



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:06 PM UTC

PDB ID : 5EFZ / pdb_00005efz
Title : Monoclinic structure of the acetyl esterase MekB
Authors : Toelzer, C.; Pal, S.; Watzlawick, H.; Altenbuchner, J.; Niefind, K.
Deposited on : 2015-10-26
Resolution : 1.82 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

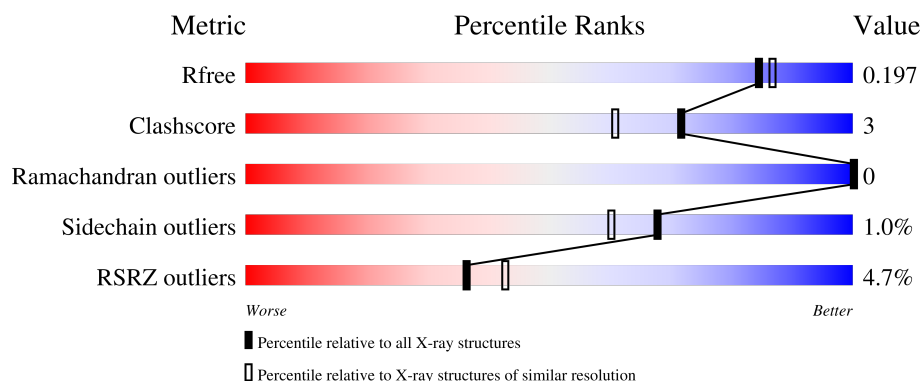
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	361	90% 5% • •
1	B	361	88% 8% •
1	C	361	89% 5% 6%
1	D	361	86% 10% •
1	E	361	88% 8% •

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Mol	Chain	Length	Quality of chain
1	F	361	%  93% . .

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	EDO	C	404	-	-	X	-
2	EDO	D	401	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17233 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 Homoserine O-acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	2	0
			2693	1709	459	509	16			
1	B	345	Total	C	N	O	S	0	2	0
			2678	1699	458	505	16			
1	C	339	Total	C	N	O	S	0	0	0
			2602	1653	448	485	16			
1	D	345	Total	C	N	O	S	0	0	0
			2661	1688	456	501	16			
1	E	345	Total	C	N	O	S	0	0	0
			2660	1689	455	500	16			
1	F	347	Total	C	N	O	S	0	0	0
			2678	1701	457	504	16			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q0MRG5
A	-10	THR	-	expression tag	UNP Q0MRG5
A	-9	MET	-	expression tag	UNP Q0MRG5
A	-8	ILE	-	expression tag	UNP Q0MRG5
A	-7	THR	-	expression tag	UNP Q0MRG5
A	-6	HIS	-	expression tag	UNP Q0MRG5
A	-5	HIS	-	expression tag	UNP Q0MRG5
A	-4	HIS	-	expression tag	UNP Q0MRG5
A	-3	HIS	-	expression tag	UNP Q0MRG5
A	-2	HIS	-	expression tag	UNP Q0MRG5
A	-1	HIS	-	expression tag	UNP Q0MRG5
A	0	GLY	-	expression tag	UNP Q0MRG5
A	1	SER	-	expression tag	UNP Q0MRG5
B	-11	MET	-	initiating methionine	UNP Q0MRG5
B	-10	THR	-	expression tag	UNP Q0MRG5
B	-9	MET	-	expression tag	UNP Q0MRG5
B	-8	ILE	-	expression tag	UNP Q0MRG5

