



Full wwPDB X-ray Structure Validation Report i

Aug 14, 2023 – 02:26 pm BST

PDB ID : 8A29
Title : Apo 1-deoxy-D-xylulose 5-phosphate synthase from *Pseudomonas aeruginosa*
Authors : Hamid, R.; Adam, S.; Lacour, A.; Monjas, L.; Hirsch, A.
Deposited on : 2022-06-02
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 types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

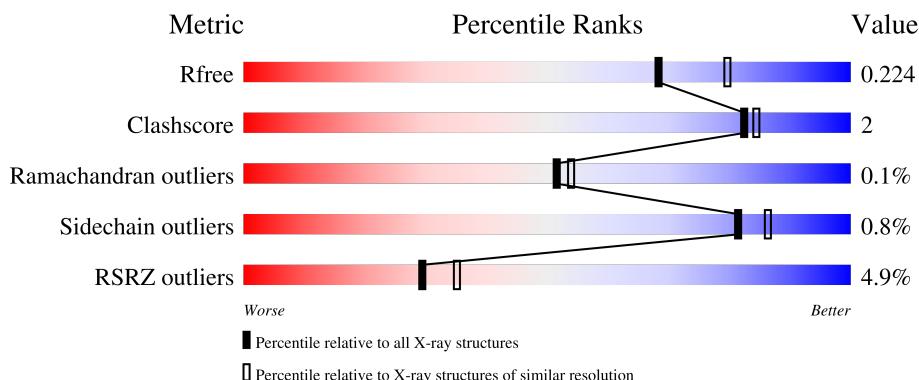
1 Overall quality at a glance

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))
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)
RSRZ outliers	127900	5083 (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 of 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 $\leq 5\%$. 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.



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Mol	Chain	Length	Quality of chain			
1	F	622	3%	85%	5%	11%

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 53080 atoms, of which 25331 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 1-deoxy-D-xylulose-5-phosphate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	557	Total	C	H	N	O	S	0	0	0
			8442	2684	4197	735	805	21			
1	B	563	Total	C	H	N	O	S	0	2	0
			8569	2719	4267	748	814	21			
1	C	559	Total	C	H	N	O	S	0	2	0
			8524	2707	4240	748	809	20			
1	D	554	Total	C	H	N	O	S	0	0	0
			8393	2669	4171	734	799	20			
1	E	560	Total	C	H	N	O	S	0	0	0
			8451	2698	4187	739	806	21			
1	F	556	Total	C	H	N	O	S	0	0	0
			8452	2685	4205	738	804	20			

