



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:20 AM UTC

PDB ID : 4QFE / pdb_00004qfe
Title : Crystal Structure of an Enoyl-CoA hydratase from Mycobacterium smegmatis
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2014-05-20
Resolution : 1.95 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

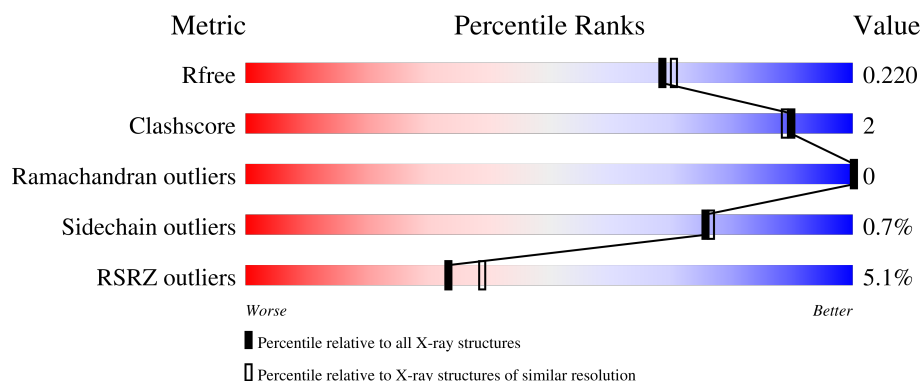
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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.



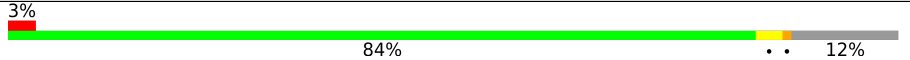
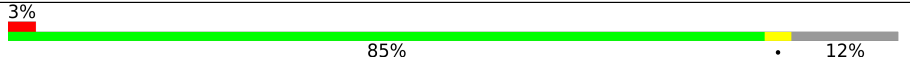
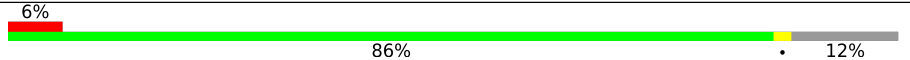
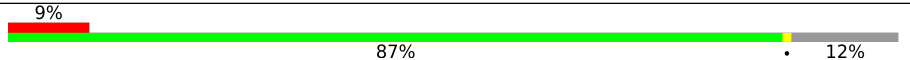
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	259	5% 83% 13%
1	B	259	3% 85% 12%
1	C	259	3% 87% 12%
1	D	259	2% 85% 11%
1	E	259	6% 85% 13%

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Mol	Chain	Length	Quality of chain
1	F	259	
1	G	259	
1	H	259	
1	I	259	
1	J	259	
1	K	259	
1	L	259	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21505 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 Enoyl-CoA hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	2	0
			1630	1013	292	315	10			
1	B	228	Total	C	N	O	S	0	2	0
			1668	1036	304	318	10			
1	C	229	Total	C	N	O	S	0	1	0
			1655	1026	302	317	10			
1	D	230	Total	C	N	O	S	0	1	0
			1666	1034	300	322	10			
1	E	225	Total	C	N	O	S	0	2	0
			1620	1005	290	315	10			
1	F	226	Total	C	N	O	S	0	1	0
			1669	1036	305	318	10			
1	G	227	Total	C	N	O	S	0	1	0
			1659	1035	298	316	10			
1	H	227	Total	C	N	O	S	0	1	0
			1639	1020	298	311	10			
1	I	228	Total	C	N	O	S	0	2	0
			1675	1040	302	323	10			
1	J	228	Total	C	N	O	S	0	2	0
			1691	1056	306	319	10			
1	K	229	Total	C	N	O	S	0	1	0
			1668	1036	300	322	10			
1	L	229	Total	C	N	O	S	0	0	0
			1626	1014	296	306	10			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP A0QS88
A	-3	PRO	-	expression tag	UNP A0QS88
A	-2	GLY	-	expression tag	UNP A0QS88
A	-1	SER	-	expression tag	UNP A0QS88
A	0	MET	-	expression tag	UNP A0QS88

