Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 04:29 pm BST

PDB ID	:	2VN8
Title	:	Crystal structure of human Reticulon 4 interacting protein 1 in complex with NADPH
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Deposited on	:	2008-01-31
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 (i) symbol.

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

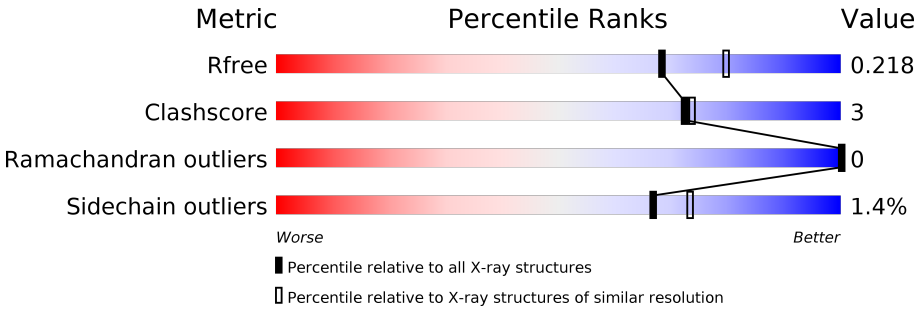
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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)

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 on 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%

Mol	Chain	Length	Quality of chain
1	A	375	91% 5% 5%
1	B	375	85% 9% • 5%

2 Entry composition

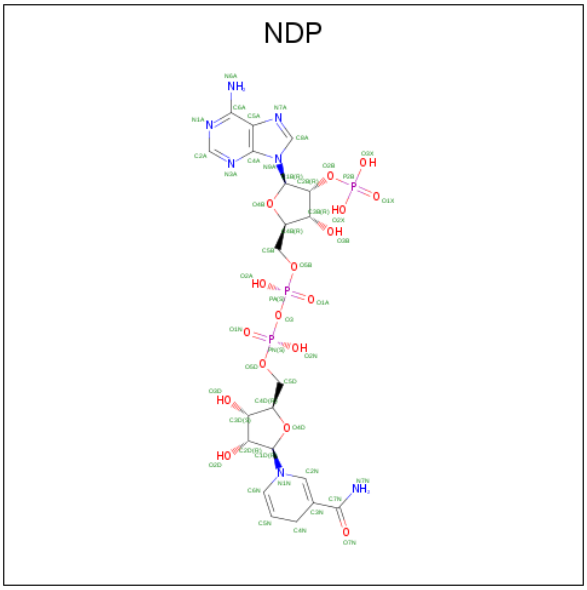
There are 6 unique types of molecules in this entry. The entry contains 5812 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RETICULON-4-INTERACTING PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2731	1758	462	497	14			
1	B	355	Total	C	N	O	S	0	3	0
			2681	1729	447	491	14			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

