



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:31 PM GMT

PDB ID : 1G0N
Title : STRUCTURE OF TRIHYDROXYNAPHTHALENE REDUCTASE IN
COMPLEX WITH NADPH AND 4,5,6,7-TETRACHLORO-PHTHALID
E
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Deposited on : 2000-10-06
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

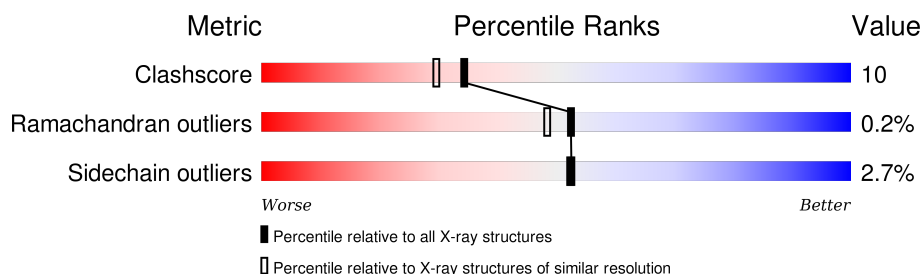
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	283	
1	B	283	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PHH	A	402	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4417 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.

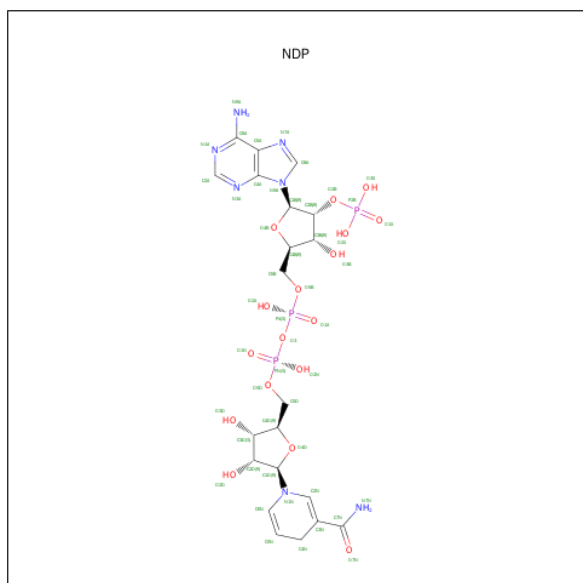
- Molecule 1 is a protein called TRIHYDROXYNAPHTHALENE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2036	1279	357	385	15			
1	B	254	Total	C	N	O	S	0	0	0
			1885	1188	331	352	14			

There are 6 discrepancies between the modelled and reference sequences:

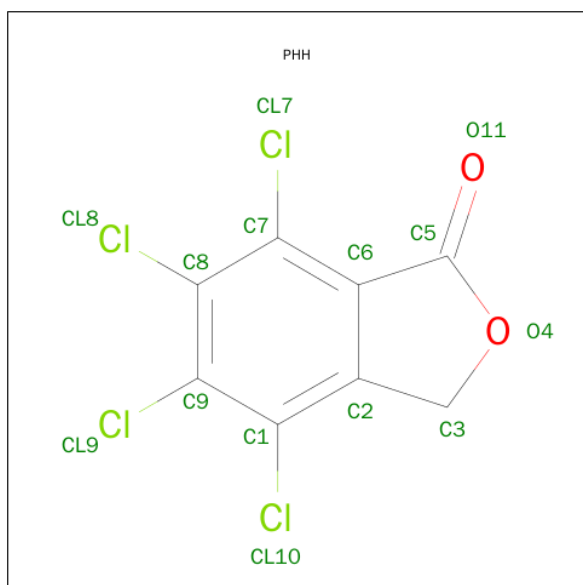
Chain	Residue	Modelled	Actual	Comment	Reference
A	241	VAL	SER	ENGINEERED	UNP Q12634
A	242	GLN	ALA	ENGINEERED	UNP Q12634
A	247	ARG	HIS	ENGINEERED	UNP Q12634
B	241	VAL	SER	ENGINEERED	UNP Q12634
B	242	GLN	ALA	ENGINEERED	UNP Q12634
B	247	ARG	HIS	ENGINEERED	UNP Q12634

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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 4,5,6,7-TETRACHLORO-PHTHALIDE (three-letter code: PHH) (formula: $C_8H_2Cl_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	O	0	0
			14	8	4	2		

- Molecule 4 is water.