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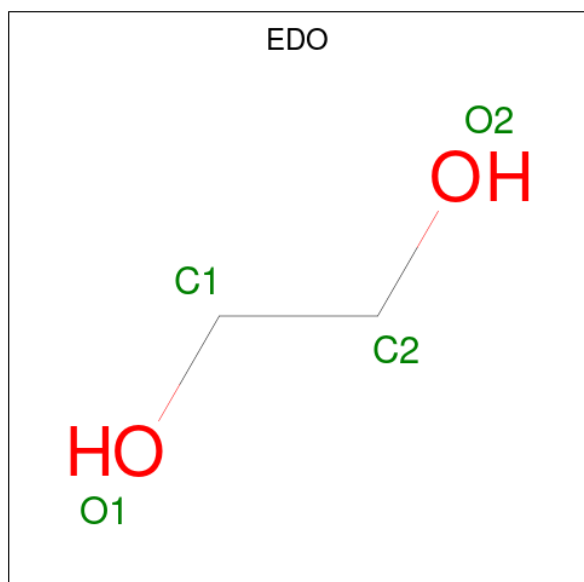
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	-	expression tag	UNP A0QS88
B	-4	GLY	-	expression tag	UNP A0QS88
B	-3	PRO	-	expression tag	UNP A0QS88
B	-2	GLY	-	expression tag	UNP A0QS88
B	-1	SER	-	expression tag	UNP A0QS88
B	0	MET	-	expression tag	UNP A0QS88
B	1	VAL	-	expression tag	UNP A0QS88
C	-4	GLY	-	expression tag	UNP A0QS88
C	-3	PRO	-	expression tag	UNP A0QS88
C	-2	GLY	-	expression tag	UNP A0QS88
C	-1	SER	-	expression tag	UNP A0QS88
C	0	MET	-	expression tag	UNP A0QS88
C	1	VAL	-	expression tag	UNP A0QS88
D	-4	GLY	-	expression tag	UNP A0QS88
D	-3	PRO	-	expression tag	UNP A0QS88
D	-2	GLY	-	expression tag	UNP A0QS88
D	-1	SER	-	expression tag	UNP A0QS88
D	0	MET	-	expression tag	UNP A0QS88
D	1	VAL	-	expression tag	UNP A0QS88
E	-4	GLY	-	expression tag	UNP A0QS88
E	-3	PRO	-	expression tag	UNP A0QS88
E	-2	GLY	-	expression tag	UNP A0QS88
E	-1	SER	-	expression tag	UNP A0QS88
E	0	MET	-	expression tag	UNP A0QS88
E	1	VAL	-	expression tag	UNP A0QS88
F	-4	GLY	-	expression tag	UNP A0QS88
F	-3	PRO	-	expression tag	UNP A0QS88
F	-2	GLY	-	expression tag	UNP A0QS88
F	-1	SER	-	expression tag	UNP A0QS88
F	0	MET	-	expression tag	UNP A0QS88
F	1	VAL	-	expression tag	UNP A0QS88
G	-4	GLY	-	expression tag	UNP A0QS88
G	-3	PRO	-	expression tag	UNP A0QS88
G	-2	GLY	-	expression tag	UNP A0QS88
G	-1	SER	-	expression tag	UNP A0QS88
G	0	MET	-	expression tag	UNP A0QS88
G	1	VAL	-	expression tag	UNP A0QS88
H	-4	GLY	-	expression tag	UNP A0QS88
H	-3	PRO	-	expression tag	UNP A0QS88
H	-2	GLY	-	expression tag	UNP A0QS88
H	-1	SER	-	expression tag	UNP A0QS88
H	0	MET	-	expression tag	UNP A0QS88

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1	VAL	-	expression tag	UNP A0QS88
I	-4	GLY	-	expression tag	UNP A0QS88
I	-3	PRO	-	expression tag	UNP A0QS88
I	-2	GLY	-	expression tag	UNP A0QS88
I	-1	SER	-	expression tag	UNP A0QS88
I	0	MET	-	expression tag	UNP A0QS88
I	1	VAL	-	expression tag	UNP A0QS88
J	-4	GLY	-	expression tag	UNP A0QS88
J	-3	PRO	-	expression tag	UNP A0QS88
J	-2	GLY	-	expression tag	UNP A0QS88
J	-1	SER	-	expression tag	UNP A0QS88
J	0	MET	-	expression tag	UNP A0QS88
J	1	VAL	-	expression tag	UNP A0QS88
K	-4	GLY	-	expression tag	UNP A0QS88
K	-3	PRO	-	expression tag	UNP A0QS88
K	-2	GLY	-	expression tag	UNP A0QS88
K	-1	SER	-	expression tag	UNP A0QS88
K	0	MET	-	expression tag	UNP A0QS88
K	1	VAL	-	expression tag	UNP A0QS88
L	-4	GLY	-	expression tag	UNP A0QS88
L	-3	PRO	-	expression tag	UNP A0QS88
L	-2	GLY	-	expression tag	UNP A0QS88
L	-1	SER	-	expression tag	UNP A0QS88
L	0	MET	-	expression tag	UNP A0QS88
L	1	VAL	-	expression tag	UNP A0QS88