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP B7V7R4
A	2	GLY	-	expression tag	UNP B7V7R4
A	3	SER	-	expression tag	UNP B7V7R4
A	4	SER	-	expression tag	UNP B7V7R4
A	5	HIS	-	expression tag	UNP B7V7R4
A	6	HIS	-	expression tag	UNP B7V7R4
A	7	HIS	-	expression tag	UNP B7V7R4
A	8	HIS	-	expression tag	UNP B7V7R4
A	9	HIS	-	expression tag	UNP B7V7R4
A	10	HIS	-	expression tag	UNP B7V7R4
A	11	SER	-	expression tag	UNP B7V7R4
A	12	SER	-	expression tag	UNP B7V7R4
A	13	GLY	-	expression tag	UNP B7V7R4
A	14	LEU	-	expression tag	UNP B7V7R4
A	15	VAL	-	expression tag	UNP B7V7R4
A	16	PRO	-	expression tag	UNP B7V7R4
A	17	ARG	-	expression tag	UNP B7V7R4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	expression tag	UNP B7V7R4
A	19	SER	-	expression tag	UNP B7V7R4
A	20	MET	-	expression tag	UNP B7V7R4
A	21	GLU	-	expression tag	UNP B7V7R4
A	22	ASN	-	expression tag	UNP B7V7R4
A	23	LEU	-	expression tag	UNP B7V7R4
A	24	TYR	-	expression tag	UNP B7V7R4
A	25	PHE	-	expression tag	UNP B7V7R4
A	26	GLN	-	expression tag	UNP B7V7R4
A	27	SER	-	expression tag	UNP B7V7R4
A	28	HIS	-	expression tag	UNP B7V7R4
A	235	GLY	-	linker	UNP B7V7R4
A	236	GLY	-	linker	UNP B7V7R4
A	237	GLY	-	linker	UNP B7V7R4
A	238	GLY	-	linker	UNP B7V7R4
A	239	GLY	-	linker	UNP B7V7R4
A	240	GLY	-	linker	UNP B7V7R4
B	1	MET	-	initiating methionine	UNP B7V7R4
B	2	GLY	-	expression tag	UNP B7V7R4
B	3	SER	-	expression tag	UNP B7V7R4
B	4	SER	-	expression tag	UNP B7V7R4
B	5	HIS	-	expression tag	UNP B7V7R4
B	6	HIS	-	expression tag	UNP B7V7R4
B	7	HIS	-	expression tag	UNP B7V7R4
B	8	HIS	-	expression tag	UNP B7V7R4
B	9	HIS	-	expression tag	UNP B7V7R4
B	10	HIS	-	expression tag	UNP B7V7R4
B	11	SER	-	expression tag	UNP B7V7R4
B	12	SER	-	expression tag	UNP B7V7R4
B	13	GLY	-	expression tag	UNP B7V7R4
B	14	LEU	-	expression tag	UNP B7V7R4
B	15	VAL	-	expression tag	UNP B7V7R4
B	16	PRO	-	expression tag	UNP B7V7R4
B	17	ARG	-	expression tag	UNP B7V7R4
B	18	GLY	-	expression tag	UNP B7V7R4
B	19	SER	-	expression tag	UNP B7V7R4
B	20	MET	-	expression tag	UNP B7V7R4
B	21	GLU	-	expression tag	UNP B7V7R4
B	22	ASN	-	expression tag	UNP B7V7R4
B	23	LEU	-	expression tag	UNP B7V7R4
B	24	TYR	-	expression tag	UNP B7V7R4
B	25	PHE	-	expression tag	UNP B7V7R4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	26	GLN	-	expression tag	UNP B7V7R4
B	27	SER	-	expression tag	UNP B7V7R4
B	28	HIS	-	expression tag	UNP B7V7R4
B	235	GLY	-	linker	UNP B7V7R4
B	236	GLY	-	linker	UNP B7V7R4
B	237	GLY	-	linker	UNP B7V7R4
B	238	GLY	-	linker	UNP B7V7R4
B	239	GLY	-	linker	UNP B7V7R4
B	240	GLY	-	linker	UNP B7V7R4
C	1	MET	-	initiating methionine	UNP B7V7R4
C	2	GLY	-	expression tag	UNP B7V7R4
C	3	SER	-	expression tag	UNP B7V7R4
C	4	SER	-	expression tag	UNP B7V7R4
C	5	HIS	-	expression tag	UNP B7V7R4
C	6	HIS	-	expression tag	UNP B7V7R4
C	7	HIS	-	expression tag	UNP B7V7R4
C	8	HIS	-	expression tag	UNP B7V7R4
C	9	HIS	-	expression tag	UNP B7V7R4
C	10	HIS	-	expression tag	UNP B7V7R4
C	11	SER	-	expression tag	UNP B7V7R4
C	12	SER	-	expression tag	UNP B7V7R4
C	13	GLY	-	expression tag	UNP B7V7R4
C	14	LEU	-	expression tag	UNP B7V7R4
C	15	VAL	-	expression tag	UNP B7V7R4
C	16	PRO	-	expression tag	UNP B7V7R4
C	17	ARG	-	expression tag	UNP B7V7R4
C	18	GLY	-	expression tag	UNP B7V7R4
C	19	SER	-	expression tag	UNP B7V7R4
C	20	MET	-	expression tag	UNP B7V7R4
C	21	GLU	-	expression tag	UNP B7V7R4
C	22	ASN	-	expression tag	UNP B7V7R4
C	23	LEU	-	expression tag	UNP B7V7R4
C	24	TYR	-	expression tag	UNP B7V7R4
C	25	PHE	-	expression tag	UNP B7V7R4
C	26	GLN	-	expression tag	UNP B7V7R4
C	27	SER	-	expression tag	UNP B7V7R4
C	28	HIS	-	expression tag	UNP B7V7R4
C	235	GLY	-	linker	UNP B7V7R4
C	236	GLY	-	linker	UNP B7V7R4
C	237	GLY	-	linker	UNP B7V7R4
C	238	GLY	-	linker	UNP B7V7R4
C	239	GLY	-	linker	UNP B7V7R4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	240	GLY	-	linker	UNP B7V7R4
D	1	MET	-	initiating methionine	UNP B7V7R4
D	2	GLY	-	expression tag	UNP B7V7R4
D	3	SER	-	expression tag	UNP B7V7R4
D	4	SER	-	expression tag	UNP B7V7R4
D	5	HIS	-	expression tag	UNP B7V7R4
D	6	HIS	-	expression tag	UNP B7V7R4
D	7	HIS	-	expression tag	UNP B7V7R4
D	8	HIS	-	expression tag	UNP B7V7R4
D	9	HIS	-	expression tag	UNP B7V7R4
D	10	HIS	-	expression tag	UNP B7V7R4
D	11	SER	-	expression tag	UNP B7V7R4
D	12	SER	-	expression tag	UNP B7V7R4
D	13	GLY	-	expression tag	UNP B7V7R4
D	14	LEU	-	expression tag	UNP B7V7R4
D	15	VAL	-	expression tag	UNP B7V7R4
D	16	PRO	-	expression tag	UNP B7V7R4
D	17	ARG	-	expression tag	UNP B7V7R4
D	18	GLY	-	expression tag	UNP B7V7R4
D	19	SER	-	expression tag	UNP B7V7R4
D	20	MET	-	expression tag	UNP B7V7R4
D	21	GLU	-	expression tag	UNP B7V7R4
D	22	ASN	-	expression tag	UNP B7V7R4
D	23	LEU	-	expression tag	UNP B7V7R4
D	24	TYR	-	expression tag	UNP B7V7R4
D	25	PHE	-	expression tag	UNP B7V7R4
D	26	GLN	-	expression tag	UNP B7V7R4
D	27	SER	-	expression tag	UNP B7V7R4
D	28	HIS	-	expression tag	UNP B7V7R4
D	235	GLY	-	linker	UNP B7V7R4
D	236	GLY	-	linker	UNP B7V7R4
D	237	GLY	-	linker	UNP B7V7R4
D	238	GLY	-	linker	UNP B7V7R4
D	239	GLY	-	linker	UNP B7V7R4
D	240	GLY	-	linker	UNP B7V7R4
E	1	MET	-	initiating methionine	UNP B7V7R4
E	2	GLY	-	expression tag	UNP B7V7R4
E	3	SER	-	expression tag	UNP B7V7R4
E	4	SER	-	expression tag	UNP B7V7R4
E	5	HIS	-	expression tag	UNP B7V7R4
E	6	HIS	-	expression tag	UNP B7V7R4
E	7	HIS	-	expression tag	UNP B7V7R4

