



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:35 PM UTC

PDB ID : 3ODM / pdb_00003odm
Title : Archaeal-type phosphoenolpyruvate carboxylase
Authors : Dunten, P.W.
Deposited on : 2010-08-11
Resolution : 2.95 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)
Xtriage (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

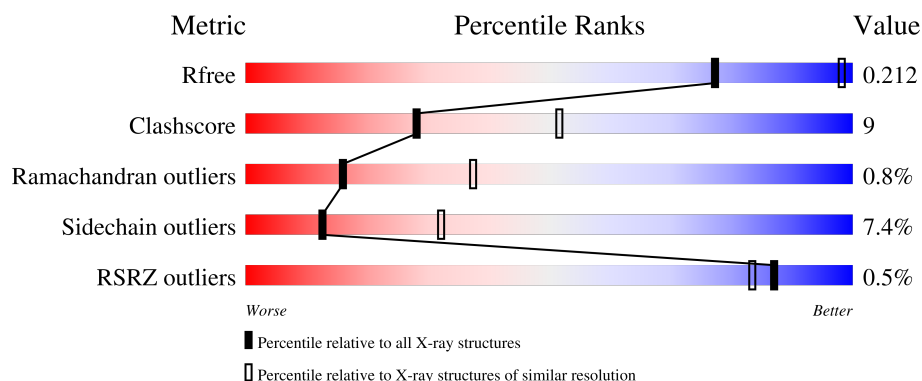
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

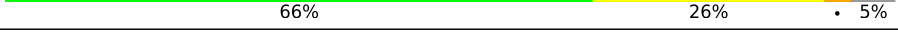
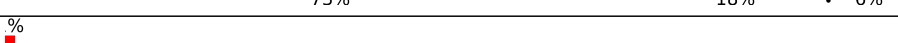
The reported resolution of this entry is 2.95 Å.

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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	560	
1	B	560	
1	C	560	
1	D	560	
1	E	560	

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Mol	Chain	Length	Quality of chain
1	F	560	 69% 24% • 6%
1	G	560	 % 65% 27% • 6%
1	H	560	 % 73% 18% • 6%

