



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 05:32 AM UTC

PDB ID : 8A29 / pdb_00008a29
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 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

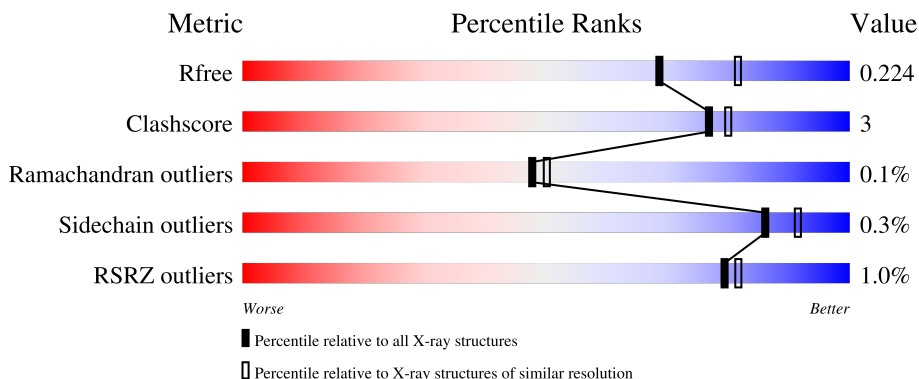
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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.

Mol	Chain	Length	Quality of chain
1	A	622	
1	B	622	
1	C	622	
1	D	622	
1	E	622	

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Mol	Chain	Length	Quality of chain
1	F	622	 84% 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	
			Total	C	H	N	O				S
1	A	557	8442	2684	4197	735	805	21	0	0	0
1	B	563	8569	2719	4267	748	814	21	0	2	0
1	C	559	8524	2707	4240	748	809	20	0	2	0
1	D	554	8393	2669	4171	734	799	20	0	0	0
1	E	560	8451	2698	4187	739	806	21	0	0	0
1	F	556	8452	2685	4205	738	804	20	0	0	0

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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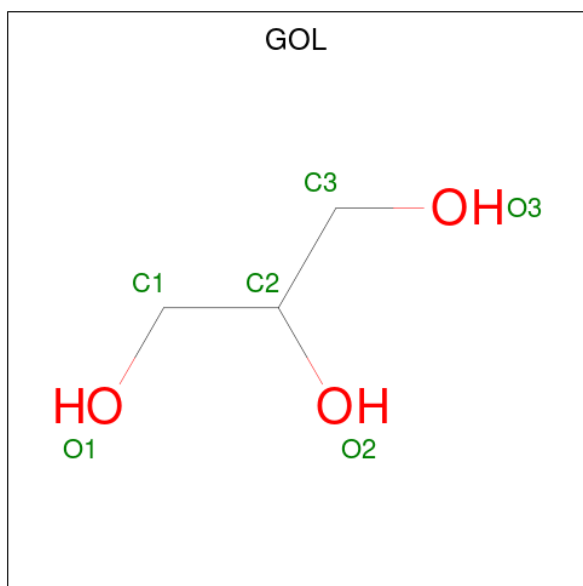
Chain	Residue	Modelled	Actual	Comment	Reference
E	8	HIS	-	expression tag	UNP B7V7R4
E	9	HIS	-	expression tag	UNP B7V7R4
E	10	HIS	-	expression tag	UNP B7V7R4
E	11	SER	-	expression tag	UNP B7V7R4
E	12	SER	-	expression tag	UNP B7V7R4
E	13	GLY	-	expression tag	UNP B7V7R4
E	14	LEU	-	expression tag	UNP B7V7R4
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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

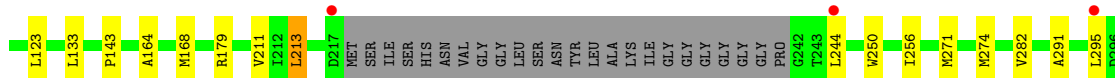
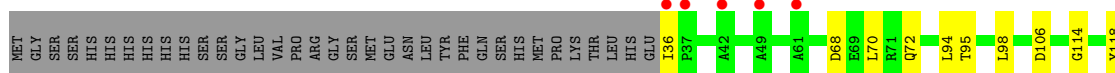
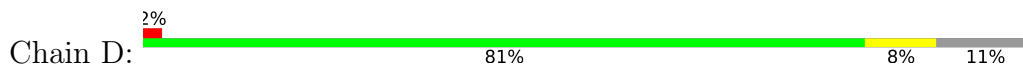
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	Ca 2	0	0
6	B	1	Total 1	Ca 1	0	0
6	C	1	Total 1	Ca 1	0	0
6	D	4	Total 4	Ca 4	0	0
6	E	2	Total 2	Ca 2	0	0
6	F	2	Total 2	Ca 2	0	0

- Molecule 7 is water.

