



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 08:52 AM UTC

PDB ID : 4MFD / pdb_00004mfd
Title : Structure of the carboxyl transferase domain from *Rhizobium etli* pyruvate carboxylase with oxalate
Authors : Lietzan, A.D.; St.Maurice, M.
Deposited on : 2013-08-27
Resolution : 2.55 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

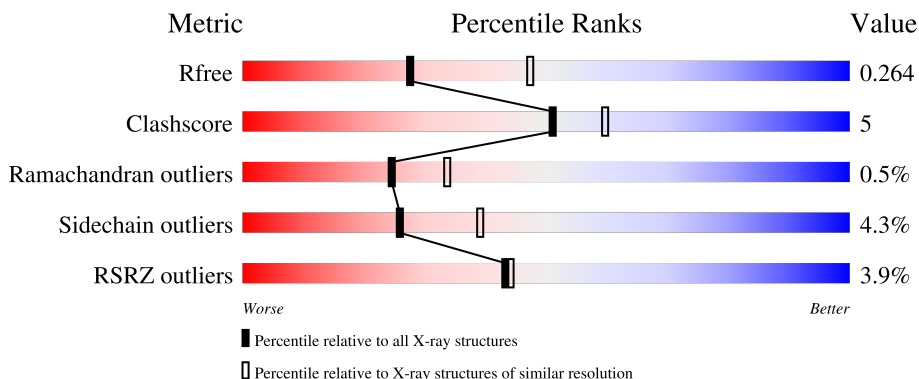
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	632	 80% 14% 6%
1	B	632	 79% 15% 6%
1	C	632	 8% 78% 14% • 6%
1	D	632	 6% 83% 11% • 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
3	OXL	A	1102	-	X	-	-
3	OXL	C	1102	-	X	-	-
3	OXL	D	1102	-	X	-	-
5	CL	C	1104	-	-	X	-

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 18052 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 PYRUVATE CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	597	4557	2897	764	873	23	0	1	0
1	B	597	4522	2878	759	862	23	0	1	0
1	C	596	4368	2767	741	837	23	0	1	0
1	D	597	4367	2752	746	846	23	0	1	0

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	MET	-	expression tag	UNP Q2K340
A	437	GLY	-	expression tag	UNP Q2K340
A	438	SER	-	expression tag	UNP Q2K340
A	439	SER	-	expression tag	UNP Q2K340
A	440	HIS	-	expression tag	UNP Q2K340
A	441	HIS	-	expression tag	UNP Q2K340
A	442	HIS	-	expression tag	UNP Q2K340
A	443	HIS	-	expression tag	UNP Q2K340
A	444	HIS	-	expression tag	UNP Q2K340
A	445	HIS	-	expression tag	UNP Q2K340
A	446	HIS	-	expression tag	UNP Q2K340
A	447	HIS	-	expression tag	UNP Q2K340
A	448	ASP	-	expression tag	UNP Q2K340
A	449	TYR	-	expression tag	UNP Q2K340
A	450	ASP	-	expression tag	UNP Q2K340
A	451	ILE	-	expression tag	UNP Q2K340
A	452	PRO	-	expression tag	UNP Q2K340
A	453	THR	-	expression tag	UNP Q2K340
A	454	SER	-	expression tag	UNP Q2K340
A	455	GLU	-	expression tag	UNP Q2K340
A	456	ASN	-	expression tag	UNP Q2K340