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	AUC	A	607	-	-	X	-
2	AUC	A	608	-	-	X	-
2	AUC	B	609	-	-	X	-
2	AUC	B	610	-	-	X	-
2	AUC	C	601	-	-	X	-
2	AUC	C	602	-	-	X	-
2	AUC	D	603	-	-	X	-
2	AUC	D	604	-	-	X	-
2	AUC	E	605	-	-	X	-
2	AUC	E	606	-	-	X	-
2	AUC	F	614	-	-	X	-
2	AUC	G	615	-	-	X	-
2	AUC	H	611	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33563 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 Phosphoenolpyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4146	2629	696	797	24			
1	B	529	Total	C	N	O	S	0	0	0
			4169	2641	701	803	24			
1	C	530	Total	C	N	O	S	0	0	1
			4171	2645	699	803	24			
1	D	526	Total	C	N	O	S	0	0	0
			4153	2634	697	798	24			
1	E	524	Total	C	N	O	S	0	0	0
			4137	2623	694	796	24			
1	F	529	Total	C	N	O	S	0	0	0
			4160	2637	696	803	24			
1	G	527	Total	C	N	O	S	0	0	0
			4156	2635	698	799	24			
1	H	527	Total	C	N	O	S	0	0	0
			4164	2643	699	798	24			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP Q8XLE8
A	-21	GLY	-	expression tag	UNP Q8XLE8
A	-20	HIS	-	expression tag	UNP Q8XLE8
A	-19	HIS	-	expression tag	UNP Q8XLE8
A	-18	HIS	-	expression tag	UNP Q8XLE8
A	-17	HIS	-	expression tag	UNP Q8XLE8
A	-16	HIS	-	expression tag	UNP Q8XLE8
A	-15	HIS	-	expression tag	UNP Q8XLE8
A	-14	HIS	-	expression tag	UNP Q8XLE8
A	-13	HIS	-	expression tag	UNP Q8XLE8
A	-12	HIS	-	expression tag	UNP Q8XLE8
A	-11	HIS	-	expression tag	UNP Q8XLE8
A	-10	SER	-	expression tag	UNP Q8XLE8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	SER	-	expression tag	UNP Q8XLE8
A	-8	GLY	-	expression tag	UNP Q8XLE8
A	-7	HIS	-	expression tag	UNP Q8XLE8
A	-6	ILE	-	expression tag	UNP Q8XLE8
A	-5	ASP	-	expression tag	UNP Q8XLE8
A	-4	ASP	-	expression tag	UNP Q8XLE8
A	-3	ASP	-	expression tag	UNP Q8XLE8
A	-2	ASP	-	expression tag	UNP Q8XLE8
A	-1	LYS	-	expression tag	UNP Q8XLE8
A	0	HIS	-	expression tag	UNP Q8XLE8
B	-22	MET	-	expression tag	UNP Q8XLE8
B	-21	GLY	-	expression tag	UNP Q8XLE8
B	-20	HIS	-	expression tag	UNP Q8XLE8
B	-19	HIS	-	expression tag	UNP Q8XLE8
B	-18	HIS	-	expression tag	UNP Q8XLE8
B	-17	HIS	-	expression tag	UNP Q8XLE8
B	-16	HIS	-	expression tag	UNP Q8XLE8
B	-15	HIS	-	expression tag	UNP Q8XLE8
B	-14	HIS	-	expression tag	UNP Q8XLE8
B	-13	HIS	-	expression tag	UNP Q8XLE8
B	-12	HIS	-	expression tag	UNP Q8XLE8
B	-11	HIS	-	expression tag	UNP Q8XLE8
B	-10	SER	-	expression tag	UNP Q8XLE8
B	-9	SER	-	expression tag	UNP Q8XLE8
B	-8	GLY	-	expression tag	UNP Q8XLE8
B	-7	HIS	-	expression tag	UNP Q8XLE8
B	-6	ILE	-	expression tag	UNP Q8XLE8
B	-5	ASP	-	expression tag	UNP Q8XLE8
B	-4	ASP	-	expression tag	UNP Q8XLE8
B	-3	ASP	-	expression tag	UNP Q8XLE8
B	-2	ASP	-	expression tag	UNP Q8XLE8
B	-1	LYS	-	expression tag	UNP Q8XLE8
B	0	HIS	-	expression tag	UNP Q8XLE8
C	-22	MET	-	expression tag	UNP Q8XLE8
C	-21	GLY	-	expression tag	UNP Q8XLE8
C	-20	HIS	-	expression tag	UNP Q8XLE8
C	-19	HIS	-	expression tag	UNP Q8XLE8
C	-18	HIS	-	expression tag	UNP Q8XLE8
C	-17	HIS	-	expression tag	UNP Q8XLE8
C	-16	HIS	-	expression tag	UNP Q8XLE8
C	-15	HIS	-	expression tag	UNP Q8XLE8
C	-14	HIS	-	expression tag	UNP Q8XLE8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	HIS	-	expression tag	UNP Q8XLE8
C	-12	HIS	-	expression tag	UNP Q8XLE8
C	-11	HIS	-	expression tag	UNP Q8XLE8
C	-10	SER	-	expression tag	UNP Q8XLE8
C	-9	SER	-	expression tag	UNP Q8XLE8
C	-8	GLY	-	expression tag	UNP Q8XLE8
C	-7	HIS	-	expression tag	UNP Q8XLE8
C	-6	ILE	-	expression tag	UNP Q8XLE8
C	-5	ASP	-	expression tag	UNP Q8XLE8
C	-4	ASP	-	expression tag	UNP Q8XLE8
C	-3	ASP	-	expression tag	UNP Q8XLE8
C	-2	ASP	-	expression tag	UNP Q8XLE8
C	-1	LYS	-	expression tag	UNP Q8XLE8
C	0	HIS	-	expression tag	UNP Q8XLE8
D	-22	MET	-	expression tag	UNP Q8XLE8
D	-21	GLY	-	expression tag	UNP Q8XLE8
D	-20	HIS	-	expression tag	UNP Q8XLE8
D	-19	HIS	-	expression tag	UNP Q8XLE8
D	-18	HIS	-	expression tag	UNP Q8XLE8
D	-17	HIS	-	expression tag	UNP Q8XLE8
D	-16	HIS	-	expression tag	UNP Q8XLE8
D	-15	HIS	-	expression tag	UNP Q8XLE8
D	-14	HIS	-	expression tag	UNP Q8XLE8
D	-13	HIS	-	expression tag	UNP Q8XLE8
D	-12	HIS	-	expression tag	UNP Q8XLE8
D	-11	HIS	-	expression tag	UNP Q8XLE8
D	-10	SER	-	expression tag	UNP Q8XLE8
D	-9	SER	-	expression tag	UNP Q8XLE8
D	-8	GLY	-	expression tag	UNP Q8XLE8
D	-7	HIS	-	expression tag	UNP Q8XLE8
D	-6	ILE	-	expression tag	UNP Q8XLE8
D	-5	ASP	-	expression tag	UNP Q8XLE8
D	-4	ASP	-	expression tag	UNP Q8XLE8
D	-3	ASP	-	expression tag	UNP Q8XLE8
D	-2	ASP	-	expression tag	UNP Q8XLE8
D	-1	LYS	-	expression tag	UNP Q8XLE8
D	0	HIS	-	expression tag	UNP Q8XLE8
E	-22	MET	-	expression tag	UNP Q8XLE8
E	-21	GLY	-	expression tag	UNP Q8XLE8
E	-20	HIS	-	expression tag	UNP Q8XLE8
E	-19	HIS	-	expression tag	UNP Q8XLE8
E	-18	HIS	-	expression tag	UNP Q8XLE8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-17	HIS	-	expression tag	UNP Q8XLE8
E	-16	HIS	-	expression tag	UNP Q8XLE8
E	-15	HIS	-	expression tag	UNP Q8XLE8
E	-14	HIS	-	expression tag	UNP Q8XLE8
E	-13	HIS	-	expression tag	UNP Q8XLE8
E	-12	HIS	-	expression tag	UNP Q8XLE8
E	-11	HIS	-	expression tag	UNP Q8XLE8
E	-10	SER	-	expression tag	UNP Q8XLE8
E	-9	SER	-	expression tag	UNP Q8XLE8
E	-8	GLY	-	expression tag	UNP Q8XLE8
E	-7	HIS	-	expression tag	UNP Q8XLE8
E	-6	ILE	-	expression tag	UNP Q8XLE8
E	-5	ASP	-	expression tag	UNP Q8XLE8
E	-4	ASP	-	expression tag	UNP Q8XLE8
E	-3	ASP	-	expression tag	UNP Q8XLE8
E	-2	ASP	-	expression tag	UNP Q8XLE8
E	-1	LYS	-	expression tag	UNP Q8XLE8
E	0	HIS	-	expression tag	UNP Q8XLE8
F	-22	MET	-	expression tag	UNP Q8XLE8
F	-21	GLY	-	expression tag	UNP Q8XLE8
F	-20	HIS	-	expression tag	UNP Q8XLE8
F	-19	HIS	-	expression tag	UNP Q8XLE8
F	-18	HIS	-	expression tag	UNP Q8XLE8
F	-17	HIS	-	expression tag	UNP Q8XLE8
F	-16	HIS	-	expression tag	UNP Q8XLE8
F	-15	HIS	-	expression tag	UNP Q8XLE8
F	-14	HIS	-	expression tag	UNP Q8XLE8
F	-13	HIS	-	expression tag	UNP Q8XLE8
F	-12	HIS	-	expression tag	UNP Q8XLE8
F	-11	HIS	-	expression tag	UNP Q8XLE8
F	-10	SER	-	expression tag	UNP Q8XLE8
F	-9	SER	-	expression tag	UNP Q8XLE8
F	-8	GLY	-	expression tag	UNP Q8XLE8
F	-7	HIS	-	expression tag	UNP Q8XLE8
F	-6	ILE	-	expression tag	UNP Q8XLE8
F	-5	ASP	-	expression tag	UNP Q8XLE8
F	-4	ASP	-	expression tag	UNP Q8XLE8
F	-3	ASP	-	expression tag	UNP Q8XLE8
F	-2	ASP	-	expression tag	UNP Q8XLE8
F	-1	LYS	-	expression tag	UNP Q8XLE8
F	0	HIS	-	expression tag	UNP Q8XLE8
G	-22	MET	-	expression tag	UNP Q8XLE8