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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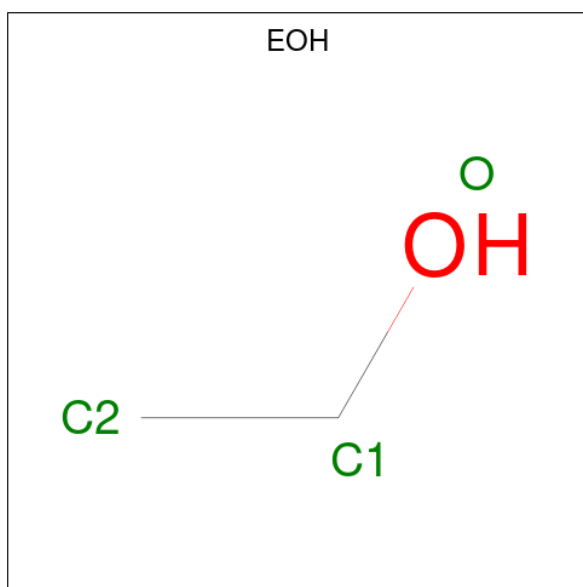
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	K	1	Total C O 4 2 2	0	0
2	K	1	Total C O 4 2 2	0	0
2	K	1	Total C O 4 2 2	0	0
2	L	1	Total C O 4 2 2	0	0
2	L	1	Total C O 4 2 2	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

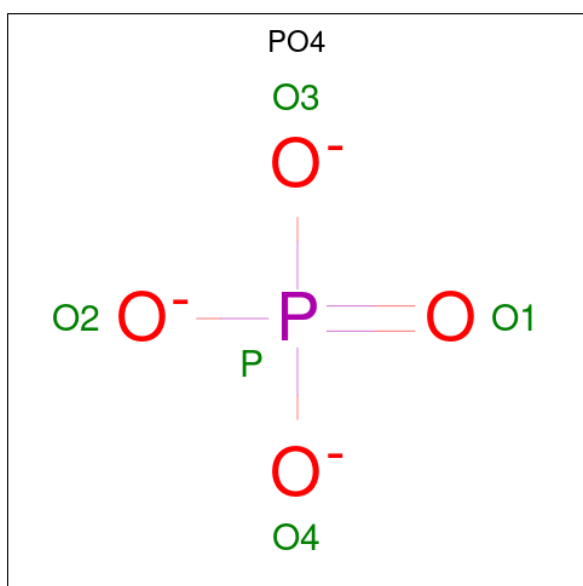
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	G	1	Total Na 1 1	0	0
3	J	1	Total Na 1 1	0	0

- Molecule 4 is ETHANOL (CCD ID: EOH) (formula: C₂H₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			3	2	1		
4	I	1	Total	C	O	0	0
			3	2	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		

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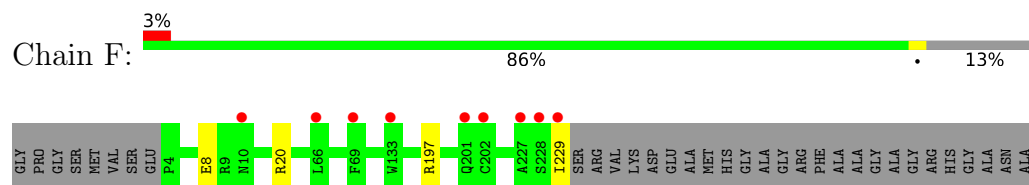
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		

