Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:29 PM GMT

PDB ID	:	4LOC
Title	:	Structure of the carboxyl transferase domain from Rhizobium etli pyruvate carboxylase with oxamate and biotin
Authors	:	Lietzan, A.D.; St. Maurice, M.
Deposited on	:	2013-07-12
Resolution	:	2.26 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

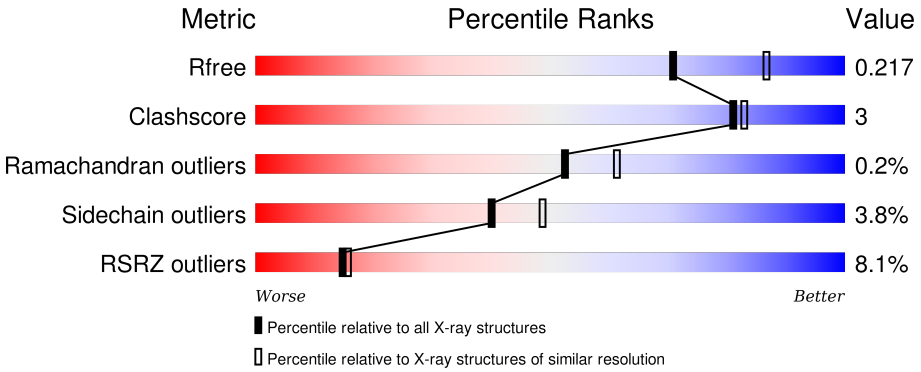
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.26 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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	2% 84% 10% • 6%
1	B	632	13% 83% 10% • 6%
1	C	632	11% 86% 7% • 6%
1	D	632	4% 84% 10% • 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	MG	B	1103	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18570 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
1	A	595	Total	C	N	O	S	0	3	0
			4572	2908	771	870	23			
1	B	593	Total	C	N	O	S	0	1	0
			4389	2784	743	839	23			
1	C	595	Total	C	N	O	S	0	1	0
			4456	2841	746	846	23			
1	D	596	Total	C	N	O	S	0	1	0
			4507	2868	761	855	23			

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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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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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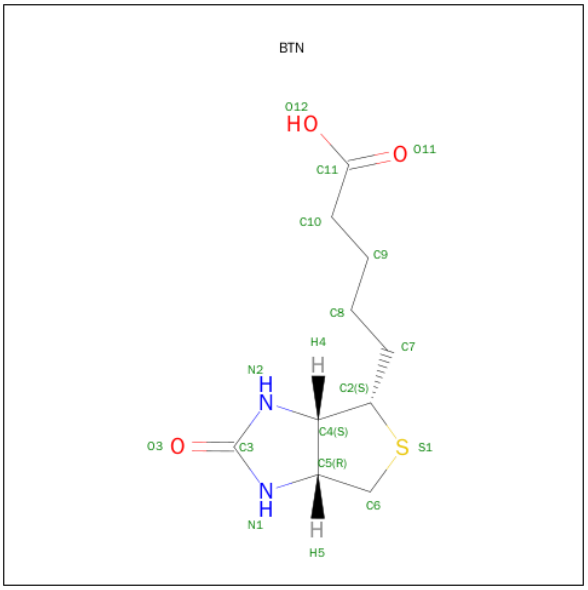
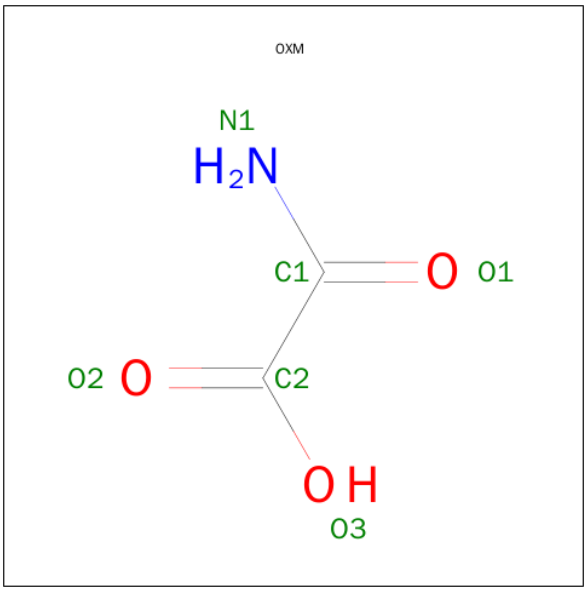
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0

- Molecule 5 is BIOTIN (three-letter code: BTN) (formula: $C_{10}H_{16}N_2O_3S$).



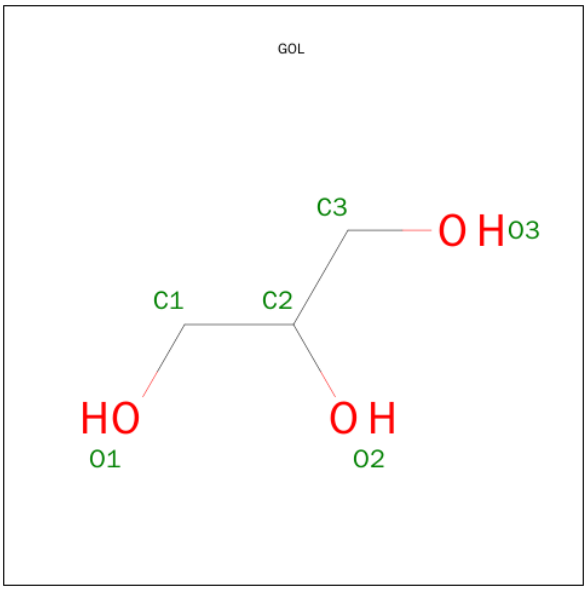
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O S 16 10 2 3 1	0	0
5	B	1	Total C N O S 16 10 2 3 1	0	0
5	C	1	Total C N O S 16 10 2 3 1	0	0
5	D	1	Total C N O S 16 10 2 3 1	0	0

- Molecule 6 is OXAMIC ACID (three-letter code: OXM) (formula: $C_2H_3NO_3$).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is water.