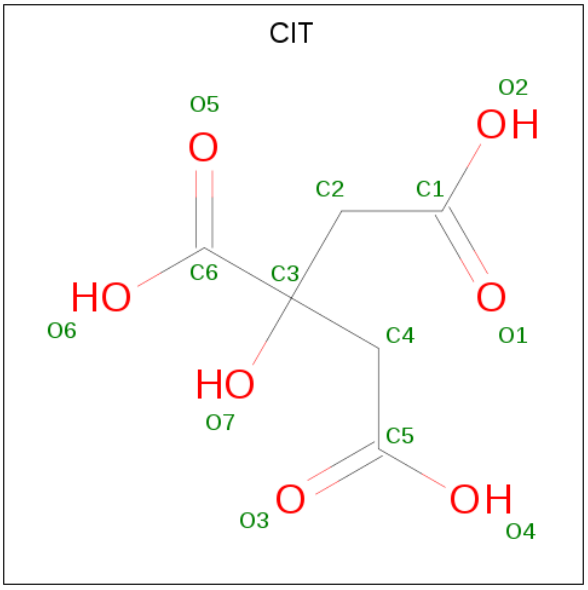


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

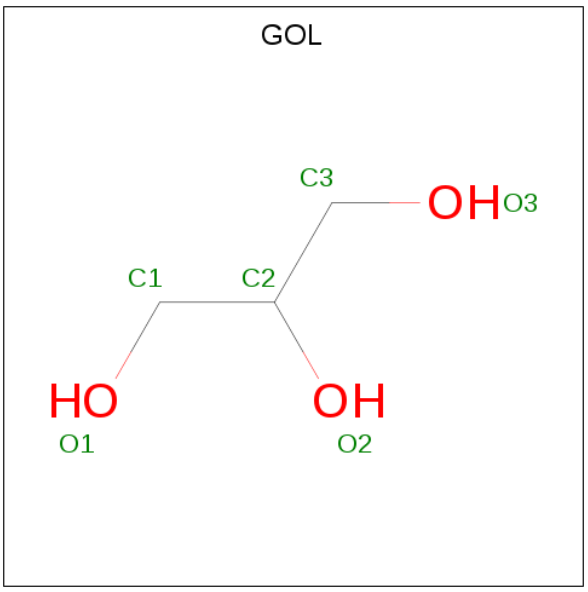
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	178	Total O 178 178	0	0
6	B	105	Total O 106 106	0	1

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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: RETICULON-4-INTERACTING PROTEIN 1

Chain A:

- Molecule 1: RETICULON-4-INTERACTING PROTEIN 1

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	106.95Å 106.95Å 177.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.10 45.80 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.10) 98.9 (45.80-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.175 , 0.213 0.180 , 0.218	Depositor DCC
R_{free} test set	1695 reflections (2.48%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 56.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5812	wwPDB-VP
Average B, all atoms (Å^2)	46.0	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, CIT, NA, NDP

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	0.73	1/2798 (0.0%)	0.73	0/3803
1	B	0.62	1/2761 (0.0%)	0.65	0/3761
All	All	0.68	2/5559 (0.0%)	0.69	0/7564

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	CYS	CB-SG	-9.59	1.66	1.82
1	A	203	CYS	CB-SG	-9.15	1.66	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2731	0	2704	8	0
1	B	2681	0	2603	22	0
2	A	48	0	26	6	0
2	B	48	0	26	4	0
3	A	1	0	0	0	0
4	A	13	0	4	1	0
5	B	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	178	0	0	1	0
6	B	106	0	0	2	0
All	All	5812	0	5371	37	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 (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:600:NDP:H52N	2:B:600:NDP:H6N	1.61	0.82
2:A:600:NDP:H52N	2:A:600:NDP:H6N	1.61	0.81
1:B:177:GLN:HA	1:B:366:ILE:HD11	1.66	0.77
1:B:97:THR:HG22	1:B:313:ILE:HD11	1.69	0.75
1:B:66:PRO:HB3	1:B:160:VAL:HG23	1.74	0.69
1:B:97:THR:HG22	1:B:313:ILE:CD1	2.25	0.67
1:A:300:LEU:O	2:A:600:NDP:H2N	1.99	0.61
2:A:600:NDP:C5D	2:A:600:NDP:H6N	2.31	0.59
1:B:45:ALA:HB3	1:B:63:MET:HG3	1.85	0.58
2:A:600:NDP:H42N	6:A:2078:HOH:O	2.04	0.58
1:B:300:LEU:O	2:B:600:NDP:H2N	2.04	0.57
1:B:147:VAL:HG22	1:B:161:VAL:HG12	1.87	0.56
2:B:600:NDP:H6N	2:B:600:NDP:C5D	2.34	0.56
1:A:177:GLN:HA	1:A:366:ILE:HD11	1.87	0.55
1:B:306:LEU:HD21	1:B:310[A]:ARG:NH2	2.23	0.54
1:B:332:PHE:CE1	5:B:1397:GOL:H2	2.44	0.52
1:B:289:LEU:HD11	1:B:297:TYR:HB2	1.91	0.52
1:B:382:VAL:HG13	6:B:2097:HOH:O	2.11	0.50
1:B:204:THR:HG23	1:B:229:ASP:OD2	2.12	0.49
1:B:53:LYS:O	1:B:56:VAL:HG22	2.12	0.49
1:B:106:LEU:HB2	1:B:108:VAL:HG23	1.94	0.49
1:B:79:HIS:HA	1:B:396:VAL:HB	1.93	0.48
1:A:110:ILE:O	1:A:113:GLU:CB	2.61	0.48
1:B:106:LEU:HD12	1:B:106:LEU:H	1.79	0.48
1:B:-1:SER:OG	6:B:2001:HOH:O	2.19	0.48
1:B:-1:SER:HA	1:B:0[B]:MET:HE1	2.00	0.44
1:A:97:THR:HG22	1:A:313:ILE:HD11	1.99	0.43
1:A:275:ASP:OD2	1:A:297:TYR:OH	2.24	0.43
1:B:292:TRP:CZ3	1:B:335:GLY:HA2	2.54	0.43
2:B:600:NDP:H52N	2:B:600:NDP:H2D	1.21	0.43
2:A:600:NDP:C6N	2:A:600:NDP:H52N	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:VAL:N	1:B:376:PRO:CD	2.82	0.42
1:A:85:PRO:HG2	2:A:600:NDP:H51N	2.01	0.41
1:B:137:PHE:CE2	1:B:166:VAL:HG13	2.56	0.41
1:A:118:THR:HG21	1:A:156:SER:HB2	2.03	0.40
1:A:79:HIS:ND1	4:A:1398:CIT:O3	2.45	0.40
1:B:225:MET:CE	1:B:225:MET:HA	2.52	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	356/375 (95%)	350 (98%)	6 (2%)	0	100	100
1	B	356/375 (95%)	348 (98%)	8 (2%)	0	100	100
All	All	712/750 (95%)	698 (98%)	14 (2%)	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	286/313 (91%)	283 (99%)	3 (1%)	76	82
1	B	271/313 (87%)	265 (98%)	6 (2%)	52	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	557/626 (89%)	548 (98%)	9 (2%)	67 69