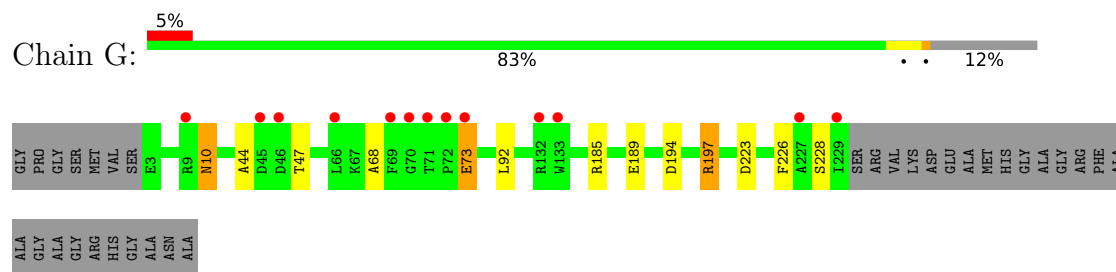
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	155	Total	O	0	0
			155	155		
6	B	119	Total	O	0	1
			120	120		
6	C	139	Total	O	0	1
			140	140		
6	D	137	Total	O	0	1
			138	138		
6	E	141	Total	O	0	0
			141	141		
6	F	108	Total	O	0	1
			109	109		
6	G	122	Total	O	0	0
			122	122		
6	H	85	Total	O	0	0
			85	85		
6	I	132	Total	O	0	2
			134	134		
6	J	146	Total	O	0	0
			146	146		
6	K	110	Total	O	0	0
			110	110		
6	L	81	Total	O	0	0
			81	81		

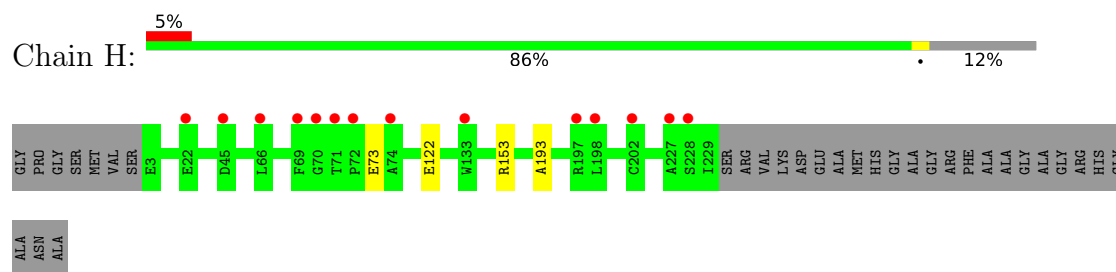
- Molecule 1: Enoyl-CoA hydratase



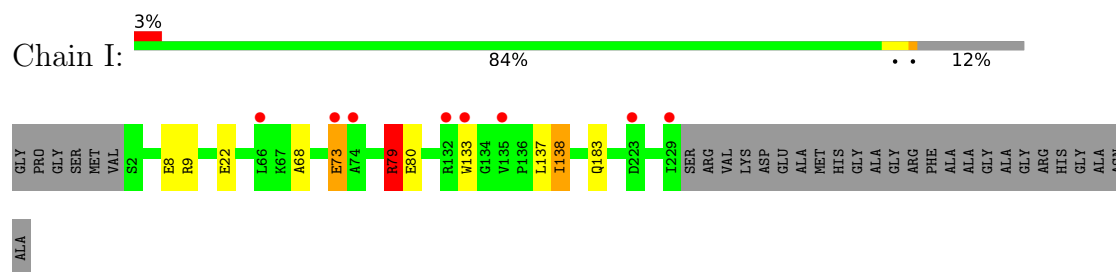
- Molecule 1: Enoyl-CoA hydratase



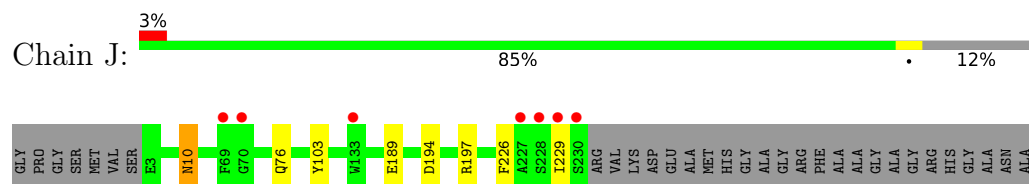
- Molecule 1: Enoyl-CoA hydratase



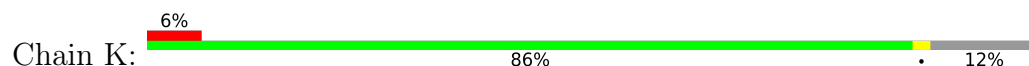
- Molecule 1: Enoyl-CoA hydratase



- Molecule 1: Enoyl-CoA hydratase

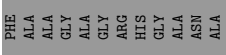
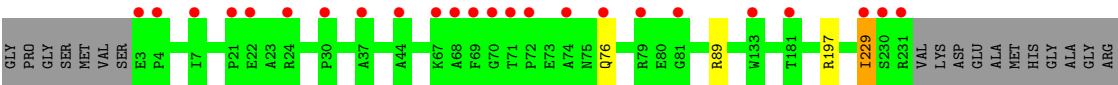
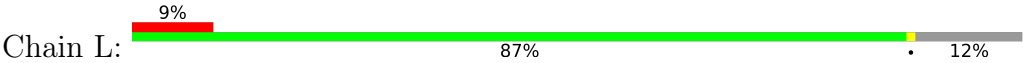