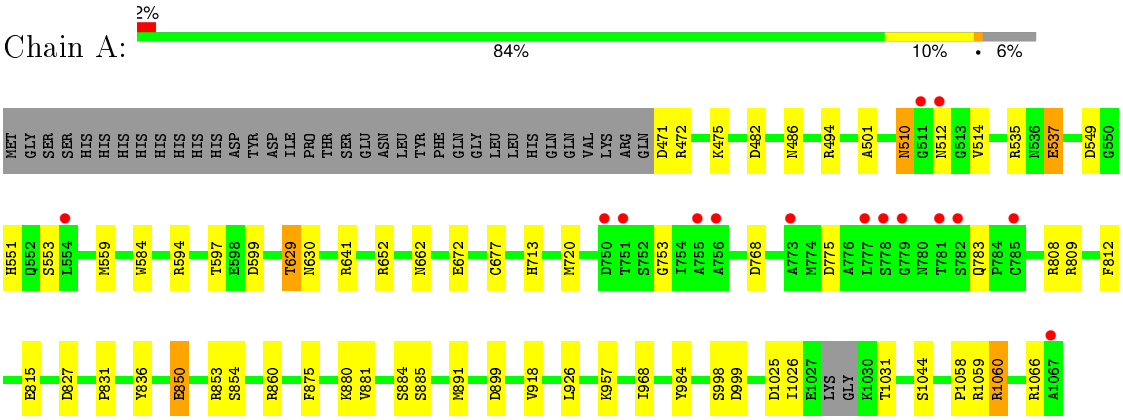
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	213	Total O 213 213	0	0
8	B	97	Total O 97 97	0	0
8	C	79	Total O 79 79	0	0
8	D	146	Total O 146 146	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

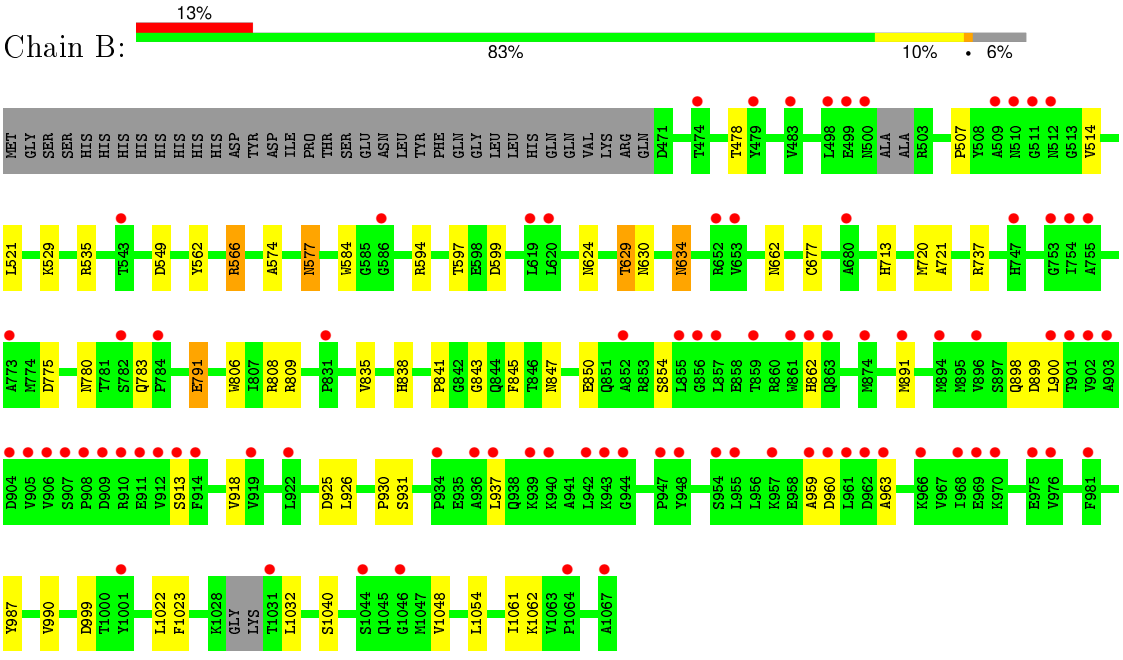
- Molecule 1: Pyruvate carboxylase

Chain A:



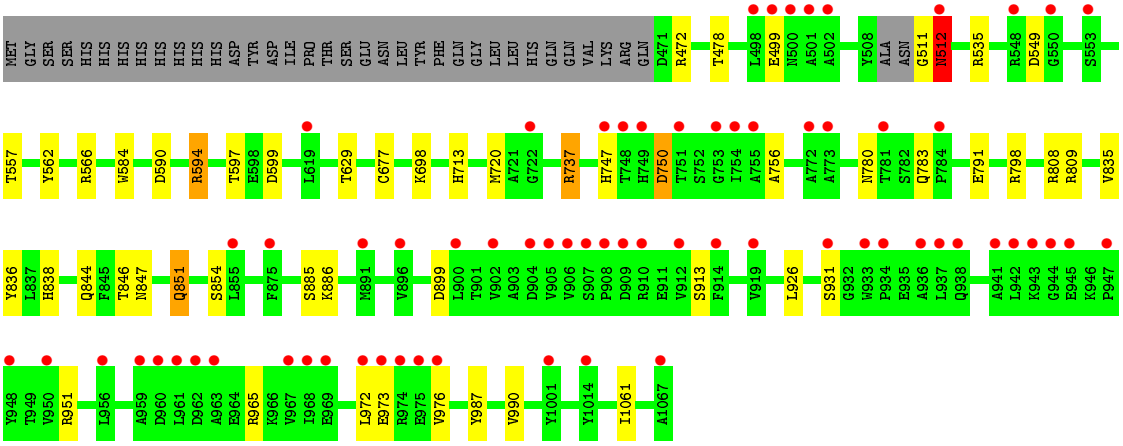
- Molecule 1: Pyruvate carboxylase

Chain B:



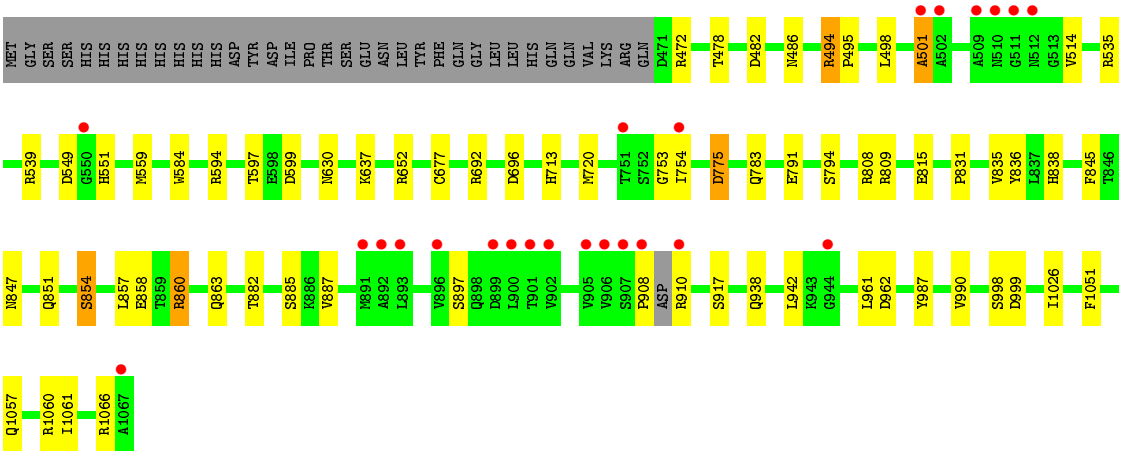
- Molecule 1: Pyruvate carboxylase

Chain C:



- Molecule 1: Pyruvate carboxylase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.87Å 157.12Å 244.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.75 – 2.26 43.71 – 2.26	Depositor EDS
% Data completeness (in resolution range)	98.0 (43.75-2.26) 98.1 (43.71-2.26)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.74 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.176 , 0.216 0.184 , 0.217	Depositor DCC
R_{free} test set	7592 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	39.4	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 148168 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18570	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, CL, ZN, OXM, BTN, KCX

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	1.01	2/4665 (0.0%)	1.03	18/6338 (0.3%)
1	B	0.80	2/4474 (0.0%)	0.89	9/6103 (0.1%)
1	C	0.74	0/4542	0.86	9/6189 (0.1%)
1	D	0.89	3/4593 (0.1%)	0.93	11/6251 (0.2%)
All	All	0.87	7/18274 (0.0%)	0.93	47/24881 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1040	SER	CB-OG	9.52	1.54	1.42
1	D	815	GLU	CD-OE2	-5.78	1.19	1.25
1	B	791	GLU	CD-OE1	-5.76	1.19	1.25
1	A	815	GLU	CD-OE1	-5.72	1.19	1.25
1	D	815	GLU	CD-OE1	-5.44	1.19	1.25
1	A	998	SER	CB-OG	-5.27	1.35	1.42
1	D	998	SER	CB-OG	-5.00	1.35	1.42

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	594[A]	ARG	NE-CZ-NH1	-10.88	114.86	120.30
1	A	594[B]	ARG	NE-CZ-NH1	-10.88	114.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	535	ARG	NE-CZ-NH2	-9.95	115.32	120.30
1	D	594	ARG	NE-CZ-NH2	9.41	125.00	120.30
1	D	594	ARG	NE-CZ-NH1	-9.40	115.60	120.30
1	A	535	ARG	NE-CZ-NH2	-9.01	115.80	120.30
1	A	768	ASP	CB-CG-OD2	-8.38	110.76	118.30
1	A	594[A]	ARG	NE-CZ-NH2	8.09	124.34	120.30
1	A	594[B]	ARG	NE-CZ-NH2	8.09	124.34	120.30
1	A	535	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	B	809	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	A	641	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	C	737	ARG	NE-CZ-NH1	-7.20	116.70	120.30
1	A	827	ASP	CB-CG-OD1	7.09	124.68	118.30
1	B	535	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	A	599	ASP	CB-CG-OD1	6.83	124.45	118.30
1	C	599	ASP	CB-CG-OD1	6.74	124.37	118.30
1	C	535	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	B	737	ARG	NE-CZ-NH1	-6.65	116.98	120.30
1	D	775	ASP	CB-CG-OD1	6.62	124.25	118.30
1	A	652	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	B	594	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	B	594	ARG	NE-CZ-NH1	-6.29	117.16	120.30
1	B	535	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	C	594	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	A	482	ASP	CB-CG-OD1	5.94	123.65	118.30
1	D	815	GLU	OE1-CD-OE2	-5.65	116.52	123.30
1	C	809	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	B	599	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	775	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	809	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	C	737	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	D	599	ASP	CB-CG-OD1	5.39	123.15	118.30
1	C	798	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	D	652	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	750	ASP	CB-CG-OD1	5.24	123.02	118.30
1	D	539	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	537	GLU	CG-CD-OE2	-5.20	107.89	118.30
1	C	951	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	B	925	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	B	775	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	482	ASP	CB-CG-OD1	5.09	122.88	118.30
1	D	696	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	860	ARG	NE-CZ-NH1	-5.06	117.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1060	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	D	809	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	652	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	512	ASN	Peptide