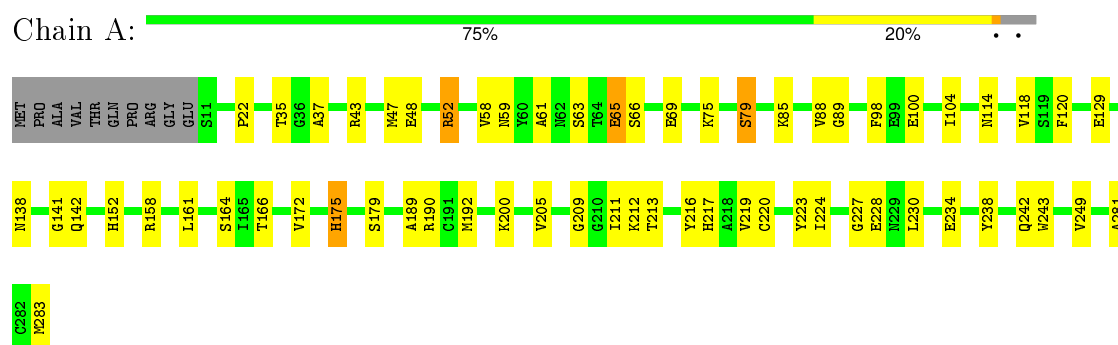
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	202	Total	O	0	0
			202	202		
4	B	184	Total	O	0	0
			184	184		

3 Residue-property plots

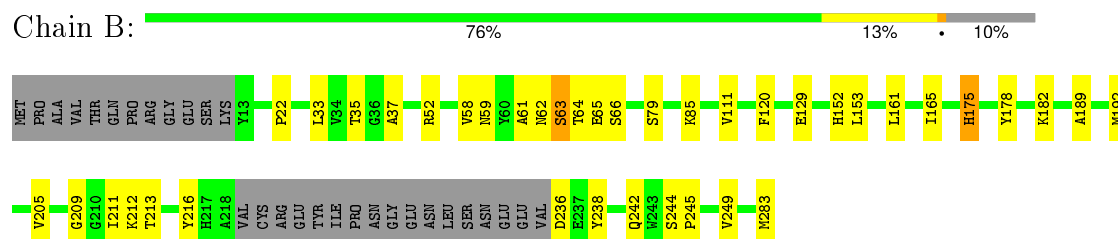
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: TRIHYDROXYNAPHTHALENE REDUCTASE



• Molecule 1: TRIHYDROXYNAPHTHALENE REDUCTASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.50 Å 140.50 Å 72.70 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.195 , 0.244	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4417	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

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: NDP, PHH

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	0.50	0/2068	0.71	1/2790 (0.0%)
1	B	0.50	0/1914	0.69	1/2580 (0.0%)
All	All	0.50	0/3982	0.70	2/5370 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	GLY	N-CA-C	-5.81	98.58	113.10
1	A	209	GLY	N-CA-C	-5.29	99.88	113.10

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	2036	0	2051	51	0
1	B	1885	0	1908	29	0
2	A	48	0	26	3	0
2	B	48	0	26	0	0
3	A	14	0	2	4	0
4	A	202	0	0	9	0
4	B	184	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4417	0	4013	80	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 10.