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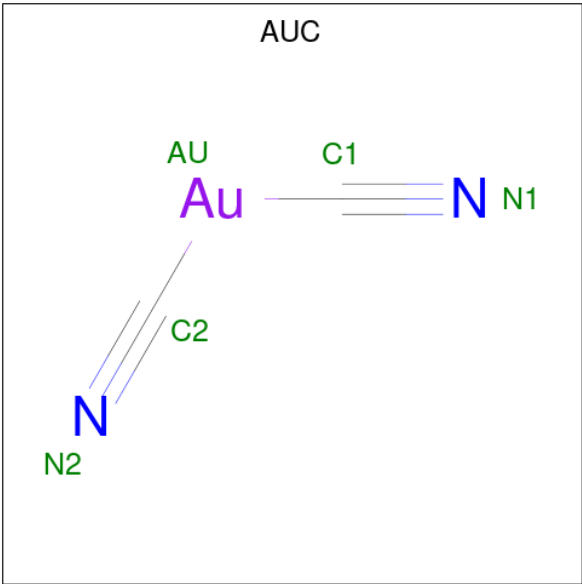
Chain	Residue	Modelled	Actual	Comment	Reference
G	-21	GLY	-	expression tag	UNP Q8XLE8
G	-20	HIS	-	expression tag	UNP Q8XLE8
G	-19	HIS	-	expression tag	UNP Q8XLE8
G	-18	HIS	-	expression tag	UNP Q8XLE8
G	-17	HIS	-	expression tag	UNP Q8XLE8
G	-16	HIS	-	expression tag	UNP Q8XLE8
G	-15	HIS	-	expression tag	UNP Q8XLE8
G	-14	HIS	-	expression tag	UNP Q8XLE8
G	-13	HIS	-	expression tag	UNP Q8XLE8
G	-12	HIS	-	expression tag	UNP Q8XLE8
G	-11	HIS	-	expression tag	UNP Q8XLE8
G	-10	SER	-	expression tag	UNP Q8XLE8
G	-9	SER	-	expression tag	UNP Q8XLE8
G	-8	GLY	-	expression tag	UNP Q8XLE8
G	-7	HIS	-	expression tag	UNP Q8XLE8
G	-6	ILE	-	expression tag	UNP Q8XLE8
G	-5	ASP	-	expression tag	UNP Q8XLE8
G	-4	ASP	-	expression tag	UNP Q8XLE8
G	-3	ASP	-	expression tag	UNP Q8XLE8
G	-2	ASP	-	expression tag	UNP Q8XLE8
G	-1	LYS	-	expression tag	UNP Q8XLE8
G	0	HIS	-	expression tag	UNP Q8XLE8
H	-22	MET	-	expression tag	UNP Q8XLE8
H	-21	GLY	-	expression tag	UNP Q8XLE8
H	-20	HIS	-	expression tag	UNP Q8XLE8
H	-19	HIS	-	expression tag	UNP Q8XLE8
H	-18	HIS	-	expression tag	UNP Q8XLE8
H	-17	HIS	-	expression tag	UNP Q8XLE8
H	-16	HIS	-	expression tag	UNP Q8XLE8
H	-15	HIS	-	expression tag	UNP Q8XLE8
H	-14	HIS	-	expression tag	UNP Q8XLE8
H	-13	HIS	-	expression tag	UNP Q8XLE8
H	-12	HIS	-	expression tag	UNP Q8XLE8
H	-11	HIS	-	expression tag	UNP Q8XLE8
H	-10	SER	-	expression tag	UNP Q8XLE8
H	-9	SER	-	expression tag	UNP Q8XLE8
H	-8	GLY	-	expression tag	UNP Q8XLE8
H	-7	HIS	-	expression tag	UNP Q8XLE8
H	-6	ILE	-	expression tag	UNP Q8XLE8
H	-5	ASP	-	expression tag	UNP Q8XLE8
H	-4	ASP	-	expression tag	UNP Q8XLE8
H	-3	ASP	-	expression tag	UNP Q8XLE8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	ASP	-	expression tag	UNP Q8XLE8
H	-1	LYS	-	expression tag	UNP Q8XLE8
H	0	HIS	-	expression tag	UNP Q8XLE8

- Molecule 2 is GOLD (I) CYANIDE ION (CCD ID: AUC) (formula: C₂AuN₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Au	C	N	0	0
			5	1	2	2		
2	A	1	Total	Au			0	0
			1	1				
2	A	1	Total	Au			0	0
			1	1				
2	A	1	Total	Au	C	N	0	0
			5	1	2	2		
2	B	1	Total	Au			0	0
			1	1				
2	B	1	Total	Au			0	0
			1	1				
2	B	1	Total	Au	C	N	0	0
			5	1	2	2		
2	B	1	Total	Au			0	0
			1	1				
2	B	1	Total	Au			0	0
			1	1				
2	B	1	Total	Au			0	0
			1	1				