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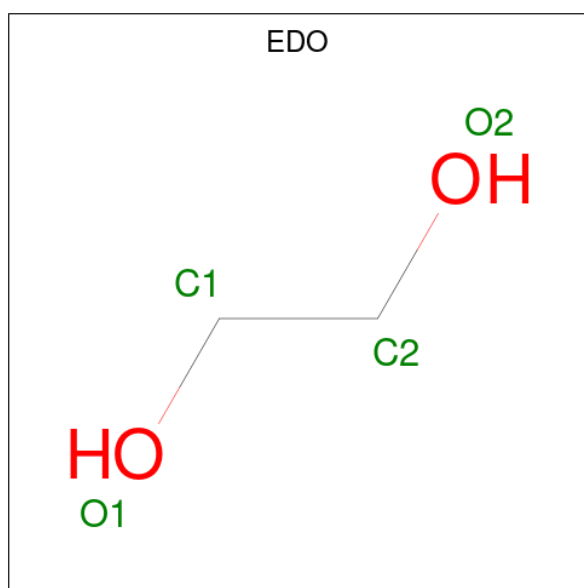
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	THR	-	expression tag	UNP Q0MRG5
B	-6	HIS	-	expression tag	UNP Q0MRG5
B	-5	HIS	-	expression tag	UNP Q0MRG5
B	-4	HIS	-	expression tag	UNP Q0MRG5
B	-3	HIS	-	expression tag	UNP Q0MRG5
B	-2	HIS	-	expression tag	UNP Q0MRG5
B	-1	HIS	-	expression tag	UNP Q0MRG5
B	0	GLY	-	expression tag	UNP Q0MRG5
B	1	SER	-	expression tag	UNP Q0MRG5
C	-11	MET	-	initiating methionine	UNP Q0MRG5
C	-10	THR	-	expression tag	UNP Q0MRG5
C	-9	MET	-	expression tag	UNP Q0MRG5
C	-8	ILE	-	expression tag	UNP Q0MRG5
C	-7	THR	-	expression tag	UNP Q0MRG5
C	-6	HIS	-	expression tag	UNP Q0MRG5
C	-5	HIS	-	expression tag	UNP Q0MRG5
C	-4	HIS	-	expression tag	UNP Q0MRG5
C	-3	HIS	-	expression tag	UNP Q0MRG5
C	-2	HIS	-	expression tag	UNP Q0MRG5
C	-1	HIS	-	expression tag	UNP Q0MRG5
C	0	GLY	-	expression tag	UNP Q0MRG5
C	1	SER	-	expression tag	UNP Q0MRG5
D	-11	MET	-	initiating methionine	UNP Q0MRG5
D	-10	THR	-	expression tag	UNP Q0MRG5
D	-9	MET	-	expression tag	UNP Q0MRG5
D	-8	ILE	-	expression tag	UNP Q0MRG5
D	-7	THR	-	expression tag	UNP Q0MRG5
D	-6	HIS	-	expression tag	UNP Q0MRG5
D	-5	HIS	-	expression tag	UNP Q0MRG5
D	-4	HIS	-	expression tag	UNP Q0MRG5
D	-3	HIS	-	expression tag	UNP Q0MRG5
D	-2	HIS	-	expression tag	UNP Q0MRG5
D	-1	HIS	-	expression tag	UNP Q0MRG5
D	0	GLY	-	expression tag	UNP Q0MRG5
D	1	SER	-	expression tag	UNP Q0MRG5
E	-11	MET	-	initiating methionine	UNP Q0MRG5
E	-10	THR	-	expression tag	UNP Q0MRG5
E	-9	MET	-	expression tag	UNP Q0MRG5
E	-8	ILE	-	expression tag	UNP Q0MRG5
E	-7	THR	-	expression tag	UNP Q0MRG5
E	-6	HIS	-	expression tag	UNP Q0MRG5
E	-5	HIS	-	expression tag	UNP Q0MRG5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP Q0MRG5
E	-3	HIS	-	expression tag	UNP Q0MRG5
E	-2	HIS	-	expression tag	UNP Q0MRG5
E	-1	HIS	-	expression tag	UNP Q0MRG5
E	0	GLY	-	expression tag	UNP Q0MRG5
E	1	SER	-	expression tag	UNP Q0MRG5
F	-11	MET	-	initiating methionine	UNP Q0MRG5
F	-10	THR	-	expression tag	UNP Q0MRG5
F	-9	MET	-	expression tag	UNP Q0MRG5
F	-8	ILE	-	expression tag	UNP Q0MRG5
F	-7	THR	-	expression tag	UNP Q0MRG5
F	-6	HIS	-	expression tag	UNP Q0MRG5
F	-5	HIS	-	expression tag	UNP Q0MRG5
F	-4	HIS	-	expression tag	UNP Q0MRG5
F	-3	HIS	-	expression tag	UNP Q0MRG5
F	-2	HIS	-	expression tag	UNP Q0MRG5
F	-1	HIS	-	expression tag	UNP Q0MRG5
F	0	GLY	-	expression tag	UNP Q0MRG5
F	1	SER	-	expression tag	UNP Q0MRG5

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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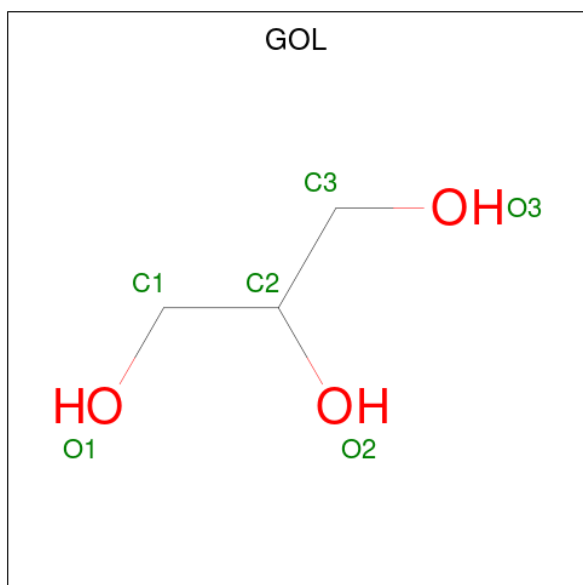
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0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

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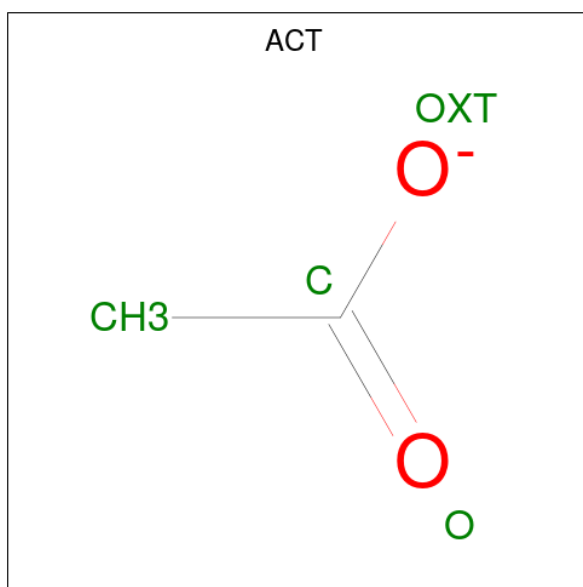
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	213	Total	O	0	0
			213	213		
5	B	207	Total	O	0	0
			207	207		
5	C	181	Total	O	0	0
			181	181		
5	D	124	Total	O	0	0
			124	124		
5	E	119	Total	O	0	0
			119	119		

