



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:36 pm GMT

PDB ID : 1X8L
Title : Crystal structure of retinol dehydratase in complex with all-trans-4-oxoretinol and inactive cofactor PAP
Authors : Pakhomova, S.; Buck, J.; Newcomer, M.E.
Deposited on : 2004-08-18
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

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

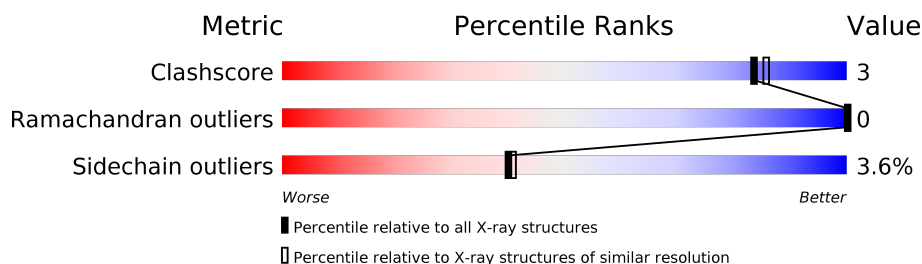
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (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. 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	351	
1	B	351	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6088 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 retinol dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2840	1835	469	521	15			
1	B	342	Total	C	N	O	S	0	0	0
			2845	1840	470	520	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	SER	PHE	SEE REMARK 999	UNP Q26490
A	258	SER	CYS	ENGINEERED	UNP Q26490
A	279	SER	CYS	ENGINEERED	UNP Q26490
B	142	SER	PHE	SEE REMARK 999	UNP Q26490
B	258	SER	CYS	ENGINEERED	UNP Q26490
B	279	SER	CYS	ENGINEERED	UNP Q26490

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

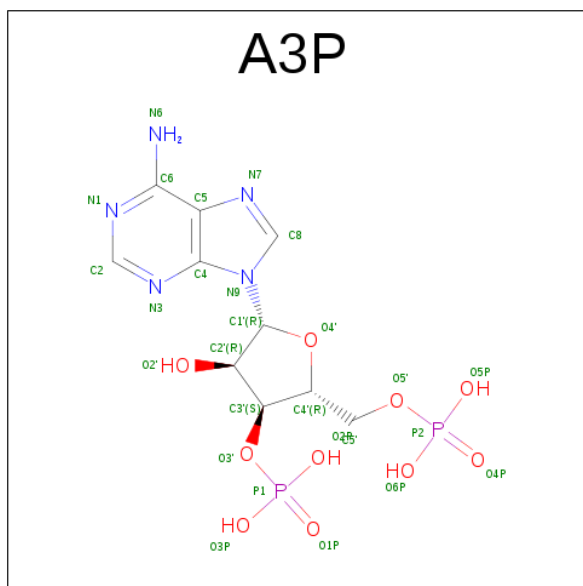
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Hg	0	0
			1	1		
2	A	1	Total	Hg	0	0
			1	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

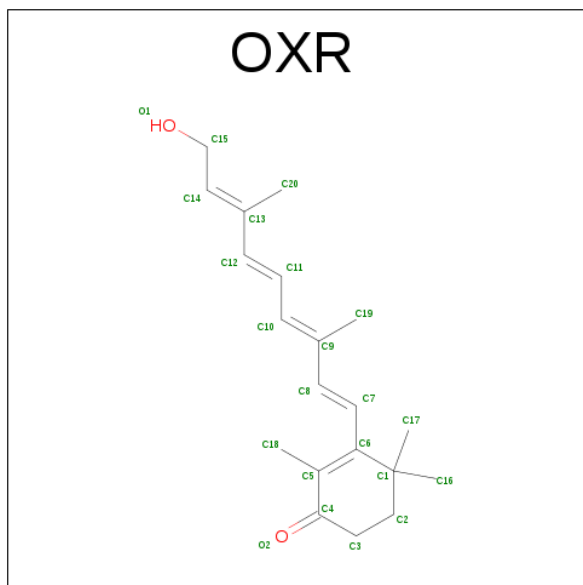
- Molecule 4 is ADENOSINE-3'-5'-DIPHOSPHATE (three-letter code: A3P) (formula:

$C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	2	Total	C	N	O	P	0	0
			54	20	10	20	4		

- Molecule 5 is 4-OXORETINOL (three-letter code: OXR) (formula: $C_{20}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			22	20	2		
5	B	1	Total	C	O	0	0
			22	20	2		

- Molecule 6 is water.