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Chain	Residue	Modelled	Actual	Comment	Reference
A	457	LEU	-	expression tag	UNP Q2K340
A	458	TYR	-	expression tag	UNP Q2K340
A	459	PHE	-	expression tag	UNP Q2K340
A	460	GLN	-	expression tag	UNP Q2K340
A	461	GLY	-	expression tag	UNP Q2K340
A	462	LEU	-	expression tag	UNP Q2K340
A	463	LEU	-	expression tag	UNP Q2K340
A	464	HIS	-	expression tag	UNP Q2K340
B	436	MET	-	expression tag	UNP Q2K340
B	437	GLY	-	expression tag	UNP Q2K340
B	438	SER	-	expression tag	UNP Q2K340
B	439	SER	-	expression tag	UNP Q2K340
B	440	HIS	-	expression tag	UNP Q2K340
B	441	HIS	-	expression tag	UNP Q2K340
B	442	HIS	-	expression tag	UNP Q2K340
B	443	HIS	-	expression tag	UNP Q2K340
B	444	HIS	-	expression tag	UNP Q2K340
B	445	HIS	-	expression tag	UNP Q2K340
B	446	HIS	-	expression tag	UNP Q2K340
B	447	HIS	-	expression tag	UNP Q2K340
B	448	ASP	-	expression tag	UNP Q2K340
B	449	TYR	-	expression tag	UNP Q2K340
B	450	ASP	-	expression tag	UNP Q2K340
B	451	ILE	-	expression tag	UNP Q2K340
B	452	PRO	-	expression tag	UNP Q2K340
B	453	THR	-	expression tag	UNP Q2K340
B	454	SER	-	expression tag	UNP Q2K340
B	455	GLU	-	expression tag	UNP Q2K340
B	456	ASN	-	expression tag	UNP Q2K340
B	457	LEU	-	expression tag	UNP Q2K340
B	458	TYR	-	expression tag	UNP Q2K340
B	459	PHE	-	expression tag	UNP Q2K340
B	460	GLN	-	expression tag	UNP Q2K340
B	461	GLY	-	expression tag	UNP Q2K340
B	462	LEU	-	expression tag	UNP Q2K340
B	463	LEU	-	expression tag	UNP Q2K340
B	464	HIS	-	expression tag	UNP Q2K340
C	436	MET	-	expression tag	UNP Q2K340
C	437	GLY	-	expression tag	UNP Q2K340
C	438	SER	-	expression tag	UNP Q2K340
C	439	SER	-	expression tag	UNP Q2K340
C	440	HIS	-	expression tag	UNP Q2K340

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Chain	Residue	Modelled	Actual	Comment	Reference
C	441	HIS	-	expression tag	UNP Q2K340
C	442	HIS	-	expression tag	UNP Q2K340
C	443	HIS	-	expression tag	UNP Q2K340
C	444	HIS	-	expression tag	UNP Q2K340
C	445	HIS	-	expression tag	UNP Q2K340
C	446	HIS	-	expression tag	UNP Q2K340
C	447	HIS	-	expression tag	UNP Q2K340
C	448	ASP	-	expression tag	UNP Q2K340
C	449	TYR	-	expression tag	UNP Q2K340
C	450	ASP	-	expression tag	UNP Q2K340
C	451	ILE	-	expression tag	UNP Q2K340
C	452	PRO	-	expression tag	UNP Q2K340
C	453	THR	-	expression tag	UNP Q2K340
C	454	SER	-	expression tag	UNP Q2K340
C	455	GLU	-	expression tag	UNP Q2K340
C	456	ASN	-	expression tag	UNP Q2K340
C	457	LEU	-	expression tag	UNP Q2K340
C	458	TYR	-	expression tag	UNP Q2K340
C	459	PHE	-	expression tag	UNP Q2K340
C	460	GLN	-	expression tag	UNP Q2K340
C	461	GLY	-	expression tag	UNP Q2K340
C	462	LEU	-	expression tag	UNP Q2K340
C	463	LEU	-	expression tag	UNP Q2K340
C	464	HIS	-	expression tag	UNP Q2K340
D	436	MET	-	expression tag	UNP Q2K340
D	437	GLY	-	expression tag	UNP Q2K340
D	438	SER	-	expression tag	UNP Q2K340
D	439	SER	-	expression tag	UNP Q2K340
D	440	HIS	-	expression tag	UNP Q2K340
D	441	HIS	-	expression tag	UNP Q2K340
D	442	HIS	-	expression tag	UNP Q2K340
D	443	HIS	-	expression tag	UNP Q2K340
D	444	HIS	-	expression tag	UNP Q2K340
D	445	HIS	-	expression tag	UNP Q2K340
D	446	HIS	-	expression tag	UNP Q2K340
D	447	HIS	-	expression tag	UNP Q2K340
D	448	ASP	-	expression tag	UNP Q2K340
D	449	TYR	-	expression tag	UNP Q2K340
D	450	ASP	-	expression tag	UNP Q2K340
D	451	ILE	-	expression tag	UNP Q2K340
D	452	PRO	-	expression tag	UNP Q2K340
D	453	THR	-	expression tag	UNP Q2K340