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	A	144	TRP
1	A	276	ASN
1	B	-1	SER
1	B	106	LEU
1	B	144	TRP
1	B	276	ASN
1	B	310[A]	ARG
1	B	310[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	331	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	NDP	A	600	-	45,52,52	1.91	12 (26%)	53,80,80	2.00	11 (20%)
2	NDP	B	600	-	45,52,52	1.64	8 (17%)	53,80,80	2.00	11 (20%)
5	GOL	B	1397	-	5,5,5	0.38	0	5,5,5	0.77	0
4	CIT	A	1398	3	3,12,12	1.51	0	3,17,17	1.81	1 (33%)

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	NDP	A	600	-	-	8/30/77/77	0/5/5/5
2	NDP	B	600	-	-	10/30/77/77	0/5/5/5
5	GOL	B	1397	-	-	4/4/4/4	-
4	CIT	A	1398	3	-	3/6/16/16	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	NDP	P2B-O1X	4.70	1.65	1.50
2	A	600	NDP	O4B-C1B	4.43	1.47	1.41
2	A	600	NDP	C7N-C3N	4.01	1.57	1.48
2	B	600	NDP	C7N-C3N	3.99	1.57	1.48
2	A	600	NDP	C6N-C5N	3.82	1.40	1.33
2	B	600	NDP	C6N-C5N	3.43	1.39	1.33
2	B	600	NDP	P2B-O1X	3.37	1.61	1.50
2	B	600	NDP	C4N-C5N	-3.24	1.40	1.48
2	B	600	NDP	C4N-C3N	3.15	1.56	1.49
2	A	600	NDP	C4N-C5N	-3.14	1.40	1.48
2	A	600	NDP	PA-O1A	3.13	1.62	1.50
2	A	600	NDP	C7N-N7N	3.11	1.41	1.33
2	B	600	NDP	C7N-N7N	3.02	1.41	1.33
2	B	600	NDP	PN-O1N	2.98	1.61	1.50
2	A	600	NDP	C4N-C3N	2.78	1.55	1.49
2	B	600	NDP	PA-O1A	2.50	1.59	1.50
2	A	600	NDP	P2B-O2B	2.46	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	NDP	P2B-O3X	-2.39	1.45	1.54
2	A	600	NDP	O3B-C3B	2.30	1.48	1.43
2	A	600	NDP	PN-O1N	2.02	1.58	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	NDP	O4D-C1D-N1N	6.60	120.97	108.06
2	A	600	NDP	C2D-C1D-N1N	-5.67	99.09	113.30
2	B	600	NDP	C2D-C1D-N1N	-5.42	99.73	113.30
2	B	600	NDP	C5D-C4D-C3D	-5.37	95.07	115.18
2	B	600	NDP	C2D-C3D-C4D	-5.03	92.86	102.64
2	A	600	NDP	N3A-C2A-N1A	-4.94	120.95	128.68
2	B	600	NDP	N3A-C2A-N1A	-4.32	121.92	128.68
2	A	600	NDP	O7N-C7N-C3N	-4.15	113.08	120.90
2	B	600	NDP	O4B-C1B-C2B	-4.08	99.51	106.59
2	B	600	NDP	O7N-C7N-C3N	-3.25	114.78	120.90
2	B	600	NDP	C1D-N1N-C2N	-3.06	116.01	121.11
2	B	600	NDP	O4D-C1D-N1N	3.05	114.01	108.06
2	A	600	NDP	O3X-P2B-O1X	2.94	122.21	110.68
2	A	600	NDP	O2B-P2B-O1X	-2.85	98.39	109.39
2	A	600	NDP	O2A-PA-O5B	2.68	120.21	107.75
4	A	1398	CIT	C3-C2-C1	-2.65	110.74	114.98
2	B	600	NDP	O5D-PN-O1N	-2.44	99.55	109.07
2	A	600	NDP	C3N-C7N-N7N	2.35	121.84	117.67
2	B	600	NDP	C4D-O4D-C1D	-2.35	104.30	109.47
2	A	600	NDP	C1D-N1N-C2N	-2.32	117.25	121.11
2	A	600	NDP	C1B-N9A-C4A	-2.24	122.70	126.64
2	A	600	NDP	O4B-C1B-C2B	-2.22	102.74	106.59
2	B	600	NDP	O2D-C2D-C1D	2.12	117.12	110.02