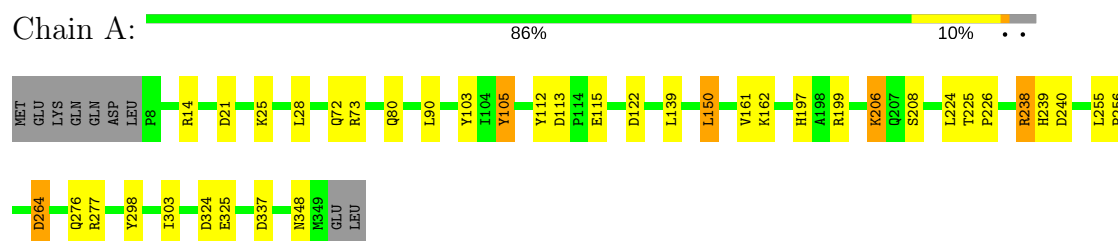
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	145	Total 145	O 145	0	0
6	B	156	Total 156	O 156	0	0

3 Residue-property plots [i](#)

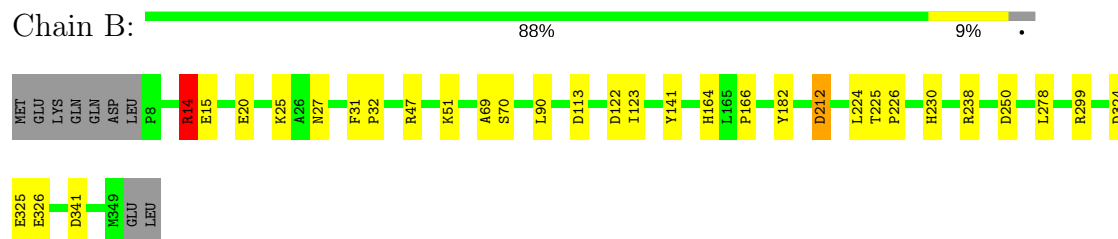
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: retinol dehydratase



- Molecule 1: retinol dehydratase



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.51Å 67.19Å 85.07Å 90.00° 111.85° 90.00°	Depositor
Resolution (Å)	15.00 – 2.10	Depositor
% Data completeness (in resolution range)	88.4 (15.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.196 , 0.231	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6088	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, A3P, HG, OXR

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	0.64	0/2921	0.84	9/3955 (0.2%)
1	B	0.66	0/2926	0.85	9/3959 (0.2%)
All	All	0.65	0/5847	0.85	18/7914 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	B	324	ASP	CB-CG-OD2	7.03	124.63	118.30
1	B	113	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	324	ASP	CB-CG-OD2	6.75	124.38	118.30
1	A	238	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	B	341	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	113	ASP	CB-CG-OD2	6.22	123.90	118.30
1	B	14	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A	337	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	122	ASP	CB-CG-OD2	5.78	123.51	118.30
1	B	14	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	299	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	250	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	264	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	240	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	212	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	73	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	122	ASP	CB-CG-OD2	5.02	122.81	118.30