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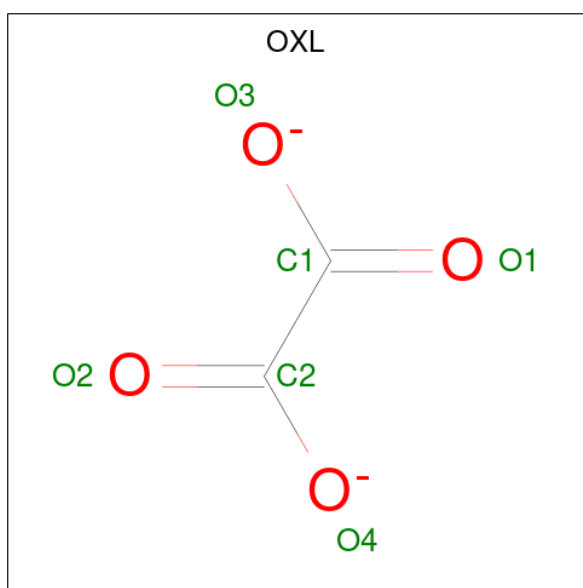
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Chain	Residue	Modelled	Actual	Comment	Reference
D	454	SER	-	expression tag	UNP Q2K340
D	455	GLU	-	expression tag	UNP Q2K340
D	456	ASN	-	expression tag	UNP Q2K340
D	457	LEU	-	expression tag	UNP Q2K340
D	458	TYR	-	expression tag	UNP Q2K340
D	459	PHE	-	expression tag	UNP Q2K340
D	460	GLN	-	expression tag	UNP Q2K340
D	461	GLY	-	expression tag	UNP Q2K340
D	462	LEU	-	expression tag	UNP Q2K340
D	463	LEU	-	expression tag	UNP Q2K340
D	464	HIS	-	expression tag	UNP Q2K340

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is OXALATE ION (CCD ID: OXL) (formula: C₂O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 2 4	0	0
3	B	1	Total C O 6 2 4	0	0
3	C	1	Total C O 6 2 4	0	0
3	D	1	Total C O 6 2 4	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

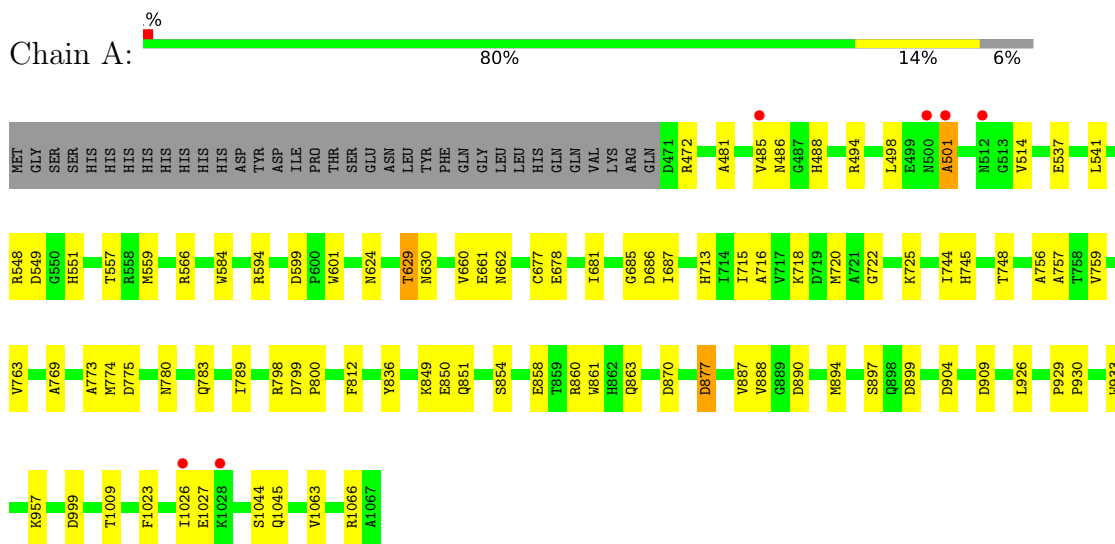
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	87	Total O 87 87	0	0
7	B	46	Total O 46 46	0	0
7	C	34	Total O 34 34	0	0
7	D	23	Total O 23 23	0	0