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	NDP	C5D-O5D-PN-O3
2	A	600	NDP	C5D-O5D-PN-O1N
2	A	600	NDP	O4D-C1D-N1N-C2N
2	B	600	NDP	C5D-O5D-PN-O3
5	B	1397	GOL	O1-C1-C2-C3
5	B	1397	GOL	C1-C2-C3-O3
4	A	1398	CIT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
5	B	1397	GOL	O2-C2-C3-O3
2	B	600	NDP	C3B-C2B-O2B-P2B
2	B	600	NDP	O4D-C1D-N1N-C2N
2	B	600	NDP	C5D-O5D-PN-O1N
2	B	600	NDP	C5D-O5D-PN-O2N
4	A	1398	CIT	C1-C2-C3-C6
5	B	1397	GOL	O1-C1-C2-O2
2	A	600	NDP	C2B-O2B-P2B-O1X
2	A	600	NDP	C2B-O2B-P2B-O2X
2	B	600	NDP	C2B-O2B-P2B-O2X
2	B	600	NDP	C2B-O2B-P2B-O3X
4	A	1398	CIT	C1-C2-C3-O7
2	A	600	NDP	C3B-C2B-O2B-P2B
2	A	600	NDP	C2N-C3N-C7N-N7N
2	B	600	NDP	C2N-C3N-C7N-N7N
2	A	600	NDP	O4B-C4B-C5B-O5B
2	B	600	NDP	O4B-C4B-C5B-O5B
2	B	600	NDP	C1B-C2B-O2B-P2B

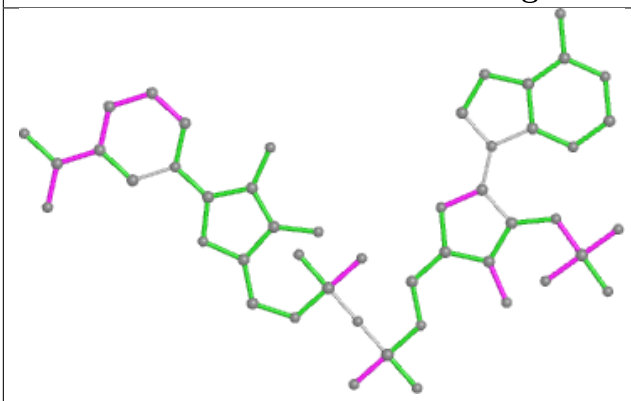
There are no ring outliers.

4 monomers are involved in 12 short contacts:

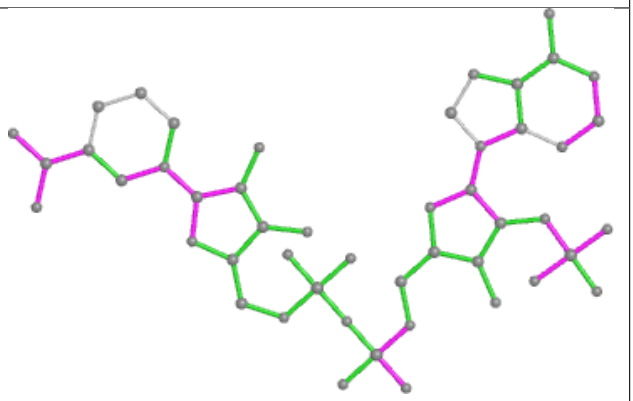
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	NDP	6	0
2	B	600	NDP	4	0
5	B	1397	GOL	1	0
4	A	1398	CIT	1	0

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.