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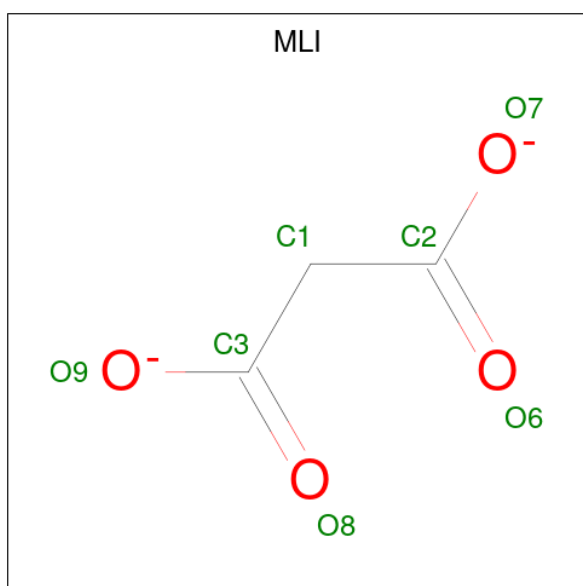
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Au 1 1	0	0
2	C	1	Total Au 1 1	0	0
2	C	1	Total Au C N 5 1 2 2	0	0
2	C	1	Total Au 1 1	0	0
2	C	1	Total Au 1 1	0	0
2	D	1	Total Au C N 5 1 2 2	0	0
2	D	1	Total Au 1 1	0	0
2	D	1	Total Au 1 1	0	0
2	D	1	Total Au 1 1	0	0
2	E	1	Total Au 1 1	0	0
2	E	1	Total Au C N 5 1 2 2	0	0
2	E	1	Total Au 1 1	0	0
2	E	1	Total Au 1 1	0	0
2	F	1	Total Au 1 1	0	0
2	F	1	Total Au 1 1	0	0
2	F	1	Total Au C N 5 1 2 2	0	0
2	F	1	Total Au 1 1	0	0
2	F	1	Total Au 1 1	0	0
2	F	1	Total Au 1 1	0	0
2	G	1	Total Au C N 5 1 2 2	0	0
2	G	1	Total Au 1 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	Au			0	0
			1	1				
2	H	1	Total	Au	C	N	0	0
			5	1	2	2		
2	H	1	Total	Au			0	0
			1	1				
2	H	1	Total	Au			0	0
			1	1				
2	H	1	Total	Au			0	0
			1	1				

- Molecule 3 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	3	4		
3	C	1	Total	C	O	0	0
			7	3	4		
3	D	1	Total	C	O	0	0
			7	3	4		
3	E	1	Total	C	O	0	0
			7	3	4		
3	H	1	Total	C	O	0	0
			7	3	4		

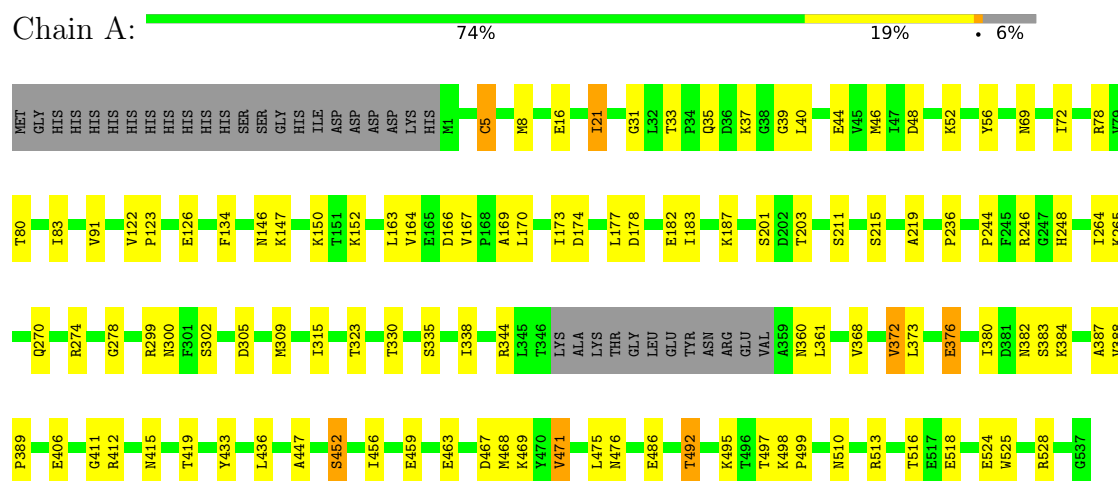
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total 34	O 34	0	0
4	B	26	Total 26	O 26	0	0
4	C	23	Total 23	O 23	0	0
4	D	22	Total 22	O 22	0	0
4	E	26	Total 26	O 26	0	0
4	F	21	Total 21	O 21	0	0
4	G	19	Total 19	O 19	0	0
4	H	29	Total 29	O 29	0	0

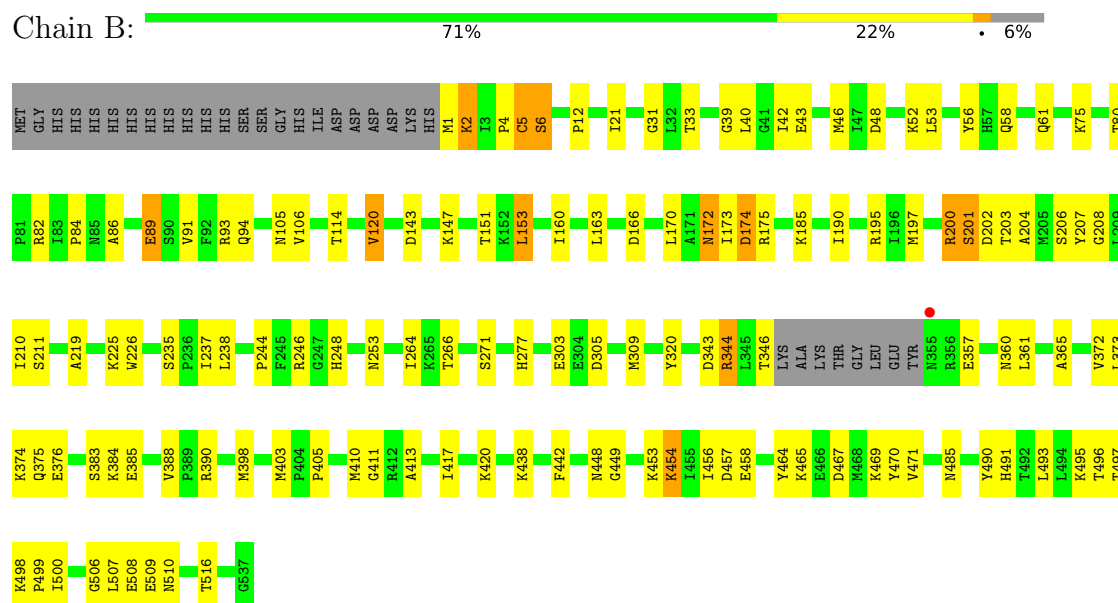
3 Residue-property plots

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.