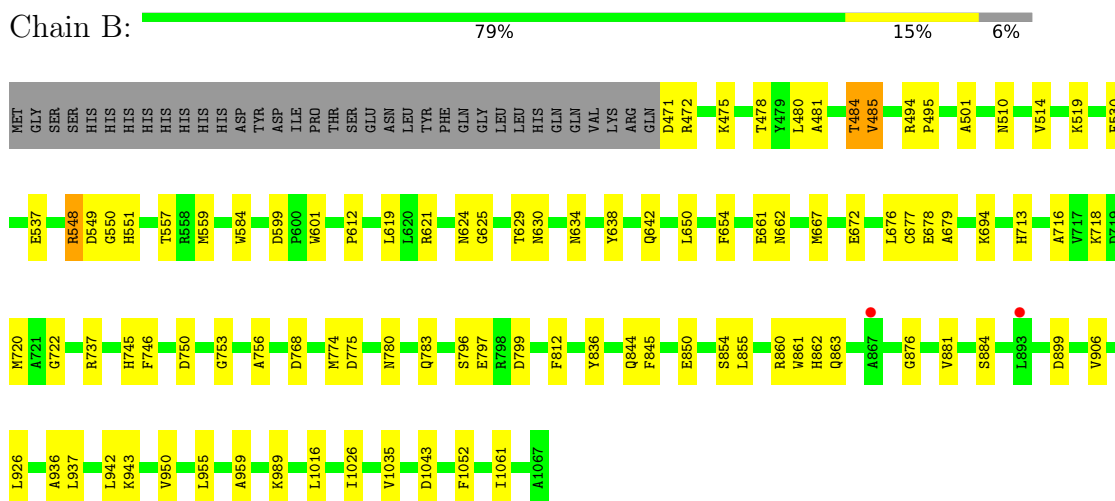
3 Residue-property plots [i](#)

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.

