Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:56 PM GMT

PDB ID	:	4JX5
Title	:	Structure of the carboxyl transferase domain from Rhizobium etli pyruvate carboxylase with pyruvate
Authors	:	Lietzan, A.D.; St Maurice, M.
Deposited on	:	2013-03-27
Resolution	:	2.55 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 (i) symbol.

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

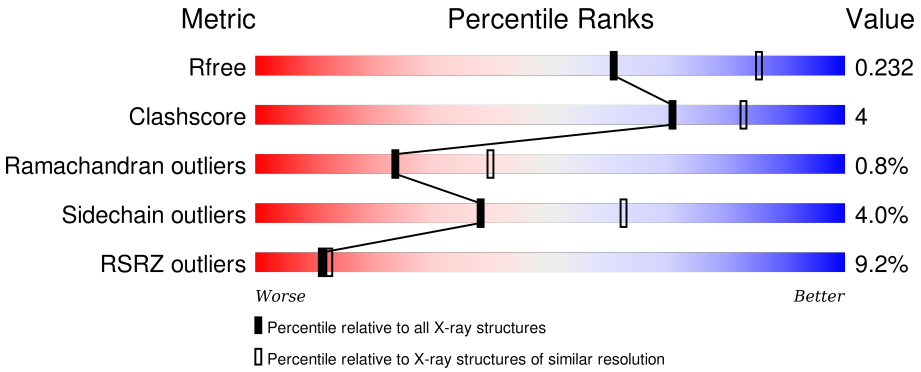
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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	3% 82% 11% • 6%
1	B	632	8% 85% 9% 6%
1	C	632	15% 81% 12% • 6%
1	D	632	9% 81% 11% • 7%

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	CL	C	1102	-	-	X	-
5	PYR	B	1105	-	-	-	X
5	PYR	C	1105	-	-	-	X
5	PYR	D	1104	-	-	-	X
6	GOL	B	1101	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17941 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	597	Total	C	N	O	S	0	2	0
			4539	2889	758	869	23			
1	B	596	Total	C	N	O	S	0	1	0
			4468	2840	747	858	23			
1	C	591	Total	C	N	O	S	0	0	0
			4357	2758	739	838	22			
1	D	590	Total	C	N	O	S	0	0	0
			4322	2733	733	834	22			

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

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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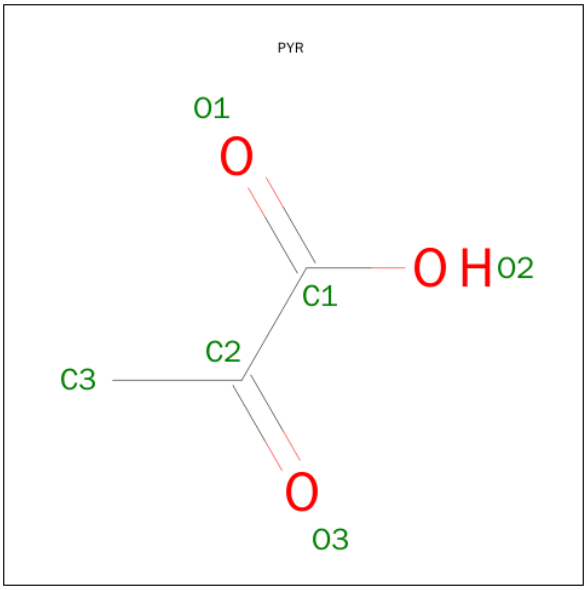
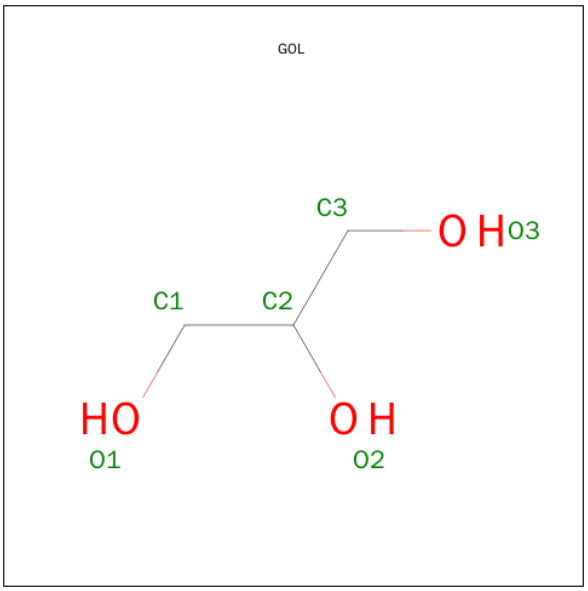
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