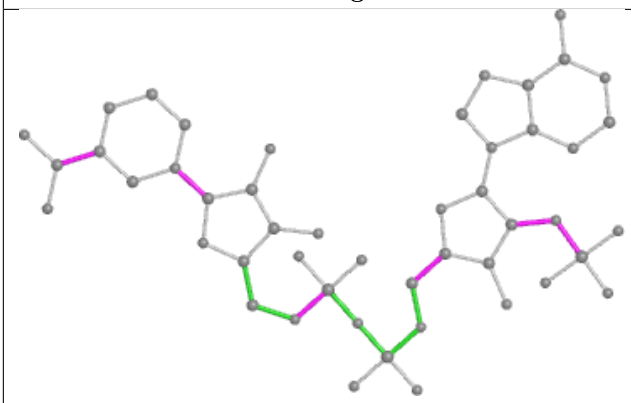
Ligand NDP A 600



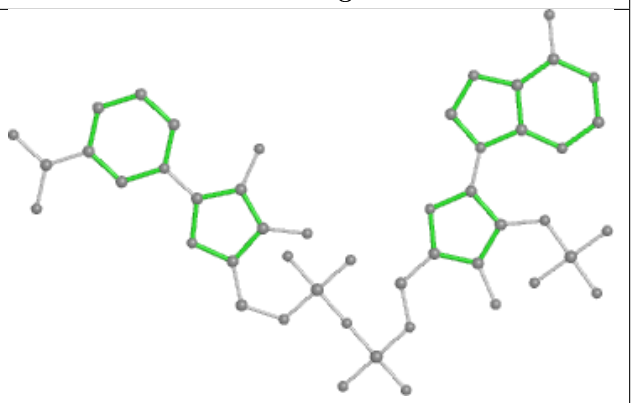
Bond lengths



Bond angles

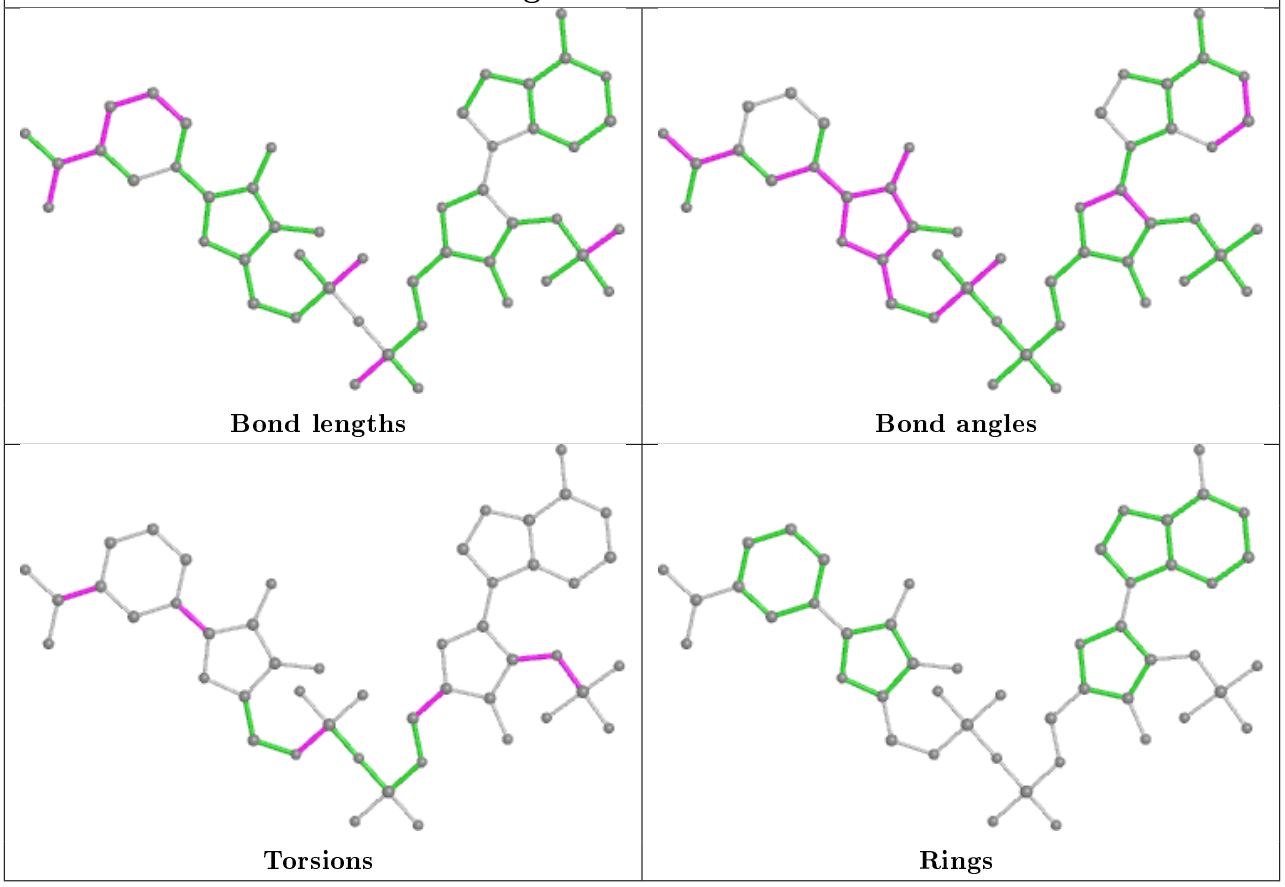


Torsions