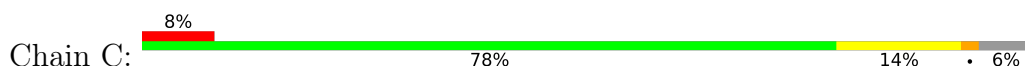
• Molecule 1: PYRUVATE CARBOXYLASE

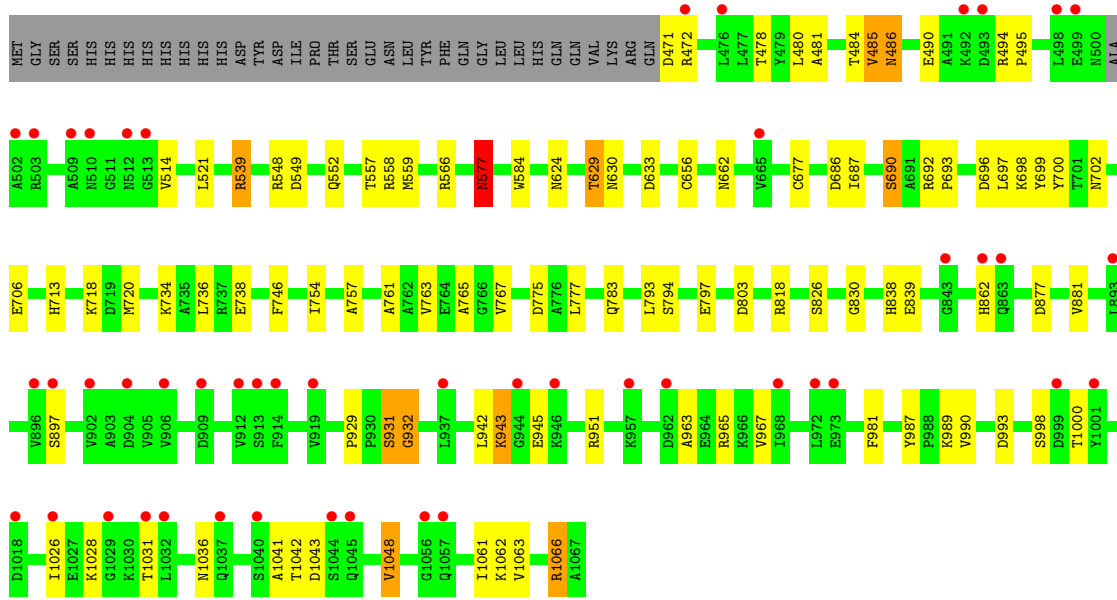


• Molecule 1: PYRUVATE CARBOXYLASE

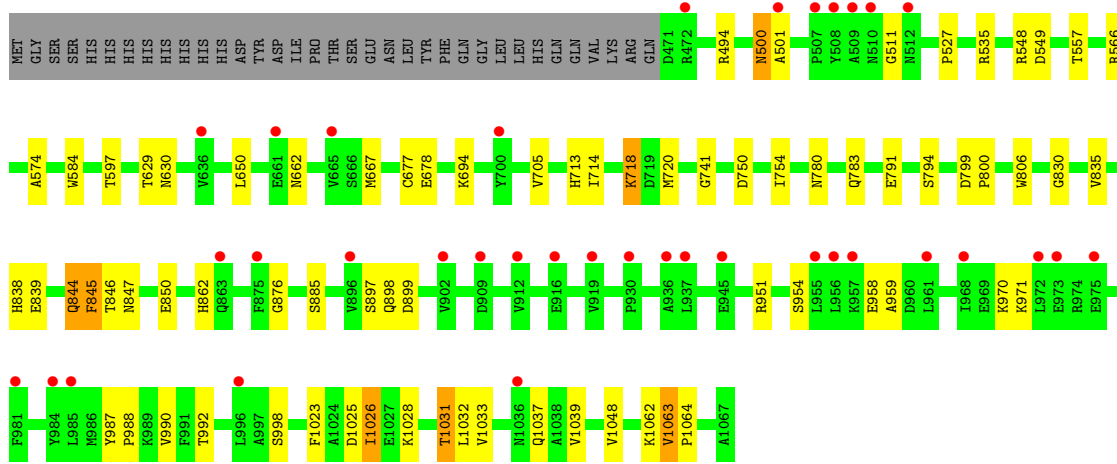
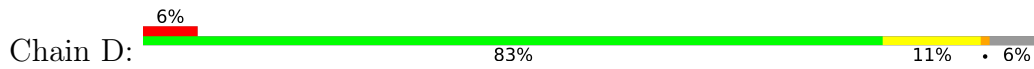


• Molecule 1: PYRUVATE CARBOXYLASE





• Molecule 1: PYRUVATE CARBOXYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.66Å 157.37Å 244.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.26 – 2.55 48.26 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.26-2.55) 99.7 (48.26-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.23 (at 2.54Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.193 , 0.240 (Not available) , 0.264	Depositor DCC
R_{free} test set	5409 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtrriage
Anisotropy	0.028	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18052	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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: KCX, ZN, CL, OXL, GOL, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.21	13/4644 (0.3%)	1.15	8/6314 (0.1%)
1	B	0.94	0/4609	1.03	4/6274 (0.1%)
1	C	1.06	12/4453 (0.3%)	1.10	11/6079 (0.2%)
1	D	0.79	2/4453 (0.0%)	0.95	5/6078 (0.1%)
All	All	1.01	27/18159 (0.1%)	1.06	28/24745 (0.1%)

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1048	VAL	C-O	8.56	1.32	1.24
1	D	799	ASP	C-N	8.52	1.40	1.33
1	A	877	ASP	N-CA	7.90	1.56	1.46
1	A	725	LYS	N-CA	6.85	1.54	1.45
1	C	761	ALA	N-CA	6.84	1.54	1.46

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	932	GLY	N-CA-C	-9.01	101.33	112.68
1	C	577	ASN	N-CA-C	7.82	121.92	112.38
1	D	511	GLY	N-CA-C	7.25	121.73	111.14
1	A	890	ASP	N-CA-C	-6.79	103.89	111.28
1	D	799	ASP	CA-C-N	-6.56	113.39	121.00

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	4557	0	4450	46	0
1	B	4522	0	4382	50	0
1	C	4368	0	4070	58	0
1	D	4367	0	4014	36	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	2	0
5	D	1	0	0	0	0
6	A	6	0	8	0	0
6	B	6	0	8	3	0
7	A	87	0	0	3	0
7	B	46	0	0	1	0
7	C	34	0	0	2	0
7	D	23	0	0	1	0
All	All	18052	0	16932	182	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 5.

