



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:54 am GMT

PDB ID : 1E18
Title : TUNGSTEN-SUBSTITUTED DMSO REDUCTASE FROM RHODOBAC-
TER CAPSULATUS
Authors : Bailey, S.; Stewart, L.J.
Deposited on : 2000-04-28
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	:	1.7.2 (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

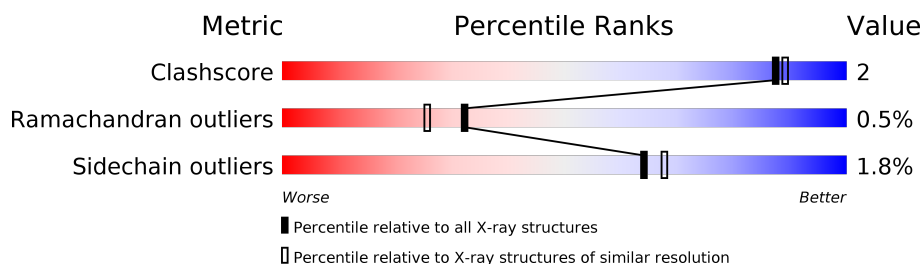
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (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	823	 86% 8% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6475 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.

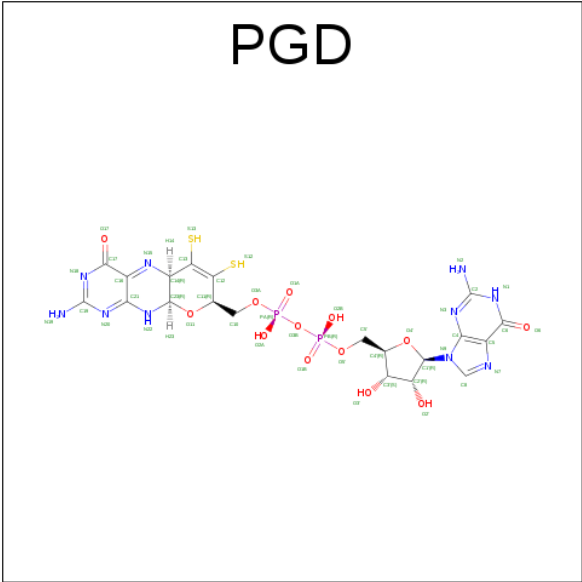
- Molecule 1 is a protein called DMSO REDUCTASE..

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	779	Total	C	N	O	S	0	0	0
			5976	3800	1012	1137	27			

There are 10 discrepancies between the modelled and reference sequences:

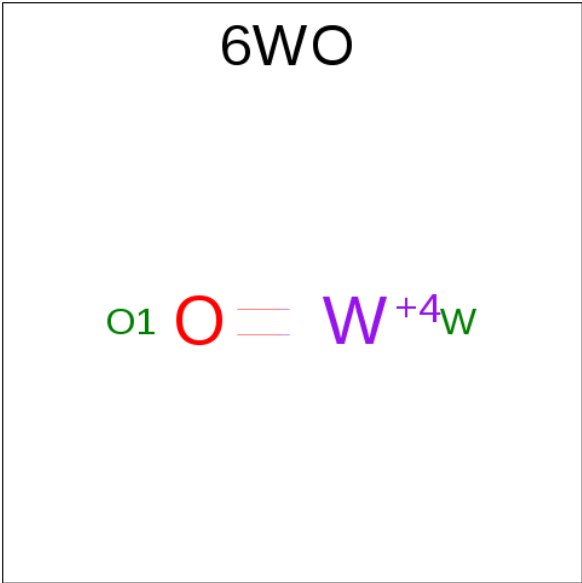
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	SER	THR	CONFLICT	UNP Q52675
A	43	ALA	GLU	CONFLICT	UNP Q52675
A	234	GLU	ASP	CONFLICT	UNP Q52675
A	236	ILE	VAL	CONFLICT	UNP Q52675
A	280	ASP	MET	CONFLICT	UNP Q52675
A	294	GLU	SER	CONFLICT	UNP Q52675
A	295	GLY	ASP	CONFLICT	UNP Q52675
A	312	GLU	LYS	CONFLICT	UNP Q52675
A	456	VAL	ILE	CONFLICT	UNP Q52675
A	552	ALA	GLY	CONFLICT	UNP Q52675

- Molecule 2 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: PGD) (formula: C₂₀H₂₄N₁₀O₁₃P₂S₂).