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	2840	0	2760	16	0
1	B	2845	0	2778	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	54	0	22	0	0
5	A	22	0	28	6	0
5	B	22	0	28	2	0
6	A	145	0	0	2	0
6	B	156	0	0	1	0
All	All	6088	0	5616	31	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 (31) 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)
5:A:1102:OXR:H181	5:A:1102:OXR:H8	1.44	1.00
5:B:2202:OXR:H8	5:B:2202:OXR:H181	1.41	0.99
1:B:27:ASN:HD21	1:B:212:ASP:HB3	1.47	0.78
5:A:1102:OXR:C8	5:A:1102:OXR:H181	2.21	0.66
5:B:2202:OXR:C8	5:B:2202:OXR:H181	2.21	0.65
1:A:199:ARG:CD	1:A:206:LYS:HZ3	2.17	0.57
1:B:225:THR:HB	1:B:226:PRO:HA	1.87	0.56
1:A:225:THR:HB	1:A:226:PRO:HA	1.86	0.56
1:A:298:TYR:HD2	1:A:303:ILE:HD11	1.73	0.52
1:A:238:ARG:HG2	1:A:239:HIS:CD2	2.45	0.52
1:A:72:GLN:NE2	6:A:1175:HOH:O	2.44	0.51
1:B:15:GLU:OE2	1:B:47:ARG:NH2	2.44	0.51
1:A:150:LEU:HD21	1:A:161:VAL:HG22	1.94	0.50
1:B:141:TYR:OH	6:B:2272:HOH:O	2.20	0.49
1:A:197:HIS:NE2	5:A:1102:OXR:H14	2.28	0.48
1:B:69:ALA:O	1:B:182:TYR:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:TYR:CE1	5:A:1102:OXR:H203	2.52	0.45
1:A:255:LEU:HB3	1:A:256:PRO:HD3	1.99	0.44
1:A:208:SER:HB2	6:A:1222:HOH:O	2.17	0.44
1:A:80:GLN:HG2	1:A:103:TYR:CE2	2.54	0.43
1:B:31:PHE:HA	1:B:32:PRO:HD3	1.92	0.42
1:A:150:LEU:HD21	1:A:161:VAL:CG2	2.49	0.42
1:B:70:SER:O	1:B:164:HIS:HA	2.19	0.42
1:B:90:LEU:HD22	1:B:278:LEU:HD21	2.02	0.41
1:A:206:LYS:HA	1:A:206:LYS:NZ	2.36	0.41
1:A:162:LYS:NZ	5:A:1102:OXR:H201	2.35	0.41
1:A:162:LYS:HZ1	5:A:1102:OXR:C15	2.33	0.41
1:B:14:ARG:NH2	1:B:20:GLU:OE1	2.53	0.41
1:A:112:TYR:CE1	1:A:139:LEU:HD22	2.55	0.40
1:B:123:ILE:O	1:B:123:ILE:HG22	2.21	0.40
1:B:166:PRO:HB3	1:B:230:HIS:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	340/351 (97%)	335 (98%)	5 (2%)	0	100	100
1	B	340/351 (97%)	337 (99%)	3 (1%)	0	100	100
All	All	680/702 (97%)	672 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	305/316 (96%)	290 (95%)	15 (5%)	29	26
1	B	306/316 (97%)	299 (98%)	7 (2%)	56	60
All	All	611/632 (97%)	589 (96%)	22 (4%)	40	41

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	21	ASP
1	A	25	LYS
1	A	28	LEU
1	A	90	LEU
1	A	105	TYR
1	A	115	GLU
1	A	150	LEU
1	A	206	LYS
1	A	224	LEU
1	A	264	ASP
1	A	276	GLN
1	A	277	ARG
1	A	325	GLU
1	A	348	ASN
1	B	14	ARG
1	B	25	LYS
1	B	51	LYS
1	B	224	LEU
1	B	238	ARG
1	B	325	GLU
1	B	326	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	239	HIS
1	B	80	GLN
1	B	207	GLN

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 8 ligands modelled in this entry, 4 are 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$
5	OXR	A	1102	-	22,22,22	0.82	1 (4%)	25,30,30	2.40	11 (44%)
4	A3P	B	1101	-	26,29,29	1.69	1 (3%)	31,45,45	2.25	12 (38%)
4	A3P	B	2201	-	26,29,29	1.59	2 (7%)	31,45,45	2.10	7 (22%)
5	OXR	B	2202	-	22,22,22	0.79	1 (4%)	25,30,30	2.30	11 (44%)

