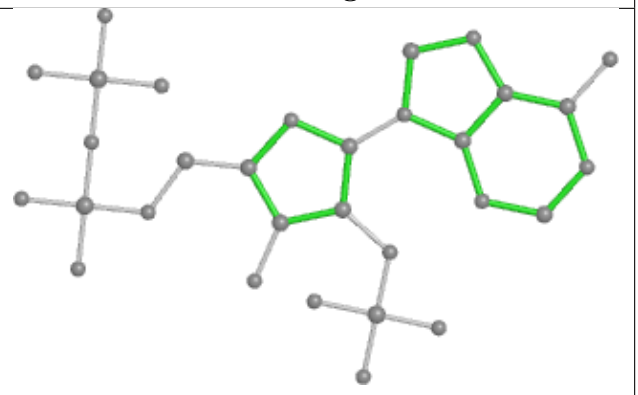
Bond lengths



Bond angles

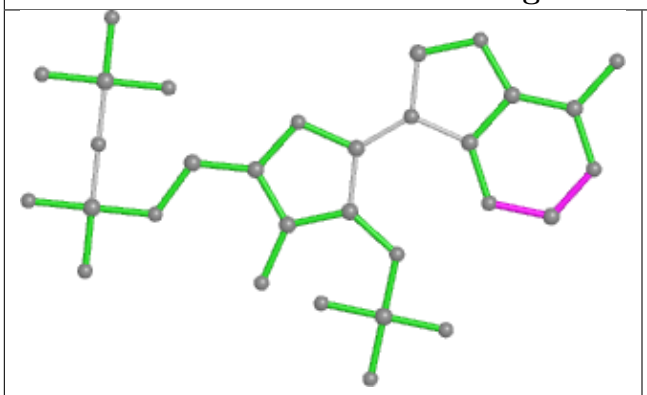


Torsions

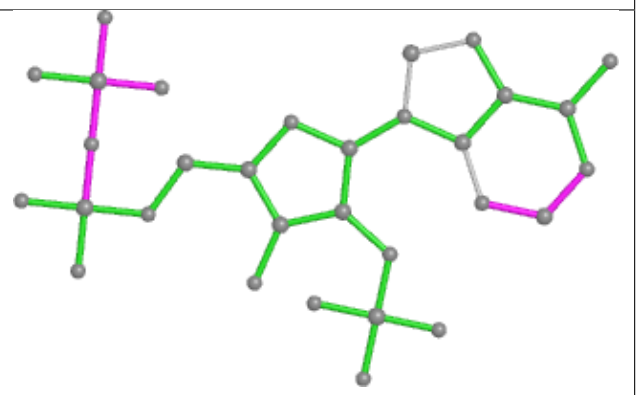


Rings

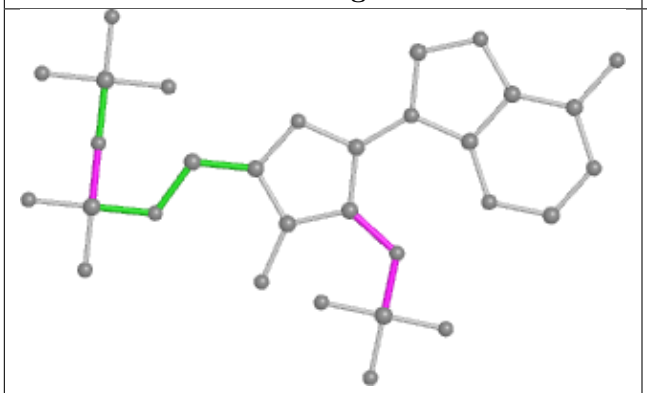
Ligand NDP B 903



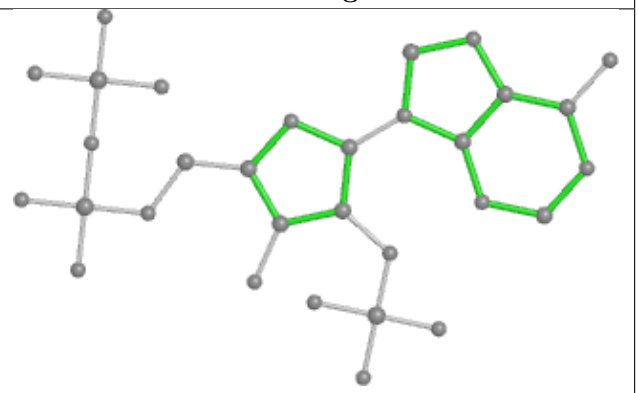
Bond lengths



Bond angles

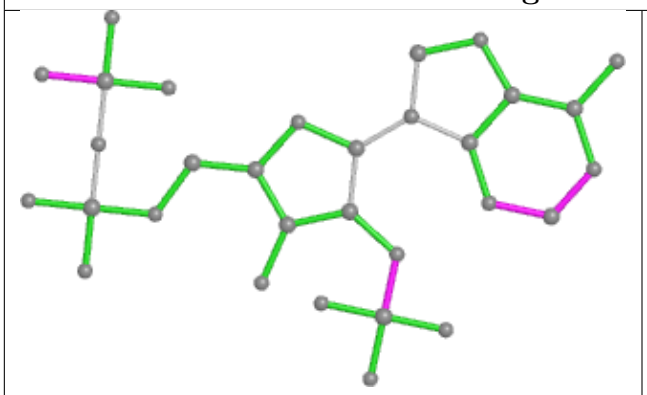


Torsions

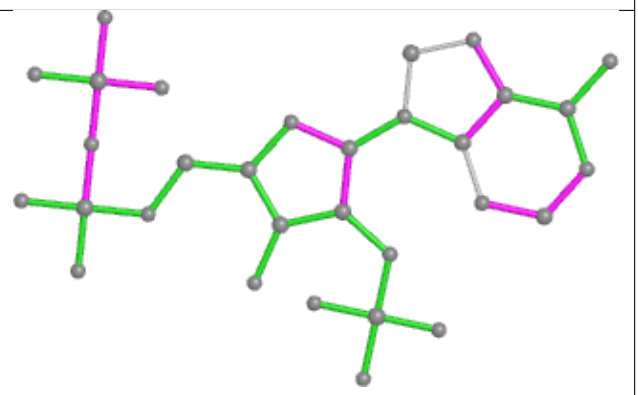


Rings

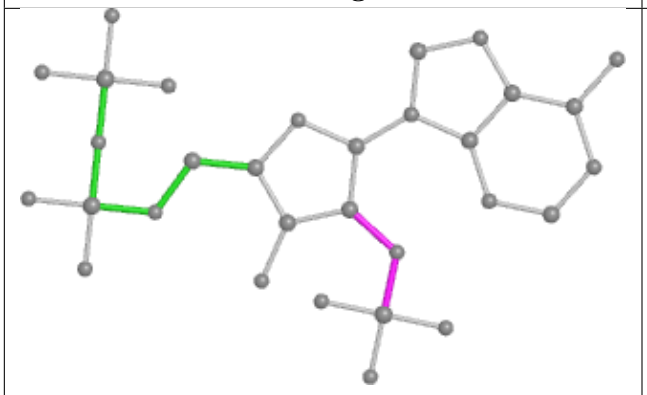
Ligand NDP A 903



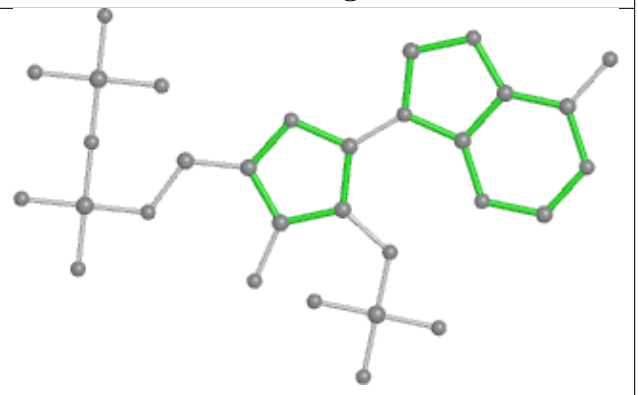
Bond lengths



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 (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	498/517 (96%)	-0.27	2 (0%)	92	91	9, 25, 38, 46	13 (2%)
1	B	498/517 (96%)	-0.29	4 (0%)	86	85	12, 26, 36, 52	12 (2%)
1	C	498/517 (96%)	-0.49	3 (0%)	89	88	7, 19, 31, 42	13 (2%)
1	D	498/517 (96%)	-0.42	2 (0%)	92	91	10, 24, 37, 47	13 (2%)