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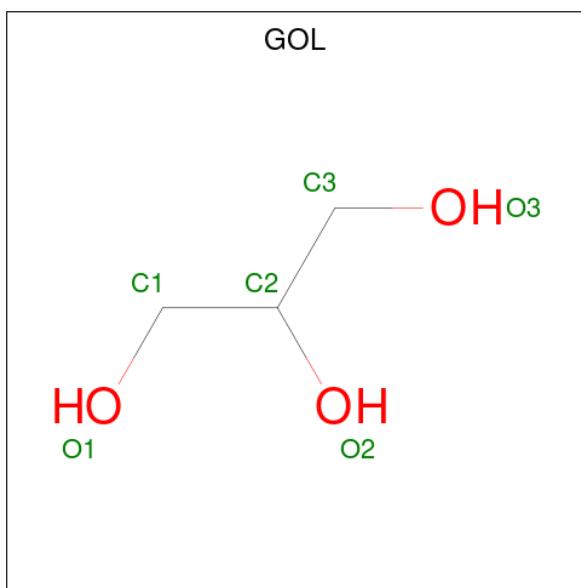
Chain	Residue	Modelled	Actual	Comment	Reference
E	8	HIS	-	expression tag	UNP B7V7R4
E	9	HIS	-	expression tag	UNP B7V7R4
E	10	HIS	-	expression tag	UNP B7V7R4
E	11	SER	-	expression tag	UNP B7V7R4
E	12	SER	-	expression tag	UNP B7V7R4
E	13	GLY	-	expression tag	UNP B7V7R4
E	14	LEU	-	expression tag	UNP B7V7R4
E	15	VAL	-	expression tag	UNP B7V7R4
E	16	PRO	-	expression tag	UNP B7V7R4
E	17	ARG	-	expression tag	UNP B7V7R4
E	18	GLY	-	expression tag	UNP B7V7R4
E	19	SER	-	expression tag	UNP B7V7R4
E	20	MET	-	expression tag	UNP B7V7R4
E	21	GLU	-	expression tag	UNP B7V7R4
E	22	ASN	-	expression tag	UNP B7V7R4
E	23	LEU	-	expression tag	UNP B7V7R4
E	24	TYR	-	expression tag	UNP B7V7R4
E	25	PHE	-	expression tag	UNP B7V7R4
E	26	GLN	-	expression tag	UNP B7V7R4
E	27	SER	-	expression tag	UNP B7V7R4
E	28	HIS	-	expression tag	UNP B7V7R4
E	235	GLY	-	linker	UNP B7V7R4
E	236	GLY	-	linker	UNP B7V7R4
E	237	GLY	-	linker	UNP B7V7R4
E	238	GLY	-	linker	UNP B7V7R4
E	239	GLY	-	linker	UNP B7V7R4
E	240	GLY	-	linker	UNP B7V7R4
F	1	MET	-	initiating methionine	UNP B7V7R4
F	2	GLY	-	expression tag	UNP B7V7R4
F	3	SER	-	expression tag	UNP B7V7R4
F	4	SER	-	expression tag	UNP B7V7R4
F	5	HIS	-	expression tag	UNP B7V7R4
F	6	HIS	-	expression tag	UNP B7V7R4
F	7	HIS	-	expression tag	UNP B7V7R4
F	8	HIS	-	expression tag	UNP B7V7R4
F	9	HIS	-	expression tag	UNP B7V7R4
F	10	HIS	-	expression tag	UNP B7V7R4
F	11	SER	-	expression tag	UNP B7V7R4
F	12	SER	-	expression tag	UNP B7V7R4
F	13	GLY	-	expression tag	UNP B7V7R4
F	14	LEU	-	expression tag	UNP B7V7R4
F	15	VAL	-	expression tag	UNP B7V7R4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	16	PRO	-	expression tag	UNP B7V7R4
F	17	ARG	-	expression tag	UNP B7V7R4
F	18	GLY	-	expression tag	UNP B7V7R4
F	19	SER	-	expression tag	UNP B7V7R4
F	20	MET	-	expression tag	UNP B7V7R4
F	21	GLU	-	expression tag	UNP B7V7R4
F	22	ASN	-	expression tag	UNP B7V7R4
F	23	LEU	-	expression tag	UNP B7V7R4
F	24	TYR	-	expression tag	UNP B7V7R4
F	25	PHE	-	expression tag	UNP B7V7R4
F	26	GLN	-	expression tag	UNP B7V7R4
F	27	SER	-	expression tag	UNP B7V7R4
F	28	HIS	-	expression tag	UNP B7V7R4
F	235	GLY	-	linker	UNP B7V7R4
F	236	GLY	-	linker	UNP B7V7R4
F	237	GLY	-	linker	UNP B7V7R4
F	238	GLY	-	linker	UNP B7V7R4
F	239	GLY	-	linker	UNP B7V7R4
F	240	GLY	-	linker	UNP B7V7R4

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C H O 14 3 8 3	0	0
2	E	1	Total C H O 14 3 8 3	0	0
2	F	1	Total C H O 14 3 8 3	0	0
2	F	1	Total C H O 14 3 8 3	0	0
2	F	1	Total C H O 14 3 8 3	0	0
2	F	1	Total C H O 14 3 8 3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	4	Total Mg 4 4	0	0
3	C	2	Total Mg 2 2	0	0
3	D	1	Total Mg 1 1	0	0
3	E	2	Total Mg 2 2	0	0
3	F	2	Total Mg 2 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Na 1 1	0	0
5	D	1	Total	Na 1 1	0	0
5	E	1	Total	Na 1 1	0	0
5	F	1	Total	Na 1 1	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Ca 2 2	0	0
6	B	1	Total	Ca 1 1	0	0
6	C	1	Total	Ca 1 1	0	0
6	D	4	Total	Ca 4 4	0	0
6	E	2	Total	Ca 2 2	0	0
6	F	2	Total	Ca 2 2	0	0

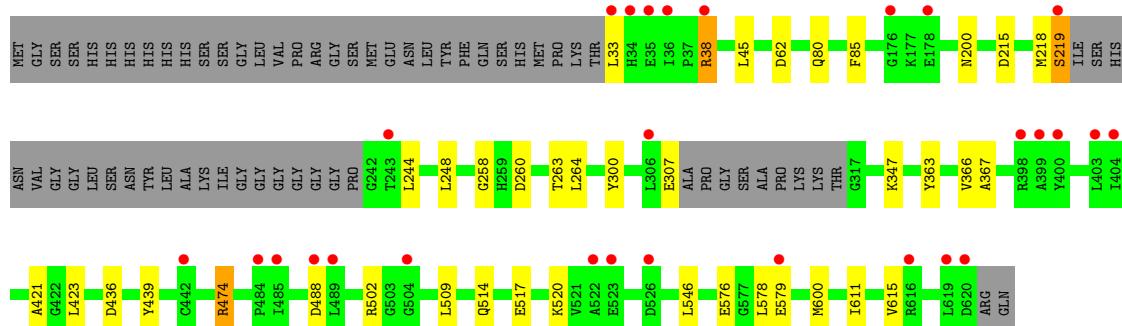
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	326	Total	O 326 326	0	0
7	B	384	Total	O 384 384	0	0
7	C	311	Total	O 311 311	0	0
7	D	337	Total	O 337 337	0	0
7	E	356	Total	O 356 356	0	0
7	F	391	Total	O 391 391	0	0