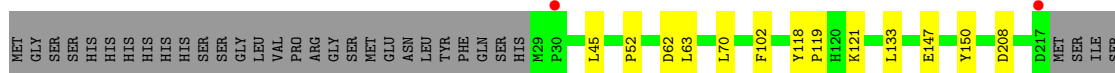
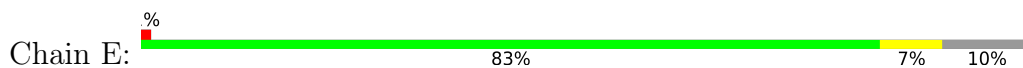
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	326	Total 326	O 326	0	0
7	B	384	Total 384	O 384	0	0
7	C	311	Total 311	O 311	0	0
7	D	337	Total 337	O 337	0	0
7	E	356	Total 356	O 356	0	0
7	F	391	Total 391	O 391	0	0



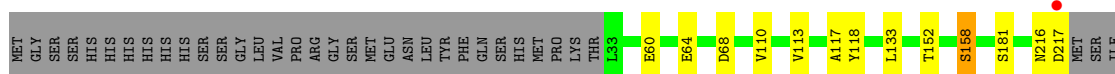
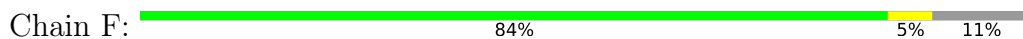
- Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase



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



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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.171 , 0.224 0.172 , 0.224	Depositor DCC
R_{free} test set	10815 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtrriage
Anisotropy	0.533	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GOL, CL, NA, MG

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	0.47	1/4329 (0.0%)	0.62	0/5869
1	B	0.50	0/4390	0.61	0/5951
1	C	0.48	0/4372	0.60	0/5926
1	D	0.49	0/4305	0.58	0/5837
1	E	0.48	0/4350	0.60	0/5899
1	F	0.52	1/4331 (0.0%)	0.62	0/5872
All	All	0.49	2/26077 (0.0%)	0.60	0/35354

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	519	MET	SD-CE	-5.55	1.65	1.79
1	A	443	ILE	CA-C	5.08	1.57	1.53

There are no bond angle outliers.

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

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	29	0
1	B	4302	4267	4274	22	0
1	C	4284	4240	4257	19	0
1	D	4222	4171	4194	36	0
1	E	4264	4187	4236	28	0
1	F	4247	4205	4214	18	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	3	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	150	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.

The worst 5 of 150 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:E:449:MET:HE3	1:E:473:VAL:HG22	1.69	0.74

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%)	43 44
1	B	559/622 (90%)	540 (97%)	19 (3%)	0	100 100
1	C	555/622 (89%)	540 (97%)	14 (2%)	1 (0%)	43 44
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%)	48 50

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%)	437 (99%)	3 (1%)	76	83
1	B	446/490 (91%)	445 (100%)	1 (0%)	87	93
1	C	444/490 (91%)	444 (100%)	0	100	100
1	D	437/490 (89%)	435 (100%)	2 (0%)	81	88
1	E	442/490 (90%)	441 (100%)	1 (0%)	87	93
1	F	440/490 (90%)	438 (100%)	2 (0%)	81	88
All	All	2649/2940 (90%)	2640 (100%)	9 (0%)	86	91

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	158	SER
1	F	181	SER
1	B	33	LEU
1	D	213	LEU
1	D	244	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	80	GLN
1	E	617	GLN
1	D	301	HIS
1	E	135	GLN
1	D	72	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 oligosaccharides 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	D	701	-	5,5,5	1.01	0	5,5,5	1.07	0
2	GOL	F	702	-	5,5,5	1.20	1 (20%)	5,5,5	0.94	0
2	GOL	F	703	-	5,5,5	2.49	1 (20%)	5,5,5	0.87	0
2	GOL	E	702	-	5,5,5	1.50	1 (20%)	5,5,5	0.45	0
2	GOL	F	704	-	5,5,5	2.67	3 (60%)	5,5,5	0.96	0
2	GOL	A	701	-	5,5,5	1.06	0	5,5,5	0.96	0
2	GOL	F	701	-	5,5,5	1.40	1 (20%)	5,5,5	0.85	0
2	GOL	E	701	-	5,5,5	1.01	0	5,5,5	1.04	1 (20%)

