



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 01:18 pm BST

PDB ID : 1M5W
Title : 1.96 Å Crystal Structure of Pyridoxine 5'-Phosphate Synthase in Complex with 1-deoxy-D-xylulose phosphate
Authors : Yeh, J.I.; Du, S.; Pohl, E.; Cane, D.E.
Deposited on : 2002-07-10
Resolution : 1.96 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

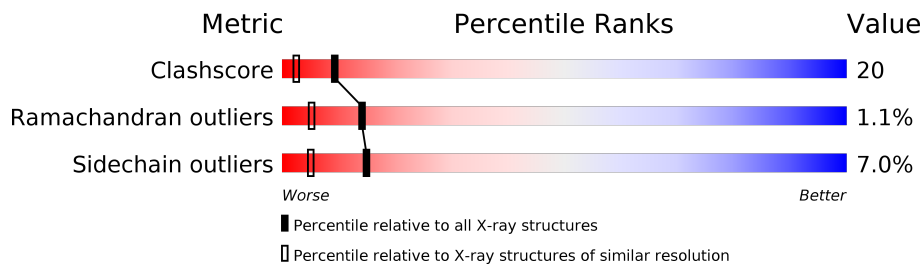
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	243	
1	B	243	
1	C	243	
1	D	243	
1	E	243	
1	F	243	
1	G	243	
1	H	243	

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
2	DXP	A	1001	-	X	-	-
2	DXP	C	1003	-	X	-	-
2	DXP	E	1005	-	-	X	-

2 Entry composition

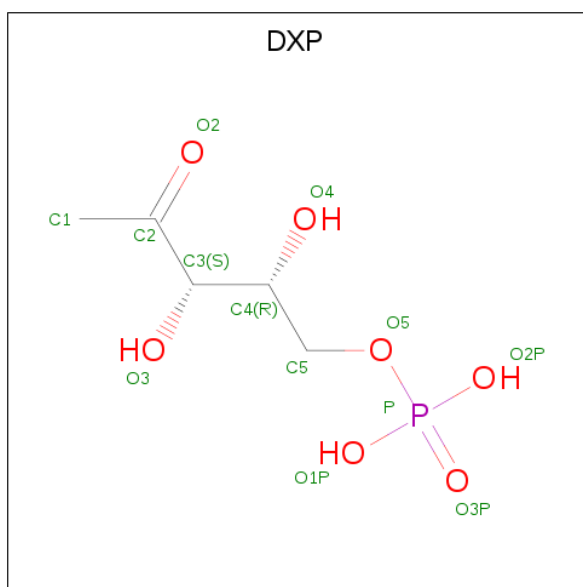
There are 4 unique types of molecules in this entry. The entry contains 15727 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyridoxal phosphate biosynthetic protein pdxJ.

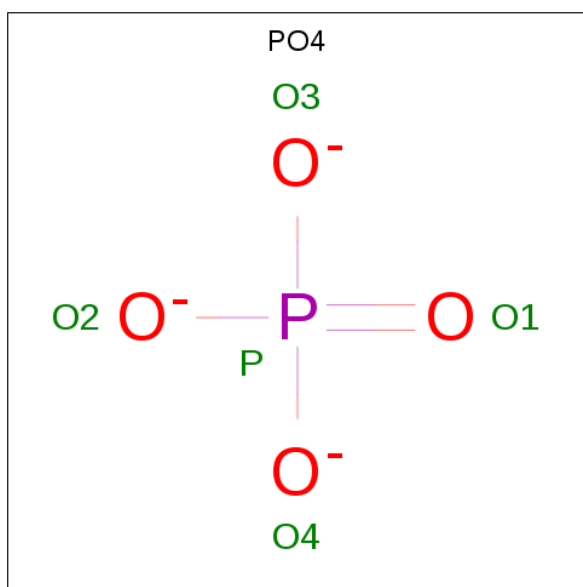
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	242	1837	1138	337	350	12	0	0	0
1	B	242	1837	1138	337	350	12	0	0	0
1	C	242	1837	1138	337	350	12	0	0	0
1	D	242	1837	1138	337	350	12	0	0	0
1	E	242	1837	1138	337	350	12	0	0	0
1	F	242	1837	1138	337	350	12	0	0	0
1	G	242	1837	1138	337	350	12	0	0	0
1	H	242	1837	1138	337	350	12	0	0	0

- Molecule 2 is 1-DEOXY-D-XYLULOSE-5-PHOSPHATE (three-letter code: DXP) (formula: C₅H₁₁O₇P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			13	5	7	1		
2	B	1	Total	C	O	P	0	0
			13	5	7	1		
2	C	1	Total	C	O	P	0	0
			13	5	7	1		
2	E	1	Total	C	O	P	0	0
			13	5	7	1		
2	F	1	Total	C	O	P	0	0
			13	5	7	1		
2	G	1	Total	C	O	P	0	0
			13	5	7	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