Rings

Ligand NDP B 600



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

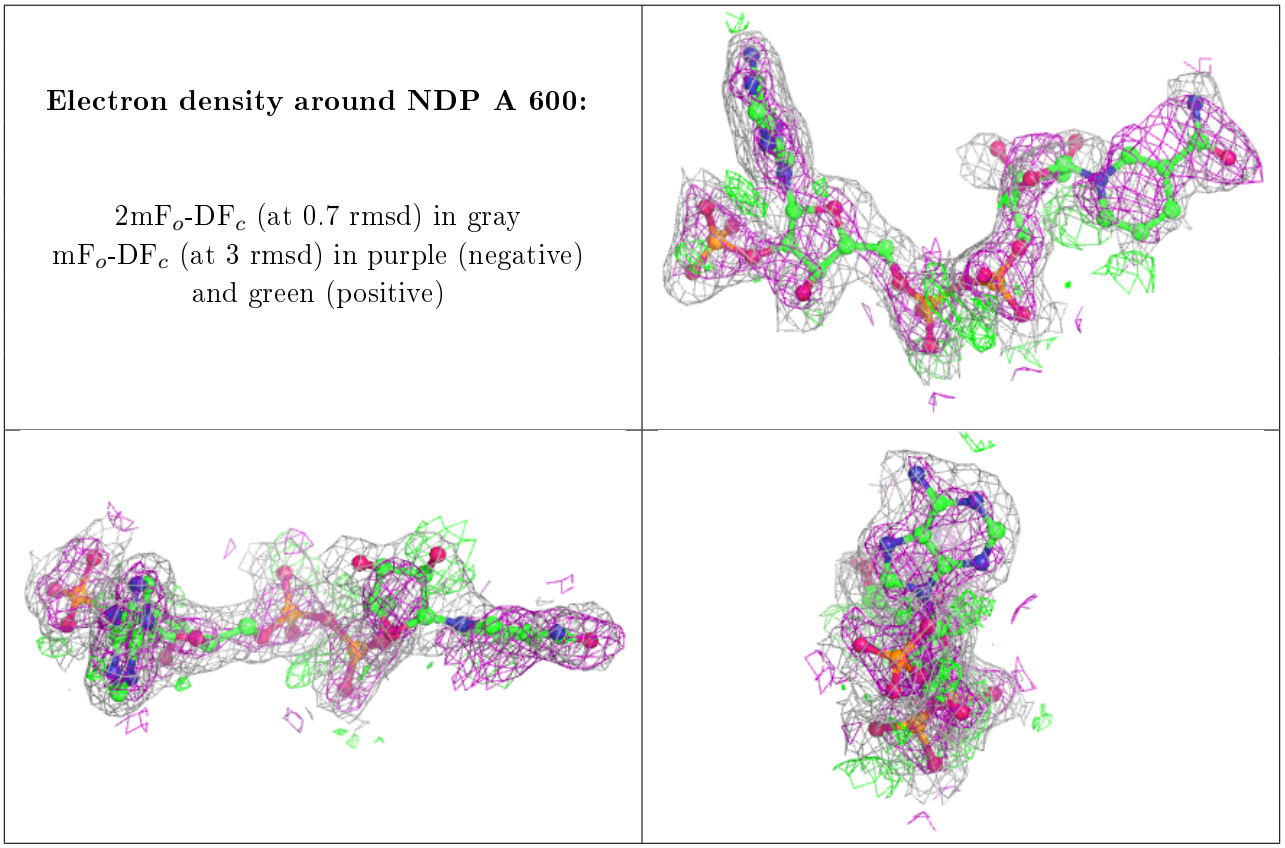
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