All	All	1992/2068 (96%)	-0.37	11 (0%)	89	88	7, 24, 36, 52	51 (2%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	405	VAL	4.7
1	B	405	VAL	4.0
1	A	405	VAL	3.8
1	B	819	ASP	2.6
1	D	415	LYS	2.4
1	B	817	ASP	2.4
1	A	795[A]	GLU	2.2
1	C	725[A]	GLN	2.2
1	C	819	ASP	2.1
1	C	405	VAL	2.1
1	B	415	LYS	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

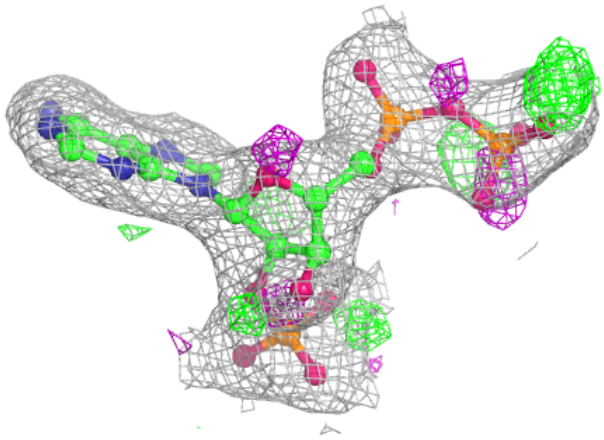
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

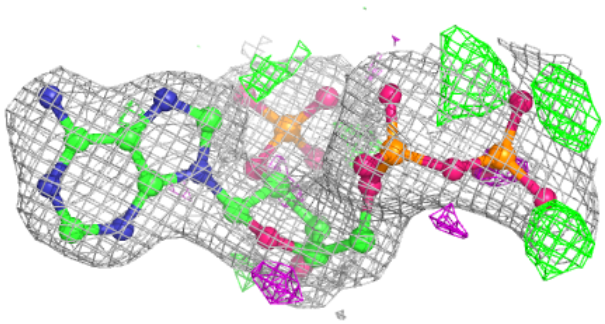
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	D	2012	5/5	0.71	0.26	55,55,56,56	5
2	SO4	A	2011	5/5	0.75	0.38	60,60,61,62	5
2	SO4	D	2021	5/5	0.82	0.16	47,48,48,49	5
2	SO4	C	2010	5/5	0.83	0.23	48,48,49,50	5
4	GOL	D	3004	6/6	0.83	0.27	65,66,67,68	0
4	GOL	C	3003	6/6	0.84	0.25	61,63,63,65	0
2	SO4	A	2019	5/5	0.84	0.18	47,47,48,49	5
2	SO4	B	2009	5/5	0.85	0.24	58,58,58,59	5