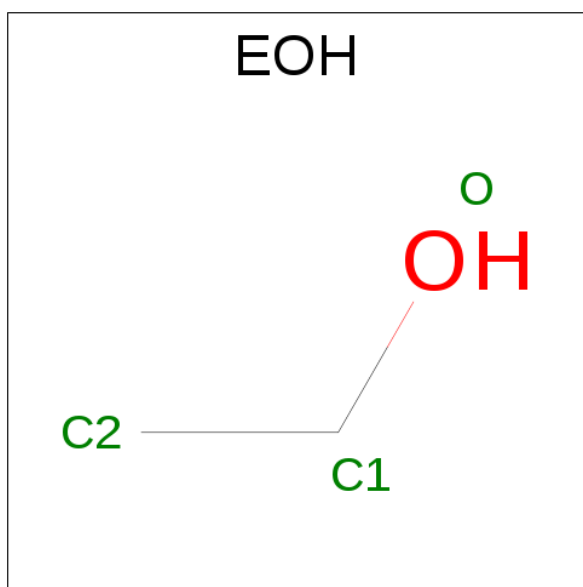
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
2	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 3 is OXO-TUNGSTEN(VI) (three-letter code: 6WO) (formula: OW).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O W	0	0
			2	1 1		

- Molecule 4 is ETHANOL (three-letter code: EOH) (formula: C₂H₆O).



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

- Molecule 5 is water.

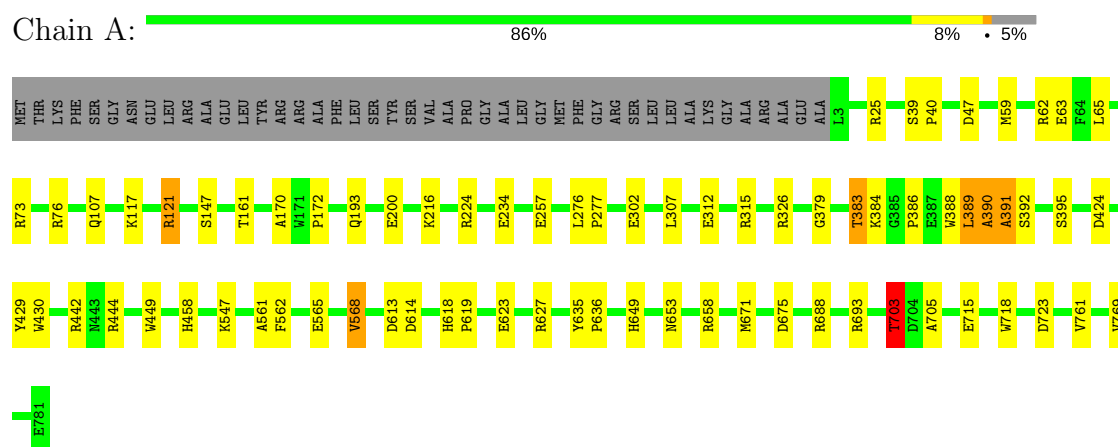
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	394	Total	O	0	0
			394	394		

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: DMSO REDUCTASE.