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	4572	0	4488	33	0
1	B	4389	0	4132	31	0
1	C	4456	0	4273	24	0
1	D	4507	0	4379	35	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	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	16	0	15	0	0
5	B	16	0	15	1	0
5	C	16	0	15	0	0
5	D	16	0	15	1	0
6	A	6	0	2	0	0
6	B	6	0	2	0	0
6	C	6	0	2	0	0
6	D	6	0	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	6	0	8	1	0
7	C	6	0	8	3	0
8	A	213	0	0	10	0
8	B	97	0	0	3	0
8	C	79	0	0	1	0
8	D	146	0	0	7	0
All	All	18570	0	17356	118	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 (118) 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:A:885:SER:N	8:A:1355:HOH:O	1.76	1.18
1:D:630:ASN:HB2	8:D:1268:HOH:O	1.64	0.97
1:A:677:CYS:H	1:A:713:HIS:HD2	1.19	0.90
1:C:780:ASN:H	7:C:1103:GOL:H12	1.36	0.90
1:C:677:CYS:H	1:C:713:HIS:HD2	1.22	0.88
1:D:494:ARG:HD2	8:D:1279:HOH:O	1.79	0.80
1:A:881:VAL:N	8:A:1355:HOH:O	2.14	0.80
1:B:630:ASN:HD21	1:B:662:ASN:HD21	1.34	0.75
1:B:549:ASP:HB3	1:B:783:GLN:HE22	1.51	0.75
1:C:549:ASP:HB3	1:C:783:GLN:HE22	1.52	0.75
1:D:677:CYS:H	1:D:713:HIS:HD2	1.36	0.73
1:D:808:ARG:HD3	8:D:1227:HOH:O	1.89	0.72
1:A:630:ASN:HB2	8:A:1382:HOH:O	1.90	0.72
1:A:630:ASN:HD21	1:A:662:ASN:HD21	1.37	0.70
1:B:577:ASN:ND2	1:B:577:ASN:H	1.89	0.70
1:A:553:SER:OG	8:A:1362:HOH:O	2.07	0.70
1:C:677:CYS:H	1:C:713:HIS:CD2	2.09	0.67
1:A:891[B]:MET:HE1	1:A:918:VAL:HG11	1.76	0.67
1:D:549:ASP:HB3	1:D:783:GLN:HE22	1.56	0.67
1:B:677:CYS:H	1:B:713:HIS:HD2	1.42	0.65
1:C:808:ARG:HD3	8:D:1288:HOH:O	1.98	0.64
1:B:634:ASN:HD21	1:B:959:ALA:H	1.46	0.63
1:A:472:ARG:CB	1:A:1026:ILE:HD11	2.28	0.63
1:C:590:ASP:OD2	1:C:594:ARG:NH2	2.32	0.63
1:A:472:ARG:CB	1:A:1026:ILE:CD1	2.79	0.60
1:C:750:ASP:OD2	7:C:1103:GOL:O1	2.18	0.59
1:A:677:CYS:H	1:A:713:HIS:CD2	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:ASN:HD22	1:B:577:ASN:H	1.50	0.58
1:A:812[B]:PHE:CE1	1:B:862:HIS:CD2	2.91	0.58
1:D:851:GLN:O	1:D:854:SER:HB2	2.04	0.57
1:B:808:ARG:HD3	8:B:1246:HOH:O	2.04	0.57
1:D:677:CYS:H	1:D:713:HIS:CD2	2.22	0.56
1:D:472:ARG:HB3	1:D:1026:ILE:HD11	1.86	0.56
1:C:511:GLY:O	1:C:512:ASN:CB	2.53	0.56
1:A:510:ASN:HD22	1:A:512:ASN:H	1.53	0.56
1:A:812[B]:PHE:HE1	1:B:862:HIS:CD2	2.24	0.56
1:A:880:LYS:HA	8:A:1355:HOH:O	2.06	0.55
1:D:486:ASN:ND2	1:D:1066:ARG:H	2.05	0.55
1:C:549:ASP:HB3	1:C:783:GLN:NE2	2.18	0.54
1:B:780:ASN:H	7:B:1101:GOL:H32	1.72	0.54
1:C:987:TYR:HB3	1:C:990:VAL:HB	1.90	0.54
1:A:629:THR:HG22	8:A:1215:HOH:O	2.07	0.53
1:D:637:LYS:HE2	8:D:1263:HOH:O	2.08	0.53
1:A:1025:ASP:OD2	1:A:1031:THR:OG1	2.17	0.53
1:C:590:ASP:CG	1:C:594:ARG:HH21	2.13	0.52
1:D:486:ASN:HD21	1:D:1066:ARG:H	1.56	0.52
1:A:486:ASN:ND2	1:A:1066:ARG:H	2.08	0.52
1:A:486:ASN:HD21	1:A:1066:ARG:H	1.57	0.52
1:C:549:ASP:OD2	1:C:747:HIS:CE1	2.63	0.52
1:B:562:TYR:CE2	1:B:566:ARG:HD2	2.45	0.51
1:D:860:ARG:O	1:D:863:GLN:N	2.44	0.51
1:D:987:TYR:HB3	1:D:990:VAL:HB	1.92	0.51
1:D:908:PRO:O	1:D:910:ARG:N	2.43	0.51
7:C:1103:GOL:H11	8:C:1264:HOH:O	2.10	0.50
1:C:851:GLN:O	1:C:854:SER:HB2	2.11	0.50
1:A:836:TYR:CD2	1:B:791:GLU:HG2	2.47	0.50
1:B:624:ASN:HD22	1:B:629:THR:C	2.15	0.49