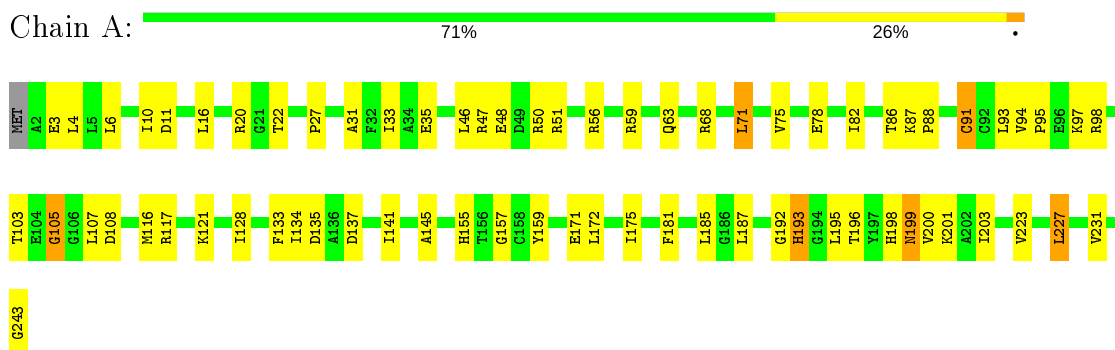
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	132	Total O 132 132	0	0
4	B	121	Total O 121 121	0	0
4	C	94	Total O 94 94	0	0
4	D	89	Total O 89 89	0	0
4	E	121	Total O 121 121	0	0
4	F	131	Total O 131 131	0	0
4	G	101	Total O 101 101	0	0
4	H	154	Total O 154 154	0	0

3 Residue-property plots [i](#)

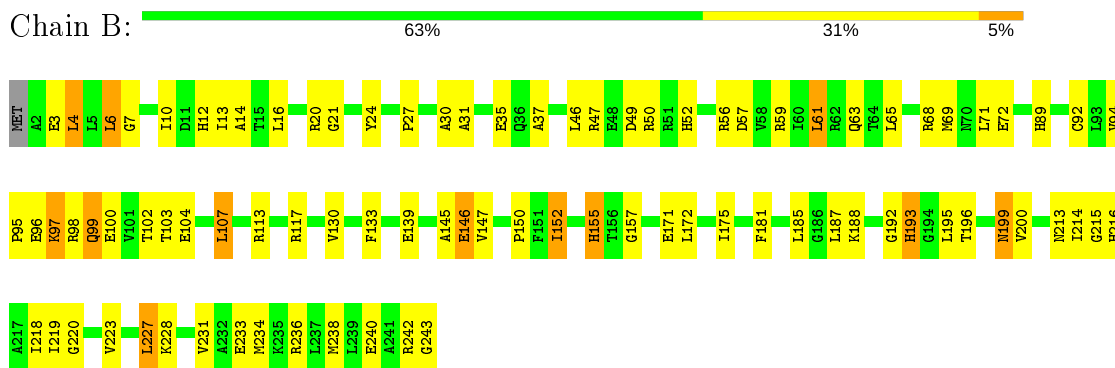
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

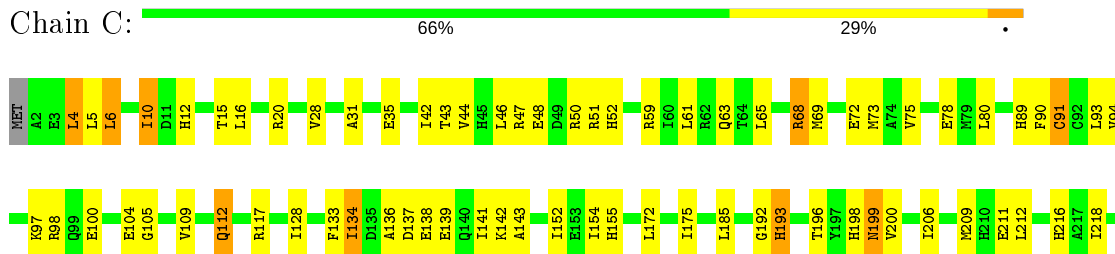
- Molecule 1: Pyridoxal phosphate biosynthetic protein pdxJ