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	80.92Å 80.92Å 229.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	98.0 (20.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.142 , 0.192	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6475	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: EOH, PGD, 6WO

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	0.55	1/6137 (0.0%)	1.21	33/8353 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	312	GLU	CD-OE1	-5.51	1.19	1.25

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	688	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	A	723	ASP	CB-CG-OD1	8.96	126.37	118.30
1	A	658	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	A	25	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	A	326	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	442	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	613	ASP	CB-CG-OD1	6.67	124.31	118.30
1	A	383	THR	C-N-CA	6.23	137.26	121.70
1	A	315	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	161	THR	CA-CB-CG2	6.16	121.02	112.40
1	A	73	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	121	ARG	CD-NE-CZ	6.14	132.20	123.60
1	A	703	THR	CB-CA-C	-6.14	95.01	111.60
1	A	47	ASP	CB-CG-OD2	6.06	123.75	118.30
1	A	62	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	458	HIS	N-CA-CB	5.88	121.18	110.60
1	A	688	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	424	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	121	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	62	ARG	NE-CZ-NH1	5.56	123.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	614	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	623	GLU	OE1-CD-OE2	-5.45	116.76	123.30
1	A	675	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	627	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	568	VAL	CB-CA-C	-5.36	101.21	111.40
1	A	444	ARG	CD-NE-CZ	5.34	131.08	123.60
1	A	444	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	63	GLU	CG-CD-OE2	-5.26	107.78	118.30
1	A	257	GLU	OE1-CD-OE2	-5.19	117.07	123.30
1	A	76	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	693	ARG	CD-NE-CZ	5.04	130.66	123.60
1	A	59	MET	CA-CB-CG	5.03	121.86	113.30
1	A	121	ARG	NE-CZ-NH1	5.01	122.80	120.30

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	5976	0	5784	28	0
2	A	94	0	40	3	0
3	A	2	0	0	0	0
4	A	9	0	18	1	0
5	A	394	0	0	1	0
All	All	6475	0	5842	28	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 2.

All (28) 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:390:ALA:O	1:A:391:ALA:HB3	1.95	0.67
1:A:703:THR:HG22	1:A:705:ALA:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:ALA:O	1:A:565:GLU:HG3	2.05	0.56
1:A:302:GLU:HG2	5:A:2154:HOH:O	2.07	0.55
1:A:390:ALA:O	1:A:391:ALA:CB	2.55	0.54
1:A:107:GLN:HG3	1:A:392:SER:HB3	1.92	0.52
1:A:193:GLN:CD	4:A:901:EOH:H21	2.33	0.48
1:A:649:HIS:CG	2:A:801:PGD:H102	2.49	0.48
1:A:390:ALA:C	1:A:391:ALA:O	2.52	0.47
1:A:671:MET:HE1	1:A:761:VAL:HG11	1.97	0.46
1:A:379:GLY:O	1:A:383:THR:HG23	2.16	0.46
1:A:147:SER:HB3	2:A:802:PGD:S12	2.55	0.45
1:A:389:LEU:HG	1:A:389:LEU:O	2.16	0.45
1:A:388:TRP:CE2	1:A:395:SER:HB3	2.52	0.45
1:A:216:LYS:NZ	1:A:234:GLU:OE1	2.50	0.45
1:A:39:SER:HA	1:A:40:PRO:HD3	1.90	0.44
1:A:618:HIS:HB2	1:A:619:PRO:HD2	2.01	0.43
1:A:391:ALA:O	1:A:392:SER:CB	2.66	0.43
1:A:121:ARG:HA	1:A:121:ARG:HD3	1.88	0.43
1:A:562:PHE:CD1	1:A:568:VAL:HG23	2.54	0.42
1:A:703:THR:CG2	1:A:705:ALA:H	2.31	0.42
1:A:276:LEU:HB3	1:A:277:PRO:HD3	2.00	0.42
1:A:635:TYR:HA	1:A:636:PRO:HD3	1.95	0.42
1:A:147:SER:CB	2:A:802:PGD:S12	3.08	0.41
1:A:653:ASN:ND2	1:A:718:TRP:H	2.18	0.41
1:A:170:ALA:HB1	1:A:172:PRO:HD2	2.03	0.40
1:A:224:ARG:HD3	1:A:224:ARG:HH11	1.72	0.40
1:A:386:PRO:HB2	1:A:388:TRP:HE3	1.86	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	777/823 (94%)	754 (97%)	19 (2%)	4 (0%)	32 26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384	LYS
1	A	390	ALA
1	A	117	LYS
1	A	391	ALA

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	618/649 (95%)	607 (98%)	11 (2%)	64 68