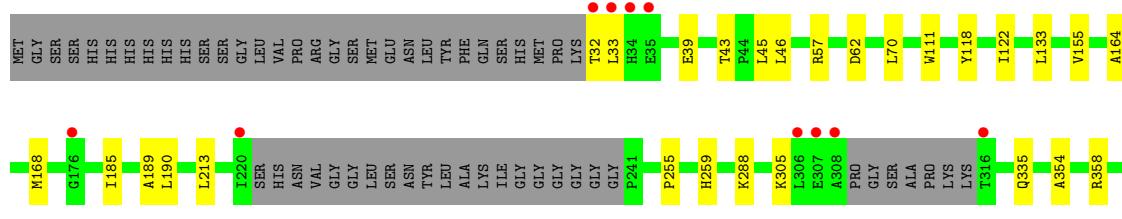
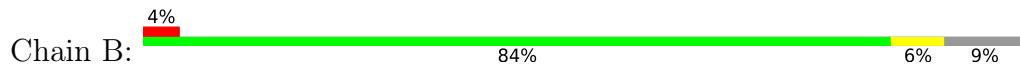
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

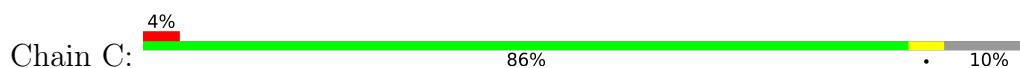
- Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase



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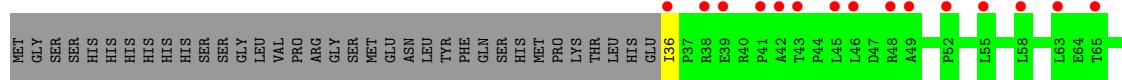
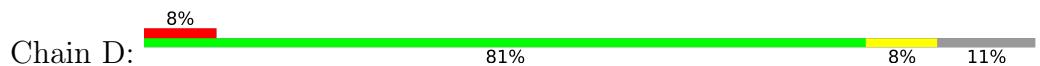


- Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase

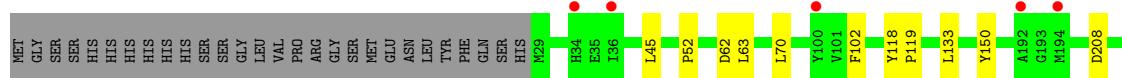
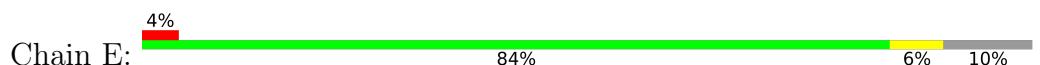




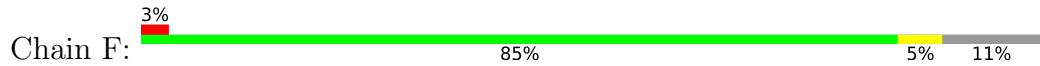
- Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase



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4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.44Å 137.63Å 232.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.59 – 2.10 48.59 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.59-2.10) 99.9 (48.59-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^{\text{1}}$	1.93 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R , R_{free}	0.171 , 0.224 0.171 , 0.224	Depositor DCC
R_{free} test set	10811 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53080	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: CL, MG, NA, GOL, CA

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	0.51	0/4329	0.70	0/5869
1	B	0.54	0/4390	0.70	0/5951
1	C	0.53	0/4372	0.70	0/5926
1	D	0.54	0/4305	0.68	0/5837
1	E	0.52	0/4350	0.70	2/5899 (0.0%)
1	F	0.55	0/4331	0.70	0/5872
All	All	0.53	0/26077	0.70	2/35354 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	453	ASP	CB-CG-OD1	6.29	123.96	118.30
1	E	531	ASP	CB-CG-OD2	-5.39	113.45	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	618	ARG	Sidechain