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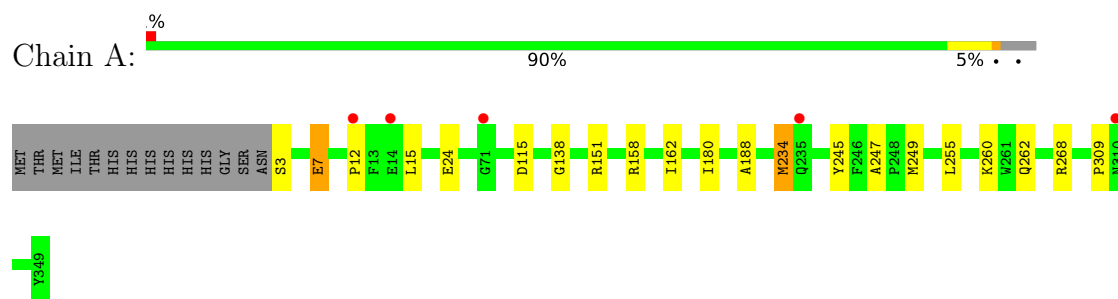
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	241	Total 241	O 241	0	0

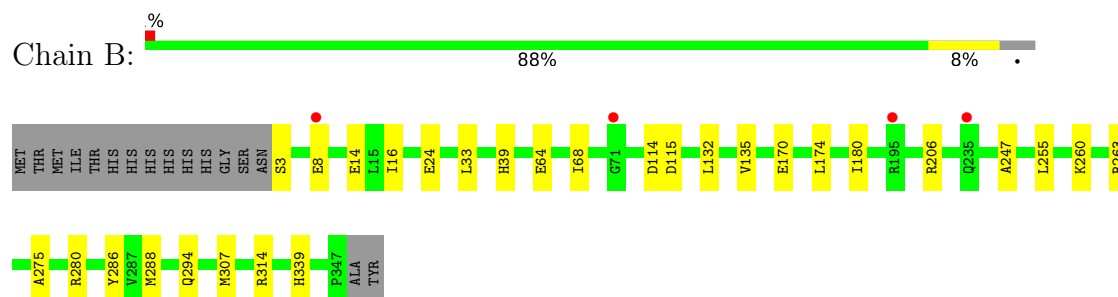
3 Residue-property plots [i](#)

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.

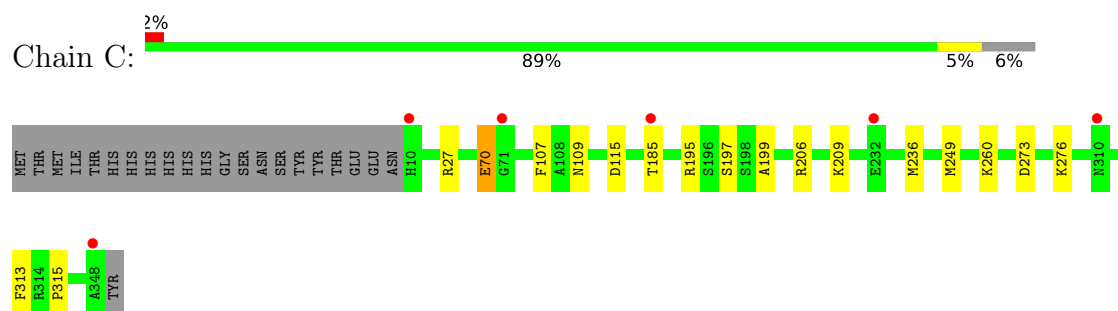
- Molecule 1: Homoserine O-acetyltransferase



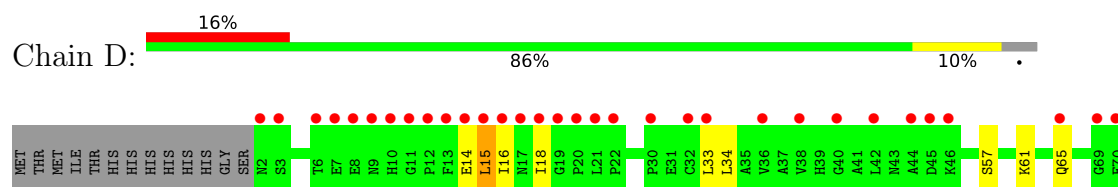
- Molecule 1: Homoserine O-acetyltransferase

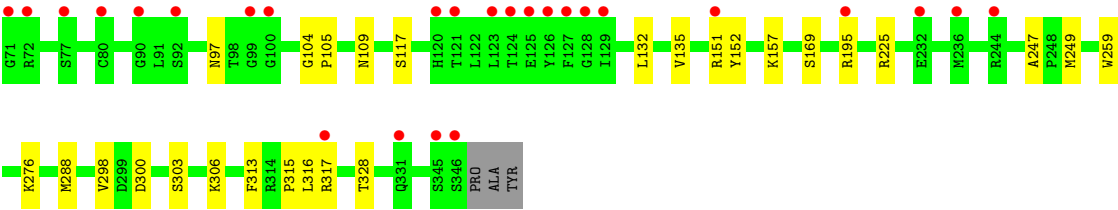


- Molecule 1: Homoserine O-acetyltransferase

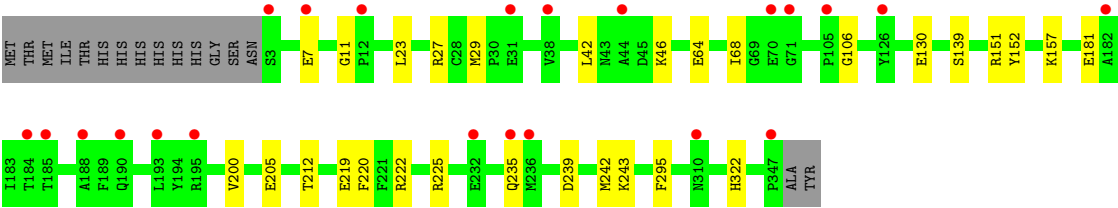
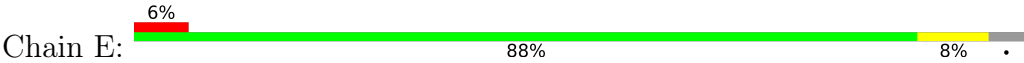