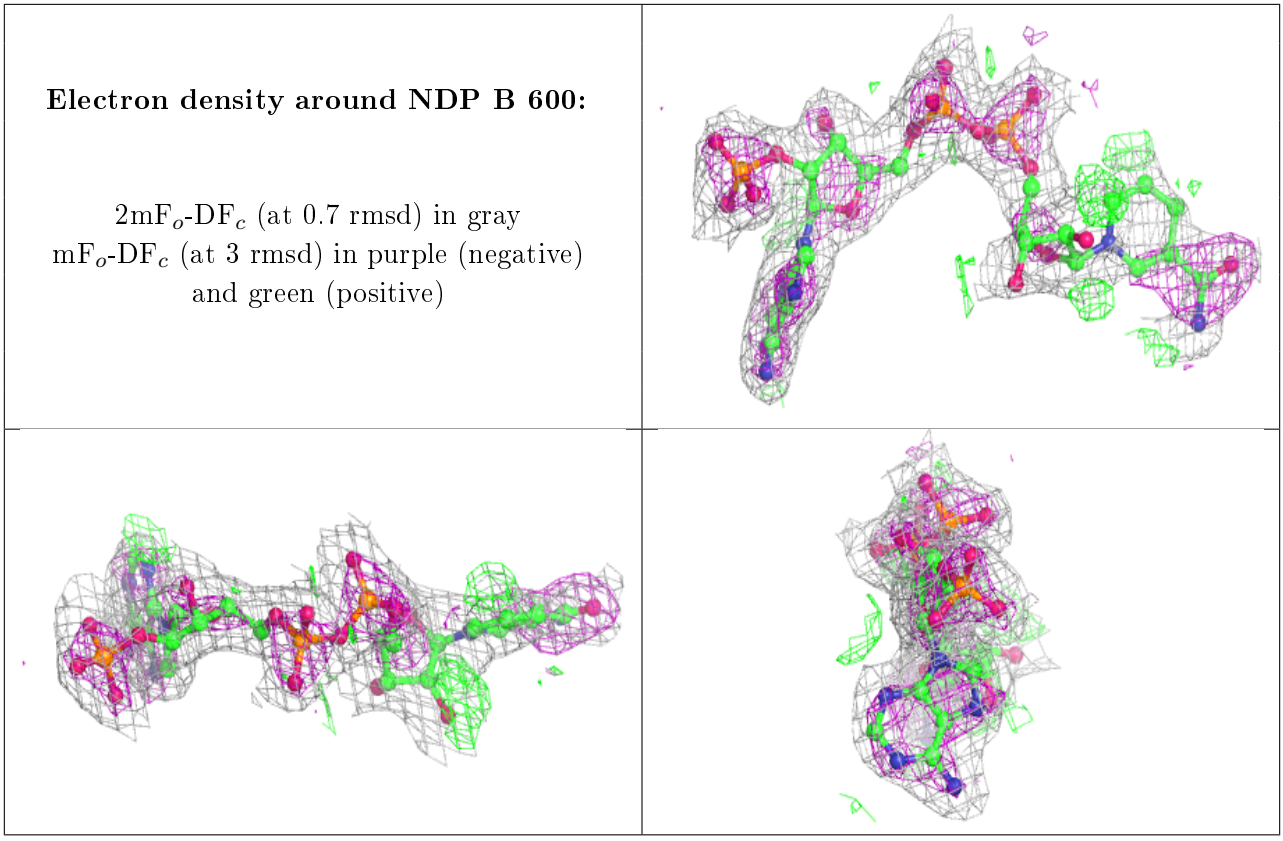
Electron density around NDP A 600:

$2mF_o$-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 600:

$2mF_o$-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

Unable to reproduce the depositors R factor - this section is therefore empty.