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	4245	4197	4210	24	0
1	B	4302	4267	4274	20	0
1	C	4284	4240	4257	13	0
1	D	4222	4171	4194	32	0
1	E	4264	4187	4236	23	0
1	F	4247	4205	4214	17	0
2	A	6	8	8	0	0
2	D	6	8	8	0	0
2	E	12	16	16	0	0
2	F	24	32	31	0	0
3	A	2	0	0	0	0
3	B	4	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	4	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
7	A	326	0	0	3	0
7	B	384	0	0	1	0
7	C	311	0	0	2	0
7	D	337	0	0	2	0
7	E	356	0	0	0	0
7	F	391	0	0	1	0
All	All	27749	25331	25448	127	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 (127) 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:D:256:ILE:HD11	1:D:282:VAL:HG22	1.48	0.93
1:A:33:LEU:O	1:A:33:LEU:HD23	1.71	0.91
1:B:39:GLU:OE1	7:B:801:HOH:O	2.00	0.79
1:A:38:ARG:HH12	1:A:307:GLU:HB2	1.48	0.78
1:A:509:LEU:HD21	1:A:546:LEU:HD13	1.80	0.64
1:D:256:ILE:CD1	1:D:282:VAL:HG22	2.27	0.64
1:E:271:MET:HA	1:E:274:MET:HE3	1.79	0.64
1:D:530:VAL:HG21	1:D:546:LEU:HD11	1.84	0.60
1:E:45:LEU:HD21	1:E:62:ASP:HB3	1.85	0.59
1:B:45:LEU:HD21	1:B:62:ASP:HB3	1.85	0.58
1:C:353:VAL:O	1:C:357:GLU:HG3	2.04	0.58
1:B:190:LEU:HD12	1:B:213:LEU:HD13	1.87	0.56
1:F:530:VAL:HG21	1:F:546:LEU:HD11	1.88	0.55
1:D:68:ASP:O	1:D:72:GLN:HG2	2.07	0.55
1:A:38:ARG:NH1	1:A:307:GLU:HB2	2.17	0.55
1:B:118:TYR:CZ	1:B:133:LEU:HD21	2.43	0.54
1:A:260:ASP:OD2	1:A:263:THR:OG1	2.21	0.54
1:E:208:ASP:OD2	1:E:275:LYS:HE3	2.08	0.53
1:F:60:GLU:OE1	1:F:269:ARG:NH1	2.31	0.53
1:B:354:ALA:O	1:B:358:ARG:HG3	2.09	0.53
1:D:502:ARG:NH1	7:D:809:HOH:O	2.41	0.53
1:F:216:ASN:O	1:F:217:ASP:HB3	2.08	0.53
1:A:215:ASP:OD1	1:A:219:SER:HB2	2.09	0.52
1:A:33:LEU:HD23	1:A:33:LEU:C	2.30	0.52
1:B:366:VAL:O	1:B:367:ALA:HB3	2.10	0.52
1:D:509:LEU:N	1:D:509:LEU:HD12	2.25	0.51
1:A:244:LEU:HD11	1:A:248:LEU:HD11	1.92	0.50
1:A:85:PHE:HB3	1:A:300:TYR:O	2.12	0.50
1:C:521:VAL:HG12	1:C:525:LEU:HD12	1.92	0.49
1:B:455:ASP:OD2	1:B:459:LYS:HE2	2.11	0.49
1:A:502:ARG:NH2	7:A:806:HOH:O	2.45	0.49
1:D:164:ALA:O	1:D:168:MET:HG3	2.13	0.49
1:F:113:VAL:CG2	1:F:158:SER:HB2	2.44	0.48
1:A:45:LEU:HD21	1:A:62:ASP:HB3	1.96	0.48
1:E:361:GLU:HG2	1:E:362:ARG:HG3	1.94	0.48
1:A:366:VAL:O	1:A:367:ALA:HB3	2.13	0.47
1:A:258:GLY:O	1:A:264:LEU:HD11	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:260:ASP:OD2	1:F:262:PRO:HD2	2.13	0.47
1:C:509:LEU:HD12	1:C:509:LEU:N	2.30	0.47
1:D:256:ILE:HD11	1:D:282:VAL:CG2	2.34	0.46
1:A:576:GLU:HB2	1:A:578:LEU:HG	1.98	0.46
1:D:270:ASN:O	1:D:274:MET:HE2	2.16	0.46
1:F:421:ALA:HB1	1:F:474:ARG:CZ	2.46	0.46
1:D:95:THR:HG22	1:D:123:LEU:HD12	1.99	0.45
1:A:33:LEU:O	1:A:33:LEU:CD2	2.56	0.45
1:D:291:ALA:O	1:D:295:LEU:HD12	2.15	0.45
1:E:118:TYR:HB2	1:E:119:PRO:HD3	1.97	0.45
1:D:36:ILE:HG21	1:D:306:LEU:HD11	1.97	0.45
1:E:291:ALA:HB3	1:E:292:PRO:HD3	1.99	0.45
1:B:70:LEU:CD1	1:B:122:ILE:HG21	2.47	0.45
1:A:436:ASP:HA	1:A:439:TYR:CE2	2.52	0.45
1:A:611:ILE:O	1:A:615:VAL:HG23	2.16	0.45
1:D:621:ARG:HH11	1:D:621:ARG:HG3	1.82	0.45
1:A:579:GLU:OE2	1:E:579:GLU:HG3	2.17	0.44
1:B:259:HIS:CE1	1:B:288:LYS:HG2	2.52	0.44
1:C:185:ILE:CG1	1:C:189:ALA:HB3	2.48	0.44
1:E:376:LEU:O	1:E:380:MET:HG3	2.17	0.44
1:C:185:ILE:HG13	1:C:189:ALA:HB3	1.99	0.44
1:D:70:LEU:HD23	1:D:70:LEU:O	2.18	0.44
1:F:68:ASP:N	1:F:68:ASP:OD1	2.50	0.44
1:D:94:LEU:O	1:D:98:LEU:HD23	2.18	0.44
1:B:32:THR:HG22	1:B:33:LEU:HD22	1.99	0.44