- Molecule 1: Homoserine O-acetyltransferase

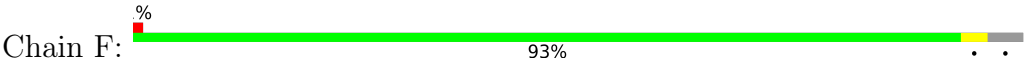




● Molecule 1: Homoserine O-acetyltransferase



● Molecule 1: Homoserine O-acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.85Å 110.34Å 122.82Å 90.00° 106.89° 90.00°	Depositor
Resolution (Å)	46.28 – 1.82 46.28 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.28-1.82) 99.6 (46.28-1.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.163 , 0.196 0.166 , 0.197	Depositor DCC
R_{free} test set	2133 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 55.6	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	0.97	EDS
Total number of atoms	17233	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: EDO, GOL, ACT

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	0.70	0/2759	0.81	3/3739 (0.1%)
1	B	0.67	0/2743	0.81	2/3718 (0.1%)
1	C	0.64	0/2665	0.83	1/3612 (0.0%)
1	D	0.59	0/2725	0.84	2/3693 (0.1%)
1	E	0.55	0/2725	0.76	0/3694
1	F	0.72	0/2744	0.82	0/3719
All	All	0.65	0/16361	0.81	8/22175 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	GLU	N-CA-C	6.67	118.55	111.28
1	D	247	ALA	CA-C-N	-5.53	114.20	120.89
1	D	247	ALA	C-N-CA	-5.53	114.20	120.89
1	A	309	PRO	CA-C-O	-5.14	115.39	121.67
1	A	247	ALA	CA-C-N	-5.04	115.15	121.00
1	A	247	ALA	C-N-CA	-5.04	115.15	121.00
1	B	247	ALA	CA-C-N	-5.00	114.84	120.89
1	B	247	ALA	C-N-CA	-5.00	114.84	120.89

There are no chirality outliers.

There are no planarity outliers.

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	2693	0	2611	16	0
1	B	2678	0	2600	25	0
1	C	2602	0	2545	12	0
1	D	2661	0	2587	29	0
1	E	2660	0	2588	19	0
1	F	2678	0	2602	8	0
2	A	28	0	42	3	0
2	B	20	0	30	3	0
2	C	24	0	36	6	0
2	D	12	0	18	7	0
2	E	8	0	12	0	0
2	F	8	0	12	0	0
3	A	6	0	8	1	0
3	C	12	0	16	2	0
3	D	12	0	16	1	0
3	F	18	0	24	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	4	0	3	0	0
4	D	4	0	3	0	0
4	E	8	0	6	1	0
4	F	4	0	3	0	0
5	A	213	0	0	1	0
5	B	207	0	0	4	0
5	C	181	0	0	1	0
5	D	124	0	0	3	0
5	E	119	0	0	0	0
5	F	241	0	0	1	0
All	All	17233	0	15768	106	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.