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	D	701	-	-	2/4/4/4	-
2	GOL	F	702	-	-	0/4/4/4	-
2	GOL	F	703	-	-	2/4/4/4	-
2	GOL	E	702	-	-	3/4/4/4	-
2	GOL	F	704	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	701	-	-	0/4/4/4	-
2	GOL	F	701	-	-	4/4/4/4	-
2	GOL	E	701	-	-	2/4/4/4	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	703	GOL	O2-C2	-5.12	1.28	1.43
2	F	704	GOL	O2-C2	4.09	1.55	1.43
2	F	704	GOL	C3-C2	2.95	1.63	1.51
2	F	701	GOL	C1-C2	2.26	1.60	1.51
2	F	704	GOL	C1-C2	-2.20	1.43	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	701	GOL	C3-C2-C1	-2.00	104.45	111.80

There are no chirality outliers.

5 of 14 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

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%)	-0.33	7 (1%) 75 77	20, 31, 53, 95	0
1	B	563/622 (90%)	-0.43	6 (1%) 78 80	18, 29, 48, 96	2 (0%)
1	C	559/622 (89%)	-0.38	4 (0%) 84 86	19, 30, 52, 83	2 (0%)
1	D	554/622 (89%)	-0.27	11 (1%) 65 67	18, 31, 62, 96	0
1	E	560/622 (90%)	-0.42	6 (1%) 78 80	20, 30, 50, 83	0
1	F	556/622 (89%)	-0.51	1 (0%) 91 92	17, 28, 49, 78	0
All	All	3349/3732 (89%)	-0.39	35 (1%) 79 81	17, 30, 54, 96	4 (0%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	THR	4.9
1	A	34	HIS	4.1
1	B	308	ALA	4.0
1	A	33	LEU	3.9
1	A	219	SER	3.9

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 oligosaccharides 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	E	702	6/6	0.66	0.21	29,46,55,66	0
2	GOL	A	701	6/6	0.72	0.15	52,62,67,72	0
2	GOL	F	703	6/6	0.76	0.15	32,40,60,60	0
2	GOL	D	701	6/6	0.77	0.13	48,57,64,66	0
2	GOL	E	701	6/6	0.78	0.17	59,73,83,87	0
6	CA	A	707	1/1	0.79	0.13	66,66,66,66	0
2	GOL	F	704	6/6	0.80	0.16	19,40,48,48	0
6	CA	C	704	1/1	0.83	0.17	67,67,67,67	0
3	MG	B	703	1/1	0.86	0.24	37,37,37,37	0
6	CA	A	706	1/1	0.87	0.12	61,61,61,61	0
4	CL	B	705	1/1	0.88	0.17	65,65,65,65	0
3	MG	C	701	1/1	0.88	0.10	40,40,40,40	0
2	GOL	F	701	6/6	0.89	0.14	35,50,66,66	0
3	MG	A	702	1/1	0.89	0.13	34,34,34,34	0
4	CL	A	704	1/1	0.91	0.10	50,50,50,50	0
6	CA	D	706	1/1	0.91	0.11	69,69,69,69	0
5	NA	D	703	1/1	0.92	0.14	54,54,54,54	0
6	CA	D	705	1/1	0.93	0.21	49,49,49,49	0
3	MG	F	706	1/1	0.93	0.15	39,39,39,39	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
2	GOL	F	702	6/6	0.95	0.07	23,36,44,53	0
6	CA	B	706	1/1	0.95	0.12	63,63,63,63	0
3	MG	B	701	1/1	0.95	0.09	28,28,28,28	0
3	MG	D	702	1/1	0.95	0.09	43,43,43,43	0
3	MG	E	703	1/1	0.95	0.09	37,37,37,37	0
6	CA	E	707	1/1	0.95	0.18	47,47,47,47	0
6	CA	F	708	1/1	0.95	0.05	39,39,39,39	0
5	NA	E	705	1/1	0.96	0.07	24,24,24,24	0
6	CA	D	704	1/1	0.96	0.12	54,54,54,54	0
6	CA	F	709	1/1	0.96	0.18	50,50,50,50	0
6	CA	E	706	1/1	0.97	0.23	49,49,49,49	0
3	MG	A	703	1/1	0.97	0.12	26,26,26,26	0
3	MG	B	702	1/1	0.97	0.05	26,26,26,26	0
6	CA	D	707	1/1	0.97	0.05	38,38,38,38	0
3	MG	B	704	1/1	0.98	0.11	51,51,51,51	0
5	NA	A	705	1/1	0.98	0.14	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NA	C	703	1/1	0.98	0.10	26,26,26,26	0
3	MG	E	704	1/1	0.99	0.11	33,33,33,33	0
3	MG	C	702	1/1	0.99	0.06	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.