- Molecule 1: Enoyl-CoA hydratase





● Molecule 1: Enoyl-CoA hydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.29Å 86.58Å 106.16Å 84.96° 73.62° 83.18°	Depositor
Resolution (Å)	46.32 – 1.95 46.32 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.2 (46.32-1.95) 96.2 (46.32-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.197 , 0.223 (Not available) , 0.220	Depositor DCC
R_{free} test set	9247 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21505	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.25% 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: EOH, EDO, PO4, NA

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	0.88	1/1663 (0.1%)	0.96	2/2265 (0.1%)
1	B	0.79	0/1704	0.85	2/2322 (0.1%)
1	C	0.79	0/1686	0.81	0/2298
1	D	0.86	0/1698	0.92	2/2315 (0.1%)
1	E	0.91	1/1653 (0.1%)	1.00	5/2253 (0.2%)
1	F	0.81	0/1699	0.86	3/2313 (0.1%)
1	G	0.78	0/1693	0.86	1/2307 (0.0%)
1	H	0.74	0/1672	0.81	0/2280
1	I	0.77	0/1711	0.84	1/2331 (0.0%)
1	J	0.84	0/1731	0.87	0/2357
1	K	0.75	0/1701	0.83	3/2318 (0.1%)
1	L	0.75	1/1656 (0.1%)	0.88	5/2262 (0.2%)
All	All	0.81	3/20267 (0.0%)	0.88	24/27621 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	129	PHE	N-CA	6.82	1.56	1.46
1	A	129	PHE	N-CA	5.94	1.57	1.46
1	L	197	ARG	CZ-NH1	-5.00	1.25	1.32

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	123	ASP	CB-CA-C	-11.66	90.62	110.09
1	E	73	GLU	CA-CB-CG	11.59	137.27	114.10
1	L	197	ARG	NE-CZ-NH2	10.98	129.08	119.20
1	E	105	VAL	CB-CA-C	-10.61	93.72	110.69
1	A	105	VAL	CB-CA-C	-10.49	93.91	110.69

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	1630	0	1584	8	0
1	B	1668	0	1620	5	0
1	C	1655	0	1600	1	0
1	D	1666	0	1607	10	0
1	E	1620	0	1552	3	0
1	F	1669	0	1632	3	0
1	G	1659	0	1611	14	0
1	H	1639	0	1580	6	0
1	I	1675	0	1625	16	0
1	J	1691	0	1669	11	0
1	K	1668	0	1611	3	0
1	L	1626	0	1558	1	0
2	A	16	0	24	0	0
2	B	8	0	12	0	0
2	C	8	0	12	0	0
2	D	4	0	6	0	0
2	E	4	0	6	0	0
2	F	8	0	12	0	0
2	G	12	0	18	2	0
2	I	24	0	36	2	0
2	J	24	0	36	4	0
2	K	12	0	18	0	0
2	L	8	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	G	1	0	0	0	0
3	J	1	0	0	0	0
4	B	3	0	6	0	0
4	I	3	0	6	0	0
5	B	5	0	0	0	0
5	D	5	0	0	0	0
5	G	5	0	0	0	0
5	H	5	0	0	0	0
6	A	155	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	120	0	0	1	0
6	C	140	0	0	0	0
6	D	138	0	0	1	0
6	E	141	0	0	1	0
6	F	109	0	0	0	0
6	G	122	0	0	1	0
6	H	85	0	0	3	0
6	I	134	0	0	7	0
6	J	146	0	0	4	0
6	K	110	0	0	0	0
6	L	81	0	0	0	0
All	All	21505	0	19453	71	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 71 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:I:9:ARG:NH2	6:I:487:HOH:O	1.90	1.02
1:H:153[A]:ARG:HG2	1:H:153[A]:ARG:HH11	1.39	0.85
1:I:73:GLU:HB3	6:I:450:HOH:O	1.79	0.82
1:I:137:LEU:O	1:I:138[A]:ILE:HD13	1.83	0.78
1:J:76:GLN:NE2	6:J:521:HOH:O	2.27	0.68