All (106) 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:B:288:MET:HE1	1:B:339:HIS:HB3	1.53	0.90
1:D:61:LYS:HG3	1:D:65:GLN:HE22	1.38	0.87
1:B:263:ARG:HE	2:B:405:EDO:H11	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:ARG:NH1	5:D:502:HOH:O	2.15	0.79
1:D:300:ASP:OD2	2:D:401:EDO:H22	1.85	0.77
1:D:151:ARG:NH1	1:D:152:TYR:OH	2.23	0.72
1:E:42:LEU:HD13	1:E:46:LYS:HD2	1.72	0.70
1:D:61:LYS:HG3	1:D:65:GLN:NE2	2.06	0.70
1:D:169:SER:OG	2:D:401:EDO:H21	1.93	0.69
1:C:109:ASN:H	2:C:404:EDO:H12	1.59	0.68
1:C:109:ASN:H	2:C:404:EDO:C1	2.08	0.67
1:D:15:LEU:HD21	1:D:33:LEU:HB3	1.78	0.66
1:A:234:MET:HE1	1:B:174:LEU:HD22	1.78	0.65
1:C:273:ASP:CG	1:C:276:LYS:HG3	2.21	0.65
2:D:401:EDO:O1	5:D:501:HOH:O	2.11	0.64
1:A:234:MET:HG3	1:B:170:GLU:HB3	1.82	0.61
3:C:408:GOL:H32	1:D:298:VAL:HG11	1.84	0.59
1:C:185:THR:HG23	1:C:206:ARG:NH2	2.18	0.59
1:B:288:MET:HE1	1:B:339:HIS:CB	2.28	0.59
1:D:306:LYS:NZ	2:D:402:EDO:H21	2.19	0.57
1:B:280:ARG:HD3	5:B:513:HOH:O	2.06	0.56
1:F:17:ASN:HD21	1:F:31:GLU:CD	2.14	0.56
1:C:199:ALA:HB2	3:C:408:GOL:H2	1.88	0.56
1:C:209:LYS:NZ	1:E:181:GLU:OE2	2.37	0.55
1:D:18:ILE:HD11	1:D:34:LEU:HD11	1.88	0.54
1:C:27:ARG:HD2	2:C:404:EDO:H22	1.89	0.54
1:B:115:ASP:OD2	1:B:260:LYS:NZ	2.39	0.54
1:D:169:SER:CB	2:D:401:EDO:H21	2.38	0.54
1:D:151:ARG:HD3	1:D:152:TYR:CE2	2.43	0.54
1:E:205:GLU:HG2	1:E:243:LYS:HE3	1.89	0.54
3:D:405:GOL:H12	1:F:210:LEU:HD11	1.90	0.53
1:A:234:MET:HE1	1:B:174:LEU:HB2	1.91	0.53
1:E:27:ARG:NH1	1:E:106:GLY:O	2.43	0.52
1:D:15:LEU:HD11	1:D:33:LEU:CG	2.39	0.52
1:B:263:ARG:HH21	2:B:405:EDO:H21	1.73	0.52
1:B:294[B]:GLN:NE2	5:B:503:HOH:O	2.42	0.52
1:B:39:HIS:NE2	1:B:64[A]:GLU:HG2	2.25	0.51
1:C:185:THR:HG23	1:C:206:ARG:HH21	1.76	0.51
1:B:288:MET:HE2	1:B:314:ARG:HB2	1.94	0.50
1:A:234:MET:CE	1:B:174:LEU:HB2	2.41	0.50
1:B:206:ARG:NH1	5:B:502:HOH:O	2.28	0.50
1:D:15:LEU:C	1:D:15:LEU:HD13	2.37	0.49
1:F:24:GLU:HG3	1:F:114:ASP:OD1	2.12	0.49
1:A:115:ASP:OD2	1:A:260:LYS:NZ	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ASP:OD2	1:C:260:LYS:NZ	2.41	0.49
1:B:286:TYR:HB3	1:B:288:MET:HE3	1.95	0.49
2:D:401:EDO:H12	1:F:218:PRO:HB3	1.95	0.49
1:A:7:GLU:OE1	1:A:12:PRO:HA	2.13	0.48
1:B:263:ARG:HH21	2:B:405:EDO:C2	2.26	0.48
1:B:275:ALA:HB2	1:B:307:MET:HE2	1.96	0.48
1:F:180:ILE:HG23	1:F:255:LEU:HD22	1.95	0.48
1:A:158:ARG:HH22	2:A:403:EDO:H11	1.79	0.48
1:D:225:ARG:NH2	1:D:328:THR:O	2.38	0.48
1:E:23:LEU:HD11	1:E:29:MET:HG3	1.95	0.48
2:C:403:EDO:H21	5:C:546:HOH:O	2.13	0.47
1:D:15:LEU:HD13	1:D:16:ILE:N	2.29	0.47
1:E:219:GLU:OE2	1:E:222:ARG:NH2	2.38	0.47
1:D:303:SER:HA	2:D:402:EDO:H22	1.97	0.47
1:E:220:PHE:CE2	1:E:225:ARG:HG2	2.49	0.47
1:A:138:GLY:HA2	1:A:162:ILE:O	2.14	0.47