All (80) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:PHE:HE1	1:A:219:VAL:HB	1.37	0.87
1:A:120:PHE:CE1	1:A:219:VAL:HB	2.14	0.82
1:A:216:TYR:HA	3:A:402:PHH:CL10	2.18	0.80
1:B:161:LEU:HD11	1:B:192:MET:HE1	1.69	0.75
1:B:189:ALA:HB2	1:B:205:VAL:HG23	1.70	0.72
1:B:238:TYR:O	1:B:242:GLN:HB2	1.90	0.70
1:A:238:TYR:O	1:A:242:GLN:HB2	1.91	0.70
1:A:48:GLU:O	1:A:52:ARG:HG2	1.95	0.67
1:B:213:THR:H	1:B:216:TYR:HB3	1.60	0.66
1:B:211:ILE:O	1:B:216:TYR:HB2	1.96	0.65
1:A:211:ILE:O	1:A:216:TYR:HB2	1.98	0.64
1:A:213:THR:O	1:A:217:HIS:HD2	1.82	0.62
1:B:61:ALA:O	1:B:85:LYS:HE3	2.00	0.61
1:A:283:MET:HE1	4:A:440:HOH:O	2.02	0.59
1:A:118:VAL:HG21	1:A:219:VAL:HG21	1.84	0.59
1:A:213:THR:H	1:A:216:TYR:HB3	1.68	0.58
1:A:100:GLU:O	1:A:104:ILE:HG13	2.05	0.57
1:A:65:GLU:O	1:A:69:GLU:HG3	2.05	0.57
1:B:212:LYS:HG3	1:B:249:VAL:HG11	1.86	0.56
1:B:238:TYR:CZ	1:B:242:GLN:HG3	2.41	0.56
1:B:161:LEU:HD11	1:B:192:MET:CE	2.34	0.56
1:A:158:ARG:NH2	4:A:463:HOH:O	2.39	0.56
1:B:189:ALA:CB	1:B:205:VAL:HG23	2.35	0.55
1:B:175:HIS:CE1	1:B:178:TYR:CD2	2.95	0.55
1:B:189:ALA:HB2	1:B:205:VAL:CG2	2.36	0.55
1:A:161:LEU:HD11	1:A:192:MET:HE1	1.89	0.55
1:A:189:ALA:HB2	1:A:205:VAL:HG23	1.88	0.55
2:A:400:NDP:H41N	3:A:402:PHH:C5	2.37	0.54
1:B:238:TYR:CE2	1:B:242:GLN:HG3	2.42	0.54
2:A:400:NDP:H52A	4:A:498:HOH:O	2.09	0.52
1:A:283:MET:CE	4:A:440:HOH:O	2.57	0.52
1:A:243:TRP:O	1:A:281:ALA:HB2	2.10	0.52
1:A:238:TYR:CZ	1:A:242:GLN:HG3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:SER:HB3	1:B:66:SER:HB2	1.93	0.51
1:A:190:ARG:NH2	4:A:447:HOH:O	2.44	0.51
1:A:227:GLY:HA2	1:A:230:LEU:HG	1.93	0.50
1:A:164:SER:OG	3:A:402:PHH:O11	2.28	0.50
1:A:172:VAL:HB	4:A:554:HOH:O	2.11	0.50
1:B:213:THR:O	1:B:216:TYR:HB3	2.11	0.50
1:A:43:ARG:NH1	4:A:587:HOH:O	2.41	0.50
1:A:63:SER:HB3	1:A:66:SER:HB2	1.93	0.49
1:A:52:ARG:HA	1:B:22:PRO:HG3	1.95	0.49
1:B:120:PHE:CE2	1:B:175:HIS:CD2	3.00	0.48
1:A:89:GLY:HA3	4:A:595:HOH:O	2.13	0.48
1:A:161:LEU:HD11	1:A:192:MET:CE	2.43	0.48
1:B:182:LYS:NZ	4:B:583:HOH:O	2.45	0.48
1:A:35:THR:HA	1:A:59:ASN:HB3	1.96	0.48
1:B:35:THR:HA	1:B:59:ASN:HB3	1.95	0.48
1:A:43:ARG:O	1:A:47:MET:HG2	2.14	0.48
1:B:152:HIS:HE1	4:B:444:HOH:O	1.97	0.48
1:A:220:CYS:HA	3:A:402:PHH:CL9	2.51	0.47
1:A:219:VAL:HG23	1:A:223:TYR:HE1	1.79	0.47
1:A:166:THR:HB	1:A:179:SER:OG	2.14	0.47
1:A:189:ALA:CB	1:A:205:VAL:HG23	2.45	0.47
1:A:114:ASN:O	2:A:400:NDP:H4D	2.16	0.46
1:B:111:VAL:HG23	1:B:153:LEU:HD21	1.98	0.46
1:A:213:THR:O	1:A:216:TYR:HB3	2.16	0.45
1:A:224:ILE:HG12	1:A:238:TYR:CE1	2.51	0.45
1:B:165:ILE:HD13	1:B:283:MET:CE	2.46	0.45
1:A:98:PHE:HB3	1:A:152:HIS:CD2	2.51	0.45
1:A:230:LEU:HD22	1:A:234:GLU:HB3	1.98	0.45
1:A:216:TYR:O	1:A:220:CYS:HB3	2.16	0.45
1:B:244:SER:HA	1:B:245:PRO:HD3	1.88	0.44
1:A:75:LYS:HA	1:A:79:SER:O	2.17	0.44
1:A:37:ALA:HB3	1:A:58:VAL:HG13	1.98	0.44
1:A:200:LYS:NZ	4:A:490:HOH:O	2.49	0.43
1:A:138:ASN:O	1:A:142:GLN:HG3	2.19	0.43
1:B:213:THR:H	1:B:216:TYR:CB	2.30	0.42
1:B:33:LEU:HD23	1:B:33:LEU:C	2.39	0.42
1:B:283:MET:CE	4:B:525:HOH:O	2.67	0.42
1:A:224:ILE:HG12	1:A:238:TYR:CD1	2.55	0.42
1:A:212:LYS:HG3	1:A:249:VAL:HG11	2.02	0.42
1:B:62:ASN:O	1:B:64:THR:N	2.53	0.42
1:A:224:ILE:HG21	1:A:230:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:VAL:CG1	1:A:141:GLY:HA3	2.50	0.41
1:B:37:ALA:HB3	1:B:58:VAL:HG13	2.03	0.41
1:A:61:ALA:O	1:A:85:LYS:HE3	2.21	0.41
1:A:238:TYR:CE2	1:A:242:GLN:HG3	2.56	0.41
1:A:22:PRO:HG3	1:B:52:ARG:HA	2.02	0.41
1:A:172:VAL:HG12	1:A:175:HIS:HB2	2.02	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	271/283 (96%)	266 (98%)	5 (2%)	0	100	100
1	B	250/283 (88%)	239 (96%)	10 (4%)	1 (0%)	39	33
All	All	521/566 (92%)	505 (97%)	15 (3%)	1 (0%)	52	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	63	SER