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	223/259 (86%)	217 (97%)	6 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	228/259 (88%)	220 (96%)	8 (4%)	0	100	100
1	C	228/259 (88%)	222 (97%)	6 (3%)	0	100	100
1	D	229/259 (88%)	221 (96%)	8 (4%)	0	100	100
1	E	223/259 (86%)	217 (97%)	6 (3%)	0	100	100
1	F	225/259 (87%)	218 (97%)	7 (3%)	0	100	100
1	G	226/259 (87%)	220 (97%)	6 (3%)	0	100	100
1	H	226/259 (87%)	220 (97%)	6 (3%)	0	100	100
1	I	228/259 (88%)	223 (98%)	5 (2%)	0	100	100
1	J	229/259 (88%)	224 (98%)	5 (2%)	0	100	100
1	K	228/259 (88%)	222 (97%)	6 (3%)	0	100	100
1	L	227/259 (88%)	222 (98%)	5 (2%)	0	100	100
All	All	2720/3108 (88%)	2646 (97%)	74 (3%)	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	159/185 (86%)	157 (99%)	2 (1%)	61	58
1	B	162/185 (88%)	161 (99%)	1 (1%)	78	79
1	C	159/185 (86%)	158 (99%)	1 (1%)	78	79
1	D	161/185 (87%)	160 (99%)	1 (1%)	78	79
1	E	155/185 (84%)	155 (100%)	0	100	100
1	F	164/185 (89%)	163 (99%)	1 (1%)	78	79
1	G	161/185 (87%)	159 (99%)	2 (1%)	63	61
1	H	156/185 (84%)	156 (100%)	0	100	100
1	I	164/185 (89%)	159 (97%)	5 (3%)	36	27
1	J	168/185 (91%)	167 (99%)	1 (1%)	78	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	162/185 (88%)	162 (100%)	0	100	100
1	L	152/185 (82%)	151 (99%)	1 (1%)	76	76
All	All	1923/2220 (87%)	1908 (99%)	15 (1%)	76	74

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	73	GLU
1	J	10	ASN
1	I	73	GLU
1	L	229	ILE
1	I	138[B]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	75	ASN
1	J	75	ASN
1	J	10	ASN
1	J	78	HIS
1	D	75	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](#)