- Molecule 5 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

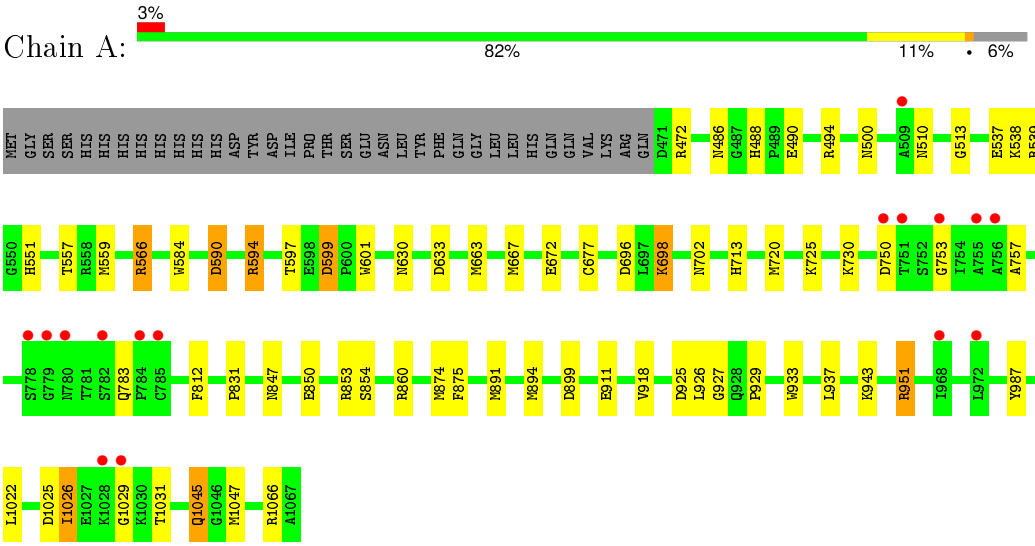
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	86	Total O 86 86	0	0
7	B	46	Total O 46 46	0	0
7	C	42	Total O 42 42	0	0
7	D	33	Total O 33 33	0	0

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.