4	GOL	A	3001	6/6	0.85	0.20	55,56,57,58	0
2	SO4	C	2018	5/5	0.86	0.21	46,47,48,48	5
4	GOL	B	3002	6/6	0.88	0.21	57,58,59,59	0
2	SO4	B	2020	5/5	0.90	0.16	49,50,51,51	5
2	SO4	A	2015	5/5	0.92	0.28	19,28,30,30	5
2	SO4	B	2005	5/5	0.93	0.20	47,47,49,49	5
2	SO4	D	2008	5/5	0.93	0.14	34,37,37,38	5
2	SO4	C	2007	5/5	0.94	0.15	38,38,41,41	5
2	SO4	A	2006	5/5	0.94	0.15	36,37,39,40	5
3	NDP	A	903	31/48	0.95	0.11	21,28,46,49	0
3	NDP	B	903	31/48	0.95	0.11	27,29,47,48	0
2	SO4	A	2002	5/5	0.95	0.17	31,32,34,34	5
3	NDP	D	903	31/48	0.96	0.10	19,22,42,44	0
2	SO4	D	2016	5/5	0.96	0.18	22,30,31,34	5
2	SO4	D	2004	5/5	0.96	0.10	37,38,38,39	5
2	SO4	C	2013	5/5	0.96	0.17	30,34,35,36	5
2	SO4	B	2014	5/5	0.96	0.16	37,43,43,45	0
3	NDP	C	903	31/48	0.97	0.10	19,21,41,42	0
2	SO4	B	2003	5/5	0.97	0.14	24,24,25,25	5
2	SO4	C	2001	5/5	0.98	0.08	48,49,50,50	5
2	SO4	C	2017	5/5	0.98	0.11	25,30,30,30	5