Of 42 ligands modelled in this entry, 4 are monoatomic - leaving 38 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	EDO	A	302	-	3,3,3	0.49	0	2,2,2	0.25	0
2	EDO	G	303	-	3,3,3	0.25	0	2,2,2	0.61	0
2	EDO	G	302	-	3,3,3	0.58	0	2,2,2	0.31	0
2	EDO	E	301	-	3,3,3	0.47	0	2,2,2	0.23	0
5	PO4	D	301	-	4,4,4	0.72	0	6,6,6	0.97	0
2	EDO	A	304	-	3,3,3	0.21	0	2,2,2	0.52	0
2	EDO	I	307	-	3,3,3	0.30	0	2,2,2	0.50	0
2	EDO	K	302	-	3,3,3	0.35	0	2,2,2	0.88	0
2	EDO	I	306	-	3,3,3	0.49	0	2,2,2	0.50	0
2	EDO	I	305	-	3,3,3	0.45	0	2,2,2	0.40	0
2	EDO	J	304	-	3,3,3	0.43	0	2,2,2	0.39	0
2	EDO	L	302	-	3,3,3	0.33	0	2,2,2	0.30	0
4	EOH	I	301	-	2,2,2	0.41	0	1,1,1	0.13	0
2	EDO	J	301	-	3,3,3	0.32	0	2,2,2	0.47	0
2	EDO	D	302	-	3,3,3	0.40	0	2,2,2	0.44	0
2	EDO	J	302	-	3,3,3	0.40	0	2,2,2	0.36	0
4	EOH	B	301	-	2,2,2	0.47	0	1,1,1	0.63	0
2	EDO	L	301	-	3,3,3	0.29	0	2,2,2	0.66	0
2	EDO	F	301	-	3,3,3	0.52	0	2,2,2	0.84	0
2	EDO	J	306	-	3,3,3	0.51	0	2,2,2	0.33	0
5	PO4	B	304	-	4,4,4	0.76	0	6,6,6	1.02	0
2	EDO	I	302	-	3,3,3	0.50	0	2,2,2	0.36	0
2	EDO	F	302	-	3,3,3	0.42	0	2,2,2	0.69	0
2	EDO	C	302	-	3,3,3	0.42	0	2,2,2	0.57	0
2	EDO	A	301	-	3,3,3	0.64	0	2,2,2	0.12	0
2	EDO	K	303	-	3,3,3	0.40	0	2,2,2	0.45	0
2	EDO	C	301	-	3,3,3	0.44	0	2,2,2	0.15	0
2	EDO	J	305	-	3,3,3	0.61	0	2,2,2	0.28	0
2	EDO	K	301	-	3,3,3	0.55	0	2,2,2	0.10	0
5	PO4	G	305	-	4,4,4	0.79	0	6,6,6	0.83	0
2	EDO	I	304	-	3,3,3	0.39	0	2,2,2	0.79	0
2	EDO	A	303	-	3,3,3	0.36	0	2,2,2	0.16	0
2	EDO	B	303	-	3,3,3	0.43	0	2,2,2	0.40	0
5	PO4	H	301	-	4,4,4	0.81	0	6,6,6	0.48	0
2	EDO	B	302	-	3,3,3	0.57	0	2,2,2	0.08	0
2	EDO	G	301	-	3,3,3	0.58	0	2,2,2	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	I	303	-	3,3,3	0.46	0	2,2,2	0.39	0
2	EDO	J	303	-	3,3,3	0.58	0	2,2,2	0.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	302	-	-	1/1/1/1	-
2	EDO	G	303	-	-	0/1/1/1	-
2	EDO	G	302	-	-	1/1/1/1	-
2	EDO	E	301	-	-	0/1/1/1	-
2	EDO	A	304	-	-	1/1/1/1	-
2	EDO	I	307	-	-	1/1/1/1	-
2	EDO	K	302	-	-	0/1/1/1	-
2	EDO	I	306	-	-	0/1/1/1	-
2	EDO	I	305	-	-	0/1/1/1	-
2	EDO	J	304	-	-	0/1/1/1	-
2	EDO	L	302	-	-	0/1/1/1	-
2	EDO	J	301	-	-	1/1/1/1	-
2	EDO	D	302	-	-	1/1/1/1	-
2	EDO	J	302	-	-	1/1/1/1	-
2	EDO	L	301	-	-	1/1/1/1	-
2	EDO	F	301	-	-	1/1/1/1	-
2	EDO	J	306	-	-	0/1/1/1	-
2	EDO	I	302	-	-	0/1/1/1	-
2	EDO	F	302	-	-	0/1/1/1	-
2	EDO	C	302	-	-	1/1/1/1	-
2	EDO	A	301	-	-	1/1/1/1	-
2	EDO	K	303	-	-	0/1/1/1	-
2	EDO	C	301	-	-	0/1/1/1	-
2	EDO	J	305	-	-	0/1/1/1	-
2	EDO	K	301	-	-	1/1/1/1	-
2	EDO	I	304	-	-	1/1/1/1	-
2	EDO	A	303	-	-	0/1/1/1	-
2	EDO	B	303	-	-	0/1/1/1	-
2	EDO	B	302	-	-	1/1/1/1	-
2	EDO	G	301	-	-	1/1/1/1	-
2	EDO	I	303	-	-	0/1/1/1	-
2	EDO	J	303	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	EDO	O1-C1-C2-O2
2	G	302	EDO	O1-C1-C2-O2
2	J	301	EDO	O1-C1-C2-O2
2	A	301	EDO	O1-C1-C2-O2
2	A	304	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	303	EDO	1	0
2	I	307	EDO	2	0
2	J	301	EDO	1	0
2	J	306	EDO	1	0
2	J	305	EDO	2	0
2	G	301	EDO	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	225/259 (86%)	0.25	13 (5%)	29	33	11, 18, 38, 49	2 (0%)
1	B	228/259 (88%)	0.29	7 (3%)	51	58	8, 22, 38, 48	2 (0%)
1	C	229/259 (88%)	0.28	8 (3%)	47	53	13, 22, 40, 50	1 (0%)
1	D	230/259 (88%)	0.18	6 (2%)	57	64	9, 19, 36, 46	1 (0%)
1	E	225/259 (86%)	0.36	16 (7%)	22	25	10, 19, 37, 55	2 (0%)
1	F	226/259 (87%)	0.35	9 (3%)	42	49	12, 23, 41, 46	1 (0%)
1	G	227/259 (87%)	0.43	13 (5%)	29	34	14, 22, 41, 56	1 (0%)
1	H	227/259 (87%)	0.61	14 (6%)	26	31	10, 27, 44, 56	1 (0%)
1	I	228/259 (88%)	0.36	8 (3%)	47	53	11, 21, 42, 53	2 (0%)
1	J	228/259 (88%)	0.10	7 (3%)	51	58	7, 18, 33, 68	2 (0%)
1	K	229/259 (88%)	0.64	15 (6%)	24	28	14, 26, 51, 65	1 (0%)
1	L	229/259 (88%)	0.81	24 (10%)	11	13	13, 30, 58, 70	0
All	All	2731/3108 (87%)	0.39	140 (5%)	33	39	7, 22, 44, 70	16 (0%)