The worst 5 of 182 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:C:486:ASN:OD1	1:C:1066:ARG:HG3	1.34	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:931:SER:OG	1:C:932:GLY:O	1.85	0.93
1:B:480:LEU:O	1:B:484:THR:OG1	1.86	0.92
1:D:500:ASN:HD22	1:D:500:ASN:H	1.21	0.88
1:C:485:VAL:HG23	1:C:486:ASN:ND2	1.89	0.88

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	595/632 (94%)	577 (97%)	16 (3%)	2 (0%)	36	45
1	B	595/632 (94%)	570 (96%)	22 (4%)	3 (0%)	24	34
1	C	592/632 (94%)	557 (94%)	32 (5%)	3 (0%)	24	34
1	D	595/632 (94%)	566 (95%)	25 (4%)	4 (1%)	18	25
All	All	2377/2528 (94%)	2270 (96%)	95 (4%)	12 (0%)	24	34

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	501	ALA
1	D	845	PHE
1	D	1028	LYS
1	A	501	ALA
1	B	501	ALA

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	467/519 (90%)	450 (96%)	17 (4%)	31	46
1	B	456/519 (88%)	440 (96%)	16 (4%)	32	48
1	C	417/519 (80%)	394 (94%)	23 (6%)	19	29
1	D	411/519 (79%)	392 (95%)	19 (5%)	24	36
All	All	1751/2076 (84%)	1676 (96%)	75 (4%)	26	39

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	500	ASN
1	D	1031	THR
1	D	566	ARG
1	D	847	ASN
1	B	661	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	847	ASN
1	D	624	ASN
1	C	1037	GLN
1	D	500	ASN
1	D	713	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	KCX	B	718	2,1	10,11,12	0.80	0	6,12,14	2.73	2 (33%)
1	KCX	C	718	2,1	10,11,12	0.78	0	6,12,14	1.87	2 (33%)
1	KCX	A	718	2,1	10,11,12	1.62	1 (10%)	6,12,14	2.55	3 (50%)
1	KCX	D	718	2,1	10,11,12	0.61	0	6,12,14	2.00	2 (33%)

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
1	KCX	B	718	2,1	-	2/9/10/12	-
1	KCX	C	718	2,1	-	4/9/10/12	-
1	KCX	A	718	2,1	-	1/9/10/12	-
1	KCX	D	718	2,1	-	2/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	718	KCX	CX-NZ	3.98	1.42	1.35

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	718	KCX	CE-NZ-CX	4.91	130.31	121.98
1	B	718	KCX	OQ1-CX-NZ	4.56	131.84	124.92
1	B	718	KCX	CE-NZ-CX	4.02	128.80	121.98
1	D	718	KCX	CE-NZ-CX	3.65	128.18	121.98
1	A	718	KCX	CD-CE-NZ	2.89	120.30	112.20

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	718	KCX	O-C-CA-CB
1	B	718	KCX	O-C-CA-CB
1	C	718	KCX	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	C	718	KCX	O-C-CA-CB
1	D	718	KCX	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	718	KCX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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$
3	OXL	C	1102	-	5,5,5	2.46	2 (40%)	6,6,6	2.23	2 (33%)
6	GOL	B	1105	-	5,5,5	0.41	0	5,5,5	1.21	1 (20%)
6	GOL	A	1105	-	5,5,5	0.42	0	5,5,5	0.99	0
3	OXL	B	1102	-	5,5,5	3.09	1 (20%)	6,6,6	0.84	0
3	OXL	A	1102	-	5,5,5	2.43	3 (60%)	6,6,6	1.29	1 (16%)
3	OXL	D	1102	-	5,5,5	2.20	2 (40%)	6,6,6	1.77	1 (16%)