1:E:151:ARG:HD3	1:E:152:TYR:CE1	2.50	0.47
1:D:97:ASN:HB3	5:D:517:HOH:O	2.15	0.47
1:E:139:SER:HG	4:E:403:ACT:C	2.25	0.47
1:E:157:LYS:HA	1:E:157:LYS:HD3	1.73	0.46
1:D:117:SER:HB2	1:D:151:ARG:NH2	2.31	0.46
1:E:235:GLN:NE2	1:E:239:ASP:OD2	2.48	0.46
1:E:212:THR:OG1	1:E:242:MET:HG3	2.16	0.46
1:C:107:PHE:HB3	2:C:403:EDO:H21	1.99	0.45
1:D:276:LYS:HE3	1:D:276:LYS:HB2	1.70	0.45
1:B:132:LEU:HD13	1:B:135:VAL:HG22	1.98	0.45
1:B:64[A]:GLU:HA	1:B:68:ILE:HD12	1.98	0.45
1:A:262:GLN:O	2:A:405:EDO:H11	2.17	0.45
1:C:109:ASN:H	2:C:404:EDO:H11	1.80	0.45
1:D:15:LEU:HD11	1:D:33:LEU:HG	1.99	0.45
1:C:313:PHE:CE2	1:C:315:PRO:HG3	2.51	0.44
1:D:15:LEU:HD11	1:D:33:LEU:HB3	1.98	0.44
1:E:64:GLU:HA	1:E:68:ILE:HD12	1.99	0.44
1:F:132:LEU:HD13	1:F:135:VAL:HG22	1.98	0.44
1:A:24[B]:GLU:OE2	1:A:151:ARG:NH2	2.41	0.44
1:E:205:GLU:OE1	1:E:243:LYS:NZ	2.36	0.44
1:A:158:ARG:HH12	2:A:403:EDO:H12	1.82	0.44
1:B:64[B]:GLU:HA	1:B:68:ILE:HD12	1.99	0.44
1:A:180:ILE:HG23	1:A:255:LEU:HD22	2.01	0.43
1:B:180:ILE:HG23	1:B:255:LEU:HD22	2.00	0.43
1:E:220:PHE:CD2	1:E:225:ARG:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:295:PHE:HZ	1:E:322:HIS:CD2	2.35	0.43
1:A:245:TYR:CZ	1:A:249:MET:HE1	2.53	0.43
1:A:3:SER:N	5:A:506:HOH:O	2.51	0.42
1:B:24:GLU:HG3	1:B:114:ASP:OD1	2.18	0.42
1:D:313:PHE:CE2	1:D:315:PRO:HG3	2.54	0.42
1:D:249:MET:HE2	1:D:249:MET:HB3	1.89	0.42
1:E:295:PHE:CZ	1:E:322:HIS:CD2	3.07	0.42
1:D:132:LEU:HD13	1:D:135:VAL:HG22	2.00	0.42
1:A:24[A]:GLU:OE2	1:A:268:ARG:NH2	2.50	0.42
1:A:188:ALA:HA	3:A:408:GOL:H12	2.01	0.42
1:B:14:GLU:CD	1:B:16:ILE:HD11	2.44	0.42
1:F:276:LYS:NZ	5:F:509:HOH:O	2.53	0.42
1:F:39:HIS:NE2	1:F:64:GLU:HG2	2.35	0.41
1:D:288:MET:CE	1:D:316:LEU:HD21	2.51	0.41
1:B:3:SER:N	5:B:514:HOH:O	2.53	0.41
1:D:57:SER:HB2	1:D:249:MET:HE1	2.02	0.41
1:E:7:GLU:HG2	1:E:11:GLY:HA3	2.03	0.40
1:D:109:ASN:HB3	1:D:259:TRP:CH2	2.56	0.40
1:E:7:GLU:CG	1:E:11:GLY:HA3	2.52	0.40
1:B:8:GLU:CD	1:B:8:GLU:H	2.30	0.40
1:D:104:GLY:HA3	1:D:105:PRO:HD3	1.95	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	347/361 (96%)	341 (98%)	6 (2%)	0	100	100
1	B	345/361 (96%)	339 (98%)	6 (2%)	0	100	100
1	C	337/361 (93%)	332 (98%)	5 (2%)	0	100	100
1	D	343/361 (95%)	335 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	343/361 (95%)	337 (98%)	6 (2%)	0	100	100
1	F	345/361 (96%)	339 (98%)	6 (2%)	0	100	100
All	All	2060/2166 (95%)	2023 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/292 (96%)	278 (99%)	3 (1%)	65	56
1	B	280/292 (96%)	279 (100%)	1 (0%)	84	81
1	C	271/292 (93%)	266 (98%)	5 (2%)	51	39
1	D	278/292 (95%)	274 (99%)	4 (1%)	59	49
1	E	278/292 (95%)	276 (99%)	2 (1%)	76	70
1	F	279/292 (96%)	278 (100%)	1 (0%)	84	81
All	All	1667/1752 (95%)	1651 (99%)	16 (1%)	68	60