The worst 5 of 140 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	ILE	4.6
1	C	229	ILE	4.5
1	H	71	THR	4.5
1	F	66	LEU	4.4
1	E	229	ILE	4.3

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 ⓘ

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	F	301	4/4	0.63	0.20	43,45,46,48	0
2	EDO	I	304	4/4	0.65	0.19	43,46,47,50	0
2	EDO	I	302	4/4	0.69	0.22	53,53,55,57	0
2	EDO	K	301	4/4	0.69	0.19	53,54,54,54	0
2	EDO	G	302	4/4	0.70	0.18	43,44,44,47	0
4	EOH	I	301	3/3	0.73	0.20	40,40,42,42	0
5	PO4	H	301	5/5	0.74	0.17	63,68,71,75	0
4	EOH	B	301	3/3	0.77	0.18	25,25,28,28	0
2	EDO	A	301	4/4	0.81	0.17	39,39,42,45	0
2	EDO	A	302	4/4	0.83	0.17	41,43,45,45	0
2	EDO	D	302	4/4	0.83	0.17	45,46,48,48	0
2	EDO	C	301	4/4	0.85	0.13	41,41,42,45	0
5	PO4	G	305	5/5	0.85	0.20	75,76,83,83	0
2	EDO	J	306	4/4	0.85	0.14	36,36,39,40	0
2	EDO	J	305	4/4	0.86	0.14	33,34,34,36	0
2	EDO	A	304	4/4	0.87	0.13	31,35,35,40	0
5	PO4	B	304	5/5	0.87	0.14	55,56,60,62	0
2	EDO	I	306	4/4	0.88	0.15	27,27,29,30	0
5	PO4	D	301	5/5	0.88	0.30	42,43,52,52	0
2	EDO	C	302	4/4	0.89	0.13	31,33,34,37	0
2	EDO	G	301	4/4	0.89	0.16	35,35,36,38	0
2	EDO	I	307	4/4	0.89	0.15	37,41,41,41	0
3	NA	B	305	1/1	0.91	0.18	26,26,26,26	0
2	EDO	J	304	4/4	0.91	0.09	23,23,23,26	0
2	EDO	B	302	4/4	0.91	0.11	34,38,39,41	0
2	EDO	J	301	4/4	0.91	0.09	25,27,27,30	0
2	EDO	J	303	4/4	0.91	0.11	33,33,33,34	0
2	EDO	K	303	4/4	0.91	0.12	39,40,40,42	0
2	EDO	L	301	4/4	0.91	0.09	27,28,28,30	0
2	EDO	F	302	4/4	0.92	0.09	26,29,31,35	0
2	EDO	L	302	4/4	0.92	0.08	23,24,25,26	0
2	EDO	I	303	4/4	0.92	0.08	20,21,22,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	B	303	4/4	0.93	0.07	22,22,22,24	0
2	EDO	K	302	4/4	0.93	0.08	20,22,24,24	0
2	EDO	G	303	4/4	0.94	0.08	21,21,23,23	0
2	EDO	J	302	4/4	0.94	0.07	18,18,19,19	0
2	EDO	I	305	4/4	0.94	0.08	25,28,28,30	0
2	EDO	E	301	4/4	0.95	0.08	21,21,22,22	0
2	EDO	A	303	4/4	0.96	0.06	16,17,17,18	0
3	NA	G	304	1/1	0.96	0.16	23,23,23,23	0
3	NA	A	305	1/1	0.97	0.13	18,18,18,18	0
3	NA	J	307	1/1	0.99	0.06	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.