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	213/221 (96%)	207 (97%)	6 (3%)	51	50
1	B	195/221 (88%)	190 (97%)	5 (3%)	54	54
All	All	408/442 (92%)	397 (97%)	11 (3%)	52	52

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	65	GLU
1	A	79	SER
1	A	129	GLU
1	A	175	HIS
1	A	228	GLU
1	B	65	GLU
1	B	79	SER
1	B	129	GLU
1	B	175	HIS
1	B	236	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	HIS
1	B	152	HIS
1	B	175	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

3 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	NDP	A	400	-	42,52,52	1.32	4 (9%)	55,80,80	2.06	6 (10%)
3	PHH	A	402	-	15,15,15	3.52	3 (20%)	20,23,23	2.19	4 (20%)
2	NDP	B	401	-	42,52,52	1.18	3 (7%)	55,80,80	2.06	7 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	A	400	-	-	0/30/77/77	0/5/5/5
3	PHH	A	402	-	-	0/0/9/9	0/2/2/2
2	NDP	B	401	-	-	0/30/77/77	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	PHH	O4-C3	-8.57	1.34	1.45
2	A	400	NDP	C4N-C5N	-3.80	1.40	1.49
2	B	401	NDP	C4N-C5N	-3.74	1.41	1.49
2	A	400	NDP	P2B-O3X	-2.16	1.46	1.54
2	B	401	NDP	C5A-N7A	-2.14	1.32	1.39
2	A	400	NDP	C2N-C3N	2.70	1.41	1.34
3	A	402	PHH	O11-C5	3.46	1.32	1.22
2	B	401	NDP	C6N-C5N	3.60	1.40	1.33
2	A	400	NDP	C6N-C5N	4.16	1.41	1.33
3	A	402	PHH	O4-C5	9.60	1.48	1.36

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NDP	N3A-C2A-N1A	-9.79	121.40	128.89
2	A	400	NDP	N3A-C2A-N1A	-9.31	121.76	128.89
2	A	400	NDP	C4B-O4B-C1B	-7.36	101.64	109.72
2	B	401	NDP	C4B-O4B-C1B	-6.47	102.61	109.72
3	A	402	PHH	C3-O4-C5	-5.04	107.16	110.59
3	A	402	PHH	O11-C5-C6	-2.60	125.27	130.94
2	B	401	NDP	O3B-C3B-C2B	-2.46	104.07	111.16
2	A	400	NDP	O3B-C3B-C2B	-2.13	105.00	111.16
2	A	400	NDP	O5B-C5B-C4B	2.15	117.06	109.12
2	B	401	NDP	PN-O3-PA	2.66	140.19	132.73
2	B	401	NDP	C4A-C5A-N7A	2.92	112.16	109.48
2	B	401	NDP	C5N-C4N-C3N	3.07	120.97	112.52
2	A	400	NDP	C5N-C4N-C3N	3.11	121.08	112.52
2	B	401	NDP	O4B-C1B-N9A	4.50	117.53	108.10
3	A	402	PHH	O4-C3-C2	4.70	109.59	104.69
2	A	400	NDP	O4B-C1B-N9A	5.01	118.59	108.10
3	A	402	PHH	O4-C5-O11	5.44	126.48	121.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	NDP	3	0
3	A	402	PHH	4	0

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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.