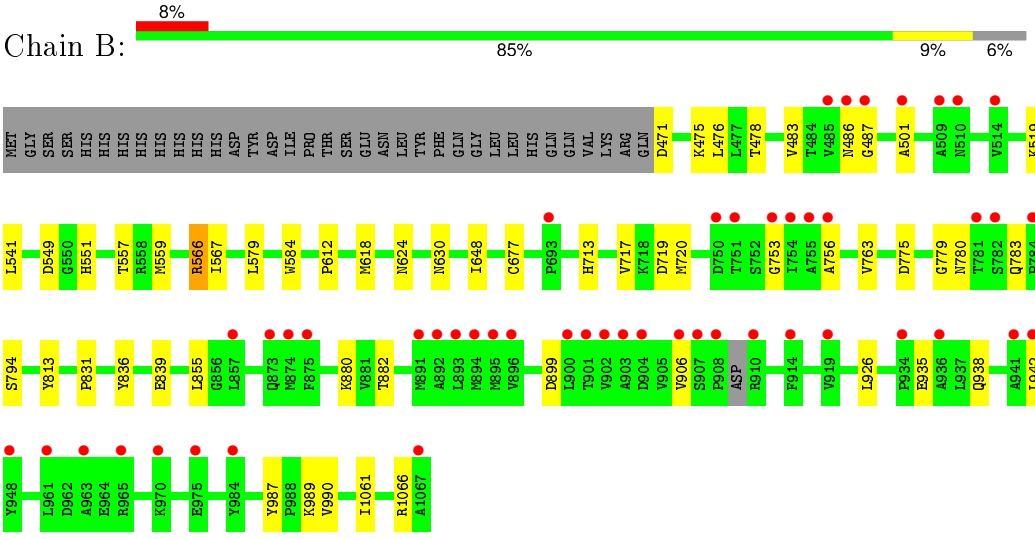
- Molecule 1: Pyruvate carboxylase

Chain A:



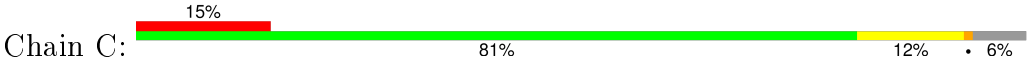
- Molecule 1: Pyruvate carboxylase

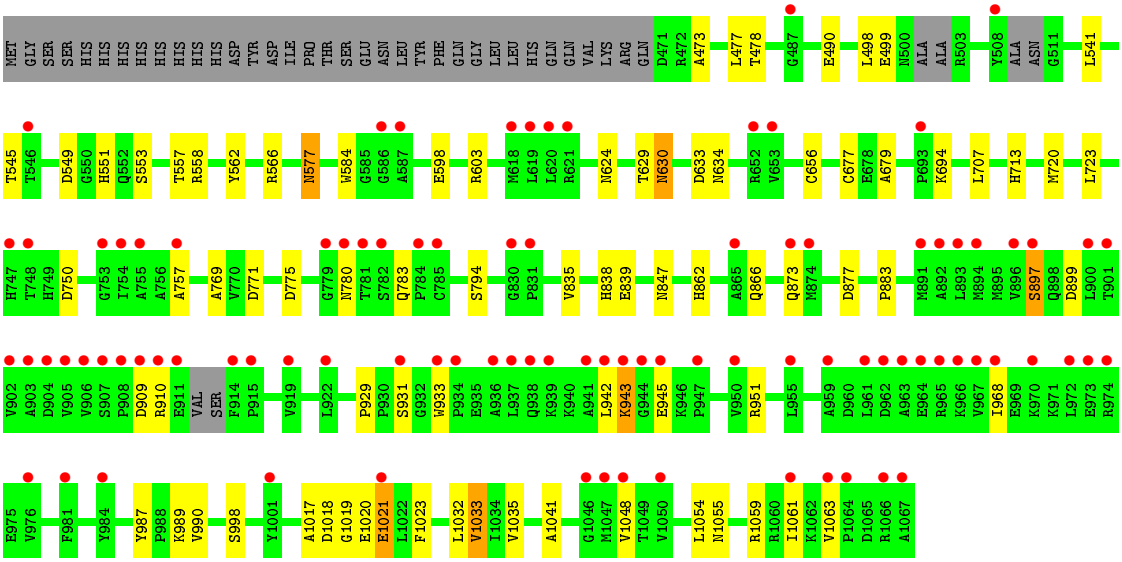
Chain B:

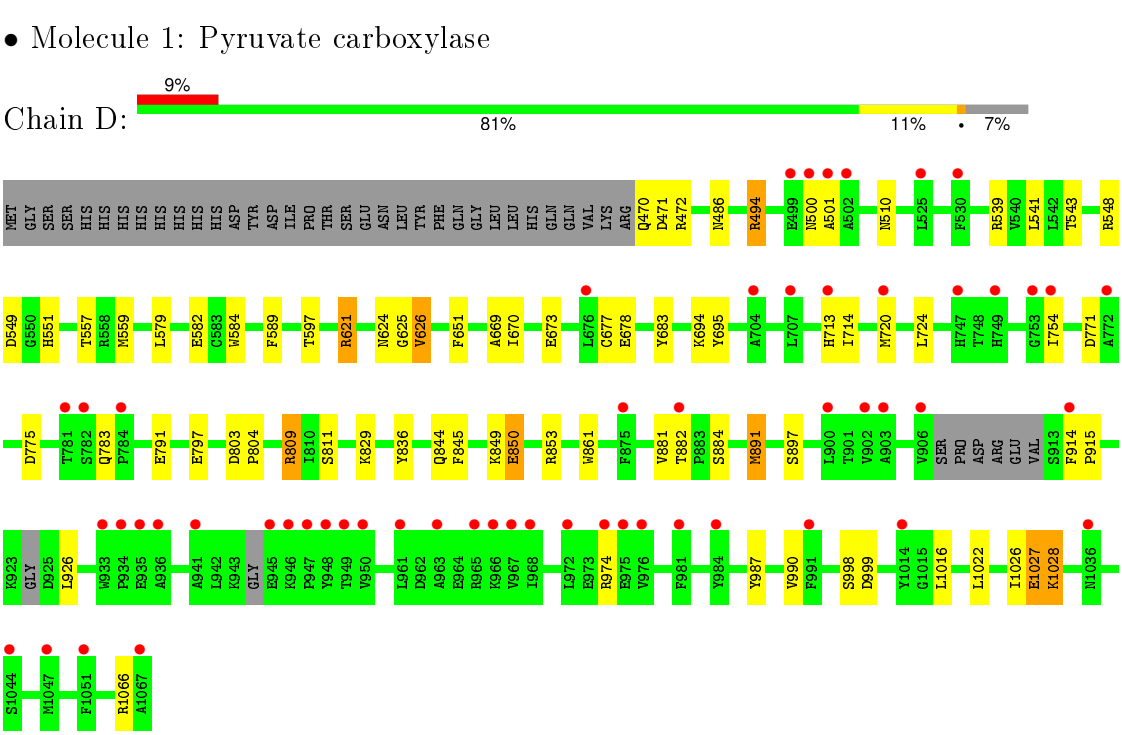


- Molecule 1: Pyruvate carboxylase

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	85.13Å 157.25Å 245.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.88 – 2.55 46.84 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.88-2.55) 99.5 (46.84-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.38 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.187 , 0.232 0.188 , 0.232	Depositor DCC
R_{free} test set	5399 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	55.9	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.5	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 107763 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17941	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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, ZN, CL, PYR, MG, 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	0.70	0/4630	0.81	5/6301 (0.1%)
1	B	0.58	0/4554	0.73	1/6210 (0.0%)
1	C	0.67	4/4438 (0.1%)	0.75	3/6056 (0.0%)
1	D	0.50	0/4402	0.66	0/6013
All	All	0.62	4/18024 (0.0%)	0.74	9/24580 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1063	VAL	C-O	10.64	1.43	1.23
1	C	910	ARG	CZ-NH1	7.20	1.42	1.33
1	C	1059	ARG	CZ-NH1	6.77	1.41	1.33
1	C	1048	VAL	C-O	6.47	1.35	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	750	ASP	CB-CG-OD1	7.65	125.18	118.30
1	C	910	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	A	599	ASP	CB-CG-OD1	6.18	123.86	118.30
1	C	910	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	B	719	ASP	CB-CG-OD1	5.59	123.33	118.30
1	C	771	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	594	ARG	NE-CZ-NH1	-5.19	117.71	120.30
1	A	951	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	A	696	ASP	CB-CG-OD1	5.08	122.88	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4539	0	4406	36	0
1	B	4468	0	4278	32	0
1	C	4357	0	4067	44	0
1	D	4322	0	3993	46	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	2	0
3	D	1	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	6	0	3	0	0
5	B	6	0	3	0	0
5	C	6	0	3	0	0
5	D	6	0	3	1	0
6	B	6	0	8	5	0
6	C	6	0	8	0	0
7	A	86	0	0	4	0
7	B	46	0	0	0	0
7	C	42	0	0	1	0
7	D	33	0	0	1	0
All	All	17941	0	16772	153	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 4.