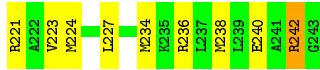


- Molecule 1: Pyridoxal phosphate biosynthetic protein pdxJ



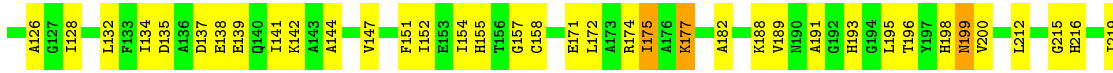
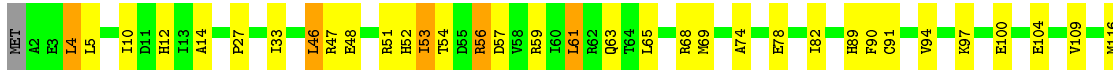
- Molecule 1: Pyridoxal phosphate biosynthetic protein pdxJ





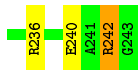
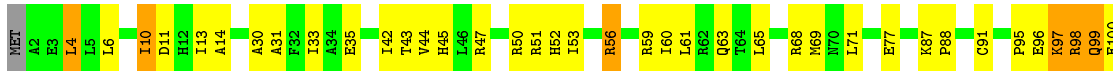
- Molecule 1: Pyridoxal phosphate biosynthetic protein pdxJ

Chain D: 68% 28%



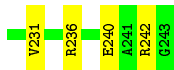
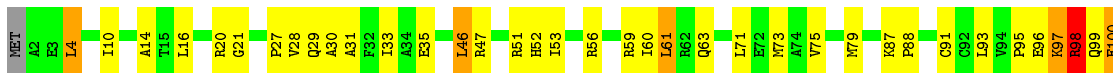
- Molecule 1: Pyridoxal phosphate biosynthetic protein pdxJ

Chain E: 68% 28%



- Molecule 1: Pyridoxal phosphate biosynthetic protein pdxJ

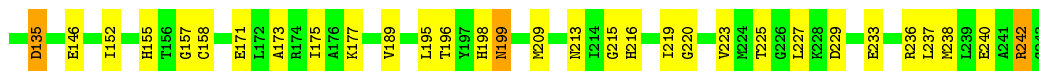
Chain F: 68% 26% 5%



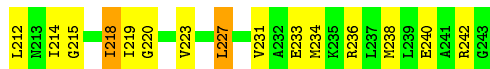
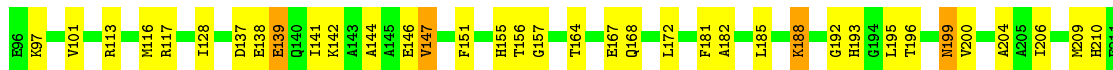
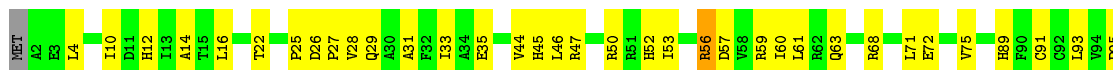
- Molecule 1: Pyridoxal phosphate biosynthetic protein pdxJ

Chain G: 72% 23% 5%





- Molecule 1: Pyridoxal phosphate biosynthetic protein pdxJ



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.01Å 129.40Å 176.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.96	Depositor
% Data completeness (in resolution range)	96.0 (6.00-1.96)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.195 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15727	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: PO4, DXP

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	0.35	0/1859	0.62	0/2509
1	B	0.34	0/1859	0.62	0/2509
1	C	0.33	0/1859	0.59	0/2509
1	D	0.33	0/1859	0.59	0/2509
1	E	0.34	0/1859	0.60	0/2509
1	F	0.35	0/1859	0.63	0/2509
1	G	0.33	0/1859	0.61	0/2509
1	H	0.35	0/1859	0.62	0/2509
All	All	0.34	0/14872	0.61	0/20072

There are no bond length outliers.

There are no bond angle outliers.

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	1837	0	1854	69	0
1	B	1837	0	1854	78	0
1	C	1837	0	1854	83	0
1	D	1837	0	1854	77	0
1	E	1837	0	1854	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1837	0	1854	76	0
1	G	1837	0	1854	58	0
1	H	1837	0	1854	88	0
2	A	13	0	7	5	0
2	B	13	0	7	3	0
2	C	13	0	6	5	0
2	E	13	0	7	7	0
2	F	13	0	7	2	0
2	G	13	0	7	5	0
3	A	5	0	0	1	0
3	C	5	0	0	1	0
4	A	132	0	0	6	0
4	B	121	0	0	8	0
4	C	94	0	0	10	0
4	D	89	0	0	3	0
4	E	121	0	0	3	0
4	F	131	0	0	7	0
4	G	101	0	0	10	0
4	H	154	0	0	3	0
All	All	15727	0	14873	587	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 20.