1:B:509:LEU:HD21	1:B:546:LEU:HD13	2.00	0.44
1:E:366:VAL:O	1:E:367:ALA:HB3	2.18	0.44
1:C:271:MET:HA	1:C:274:MET:CE	2.48	0.44
1:B:335:GLN:HA	1:B:335:GLN:NE2	2.33	0.43
1:F:117:ALA:HA	7:F:954:HOH:O	2.17	0.43
1:F:366:VAL:O	1:F:367:ALA:HB3	2.18	0.43
1:A:517:GLU:OE2	1:A:520:LYS:NZ	2.47	0.43
1:B:43:THR:HB	1:B:46:LEU:HB3	2.00	0.43
1:B:111:TRP:O	1:B:155:VAL:HG11	2.18	0.43
1:E:366:VAL:HG21	1:E:373:ALA:HB2	2.01	0.43
1:A:423:LEU:HD13	1:A:600:MET:HB3	2.01	0.43
1:F:509:LEU:HD12	1:F:509:LEU:N	2.34	0.43
1:E:261:LEU:O	1:E:265:VAL:HG23	2.18	0.43
1:F:113:VAL:HG22	1:F:158:SER:HB2	2.00	0.43
1:D:391:ILE:O	1:D:418:ILE:HA	2.19	0.43
1:E:118:TYR:CZ	1:E:133:LEU:HD21	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:TYR:CZ	1:D:133:LEU:HD21	2.54	0.42
1:D:494:ILE:HA	1:D:534:PHE:CZ	2.54	0.42
1:F:64:GLU:O	1:F:68:ASP:OD1	2.37	0.42
1:F:436:ASP:HA	1:F:439:TYR:CE2	2.54	0.42
1:C:421:ALA:HB1	1:C:474:ARG:CZ	2.49	0.42
1:D:211:VAL:HG23	1:D:250:TRP:CZ3	2.53	0.42
1:C:106:ASP:O	1:C:179:ARG:HD3	2.19	0.42
1:E:70:LEU:HD23	1:E:70:LEU:O	2.18	0.42
1:E:530:VAL:HG21	1:E:546:LEU:HD11	2.01	0.42
7:A:995:HOH:O	1:E:563:GLY:HA3	2.19	0.42
1:B:421:ALA:HB1	1:B:474:ARG:CZ	2.49	0.42
1:E:52:PRO:HG2	1:E:150:TYR:CE1	2.55	0.42
1:F:110:VAL:HG22	1:F:152:THR:OG1	2.20	0.42
1:B:185:ILE:HG13	1:B:189:ALA:HB3	2.01	0.42
1:D:578:LEU:O	7:D:801:HOH:O	2.21	0.42
1:E:271:MET:CA	1:E:274:MET:HE3	2.48	0.42
1:E:252:TYR:O	1:E:253:ILE:HD13	2.20	0.42
1:D:114:GLY:HA3	1:D:143:PRO:HD2	2.01	0.42
1:D:352:LEU:HD12	1:D:352:LEU:N	2.34	0.42
1:E:70:LEU:HD23	1:E:70:LEU:C	2.40	0.42
1:D:436:ASP:HA	1:D:439:TYR:CE2	2.55	0.42
1:A:421:ALA:HB1	1:A:474:ARG:CZ	2.49	0.42
1:B:504:GLY:O	1:B:505:ARG:HB3	2.20	0.41
1:A:200:ASN:OD1	1:A:248:LEU:HD22	2.19	0.41
1:B:164:ALA:O	1:B:168:MET:HG3	2.20	0.41
1:C:149:GLU:HG2	7:C:1017:HOH:O	2.21	0.41
1:C:506:VAL:HG11	1:C:619:LEU:HD11	2.03	0.41
1:D:451:PRO:HB3	1:D:460:LEU:HD12	2.02	0.41
1:D:366:VAL:O	1:D:367:ALA:HB3	2.19	0.41
1:D:509:LEU:N	1:D:509:LEU:CD1	2.83	0.41
1:F:339:LEU:HD23	1:F:339:LEU:C	2.41	0.41
1:D:106:ASP:O	1:D:179:ARG:HD3	2.21	0.41
1:B:489:LEU:HD23	1:B:489:LEU:HA	1.93	0.41
1:C:366:VAL:HG21	1:C:373:ALA:HB2	2.03	0.41
1:D:256:ILE:C	1:D:256:ILE:HD12	2.41	0.41
1:E:451:PRO:HB3	1:E:460:LEU:HD12	2.02	0.41
1:F:118:TYR:CZ	1:F:133:LEU:HD21	2.56	0.41
1:F:243:THR:HG22	1:F:245:PHE:H	1.86	0.41
1:D:211:VAL:HG23	1:D:250:TRP:CH2	2.57	0.41
1:D:347:LYS:HB2	1:D:363:TYR:OH	2.21	0.41
1:E:63:LEU:HB3	1:E:261:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:391:ILE:O	1:E:418:ILE:HA	2.21	0.41
1:B:567:SER:OG	1:D:571:GLU:OE1	2.21	0.40
1:A:514:GLN:HB2	7:A:801:HOH:O	2.21	0.40
1:C:613:LYS:O	1:C:617:GLN:HG3	2.21	0.40
1:E:102:PHE:CE2	1:E:272:ARG:HG3	2.56	0.40
1:A:347:LYS:HB2	1:A:363:TYR:OH	2.22	0.40
1:C:62:ASP:OD2	7:C:801:HOH:O	2.22	0.40
1:D:366:VAL:HG21	1:D:373:ALA:HB2	2.03	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	551/622 (89%)	534 (97%)	16 (3%)	1 (0%)	47 49
1	B	559/622 (90%)	540 (97%)	19 (3%)	0	100 100
1	C	555/622 (89%)	540 (97%)	14 (2%)	1 (0%)	47 49
1	D	548/622 (88%)	531 (97%)	17 (3%)	0	100 100
1	E	554/622 (89%)	537 (97%)	17 (3%)	0	100 100
1	F	550/622 (88%)	532 (97%)	18 (3%)	0	100 100
All	All	3317/3732 (89%)	3214 (97%)	101 (3%)	2 (0%)	51 54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	526	ASP
1	A	218	MET