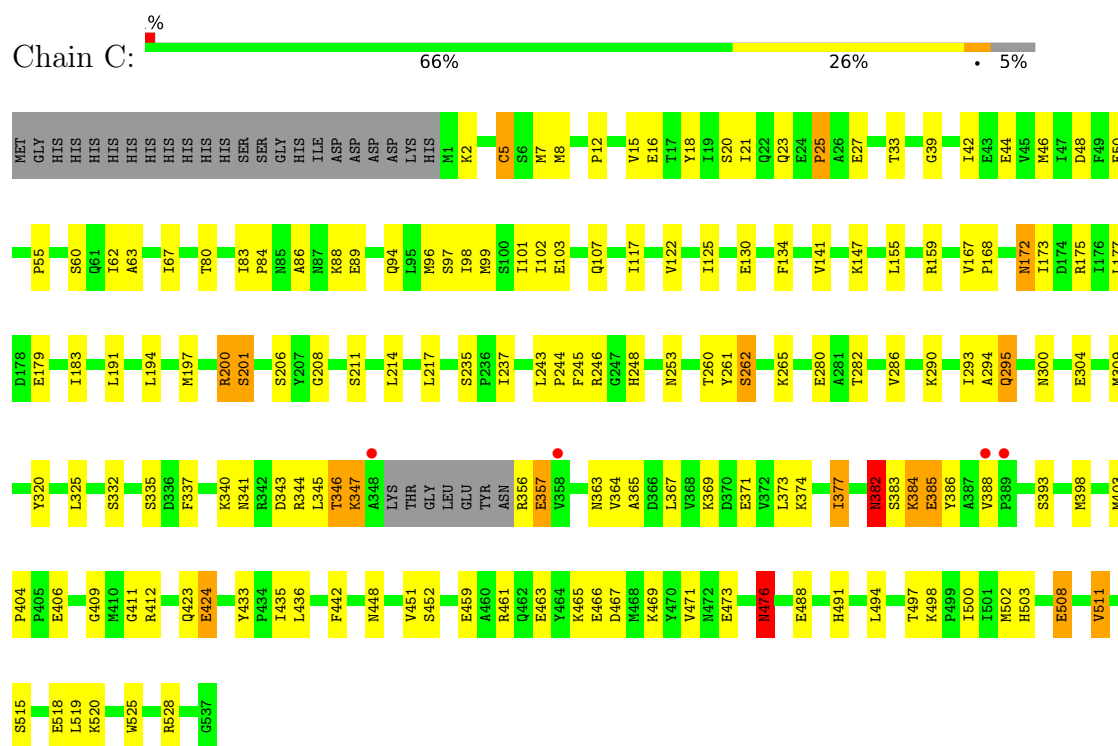
• Molecule 1: Phosphoenolpyruvate carboxylase



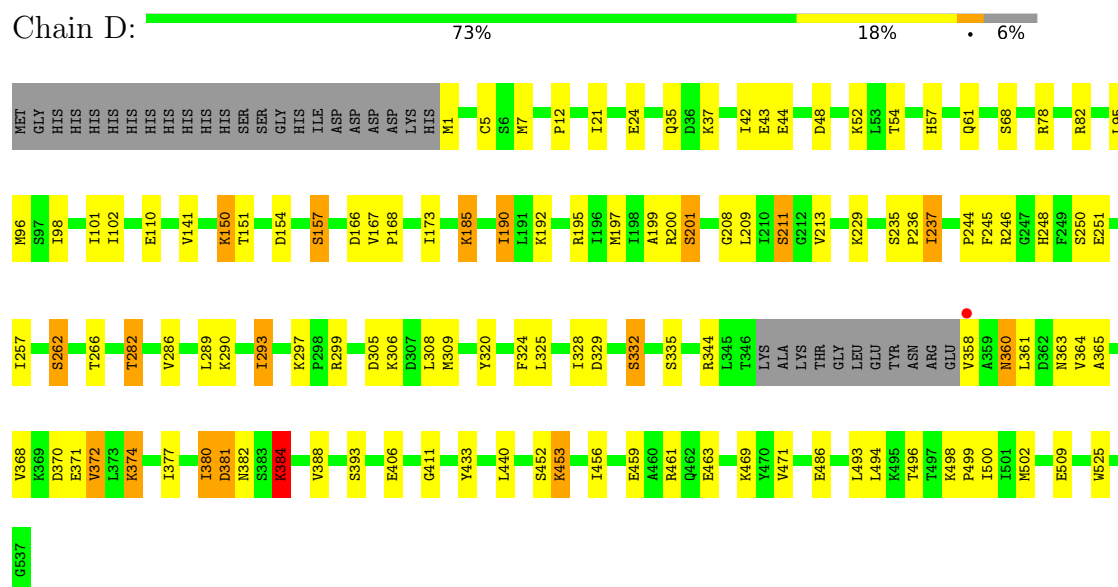
• Molecule 1: Phosphoenolpyruvate carboxylase



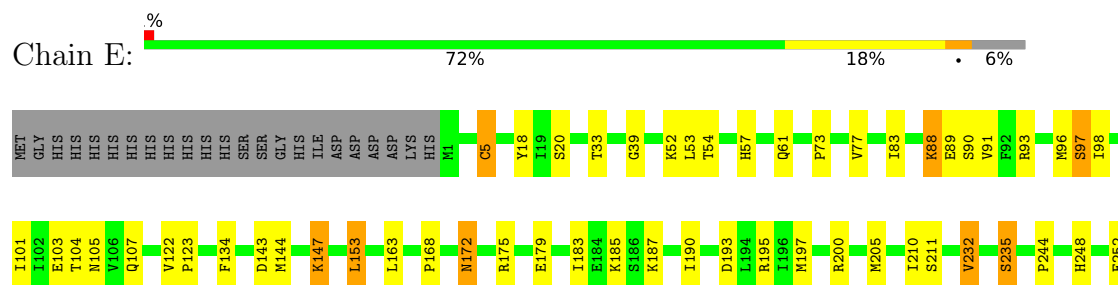
• Molecule 1: Phosphoenolpyruvate carboxylase