The worst 5 of 587 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:G:1007:DXP:C1	4:G:1107:HOH:O	1.67	1.25
1:C:72:GLU:OE2	4:C:1196:HOH:O	1.57	1.17
1:H:95:PRO:HB2	1:H:101:VAL:HG22	1.30	1.07
2:C:1003:DXP:H52	4:C:1197:HOH:O	1.55	1.06
2:C:1003:DXP:HC13	4:C:1195:HOH:O	1.55	1.05

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	240/243 (99%)	231 (96%)	7 (3%)	2 (1%)	19	9
1	B	240/243 (99%)	230 (96%)	7 (3%)	3 (1%)	12	3
1	C	240/243 (99%)	230 (96%)	6 (2%)	4 (2%)	9	2
1	D	240/243 (99%)	233 (97%)	5 (2%)	2 (1%)	19	9
1	E	240/243 (99%)	222 (92%)	16 (7%)	2 (1%)	19	9
1	F	240/243 (99%)	230 (96%)	6 (2%)	4 (2%)	9	2
1	G	240/243 (99%)	226 (94%)	13 (5%)	1 (0%)	34	22
1	H	240/243 (99%)	231 (96%)	6 (2%)	3 (1%)	12	3
All	All	1920/1944 (99%)	1833 (96%)	66 (3%)	21 (1%)	14	5

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	100	GLU
1	A	105	GLY
1	B	97	LYS
1	B	99	GLN
1	C	104	GLU

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	185/186 (100%)	173 (94%)	12 (6%)	17	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	185/186 (100%)	170 (92%)	15 (8%)	11	3
1	C	185/186 (100%)	171 (92%)	14 (8%)	13	4
1	D	185/186 (100%)	174 (94%)	11 (6%)	19	8
1	E	185/186 (100%)	170 (92%)	15 (8%)	11	3
1	F	185/186 (100%)	172 (93%)	13 (7%)	15	5
1	G	185/186 (100%)	171 (92%)	14 (8%)	13	4
1	H	185/186 (100%)	175 (95%)	10 (5%)	22	10
All	All	1480/1488 (100%)	1376 (93%)	104 (7%)	15	5

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	91	CYS
1	E	71	LEU
1	H	56	ARG
1	D	175	ILE
1	E	4	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	155	HIS
1	E	63	GLN
1	H	63	GLN
1	D	198	HIS
1	D	216	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	DXP	G	1007	-	11,12,12	4.81	5 (45%)	13,17,17	2.60	7 (53%)
3	PO4	A	1101	-	4,4,4	1.28	0	6,6,6	0.88	0
2	DXP	F	1006	-	11,12,12	4.83	5 (45%)	13,17,17	2.59	7 (53%)
2	DXP	B	1002	-	11,12,12	4.82	5 (45%)	13,17,17	2.61	7 (53%)
2	DXP	C	1003	-	11,12,12	4.95	5 (45%)	13,17,17	3.03	7 (53%)
2	DXP	A	1001	-	11,12,12	4.95	5 (45%)	13,17,17	2.86	7 (53%)
3	PO4	C	1103	-	4,4,4	0.91	0	6,6,6	0.83	0
2	DXP	E	1005	-	11,12,12	4.79	5 (45%)	13,17,17	2.60	7 (53%)

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	DXP	G	1007	-	-	5/14/14/14	-
2	DXP	B	1002	-	-	5/14/14/14	-
2	DXP	F	1006	-	-	5/14/14/14	-
2	DXP	E	1005	-	-	5/14/14/14	-
2	DXP	A	1001	-	-	10/14/14/14	-
2	DXP	C	1003	-	-	8/14/14/14	-

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1003	DXP	C3-C2	-13.65	1.42	1.52
2	A	1001	DXP	C3-C2	-13.60	1.42	1.52
2	F	1006	DXP	C3-C2	-13.15	1.42	1.52
2	B	1002	DXP	C3-C2	-13.07	1.42	1.52
2	G	1007	DXP	C3-C2	-13.06	1.42	1.52

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1003	DXP	C1-C2-C3	-6.00	114.29	118.39
2	A	1001	DXP	C1-C2-C3	-5.08	114.92	118.39
2	C	1003	DXP	O3-C3-C2	-4.61	103.62	111.04
2	A	1001	DXP	O3-C3-C2	-4.51	103.80	111.04
2	B	1002	DXP	O5-C5-C4	4.50	121.36	109.36

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1007	DXP	O2-C2-C3-O3
2	G	1007	DXP	O4-C4-C5-O5
2	F	1006	DXP	O2-C2-C3-O3
2	F	1006	DXP	O4-C4-C5-O5
2	B	1002	DXP	O2-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1007	DXP	5	0
3	A	1101	PO4	1	0
2	F	1006	DXP	2	0
2	B	1002	DXP	3	0
2	C	1003	DXP	5	0
2	A	1001	DXP	5	0
3	C	1103	PO4	1	0
2	E	1005	DXP	7	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.