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	15	LEU
1	A	234	MET
1	B	33	LEU
1	C	70	GLU
1	C	195	ARG
1	C	197	SER
1	C	236	MET
1	C	249	MET
1	D	14	GLU
1	D	15	LEU
1	D	157	LYS

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Mol	Chain	Res	Type
1	D	317	ARG
1	E	130	GLU
1	E	200	VAL
1	F	276	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	A	190	GLN
1	B	168	ASN
1	B	310	ASN
1	C	65	GLN
1	D	168	ASN
1	E	39	HIS
1	E	65	GLN
1	E	168	ASN
1	E	310	ASN
1	F	168	ASN

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](#)

40 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	D	404	-	5,5,5	0.33	0	5,5,5	0.53	0
3	GOL	C	407	-	5,5,5	0.33	0	5,5,5	0.25	0
4	ACT	C	409	-	3,3,3	0.94	0	3,3,3	1.27	0
2	EDO	A	403	-	3,3,3	0.51	0	2,2,2	0.19	0
2	EDO	C	402	-	3,3,3	0.31	0	2,2,2	0.70	0
2	EDO	C	403	-	3,3,3	0.56	0	2,2,2	0.26	0
2	EDO	D	403	-	3,3,3	0.46	0	2,2,2	0.31	0
4	ACT	B	406	-	3,3,3	1.01	0	3,3,3	1.08	0
2	EDO	C	401	-	3,3,3	0.46	0	2,2,2	0.37	0
2	EDO	C	405	-	3,3,3	0.48	0	2,2,2	0.38	0
2	EDO	B	403	-	3,3,3	0.35	0	2,2,2	0.84	0
2	EDO	A	405	-	3,3,3	0.66	0	2,2,2	0.28	0
2	EDO	A	402	-	3,3,3	0.51	0	2,2,2	0.39	0
2	EDO	E	401	-	3,3,3	0.43	0	2,2,2	0.51	0
3	GOL	D	405	-	5,5,5	0.33	0	5,5,5	0.38	0
2	EDO	D	402	-	3,3,3	0.45	0	2,2,2	0.29	0
4	ACT	A	409	-	3,3,3	0.69	0	3,3,3	1.27	0
2	EDO	B	401	-	3,3,3	0.42	0	2,2,2	0.45	0
3	GOL	F	405	-	5,5,5	0.37	0	5,5,5	0.13	0
2	EDO	F	401	-	3,3,3	0.50	0	2,2,2	0.44	0
2	EDO	F	402	-	3,3,3	0.44	0	2,2,2	0.37	0
2	EDO	E	402	-	3,3,3	0.42	0	2,2,2	0.45	0
2	EDO	C	406	-	3,3,3	0.54	0	2,2,2	0.32	0
4	ACT	E	403	-	3,3,3	0.81	0	3,3,3	1.47	0
2	EDO	A	401	-	3,3,3	0.48	0	2,2,2	0.37	0
4	ACT	D	406	-	3,3,3	0.46	0	3,3,3	1.77	1 (33%)
2	EDO	D	401	-	3,3,3	0.49	0	2,2,2	0.74	0
2	EDO	A	407	-	3,3,3	0.43	0	2,2,2	0.38	0
4	ACT	F	406	-	3,3,3	1.15	0	3,3,3	1.08	0
3	GOL	F	403	-	5,5,5	0.40	0	5,5,5	0.71	0
2	EDO	C	404	-	3,3,3	0.34	0	2,2,2	0.47	0
2	EDO	A	404	-	3,3,3	0.39	0	2,2,2	0.44	0
2	EDO	B	405	-	3,3,3	0.39	0	2,2,2	0.38	0
2	EDO	B	402	-	3,3,3	0.43	0	2,2,2	0.39	0
4	ACT	E	404	-	3,3,3	0.90	0	3,3,3	1.32	0
2	EDO	B	404	-	3,3,3	0.49	0	2,2,2	0.30	0
3	GOL	A	408	-	5,5,5	0.36	0	5,5,5	0.46	0
3	GOL	C	408	-	5,5,5	0.41	0	5,5,5	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	406	-	3,3,3	0.67	0	2,2,2	0.42	0
3	GOL	F	404	-	5,5,5	0.29	0	5,5,5	0.43	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
3	GOL	D	404	-	-	2/4/4/4	-
3	GOL	C	407	-	-	1/4/4/4	-
2	EDO	A	403	-	-	0/1/1/1	-
2	EDO	C	402	-	-	0/1/1/1	-
2	EDO	C	403	-	-	0/1/1/1	-
2	EDO	D	403	-	-	0/1/1/1	-
2	EDO	C	401	-	-	0/1/1/1	-
2	EDO	C	405	-	-	1/1/1/1	-
2	EDO	B	403	-	-	1/1/1/1	-
2	EDO	A	405	-	-	1/1/1/1	-
2	EDO	A	402	-	-	1/1/1/1	-
2	EDO	E	401	-	-	0/1/1/1	-
3	GOL	D	405	-	-	0/4/4/4	-
2	EDO	D	402	-	-	1/1/1/1	-
2	EDO	B	401	-	-	1/1/1/1	-
3	GOL	F	405	-	-	0/4/4/4	-
2	EDO	F	401	-	-	0/1/1/1	-
2	EDO	F	402	-	-	0/1/1/1	-
2	EDO	E	402	-	-	0/1/1/1	-
2	EDO	C	406	-	-	0/1/1/1	-
2	EDO	A	401	-	-	1/1/1/1	-
2	EDO	D	401	-	-	1/1/1/1	-
2	EDO	A	407	-	-	0/1/1/1	-
3	GOL	F	403	-	-	2/4/4/4	-
2	EDO	C	404	-	-	0/1/1/1	-
2	EDO	A	404	-	-	1/1/1/1	-
2	EDO	B	405	-	-	0/1/1/1	-
2	EDO	B	402	-	-	0/1/1/1	-
2	EDO	B	404	-	-	1/1/1/1	-
3	GOL	A	408	-	-	2/4/4/4	-
3	GOL	C	408	-	-	4/4/4/4	-
2	EDO	A	406	-	-	1/1/1/1	-
3	GOL	F	404	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	D	406	ACT	OXT-C-CH3	2.45	125.31	115.05