• Molecule 1: Phosphoenolpyruvate carboxylase

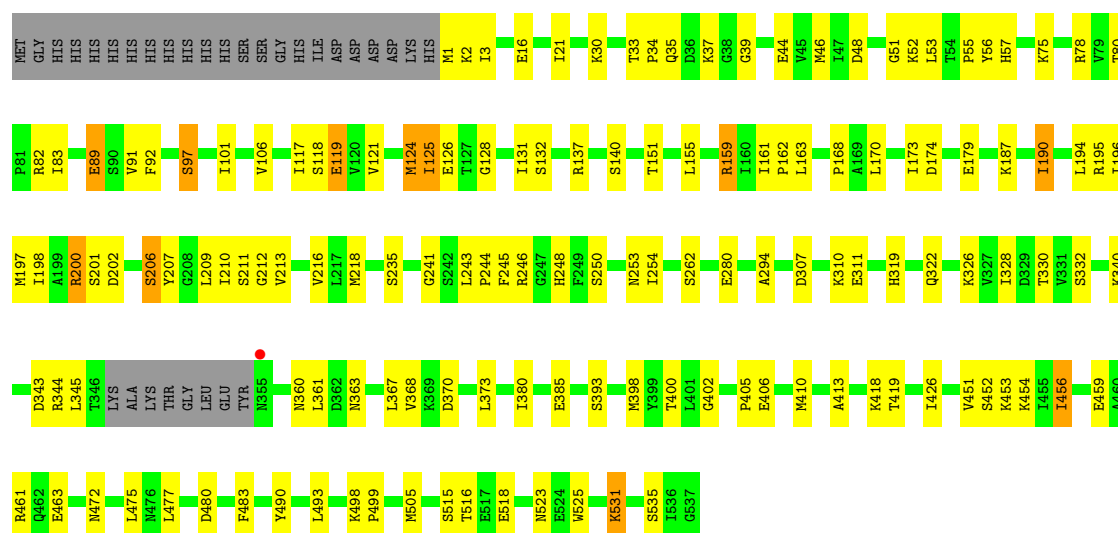


• Molecule 1: Phosphoenolpyruvate carboxylase

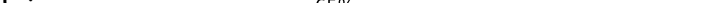


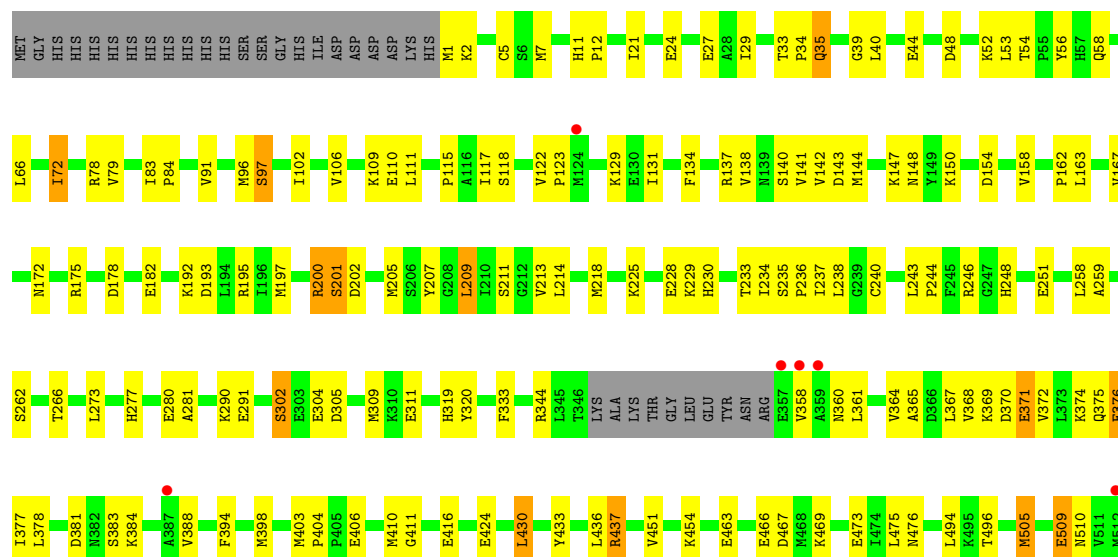
- Molecule 1: Phosphoenolpyruvate carboxylase

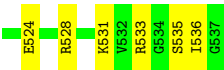
Chain F:  69% 24% • 6%



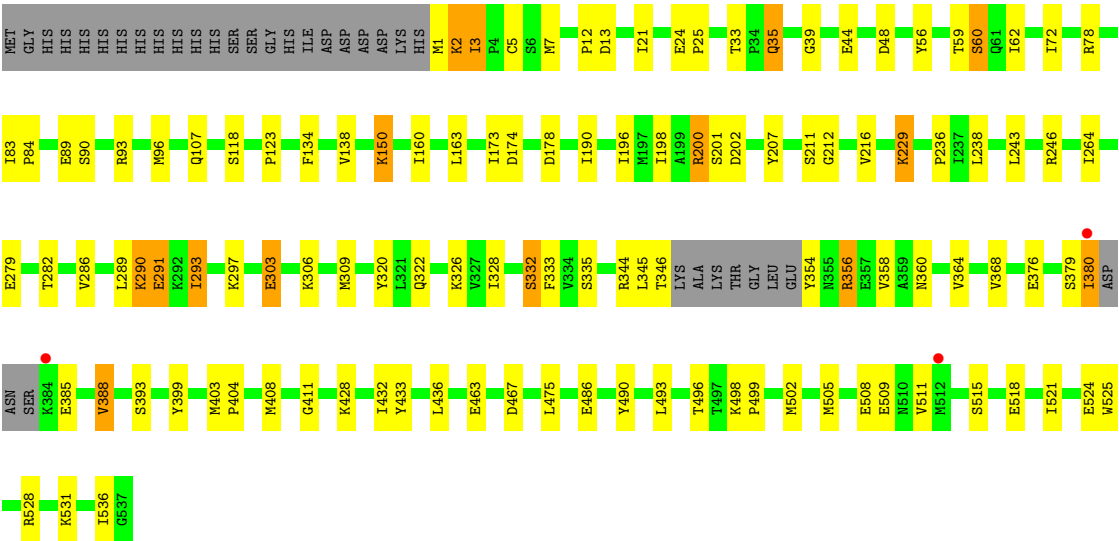
- Molecule 1: Phosphoenolpyruvate carboxylase