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	OXL	C	1102	-	-	4/4/4/4	-
6	GOL	B	1105	-	-	1/4/4/4	-
6	GOL	A	1105	-	-	0/4/4/4	-
3	OXL	B	1102	-	-	4/4/4/4	-
3	OXL	A	1102	-	-	4/4/4/4	-
3	OXL	D	1102	-	-	4/4/4/4	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1102	OXL	C2-C1	-5.98	1.44	1.54
3	C	1102	OXL	C2-C1	-4.32	1.47	1.54
3	A	1102	OXL	C2-C1	-4.08	1.47	1.54
3	D	1102	OXL	C2-C1	-3.26	1.49	1.54
3	C	1102	OXL	O1-C1	2.68	1.29	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1102	OXL	O4-C2-C1	3.81	120.22	112.83
3	D	1102	OXL	O4-C2-C1	3.15	118.93	112.83
3	C	1102	OXL	O3-C1-C2	2.80	118.25	112.83
3	A	1102	OXL	O3-C1-C2	2.62	117.91	112.83
6	B	1105	GOL	C3-C2-C1	-2.35	103.17	111.80

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	OXL	O1-C1-C2-O4
3	A	1102	OXL	O3-C1-C2-O4
3	B	1102	OXL	O1-C1-C2-O2
3	B	1102	OXL	O1-C1-C2-O4
3	B	1102	OXL	O3-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1105	GOL	3	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	596/632 (94%)	-0.30	6 (1%) 79 80	22, 50, 82, 122	10 (1%)
1	B	596/632 (94%)	-0.01	2 (0%) 90 92	44, 64, 108, 153	8 (1%)
1	C	595/632 (94%)	0.57	48 (8%) 18 17	35, 96, 182, 235	5 (0%)
1	D	596/632 (94%)	0.49	36 (6%) 27 27	51, 92, 142, 166	7 (1%)
All	All	2383/2528 (94%)	0.19	92 (3%) 43 44	22, 70, 150, 235	30 (1%)

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	510	ASN	4.3
1	C	510	ASN	4.3
1	D	968	ILE	4.0
1	C	472	ARG	3.9
1	D	661	GLU	3.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KCX	C	718	12/13	0.93	0.13	65,73,85,90	0
1	KCX	D	718	12/13	0.94	0.11	71,75,79,80	0
1	KCX	A	718	12/13	0.96	0.08	33,37,42,44	0
1	KCX	B	718	12/13	0.97	0.08	49,54,55,59	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OXL	C	1102	6/6	0.87	0.16	63,74,78,80	0
5	CL	C	1104	1/1	0.88	0.11	78,78,78,78	0
3	OXL	D	1102	6/6	0.89	0.18	66,72,74,76	0
5	CL	D	1104	1/1	0.89	0.10	104,104,104,104	0
5	CL	B	1104	1/1	0.92	0.13	67,67,67,67	0
3	OXL	B	1102	6/6	0.92	0.20	47,54,57,63	0
4	MG	C	1103	1/1	0.92	0.15	44,44,44,44	0
4	MG	A	1103	1/1	0.94	0.08	49,49,49,49	0
4	MG	B	1103	1/1	0.94	0.07	51,51,51,51	0
4	MG	D	1103	1/1	0.95	0.10	66,66,66,66	0
6	GOL	B	1105	6/6	0.95	0.12	55,59,66,73	0
6	GOL	A	1105	6/6	0.96	0.09	49,53,54,57	0
5	CL	A	1104	1/1	0.97	0.06	56,56,56,56	0
3	OXL	A	1102	6/6	0.97	0.09	40,48,53,55	0
2	ZN	B	1101	1/1	0.98	0.03	42,42,42,42	1
2	ZN	C	1101	1/1	0.98	0.04	58,58,58,58	1
2	ZN	D	1101	1/1	0.99	0.06	56,56,56,56	1
2	ZN	A	1101	1/1	1.00	0.03	37,37,37,37	1

6.5 Other polymers [i](#)

There are no such residues in this entry.