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	408	GOL	O1-C1-C2-C3
3	C	408	GOL	O1-C1-C2-C3
3	C	408	GOL	C1-C2-C3-O3
3	F	403	GOL	O1-C1-C2-C3
3	F	403	GOL	O1-C1-C2-O2
3	A	408	GOL	O1-C1-C2-O2
3	C	408	GOL	O2-C2-C3-O3
3	D	404	GOL	O2-C2-C3-O3
2	A	404	EDO	O1-C1-C2-O2
2	B	404	EDO	O1-C1-C2-O2
3	C	407	GOL	O1-C1-C2-O2
2	A	402	EDO	O1-C1-C2-O2
2	A	406	EDO	O1-C1-C2-O2
2	B	403	EDO	O1-C1-C2-O2
2	C	405	EDO	O1-C1-C2-O2
2	D	401	EDO	O1-C1-C2-O2
2	A	405	EDO	O1-C1-C2-O2
2	B	401	EDO	O1-C1-C2-O2
2	A	401	EDO	O1-C1-C2-O2
2	D	402	EDO	O1-C1-C2-O2
3	D	404	GOL	O1-C1-C2-C3
3	C	408	GOL	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	403	EDO	2	0
2	C	403	EDO	2	0
2	A	405	EDO	1	0
3	D	405	GOL	1	0
2	D	402	EDO	2	0
4	E	403	ACT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	EDO	5	0
2	C	404	EDO	4	0
2	B	405	EDO	3	0
3	A	408	GOL	1	0
3	C	408	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	347/361 (96%)	-0.41	5 (1%)	73 79	14, 23, 39, 57	2 (0%)
1	B	345/361 (95%)	-0.31	4 (1%)	76 82	9, 25, 43, 64	2 (0%)
1	C	339/361 (93%)	-0.17	6 (1%)	67 73	17, 27, 45, 67	0
1	D	345/361 (95%)	0.70	58 (16%)	4 5	17, 39, 67, 83	0
1	E	345/361 (95%)	0.47	22 (6%)	25 29	22, 39, 63, 83	0
1	F	347/361 (96%)	-0.50	2 (0%)	85 89	13, 22, 37, 53	0
All	All	2068/2166 (95%)	-0.04	97 (4%)	36 43	9, 28, 57, 83	4 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	18	ILE	6.1
1	D	15	LEU	5.2
1	C	348	ALA	4.4
1	D	30	PRO	4.3
1	D	2	ASN	3.8
1	D	38	VAL	3.5
1	D	20	PRO	3.5
1	D	17	ASN	3.5
1	D	19	GLY	3.4
1	B	195	ARG	3.4
1	D	244	ARG	3.3
1	D	16	ILE	3.2
1	D	128	GLY	3.2
1	D	124	THR	3.2
1	D	11	GLY	3.2
1	D	125	GLU	3.1
1	D	92	SER	3.1
1	D	100	GLY	3.1
1	A	71	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	99	GLY	3.1
1	E	126	TYR	3.1
1	D	36	VAL	3.1
1	F	310	ASN	3.1
1	D	33	LEU	3.0
1	C	71	GLY	3.0
1	D	44	ALA	3.0
1	D	42	LEU	2.9
1	E	71	GLY	2.9
1	E	347	PRO	2.9
1	D	7	GLU	2.9
1	D	195	ARG	2.9
1	D	121	THR	2.8
1	D	129	ILE	2.8
1	E	185	THR	2.8
1	D	123	LEU	2.8
1	D	32	CYS	2.7
1	D	331	GLN	2.6
1	D	126	TYR	2.6
1	E	193	LEU	2.6
1	E	38	VAL	2.6
1	A	310	ASN	2.6
1	E	236	MET	2.6
1	D	3	SER	2.5
1	D	13	PHE	2.5
1	D	71	GLY	2.5
1	D	90	GLY	2.5
1	D	120	HIS	2.5
1	B	8	GLU	2.5
1	E	7	GLU	2.5
1	D	40	GLY	2.4
1	D	10	HIS	2.4
1	D	21	LEU	2.4
1	D	346	SER	2.4
1	D	127	PHE	2.4
1	C	10	HIS	2.4
1	E	182	ALA	2.4
1	D	45	ASP	2.3
1	D	6	THR	2.3
1	C	310	ASN	2.3
1	E	105	PRO	2.3
1	E	232	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	3	SER	2.3
1	F	28	CYS	2.3
1	C	185	THR	2.3
1	D	72	ARG	2.2
1	E	44	ALA	2.2
1	D	46	LYS	2.2
1	D	8	GLU	2.2
1	B	71	GLY	2.2
1	E	235	GLN	2.2
1	D	69	GLY	2.2
1	D	9	ASN	2.2
1	D	317	ARG	2.2
1	D	70	GLU	2.2
1	D	345	SER	2.2
1	E	12	PRO	2.2
1	E	188	ALA	2.2
1	C	232	GLU	2.1
1	E	31	GLU	2.1
1	B	235	GLN	2.1
1	A	14	GLU	2.1
1	E	195	ARG	2.1
1	D	14	GLU	2.1
1	E	70	GLU	2.1
1	D	22	PRO	2.1
1	E	190	GLN	2.1
1	D	232	GLU	2.1
1	E	184	THR	2.1
1	E	310	ASN	2.1
1	D	65	GLN	2.1
1	D	77	SER	2.0
1	D	236	MET	2.0
1	A	235	GLN	2.0
1	A	12	PRO	2.0
1	D	80	CYS	2.0
1	D	12	PRO	2.0
1	D	151	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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	EDO	B	405	4/4	0.60	0.26	70,70,71,71	0
4	ACT	E	404	4/4	0.71	0.22	43,45,47,47	0
3	GOL	F	404	6/6	0.73	0.21	52,55,55,56	0
2	EDO	B	404	4/4	0.74	0.22	58,59,59,59	0
3	GOL	D	404	6/6	0.77	0.20	64,66,67,69	0
2	EDO	B	403	4/4	0.78	0.20	43,43,43,47	0
2	EDO	A	405	4/4	0.78	0.18	37,42,44,47	0
2	EDO	C	406	4/4	0.79	0.19	52,53,53,54	0
2	EDO	A	403	4/4	0.79	0.21	51,53,56,56	0
3	GOL	D	405	6/6	0.81	0.17	45,53,54,54	0
3	GOL	C	408	6/6	0.82	0.18	50,54,56,57	0
2	EDO	C	402	4/4	0.82	0.18	39,45,49,51	0
2	EDO	C	401	4/4	0.82	0.20	53,53,53,54	0
2	EDO	D	402	4/4	0.82	0.16	57,59,59,59	0
3	GOL	A	408	6/6	0.82	0.16	50,50,51,52	0
2	EDO	A	402	4/4	0.84	0.16	49,49,49,50	0
2	EDO	B	402	4/4	0.85	0.16	55,55,56,56	0
2	EDO	D	403	4/4	0.85	0.15	51,54,55,57	0
2	EDO	E	401	4/4	0.85	0.15	39,43,45,46	0
2	EDO	C	405	4/4	0.86	0.15	55,55,55,56	0
2	EDO	F	401	4/4	0.86	0.15	40,44,44,45	0
2	EDO	C	404	4/4	0.87	0.17	44,47,49,51	0
2	EDO	A	401	4/4	0.87	0.15	48,50,51,51	0
3	GOL	C	407	6/6	0.87	0.15	57,57,57,57	0
3	GOL	F	405	6/6	0.87	0.16	54,54,55,56	0
4	ACT	E	403	4/4	0.87	0.14	33,33,37,40	0
2	EDO	A	406	4/4	0.87	0.17	37,40,41,42	0
2	EDO	B	401	4/4	0.88	0.13	56,56,56,57	0
4	ACT	F	406	4/4	0.88	0.11	24,25,27,27	0
3	GOL	F	403	6/6	0.89	0.14	34,43,46,47	0
2	EDO	D	401	4/4	0.89	0.14	28,29,30,37	0
2	EDO	A	404	4/4	0.89	0.13	37,38,41,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	E	402	4/4	0.90	0.16	54,56,58,59	0
4	ACT	D	406	4/4	0.91	0.10	30,31,31,35	0
2	EDO	A	407	4/4	0.91	0.12	26,34,38,39	0
2	EDO	F	402	4/4	0.92	0.12	52,53,55,55	0
4	ACT	C	409	4/4	0.92	0.10	27,30,31,32	0
4	ACT	B	406	4/4	0.93	0.09	26,26,29,31	0
2	EDO	C	403	4/4	0.93	0.10	38,40,40,40	0
4	ACT	A	409	4/4	0.93	0.10	23,25,26,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.