1:C:844:GLN:HG2	1:C:844:GLN:O	2.13	0.49
1:A:884:SER:C	8:A:1355:HOH:O	2.32	0.48
1:B:529:LYS:HE3	8:B:1236:HOH:O	2.12	0.48
1:B:898:GLN:O	1:B:900:LEU:HG	2.14	0.48
1:B:835:VAL:HA	1:B:838:HIS:CE1	2.49	0.48
1:A:885:SER:CA	8:A:1355:HOH:O	2.47	0.48
1:C:590:ASP:OD1	1:C:594:ARG:NH2	2.46	0.48
1:B:574:ALA:HB1	1:B:806:TRP:CG	2.49	0.48
1:D:498:LEU:O	1:D:501:ALA:HB2	2.14	0.48
1:D:692:ARG:HB2	8:D:1245:HOH:O	2.12	0.48
1:C:836:TYR:CD2	1:D:791:GLU:HG2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:968:ILE:HD13	1:A:984:TYR:CD1	2.49	0.47
1:B:891[B]:MET:HE1	1:B:918:VAL:HG11	1.97	0.47
1:D:597:THR:OG1	5:D:1104:BTN:H102	2.14	0.47
1:D:938:GLN:HG2	1:D:942:LEU:HD12	1.97	0.47
1:A:551:HIS:ND1	1:A:559:MET:HB3	2.30	0.47
1:C:478:THR:HA	1:C:1061:ILE:HG21	1.96	0.47
1:D:478:THR:HA	1:D:1061:ILE:HG21	1.96	0.47
1:A:549:ASP:HB3	1:A:783:GLN:HE22	1.79	0.47
1:A:808:ARG:HD3	8:A:1351:HOH:O	2.15	0.47
1:C:756:ALA:CB	1:D:754:ILE:HG22	2.45	0.47
1:C:562:TYR:CE2	1:C:566:ARG:HD2	2.50	0.46
1:D:692:ARG:CB	8:D:1245:HOH:O	2.63	0.46
1:B:987:TYR:HB3	1:B:990:VAL:HB	1.97	0.46
1:C:791:GLU:HG2	1:D:836:TYR:CD2	2.52	0.45
1:D:845:PHE:CD2	1:D:845:PHE:C	2.89	0.45
1:D:1051:PHE:CE1	1:D:1060:ARG:HD2	2.51	0.45
1:D:753:GLY:HA3	1:D:831:PRO:HB3	1.99	0.45
1:B:597:THR:OG1	5:B:1104:BTN:O12	2.29	0.45
1:A:713:HIS:HE1	8:A:1368:HOH:O	1.99	0.44
1:A:471:ASP:O	1:A:475:LYS:HG3	2.16	0.44
1:A:850:GLU:OE2	1:A:853:ARG:NE	2.50	0.44
1:B:960:ASP:HB3	1:B:963:ALA:HB3	1.99	0.44
1:C:972:LEU:O	1:C:973:GLU:C	2.55	0.44
1:B:597:THR:HG22	1:B:597:THR:O	2.17	0.44
1:D:835:VAL:HA	1:D:838:HIS:CE1	2.52	0.44
1:A:510:ASN:HD21	1:A:512:ASN:HB2	1.83	0.44
1:B:721:ALA:HA	1:B:841:PRO:HA	2.00	0.44
1:A:510:ASN:ND2	1:A:512:ASN:H	2.13	0.44
1:D:1051:PHE:CD2	1:D:1051:PHE:N	2.86	0.44
1:B:549:ASP:HB3	1:B:783:GLN:NE2	2.28	0.43
1:D:961:LEU:O	1:D:962:ASP:C	2.56	0.43
1:D:551:HIS:ND1	1:D:559:MET:HB3	2.34	0.43
1:C:835:VAL:HA	1:C:838:HIS:CE1	2.54	0.43
1:D:494:ARG:HB3	1:D:495:PRO:CD	2.49	0.42
1:B:713:HIS:HE1	8:B:1290:HOH:O	2.01	0.42
1:C:965:ARG:NH2	1:C:976:VAL:O	2.46	0.42
1:C:590:ASP:CG	1:C:594:ARG:NH2	2.73	0.42
1:B:1023:PHE:HA	1:B:1032:LEU:O	2.20	0.42
1:A:1058:PRO:O	1:A:1059:ARG:HD2	2.20	0.42
1:B:845:PHE:C	1:B:845:PHE:CD2	2.93	0.41
1:D:551:HIS:CE1	1:D:559:MET:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1032:LEU:HD22	1:B:1054:LEU:HD11	2.02	0.41
1:D:857:LEU:O	1:D:858:GLU:C	2.59	0.41
1:A:753:GLY:HA3	1:A:831:PRO:HB3	2.03	0.41
1:B:1048:VAL:O	1:B:1062:LYS:HA	2.21	0.41
1:D:677:CYS:N	1:D:713:HIS:HD2	2.10	0.40
1:B:478:THR:HA	1:B:1061:ILE:HG21	2.02	0.40
1:D:887:VAL:HG22	1:D:917:SER:HB2	2.02	0.40
1:B:577:ASN:N	1:B:577:ASN:ND2	2.60	0.40
1:A:875:PHE:CZ	1:A:891[B]:MET:HE2	2.56	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	593/632 (94%)	577 (97%)	15 (2%)	1 (0%)	52	61
1	B	587/632 (93%)	567 (97%)	18 (3%)	2 (0%)	46	52
1	C	591/632 (94%)	563 (95%)	27 (5%)	1 (0%)	52	61
1	D	592/632 (94%)	573 (97%)	18 (3%)	1 (0%)	52	61
All	All	2363/2528 (94%)	2280 (96%)	78 (3%)	5 (0%)	52	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	ALA
1	C	512	ASN
1	D	501	ALA
1	B	930	PRO
1	B	843	GLY