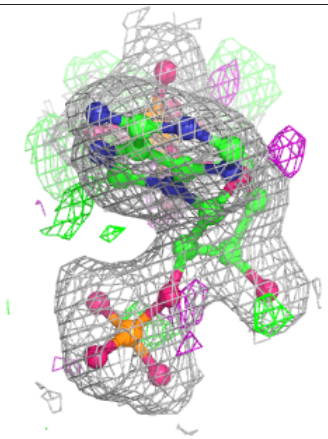
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP 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)

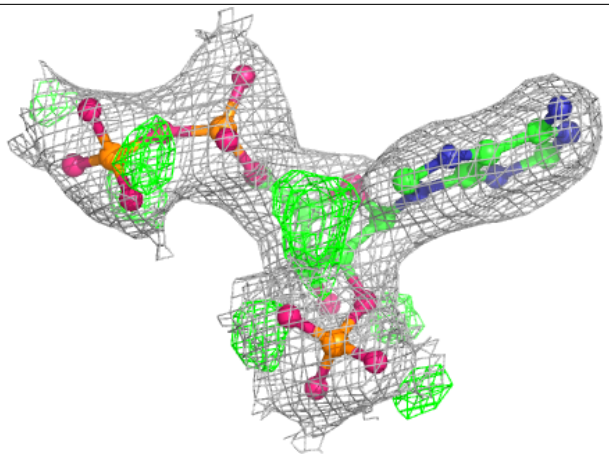


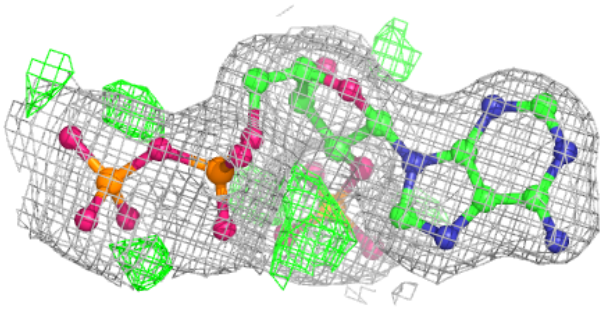


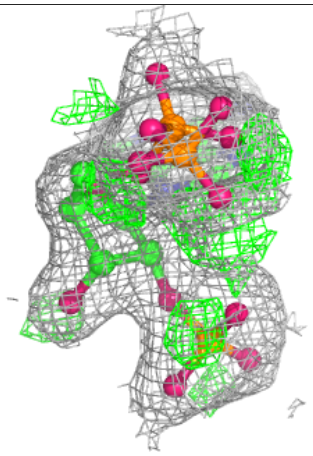


Electron density around NDP B 903:

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

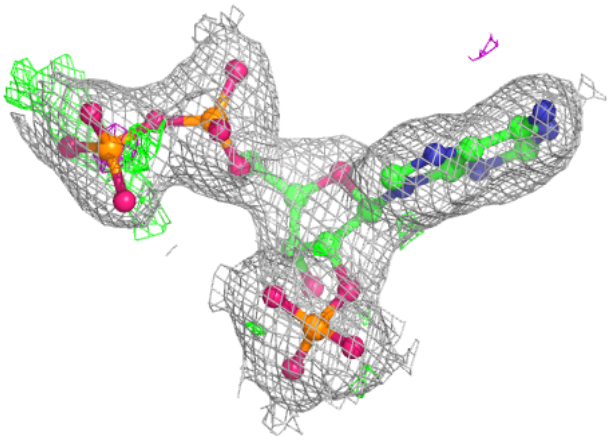


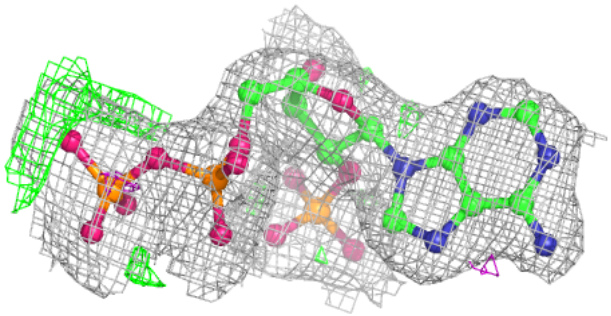


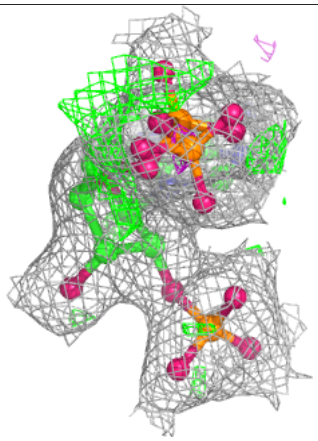


Electron density around NDP D 903:

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

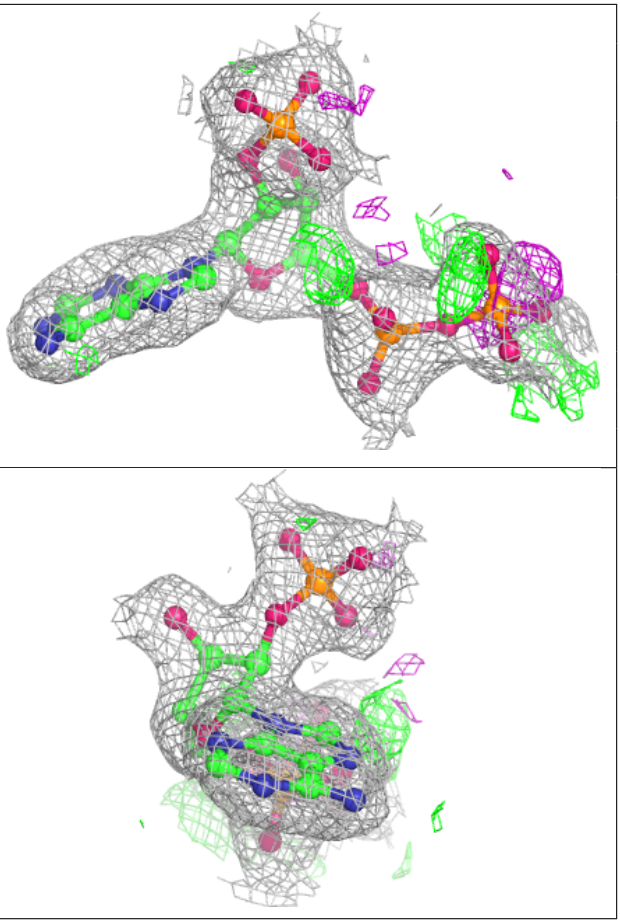






Electron density around NDP C 903:

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



6.5 Other polymers (i)

There are no such residues in this entry.