Chain G:  %





● Molecule 1: Phosphoenolpyruvate carboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.42Å 161.58Å 279.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.84 – 2.95 56.84 – 2.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (56.84-2.95) 99.8 (56.84-2.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.178 , 0.223 0.177 , 0.212	Depositor DCC
R_{free} test set	1135 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	67.1	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33563	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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: MLI, AUC

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	0.78	0/4214	0.99	6/5678 (0.1%)
1	B	0.68	0/4237	0.99	4/5711 (0.1%)
1	C	0.74	0/4239	0.97	4/5712 (0.1%)
1	D	0.76	0/4221	0.96	5/5688 (0.1%)
1	E	0.77	0/4205	0.99	4/5667 (0.1%)
1	F	0.67	0/4228	0.94	1/5700 (0.0%)
1	G	0.69	0/4224	1.00	4/5692 (0.1%)
1	H	0.73	0/4232	1.00	8/5702 (0.1%)
All	All	0.73	0/33800	0.98	36/45550 (0.1%)

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	388	VAL	N-CA-C	7.78	115.32	108.63
1	C	383	SER	N-CA-C	7.17	119.20	107.23
1	G	360	ASN	N-CA-C	7.10	120.30	110.35
1	C	382	ASN	N-CA-C	6.94	118.59	110.41
1	A	72	ILE	N-CA-C	6.37	113.36	107.56

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	4146	0	4209	57	0
1	B	4169	0	4212	73	0
1	C	4171	0	4224	97	0
1	D	4153	0	4218	78	0
1	E	4137	0	4193	70	0
1	F	4160	0	4198	73	0
1	G	4156	0	4213	87	0
1	H	4164	0	4221	65	0
2	A	12	0	0	4	0
2	B	10	0	0	6	0
2	C	9	0	0	4	0
2	D	8	0	0	4	0
2	E	8	0	0	4	0
2	F	10	0	0	4	0
2	G	7	0	0	5	0
2	H	8	0	0	5	0
3	A	7	0	2	0	0
3	C	7	0	2	0	0
3	D	7	0	2	1	0
3	E	7	0	2	0	0
3	H	7	0	2	0	0
4	A	34	0	0	1	0
4	B	26	0	0	1	0
4	C	23	0	0	2	0
4	D	22	0	0	0	0
4	E	26	0	0	2	0
4	F	21	0	0	0	0
4	G	19	0	0	0	0
4	H	29	0	0	0	0
All	All	33563	0	33698	593	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 9.

The worst 5 of 593 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:E:5:CYS:SG	2:E:605:AUC:AU	1.32	1.56
1:A:5:CYS:SG	2:A:608:AUC:AU	1.54	1.34
1:B:5:CYS:SG	2:B:609:AUC:AU	1.56	1.34
1:C:5:CYS:SG	2:C:601:AUC:AU	1.65	1.24
1:D:5:CYS:SG	2:D:604:AUC:AU	1.64	1.24

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	521/560 (93%)	496 (95%)	24 (5%)	1 (0%)	43	66
1	B	525/560 (94%)	486 (93%)	38 (7%)	1 (0%)	43	66
1	C	526/560 (94%)	483 (92%)	31 (6%)	12 (2%)	5	14
1	D	522/560 (93%)	484 (93%)	34 (6%)	4 (1%)	16	37
1	E	520/560 (93%)	484 (93%)	28 (5%)	8 (2%)	8	23
1	F	525/560 (94%)	486 (93%)	35 (7%)	4 (1%)	16	37
1	G	523/560 (93%)	478 (91%)	42 (8%)	3 (1%)	21	45
1	H	521/560 (93%)	496 (95%)	23 (4%)	2 (0%)	30	53
All	All	4183/4480 (93%)	3893 (93%)	255 (6%)	35 (1%)	16	37

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	346	THR
1	C	347	LYS
1	C	357	GLU
1	D	384	LYS
1	C	385	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	462/493 (94%)	433 (94%)	29 (6%)	16	38
1	B	462/493 (94%)	427 (92%)	35 (8%)	12	31
1	C	463/493 (94%)	426 (92%)	37 (8%)	11	28
1	D	463/493 (94%)	432 (93%)	31 (7%)	15	36
1	E	461/493 (94%)	430 (93%)	31 (7%)	15	36
1	F	461/493 (94%)	416 (90%)	45 (10%)	7	21
1	G	462/493 (94%)	427 (92%)	35 (8%)	12	31
1	H	462/493 (94%)	432 (94%)	30 (6%)	15	37
All	All	3696/3944 (94%)	3423 (93%)	273 (7%)	13	32

5 of 273 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	381	ASP
1	G	454	LYS
1	H	332	SER
1	C	502	MET
1	C	466	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	415	ASN
1	F	253	ASN
1	H	503	HIS
1	H	69	ASN
1	E	476	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 27 are modelled with single atom - leaving 14 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	AUC	G	615	1	4,4,4	1.57	2 (50%)	-		
2	AUC	E	606	-	4,4,4	1.68	2 (50%)	-		
2	AUC	D	603	-	4,4,4	1.67	2 (50%)	-		
3	MLI	A	901	-	6,6,6	1.16	0	7,7,7	1.35	0
3	MLI	C	901	-	6,6,6	1.09	0	7,7,7	1.20	1 (14%)
2	AUC	H	611	-	4,4,4	1.62	2 (50%)	-		
2	AUC	A	631	-	4,4,4	1.65	2 (50%)	-		
2	AUC	B	610	-	4,4,4	1.61	2 (50%)	-		
3	MLI	H	901	-	6,6,6	1.10	0	7,7,7	1.04	0
2	AUC	F	614	-	4,4,4	1.59	2 (50%)	-		
2	AUC	C	602	-	4,4,4	1.64	2 (50%)	-		
2	AUC	A	607	-	4,4,4	1.64	2 (50%)	-		
3	MLI	E	901	-	6,6,6	1.20	0	7,7,7	1.48	1 (14%)
3	MLI	D	901	-	6,6,6	1.20	0	7,7,7	1.08	1 (14%)