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	440/490 (90%)	435 (99%)	5 (1%)	73 79
1	B	446/490 (91%)	443 (99%)	3 (1%)	84 88
1	C	444/490 (91%)	441 (99%)	3 (1%)	84 88
1	D	437/490 (89%)	432 (99%)	5 (1%)	73 79
1	E	442/490 (90%)	440 (100%)	2 (0%)	88 92
1	F	440/490 (90%)	436 (99%)	4 (1%)	78 84
All	All	2649/2940 (90%)	2627 (99%)	22 (1%)	81 86

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

Mol	Chain	Res	Type
1	A	38	ARG
1	A	80	GLN
1	A	219	SER
1	A	474	ARG
1	A	488	ASP
1	B	57	ARG
1	B	255	PRO
1	B	305	LYS
1	C	320	LYS
1	C	470	PRO
1	C	505	ARG
1	D	178	GLU
1	D	179	ARG
1	D	213	LEU
1	D	244	LEU
1	D	305	LYS
1	E	474	ARG
1	E	524	SER
1	F	68	ASP
1	F	158	SER
1	F	273	ASP
1	F	307	GLU

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

Mol	Chain	Res	Type
1	A	490	GLN
1	E	135	GLN
1	E	617	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 40 ligands modelled in this entry, 32 are monoatomic - leaving 8 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	GOL	E	702	-	5,5,5	1.46	0	5,5,5	0.42	0
2	GOL	A	701	-	5,5,5	1.00	0	5,5,5	0.90	0
2	GOL	E	701	-	5,5,5	0.95	0	5,5,5	0.97	0
2	GOL	F	702	-	5,5,5	1.17	1 (20%)	5,5,5	0.86	0
2	GOL	D	701	-	5,5,5	0.95	0	5,5,5	1.00	0
2	GOL	F	701	-	5,5,5	1.33	1 (20%)	5,5,5	0.80	0
2	GOL	F	703	-	5,5,5	2.43	1 (20%)	5,5,5	0.80	0
2	GOL	F	704	-	5,5,5	2.56	3 (60%)	5,5,5	0.90	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	GOL	E	702	-	-	4/4/4/4	-
2	GOL	A	701	-	-	0/4/4/4	-
2	GOL	E	701	-	-	2/4/4/4	-
2	GOL	F	702	-	-	1/4/4/4	-
2	GOL	D	701	-	-	2/4/4/4	-
2	GOL	F	701	-	-	4/4/4/4	-
2	GOL	F	703	-	-	2/4/4/4	-
2	GOL	F	704	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	703	GOL	O2-C2	-4.99	1.28	1.43
2	F	704	GOL	O2-C2	3.97	1.55	1.43
2	F	704	GOL	C3-C2	2.75	1.63	1.51
2	F	701	GOL	C1-C2	2.11	1.60	1.51
2	F	702	GOL	O2-C2	-2.10	1.37	1.43
2	F	704	GOL	C1-C2	-2.03	1.43	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	702	GOL	C1-C2-C3-O3
2	D	701	GOL	C1-C2-C3-O3
2	E	701	GOL	C1-C2-C3-O3
2	F	701	GOL	O1-C1-C2-C3
2	F	701	GOL	C1-C2-C3-O3
2	F	703	GOL	O1-C1-C2-C3
2	E	702	GOL	O2-C2-C3-O3
2	D	701	GOL	O2-C2-C3-O3
2	E	701	GOL	O2-C2-C3-O3
2	F	703	GOL	O1-C1-C2-O2
2	F	701	GOL	O1-C1-C2-O2
2	F	704	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	E	702	GOL	O1-C1-C2-C3
2	F	704	GOL	O1-C1-C2-C3
2	E	702	GOL	O1-C1-C2-O2
2	F	701	GOL	O2-C2-C3-O3
2	F	702	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	557/622 (89%)	0.28	28 (5%) 28 34	19, 29, 49, 88	0
1	B	563/622 (90%)	0.23	24 (4%) 35 41	17, 26, 43, 90	0
1	C	559/622 (89%)	0.25	22 (3%) 39 45	17, 28, 47, 79	0
1	D	554/622 (89%)	0.52	52 (9%) 8 11	17, 29, 57, 90	0
1	E	560/622 (90%)	0.28	23 (4%) 37 43	18, 27, 46, 83	0
1	F	556/622 (89%)	0.26	16 (2%) 51 57	16, 25, 44, 71	0
All	All	3349/3732 (89%)	0.30	165 (4%) 29 35	16, 27, 49, 90	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	621	ARG	5.7
1	D	75	LEU	5.2
1	F	307	GLU	4.9
1	D	306	LEU	4.8
1	A	219	SER	4.8
1	D	295	LEU	4.6
1	B	316	THR	4.6
1	A	33	LEU	4.3
1	B	32	THR	4.1
1	A	34	HIS	4.1
1	D	63	LEU	3.9
1	F	38	ARG	3.9
1	D	48	ARG	3.8
1	D	217	ASP	3.7
1	D	298	ILE	3.5
1	D	297	PRO	3.5
1	D	46	LEU	3.5
1	F	439	TYR	3.5
1	F	306	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	439	TYR	3.5
1	D	38	ARG	3.4
1	D	316	THR	3.4
1	D	303	ILE	3.4
1	D	100	TYR	3.4
1	E	240	GLY	3.4
1	E	369	ALA	3.3
1	B	484	PRO	3.3
1	E	100	TYR	3.3
1	A	403	LEU	3.3
1	C	306	LEU	3.3
1	D	74	LEU	3.3
1	C	621	ARG	3.2
1	D	78	VAL	3.2
1	D	400	TYR	3.2
1	A	619	LEU	3.2
1	E	400	TYR	3.2
1	C	521	VAL	3.2
1	A	504	GLY	3.1
1	A	488	ASP	3.1
1	C	33	LEU	3.1
1	D	41	PRO	3.1
1	D	68	ASP	3.1
1	A	400	TYR	3.1
1	C	400	TYR	3.1
1	C	38	ARG	3.0
1	D	45	LEU	3.0
1	C	617	GLN	3.0
1	B	308	ALA	3.0
1	D	42	ALA	3.0
1	B	400	TYR	2.9
1	D	49	ALA	2.9
1	D	272	ARG	2.9
1	F	400	TYR	2.9