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
5	OXR	A	1102	-	-	0/14/34/34	0/1/1/1
4	A3P	B	1101	-	-	0/11/31/31	0/3/3/3
4	A3P	B	2201	-	-	0/11/31/31	0/3/3/3
5	OXR	B	2202	-	-	0/14/34/34	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2201	A3P	P2-O4P	2.09	1.57	1.50
5	A	1102	OXR	C15-C14	2.43	1.53	1.50
5	B	2202	OXR	C15-C14	2.52	1.53	1.50
4	B	2201	A3P	C4-N3	5.81	1.44	1.35
4	B	1101	A3P	C4-N3	6.73	1.45	1.35

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1101	A3P	N3-C2-N1	-8.44	121.51	128.86
4	B	2201	A3P	N3-C2-N1	-7.11	122.67	128.86
4	B	2201	A3P	C4-C5-N7	-3.93	105.61	109.41
5	B	2202	OXR	C8-C9-C10	-3.91	112.94	118.94
4	B	2201	A3P	O3'-C3'-C4'	-3.52	96.82	110.04
5	A	1102	OXR	C16-C1-C6	-3.33	104.90	110.31
5	B	2202	OXR	O2-C4-C3	-3.20	115.31	120.82
5	A	1102	OXR	C8-C9-C10	-3.06	114.24	118.94
5	A	1102	OXR	O2-C4-C3	-2.77	116.04	120.82
5	B	2202	OXR	C10-C11-C12	-2.75	114.80	123.23
4	B	1101	A3P	O3'-C3'-C4'	-2.73	99.78	110.04
5	B	2202	OXR	C17-C1-C6	-2.53	106.20	110.31
5	A	1102	OXR	C7-C8-C9	-2.51	122.45	126.21
5	A	1102	OXR	C10-C11-C12	-2.50	115.57	123.23
4	B	1101	A3P	O3'-C3'-C2'	-2.41	102.72	111.63
5	B	2202	OXR	C7-C8-C9	-2.32	122.73	126.21
4	B	1101	A3P	C4-C5-N7	-2.25	107.24	109.41
5	B	2202	OXR	C16-C1-C6	-2.20	106.74	110.31
4	B	1101	A3P	C5-C6-N6	-2.20	115.99	120.47
5	A	1102	OXR	C11-C10-C9	-2.18	124.19	127.31
5	A	1102	OXR	C17-C1-C6	-2.16	106.81	110.31
4	B	1101	A3P	C5'-C4'-C3'	-2.15	107.02	114.30
4	B	1101	A3P	O3P-P1-O2P	2.23	116.62	107.61
4	B	1101	A3P	C2'-C3'-C4'	2.27	107.30	103.23
4	B	2201	A3P	N6-C6-N1	2.39	123.51	118.77
4	B	2201	A3P	C2-N1-C6	2.44	123.03	118.77
5	B	2202	OXR	O1-C15-C14	2.54	116.28	110.71
4	B	1101	A3P	N6-C6-N1	2.79	124.30	118.77
4	B	1101	A3P	O2'-C2'-C3'	2.82	119.21	111.18
5	B	2202	OXR	C19-C9-C8	2.84	122.62	118.10
4	B	1101	A3P	O2'-C2'-C1'	2.84	120.49	111.61
4	B	1101	A3P	C2-N1-C6	2.96	123.95	118.77
4	B	2201	A3P	O2'-C2'-C3'	3.12	120.06	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2201	A3P	C2'-C3'-C4'	3.13	108.84	103.23
5	A	1102	OXR	C3-C2-C1	3.82	120.18	113.11
5	B	2202	OXR	C3-C2-C1	4.13	120.76	113.11
5	B	2202	OXR	C2-C1-C6	4.17	117.00	110.48
5	A	1102	OXR	C19-C9-C8	4.32	124.97	118.10
5	A	1102	OXR	C2-C1-C6	4.35	117.29	110.48
5	A	1102	OXR	C3-C4-C5	4.79	123.08	118.80
5	B	2202	OXR	C3-C4-C5	4.92	123.18	118.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1102	OXR	6	0
5	B	2202	OXR	2	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.