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	472/519 (91%)	455 (96%)	17 (4%)	42	51
1	B	427/519 (82%)	408 (96%)	19 (4%)	35	40
1	C	439/519 (85%)	421 (96%)	18 (4%)	37	44
1	D	455/519 (88%)	441 (97%)	14 (3%)	47	58
All	All	1793/2076 (86%)	1725 (96%)	68 (4%)	40	49

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	494	ARG
1	A	510	ASN
1	A	514	VAL
1	A	537	GLU
1	A	584	TRP
1	A	597	THR
1	A	629	THR
1	A	672	GLU
1	A	720	MET
1	A	850	GLU
1	A	854	SER
1	A	899	ASP
1	A	926	LEU
1	A	957	LYS
1	A	999	ASP
1	A	1044	SER
1	A	1060	ARG
1	B	507	PRO
1	B	514	VAL
1	B	521	LEU
1	B	566	ARG
1	B	577	ASN
1	B	584	TRP
1	B	629	THR

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Mol	Chain	Res	Type
1	B	634	ASN
1	B	720	MET
1	B	847	ASN
1	B	850	GLU
1	B	854	SER
1	B	899	ASP
1	B	913	SER
1	B	926	LEU
1	B	931	SER
1	B	937	LEU
1	B	999	ASP
1	B	1022	LEU
1	C	472	ARG
1	C	499	GLU
1	C	557	THR
1	C	584	TRP
1	C	597	THR
1	C	629	THR
1	C	698	LYS
1	C	720	MET
1	C	737	ARG
1	C	846	THR
1	C	847	ASN
1	C	851	GLN
1	C	885	SER
1	C	886	LYS
1	C	899	ASP
1	C	913	SER
1	C	926	LEU
1	C	931	SER
1	D	494	ARG
1	D	514	VAL
1	D	584	TRP
1	D	720	MET
1	D	775	ASP
1	D	794	SER
1	D	847	ASN
1	D	854	SER
1	D	860	ARG
1	D	882	THR
1	D	885	SER
1	D	897	SER

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Mol	Chain	Res	Type
1	D	999	ASP
1	D	1057	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	486	ASN
1	A	510	ASN
1	A	577	ASN
1	A	624	ASN
1	A	630	ASN
1	A	713	HIS
1	A	783	GLN
1	A	1055	ASN
1	B	486	ASN
1	B	577	ASN
1	B	624	ASN
1	B	630	ASN
1	B	713	HIS
1	B	783	GLN
1	B	862	HIS
1	B	1057	GLN
1	C	486	ASN
1	C	577	ASN
1	C	624	ASN
1	C	642	GLN
1	C	713	HIS
1	C	783	GLN
1	C	851	GLN
1	D	486	ASN
1	D	510	ASN
1	D	577	ASN
1	D	713	HIS
1	D	783	GLN
1	D	820	GLN

5.3.3 RNA

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	A	718	1,2	7,11,12	1.23	0	7,12,14	2.60	2 (28%)
1	KCX	B	718	1,2	7,11,12	0.68	0	7,12,14	3.18	2 (28%)
1	KCX	C	718	1,2	7,11,12	0.94	0	7,12,14	2.71	2 (28%)
1	KCX	D	718	1,2	7,11,12	0.80	0	7,12,14	1.65	2 (28%)

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	A	718	1,2	-	0/6/10/12	0/0/0/0
1	KCX	B	718	1,2	-	0/6/10/12	0/0/0/0
1	KCX	C	718	1,2	-	0/6/10/12	0/0/0/0
1	KCX	D	718	1,2	-	0/6/10/12	0/0/0/0

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	718	KCX	CD-CE-NZ	2.74	118.88	111.46
1	D	718	KCX	CE-NZ-CX	2.75	126.61	123.49
1	B	718	KCX	CD-CE-NZ	3.24	120.22	111.46
1	A	718	KCX	CD-CE-NZ	3.28	120.33	111.46
1	C	718	KCX	CD-CE-NZ	3.40	120.66	111.46
1	A	718	KCX	CE-NZ-CX	5.73	129.98	123.49
1	C	718	KCX	CE-NZ-CX	6.09	130.39	123.49
1	B	718	KCX	CE-NZ-CX	7.53	132.02	123.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 11 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
5	BTN	A	1104	-	12,17,17	1.30	1 (8%)	13,23,23	1.94	4 (30%)
6	OXM	A	1105	-	2,5,5	1.86	1 (50%)	2,6,6	1.06	0
7	GOL	B	1101	-	5,5,5	0.51	0	5,5,5	1.88	2 (40%)
5	BTN	B	1104	-	12,17,17	0.91	0	13,23,23	2.42	5 (38%)
6	OXM	B	1105	-	2,5,5	0.81	0	2,6,6	1.81	1 (50%)
7	GOL	C	1103	-	5,5,5	0.70	0	5,5,5	1.52	1 (20%)
5	BTN	C	1105	-	12,17,17	1.03	1 (8%)	13,23,23	0.83	1 (7%)
6	OXM	C	1106	-	2,5,5	0.62	0	2,6,6	0.82	0
5	BTN	D	1104	-	12,17,17	1.07	0	13,23,23	1.49	3 (23%)
6	OXM	D	1105	-	2,5,5	0.30	0	2,6,6	2.01	1 (50%)