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

Mol	Chain	Res	Type
1	A	65	LEU
1	A	200	GLU
1	A	307	LEU
1	A	389	LEU
1	A	429	TYR
1	A	430	TRP
1	A	449	TRP
1	A	547	LYS
1	A	703	THR
1	A	715	GLU
1	A	769	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN

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Mol	Chain	Res	Type
1	A	653	ASN

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 ⓘ

6 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	PGD	A	801	3	39,52,52	2.32	12 (30%)	35,81,81	1.59	3 (8%)
2	PGD	A	802	3	39,52,52	2.36	11 (28%)	35,81,81	2.28	9 (25%)
3	6WO	A	803	1,2	0,1,1	0.00	-	0,0,0	0.00	-
4	EOH	A	901	-	2,2,2	0.34	0	1,1,1	0.93	0
4	EOH	A	902	-	2,2,2	0.19	0	1,1,1	0.36	0
4	EOH	A	903	-	2,2,2	0.19	0	1,1,1	0.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGD	A	801	3	-	0/18/82/82	0/6/6/6
2	PGD	A	802	3	-	0/18/82/82	0/6/6/6
3	6WO	A	803	1,2	-	0/0/0/0	0/0/0/0
4	EOH	A	901	-	-	0/0/0/0	0/0/0/0
4	EOH	A	902	-	-	0/0/0/0	0/0/0/0
4	EOH	A	903	-	-	0/0/0/0	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	PGD	O11-C11	-2.12	1.40	1.43
2	A	801	PGD	C5-C4	-2.05	1.35	1.40
2	A	802	PGD	C21-N20	2.17	1.37	1.32
2	A	801	PGD	C21-N20	2.29	1.38	1.32
2	A	801	PGD	C2-N1	2.36	1.39	1.35
2	A	801	PGD	PB-O2B	2.50	1.67	1.55
2	A	802	PGD	PA-O2A	2.58	1.68	1.55
2	A	801	PGD	C19-N19	2.74	1.41	1.34
2	A	802	PGD	PB-O2B	2.94	1.70	1.55
2	A	802	PGD	PB-O5'	2.99	1.71	1.59
2	A	801	PGD	PB-O5'	3.25	1.73	1.59
2	A	802	PGD	C19-N19	3.39	1.42	1.34
2	A	801	PGD	C2-N2	3.47	1.41	1.34
2	A	801	PGD	PA-O3A	3.60	1.74	1.59
2	A	802	PGD	PA-O3A	3.68	1.74	1.59
2	A	802	PGD	C2-N2	4.03	1.42	1.34
2	A	802	PGD	C10-C11	4.12	1.57	1.52
2	A	801	PGD	PA-O1A	4.93	1.69	1.50
2	A	802	PGD	PA-O1A	5.14	1.70	1.50
2	A	802	PGD	PB-O1B	5.39	1.71	1.50
2	A	801	PGD	PB-O1B	5.42	1.71	1.50
2	A	802	PGD	C16-N15	6.59	1.45	1.28
2	A	801	PGD	C16-N15	6.62	1.45	1.28

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	802	PGD	C4'-O4'-C1'	-6.29	103.08	109.77
2	A	802	PGD	N3-C2-N1	-4.56	120.80	127.46
2	A	802	PGD	N20-C19-N18	-4.33	119.76	126.41
2	A	801	PGD	C5-C6-N1	-3.80	118.07	123.48
2	A	802	PGD	C5-C6-N1	-3.53	118.45	123.48
2	A	801	PGD	N20-C19-N18	-2.66	122.34	126.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	802	PGD	C6-C5-C4	-2.04	118.81	120.84
2	A	802	PGD	C16-C21-N22	2.35	122.71	116.53
2	A	802	PGD	C6-N1-C2	3.60	121.23	116.06
2	A	802	PGD	N19-C19-N18	4.54	123.22	117.09
2	A	802	PGD	C17-C16-N15	5.14	123.71	118.06
2	A	801	PGD	C17-C16-N15	5.75	124.37	118.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	PGD	1	0
2	A	802	PGD	2	0
4	A	901	EOH	1	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.