1	B	306	LEU	2.9
1	D	268	LEU	2.9
1	C	579	GLU	2.9
1	C	622	GLN	2.9
1	E	298	ILE	2.8
1	A	399	ALA	2.8
1	A	176	GLY	2.8
1	D	435	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	273	ASP	2.8
1	C	36	ILE	2.8
1	C	316	THR	2.8
1	B	176	GLY	2.8
1	D	65	THR	2.8
1	D	58	LEU	2.7
1	F	399	ALA	2.7
1	D	52	PRO	2.7
1	D	43	THR	2.7
1	D	304	THR	2.7
1	D	267	THR	2.7
1	D	36	ILE	2.7
1	F	55	LEU	2.7
1	A	522	ALA	2.7
1	E	373	ALA	2.7
1	B	403	LEU	2.7
1	A	620	ASP	2.6
1	C	442	CYS	2.6
1	A	404	ILE	2.6
1	B	34	HIS	2.6
1	A	523	GLU	2.6
1	B	620	ASP	2.6
1	E	253	ILE	2.6
1	E	295	LEU	2.6
1	E	399	ALA	2.5
1	F	272	ARG	2.5
1	B	33	LEU	2.5
1	A	484	PRO	2.5
1	C	403	LEU	2.5
1	D	291	ALA	2.5
1	D	399	ALA	2.5
1	E	192	ALA	2.5
1	B	487	PRO	2.5
1	D	261	LEU	2.5
1	E	396	LEU	2.4
1	A	442	CYS	2.4
1	B	490	GLN	2.4
1	B	404	ILE	2.4
1	B	399	ALA	2.4
1	E	34	HIS	2.4
1	E	395	PHE	2.4
1	D	369	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	35	GLU	2.3
1	F	396	LEU	2.3
1	C	34	HIS	2.3
1	B	307	GLU	2.3
1	D	39	GLU	2.3
1	E	439	TYR	2.3
1	D	395	PHE	2.3
1	B	442	CYS	2.3
1	B	220	ILE	2.3
1	A	306	LEU	2.3
1	D	178	GLU	2.3
1	D	73	TYR	2.2
1	A	526	ASP	2.2
1	A	616	ARG	2.2
1	D	55	LEU	2.2
1	D	76	TYR	2.2
1	D	292	PRO	2.2
1	F	268	LEU	2.2
1	D	260	ASP	2.2
1	B	401	ASP	2.2
1	F	369	ALA	2.2
1	A	36	ILE	2.2
1	A	485	ILE	2.2
1	B	617	GLN	2.2
1	B	488	ASP	2.2
1	C	399	ALA	2.2
1	C	404	ILE	2.1
1	E	36	ILE	2.1
1	D	293	ALA	2.1
1	A	38	ARG	2.1
1	C	505	ARG	2.1
1	A	243	THR	2.1
1	D	440	LEU	2.1
1	D	194	MET	2.1
1	B	439	TYR	2.1
1	B	35	GLU	2.1
1	A	489	LEU	2.1
1	E	403	LEU	2.1
1	C	374	VAL	2.1
1	F	374	VAL	2.1
1	D	263	THR	2.1
1	D	270	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	526	ASP	2.1
1	E	273	ASP	2.1
1	C	244	LEU	2.1
1	F	270	ASN	2.1
1	C	398	ARG	2.1
1	E	402	GLN	2.1
1	F	395	PHE	2.1
1	C	620	ASP	2.0
1	E	272	ARG	2.0
1	E	194	MET	2.0
1	F	192	ALA	2.0
1	A	178	GLU	2.0
1	A	579	GLU	2.0
1	E	404	ILE	2.0
1	D	374	VAL	2.0
1	A	398	ARG	2.0
1	D	289	GLY	2.0
1	D	72	GLN	2.0
1	E	401	ASP	2.0
1	E	274	MET	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	A	701	6/6	0.69	0.31	52,62,67,72	0
2	GOL	D	701	6/6	0.74	0.26	48,57,64,66	0
2	GOL	E	701	6/6	0.75	0.22	59,73,83,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	E	702	6/6	0.75	0.22	29,46,55,66	0
2	GOL	F	701	6/6	0.77	0.26	35,50,66,66	0
2	GOL	F	703	6/6	0.81	0.18	32,40,60,60	0
3	MG	C	701	1/1	0.82	0.13	40,40,40,40	0
3	MG	B	703	1/1	0.83	0.35	37,37,37,37	0
2	GOL	F	704	6/6	0.83	0.17	19,40,48,48	0
6	CA	A	707	1/1	0.83	0.11	66,66,66,66	0
5	NA	D	703	1/1	0.85	0.05	54,54,54,54	0
6	CA	A	706	1/1	0.86	0.14	61,61,61,61	0
4	CL	B	705	1/1	0.89	0.14	65,65,65,65	0
6	CA	C	704	1/1	0.91	0.18	67,67,67,67	0
3	MG	F	706	1/1	0.93	0.30	39,39,39,39	0
3	MG	A	702	1/1	0.93	0.23	34,34,34,34	0
3	MG	B	701	1/1	0.93	0.12	28,28,28,28	0
3	MG	D	702	1/1	0.94	0.22	43,43,43,43	0
3	MG	E	703	1/1	0.94	0.27	37,37,37,37	0
5	NA	F	707	1/1	0.95	0.08	37,37,37,37	0
3	MG	F	705	1/1	0.95	0.11	35,35,35,35	0
5	NA	A	705	1/1	0.95	0.17	29,29,29,29	0
4	CL	A	704	1/1	0.95	0.15	50,50,50,50	0
6	CA	F	709	1/1	0.95	0.20	50,50,50,50	0
6	CA	D	704	1/1	0.96	0.07	54,54,54,54	0
6	CA	D	705	1/1	0.96	0.25	49,49,49,49	0
6	CA	F	708	1/1	0.96	0.06	39,39,39,39	0
3	MG	B	702	1/1	0.96	0.13	26,26,26,26	0
6	CA	B	706	1/1	0.97	0.05	63,63,63,63	0
6	CA	D	706	1/1	0.97	0.14	69,69,69,69	0
6	CA	D	707	1/1	0.97	0.06	38,38,38,38	0
6	CA	E	706	1/1	0.97	0.20	49,49,49,49	0
6	CA	E	707	1/1	0.97	0.20	47,47,47,47	0
5	NA	E	705	1/1	0.97	0.07	24,24,24,24	0
3	MG	A	703	1/1	0.97	0.22	26,26,26,26	0
5	NA	C	703	1/1	0.98	0.10	26,26,26,26	0
3	MG	E	704	1/1	0.98	0.14	33,33,33,33	0
2	GOL	F	702	6/6	0.98	0.10	23,36,44,53	0
3	MG	C	702	1/1	0.98	0.14	22,22,22,22	0
3	MG	B	704	1/1	0.99	0.50	51,51,51,51	0

6.5 Other polymers

There are no such residues in this entry.