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
5	BTN	A	1104	-	-	0/5/28/28	0/2/2/2
6	OXM	A	1105	-	-	0/0/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	1101	-	-	0/4/4/4	0/0/0/0
5	BTN	B	1104	-	-	0/5/28/28	0/2/2/2
6	OXM	B	1105	-	-	0/0/4/4	0/0/0/0
7	GOL	C	1103	-	-	0/4/4/4	0/0/0/0
5	BTN	C	1105	-	-	0/5/28/28	0/2/2/2
6	OXM	C	1106	-	-	0/0/4/4	0/0/0/0
5	BTN	D	1104	-	-	0/5/28/28	0/2/2/2
6	OXM	D	1105	-	-	0/0/4/4	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1105	OXM	O1-C1	-2.56	1.18	1.24
5	C	1105	BTN	C5-C4	-2.08	1.52	1.56
5	A	1104	BTN	C7-C2	2.50	1.58	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1104	BTN	C5-N1-C3	-3.88	109.59	112.49
5	B	1104	BTN	C5-C4-N2	-3.53	98.96	102.52
5	A	1104	BTN	C5-C4-N2	-3.44	99.05	102.52
5	A	1104	BTN	C5-N1-C3	-3.33	109.99	112.49
5	B	1104	BTN	C7-C2-S1	-3.26	104.59	112.33
7	B	1101	GOL	C3-C2-C1	-2.98	99.45	111.12
6	D	1105	OXM	C2-C1-N1	-2.47	111.67	115.90
7	C	1103	GOL	O3-C3-C2	-2.17	99.66	110.18
5	D	1104	BTN	C4-N2-C3	2.02	114.59	112.66
6	B	1105	OXM	C2-C1-N1	2.06	119.42	115.90
5	B	1104	BTN	C6-S1-C2	2.06	94.87	90.33
5	D	1104	BTN	C8-C7-C2	2.10	118.59	113.70
5	C	1105	BTN	C6-S1-C2	2.11	94.97	90.33
5	D	1104	BTN	C9-C8-C7	2.31	121.86	113.66
5	A	1104	BTN	C4-C5-N1	2.71	105.43	102.37
7	B	1101	GOL	O2-C2-C1	2.77	121.33	108.65
5	A	1104	BTN	C4-N2-C3	3.20	115.72	112.66
5	B	1104	BTN	C8-C7-C2	5.23	125.86	113.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1101	GOL	1	0
5	B	1104	BTN	1	0
7	C	1103	GOL	3	0
5	D	1104	BTN	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	594/632 (93%)	-0.16	15 (2%) 61 65	23, 34, 57, 82	12 (2%)
1	B	592/632 (93%)	0.61	85 (14%) 3 4	26, 61, 122, 160	7 (1%)
1	C	594/632 (93%)	0.45	69 (11%) 6 6	33, 59, 96, 129	6 (1%)
1	D	595/632 (94%)	0.07	24 (4%) 42 45	29, 44, 80, 106	3 (0%)
All	All	2375/2528 (93%)	0.24	193 (8%) 15 16	23, 47, 101, 160	28 (1%)