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
3	MLI	C	901	-	-	4/4/4/4	-
3	MLI	A	901	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLI	H	901	-	-	2/4/4/4	-
3	MLI	E	901	-	-	2/4/4/4	-
3	MLI	D	901	-	-	2/4/4/4	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	606	AUC	AU-C1	-2.47	1.79	1.97
2	D	603	AUC	AU-C1	-2.39	1.79	1.97
2	A	607	AUC	AU-C2	-2.36	1.80	1.97
2	H	611	AUC	AU-C2	-2.36	1.80	1.97
2	A	631	AUC	AU-C2	-2.36	1.80	1.97

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	901	MLI	O8-C3-C1	-2.69	114.46	122.11
3	D	901	MLI	C3-C1-C2	-2.11	105.49	112.95
3	C	901	MLI	C3-C1-C2	-2.06	105.69	112.95

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	901	MLI	C3-C1-C2-O6
3	E	901	MLI	C3-C1-C2-O7
3	C	901	MLI	C2-C1-C3-O9
3	A	901	MLI	C2-C1-C3-O8
3	A	901	MLI	C2-C1-C3-O9

There are no ring outliers.

9 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	615	AUC	5	0
2	E	606	AUC	2	0
2	D	603	AUC	2	0
2	H	611	AUC	4	0
2	B	610	AUC	4	0
2	F	614	AUC	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	602	AUC	2	0
2	A	607	AUC	2	0
3	D	901	MLI	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 [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	525/560 (93%)	-0.66	0 100 100	37, 55, 74, 101	1 (0%)
1	B	529/560 (94%)	-0.50	1 (0%) 91 90	44, 67, 99, 110	0
1	C	530/560 (94%)	-0.49	4 (0%) 82 78	42, 64, 116, 128	1 (0%)
1	D	526/560 (93%)	-0.51	1 (0%) 91 90	40, 59, 95, 122	0
1	E	524/560 (93%)	-0.49	5 (0%) 79 74	37, 58, 101, 169	1 (0%)
1	F	529/560 (94%)	-0.44	1 (0%) 91 90	51, 69, 110, 118	2 (0%)
1	G	527/560 (94%)	-0.29	6 (1%) 78 73	57, 75, 103, 123	1 (0%)
1	H	527/560 (94%)	-0.52	3 (0%) 85 82	42, 62, 82, 125	4 (0%)
All	All	4217/4480 (94%)	-0.49	21 (0%) 87 83	37, 64, 98, 169	10 (0%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	393	SER	6.5
1	C	348	ALA	4.7
1	E	391	ALA	4.2
1	E	390	ARG	3.8
1	E	392	ILE	3.8

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 ⓘ

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	AUC	D	640	1/5	0.76	0.29	99,99,99,99	1
2	AUC	F	637	1/5	0.76	0.17	85,85,85,85	1
3	MLI	H	901	7/7	0.79	0.25	58,59,61,61	7
3	MLI	D	901	7/7	0.84	0.18	52,54,55,55	7
2	AUC	C	634	1/5	0.84	0.23	82,82,82,82	1
2	AUC	A	631	5/5	0.85	0.51	57,58,58,59	5
2	AUC	B	630	1/5	0.87	0.17	107,107,107,107	1
2	AUC	B	638	1/5	0.88	0.24	86,86,86,86	1
2	AUC	F	627	1/5	0.88	0.20	85,85,85,85	1
2	AUC	F	641	1/5	0.88	0.17	108,108,108,108	1
2	AUC	H	629	1/5	0.88	0.16	85,85,85,85	1
3	MLI	C	901	7/7	0.88	0.17	47,48,49,50	7
2	AUC	B	640	1/5	0.88	0.11	93,93,93,93	1
2	AUC	E	628	1/5	0.88	0.24	80,80,80,80	1
2	AUC	C	635	1/5	0.89	0.21	76,76,76,76	1
3	MLI	E	901	7/7	0.90	0.16	41,43,43,44	7
3	MLI	A	901	7/7	0.90	0.12	40,41,43,43	7
2	AUC	E	619	1/5	0.91	0.13	68,68,68,68	1
2	AUC	C	621	1/5	0.92	0.09	70,70,70,70	1
2	AUC	H	617	1/5	0.93	0.07	74,74,74,74	1
2	AUC	A	624	1/5	0.94	0.10	71,71,71,71	1
2	AUC	F	620	1/5	0.95	0.12	69,69,69,69	1
2	AUC	B	622	1/5	0.95	0.10	69,69,69,69	1
2	AUC	G	626	1/5	0.96	0.08	76,76,76,76	1
2	AUC	D	618	1/5	0.97	0.08	82,82,82,82	1
2	AUC	B	610	5/5	0.97	0.14	82,83,84,86	5
2	AUC	F	613	1/5	0.98	0.04	80,80,80,80	0
2	AUC	G	616	1/5	0.98	0.04	86,86,86,86	0
2	AUC	A	608	1/5	0.99	0.02	74,74,74,74	0
2	AUC	D	604	1/5	0.99	0.03	85,85,85,85	0
2	AUC	C	601	1/5	0.99	0.02	75,75,75,75	0
2	AUC	G	615	5/5	0.99	0.06	69,70,70,73	1
2	AUC	B	609	1/5	0.99	0.02	79,79,79,79	0
2	AUC	F	614	5/5	0.99	0.08	80,82,83,83	5
2	AUC	H	612	1/5	0.99	0.03	80,80,80,80	0
2	AUC	E	605	1/5	1.00	0.02	72,72,72,72	0
2	AUC	E	606	5/5	1.00	0.04	72,73,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AUC	A	607	5/5	1.00	0.03	65,65,66,67	0
2	AUC	H	611	5/5	1.00	0.04	73,75,75,76	0
2	AUC	C	602	5/5	1.00	0.04	73,74,77,78	0
2	AUC	D	603	5/5	1.00	0.04	75,76,77,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.