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	512	ASN	6.7
1	B	908	PRO	6.1
1	C	944	GLY	5.9
1	C	906	VAL	5.9
1	C	959	ALA	5.8
1	B	896	VAL	5.5
1	D	902	VAL	5.4
1	C	907	SER	5.4
1	B	500	ASN	5.1
1	C	502	ALA	5.0
1	C	909	ASP	5.0
1	C	501	ALA	4.9
1	C	499	GLU	4.9
1	C	908	PRO	4.8
1	C	937	LEU	4.8
1	B	912	VAL	4.8
1	C	910	ARG	4.8
1	B	902	VAL	4.8
1	B	937	LEU	4.6
1	C	960	ASP	4.6
1	B	509	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	963	ALA	4.4
1	C	947	PRO	4.4
1	C	976	VAL	4.3
1	C	943	LYS	4.3
1	B	511	GLY	4.3
1	B	914	PHE	4.3
1	B	510	ASN	4.2
1	B	909	ASP	4.1
1	C	498	LEU	4.1
1	C	972	LEU	4.1
1	D	501	ALA	4.0
1	B	947	PRO	4.0
1	C	941	ALA	4.0
1	B	903	ALA	4.0
1	B	944	GLY	4.0
1	B	976	VAL	3.9
1	D	907	SER	3.9
1	C	919	VAL	3.9
1	B	863	GLN	3.9
1	C	942	LEU	3.9
1	B	906	VAL	3.8
1	D	502	ALA	3.8
1	B	959	ALA	3.7
1	B	934	PRO	3.7
1	B	859	THR	3.7
1	D	1067	ALA	3.6
1	B	942	LEU	3.6
1	C	905	VAL	3.6
1	D	906	VAL	3.6
1	B	900	LEU	3.6
1	C	914	PHE	3.6
1	B	619	LEU	3.5
1	D	509	ALA	3.5
1	B	474	THR	3.5
1	B	905	VAL	3.5
1	B	907	SER	3.5
1	B	1001	TYR	3.5
1	B	891[A]	MET	3.4
1	C	967	VAL	3.4
1	D	511	GLY	3.4
1	C	500	ASN	3.4
1	B	962	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	936	ALA	3.4
1	C	968	ILE	3.4
1	B	966	LYS	3.4
1	C	975	GLU	3.3
1	C	961	LEU	3.3
1	B	955	LEU	3.3
1	B	913	SER	3.3
1	B	901	THR	3.2
1	B	910	ARG	3.2
1	D	908	PRO	3.2
1	B	483	VAL	3.2
1	C	896	VAL	3.1
1	D	512	ASN	3.1
1	D	900	LEU	3.1
1	C	748	THR	3.1
1	B	970	LYS	3.1
1	C	945	GLU	3.0
1	B	862	HIS	3.0
1	B	969	GLU	3.0
1	B	975	GLU	3.0
1	C	933	TRP	3.0
1	C	754	ILE	3.0
1	D	944	GLY	2.9
1	C	973	GLU	2.9
1	C	912	VAL	2.9
1	B	857	LEU	2.9
1	C	900	LEU	2.9
1	C	781	THR	2.9
1	D	905	VAL	2.8
1	C	934	PRO	2.8
1	C	931	SER	2.8
1	C	962	ASP	2.7
1	B	855	LEU	2.7
1	C	963	ALA	2.7
1	A	511	GLY	2.7
1	B	948	TYR	2.7
1	C	512	ASN	2.7
1	B	968	ILE	2.7
1	B	499	GLU	2.7
1	C	904	ASP	2.7
1	B	922	LEU	2.6
1	A	779	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	753	GLY	2.6
1	C	948	TYR	2.6
1	D	896	VAL	2.6
1	C	875	PHE	2.6
1	C	1001	TYR	2.6
1	C	936	ALA	2.6
1	A	1067	ALA	2.6
1	B	894	MET	2.6
1	D	891[A]	MET	2.6
1	C	619	LEU	2.6
1	B	754	ILE	2.5
1	C	969	GLU	2.5
1	C	938	GLN	2.5
1	C	855	LEU	2.5
1	B	1046	GLY	2.5
1	A	756	ALA	2.5
1	B	1044	SER	2.5
1	C	1067	ALA	2.4
1	B	961	LEU	2.4
1	D	899	ASP	2.4
1	B	919	VAL	2.4
1	C	974	ARG	2.4
1	D	910	ARG	2.4
1	A	512	ASN	2.4
1	D	754	ILE	2.4
1	C	902	VAL	2.4
1	C	749	HIS	2.4
1	B	1064	PRO	2.4
1	C	773	ALA	2.3
1	A	785	CYS	2.3
1	B	904	ASP	2.3
1	B	747	HIS	2.3
1	B	782	SER	2.3
1	B	861	TRP	2.3
1	C	784	PRO	2.3
1	B	960	ASP	2.3
1	B	957	LYS	2.3
1	C	550	GLY	2.3
1	D	550	GLY	2.2
1	A	781	THR	2.2
1	B	755	ALA	2.2
1	C	747	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	943	LYS	2.2
1	A	750	ASP	2.2
1	B	911	GLU	2.2
1	D	751	THR	2.2
1	B	954	SER	2.2
1	D	901	THR	2.2
1	B	852	ALA	2.2
1	B	856	GLY	2.2
1	B	652	ARG	2.2
1	C	891[A]	MET	2.2
1	D	893	LEU	2.2
1	B	680	ALA	2.2
1	B	1067	ALA	2.2
1	D	892	ALA	2.2
1	A	778	SER	2.2
1	A	751	THR	2.2
1	B	773	ALA	2.2
1	A	554	LEU	2.1
1	B	543	THR	2.1
1	A	773	ALA	2.1
1	C	753	GLY	2.1
1	B	784	PRO	2.1
1	B	874	MET	2.1
1	B	586	GLY	2.1
1	C	553	SER	2.1
1	B	981	PHE	2.1
1	A	777	LEU	2.1
1	B	479	TYR	2.1
1	B	940	LYS	2.1
1	A	782	SER	2.1
1	C	956	LEU	2.1
1	C	1014	TYR	2.1
1	C	755	ALA	2.1
1	C	950	VAL	2.1
1	C	722	GLY	2.0
1	B	1031	THR	2.0
1	C	772	ALA	2.0
1	B	653	VAL	2.0
1	D	510	ASN	2.0
1	B	498	LEU	2.0
1	B	620	LEU	2.0
1	B	939	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	831	PRO	2.0
1	C	548	ARG	2.0
1	C	751	THR	2.0
1	A	755	ALA	2.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
1	KCX	C	718	12/13	0.96	0.29	-	40,41,43,46	0
1	KCX	B	718	12/13	0.96	0.20	-	38,41,48,48	0
1	KCX	D	718	12/13	0.99	0.21	-	31,32,34,35	0
1	KCX	A	718	12/13	0.99	0.18	-	21,23,25,26	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	MG	B	1103	1/1	0.87	0.17	4.19	32,32,32,32	0
5	BTN	B	1104	16/16	0.73	0.28	1.66	55,71,80,82	0
5	BTN	A	1104	16/16	0.90	0.16	1.26	44,55,73,74	0
5	BTN	D	1104	16/16	0.91	0.14	0.89	51,57,81,87	0
7	GOL	B	1101	6/6	0.89	0.26	0.58	42,45,49,51	0
6	OXM	A	1105	6/6	0.98	0.18	0.54	30,36,37,42	0
7	GOL	C	1103	6/6	0.90	0.24	0.50	42,50,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	OXM	D	1105	6/6	0.95	0.20	0.37	33,38,41,41	0
5	BTN	C	1105	16/16	0.90	0.16	0.29	53,62,72,78	0
3	MG	C	1102	1/1	0.92	0.11	0.15	41,41,41,41	0
6	OXM	C	1106	6/6	0.96	0.19	-0.77	42,44,48,49	0
6	OXM	B	1105	6/6	0.96	0.17	-0.84	40,43,45,45	0
3	MG	D	1102	1/1	0.95	0.07	-3.09	33,33,33,33	0
3	MG	A	1102	1/1	0.97	0.05	-3.24	34,34,34,34	0
2	ZN	D	1101	1/1	1.00	0.11	-3.58	34,34,34,34	0
2	ZN	A	1101	1/1	0.99	0.12	-3.59	30,30,30,30	0
2	ZN	B	1102	1/1	0.95	0.12	-4.33	41,41,41,41	0
2	ZN	C	1101	1/1	0.99	0.11	-4.38	41,41,41,41	0
4	CL	D	1103	1/1	0.94	0.10	-	49,49,49,49	0
4	CL	C	1104	1/1	0.95	0.15	-	58,58,58,58	0
4	CL	A	1103	1/1	1.00	0.07	-	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.