All (153) 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:D:809:ARG:HH11	1:D:809:ARG:HG2	1.17	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:GLN:HG3	1:D:472:ARG:HB2	1.43	1.01
1:C:677:CYS:H	1:C:713:HIS:HD2	1.10	0.99
1:B:566:ARG:HG3	1:B:566:ARG:HH11	1.27	0.99
1:D:677:CYS:H	1:D:713:HIS:HD2	1.00	0.97
1:C:562:TYR:O	1:C:566:ARG:HG3	1.68	0.94
1:A:677:CYS:H	1:A:713:HIS:HD2	1.02	0.92
1:D:677:CYS:H	1:D:713:HIS:CD2	1.88	0.90
1:D:494:ARG:HH11	1:D:494:ARG:HG2	1.37	0.89
1:B:780:ASN:H	6:B:1101:GOL:H11	1.37	0.88
1:A:677:CYS:H	1:A:713:HIS:CD2	1.92	0.86
1:B:677:CYS:H	1:B:713:HIS:HD2	1.22	0.85
1:C:677:CYS:H	1:C:713:HIS:CD2	1.95	0.83
1:D:549:ASP:HB3	1:D:783:GLN:HE22	1.44	0.83
1:B:566:ARG:CG	1:B:566:ARG:HH11	1.97	0.76
1:C:490:GLU:OE1	1:C:558:ARG:NH2	2.21	0.73
1:D:677:CYS:N	1:D:713:HIS:HD2	1.82	0.72
1:D:470:GLN:CG	1:D:472:ARG:HB2	2.20	0.70
1:D:809:ARG:NH1	1:D:809:ARG:HG2	1.94	0.70
1:A:472:ARG:CB	1:A:1026:ILE:HD11	2.22	0.70
1:C:577:ASN:HB2	7:C:1208:HOH:O	1.92	0.70
1:C:990:VAL:N	3:C:1102:CL:CL	2.60	0.68
1:D:621:ARG:HB3	1:D:624:ASN:HB2	1.75	0.67
1:C:1021:GLU:HG2	1:C:1035:VAL:HG22	1.76	0.67
1:B:677:CYS:H	1:B:713:HIS:CD2	2.11	0.65
1:B:549:ASP:HB3	1:B:783:GLN:HE22	1.62	0.65
1:C:549:ASP:HB3	1:C:783:GLN:HE22	1.64	0.63
1:C:679:ALA:HB1	1:C:707:LEU:HD22	1.81	0.62
1:D:486:ASN:HD21	1:D:1066:ARG:H	1.47	0.61
1:A:730:LYS:HG2	7:A:1270:HOH:O	2.01	0.60
1:A:753:GLY:HA3	1:A:831:PRO:HB3	1.84	0.60
1:B:780:ASN:H	6:B:1101:GOL:C1	2.13	0.60
1:D:549:ASP:HB3	1:D:783:GLN:NE2	2.16	0.60
1:A:847:ASN:HB2	7:A:1242:HOH:O	2.03	0.59
1:A:677:CYS:N	1:A:713:HIS:HD2	1.87	0.58
1:A:850:GLU:OE2	1:A:853:ARG:NE	2.37	0.58
1:D:486:ASN:ND2	1:D:1066:ARG:H	2.02	0.58
1:B:566:ARG:CG	1:B:566:ARG:NH1	2.59	0.57
1:A:891[B]:MET:HE1	1:A:918:VAL:HG11	1.87	0.57
1:C:545:THR:OG1	1:C:783:GLN:NE2	2.38	0.57
1:D:589:PHE:CG	1:D:626:VAL:HG11	2.40	0.56
1:C:677:CYS:N	1:C:713:HIS:HD2	1.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:THR:HA	1:B:1061:ILE:HG21	1.87	0.56
1:D:850:GLU:O	1:D:853:ARG:HB3	2.06	0.56
1:D:539:ARG:NH1	7:D:1202:HOH:O	2.32	0.56
1:B:779:GLY:HA2	6:B:1101:GOL:H12	1.87	0.56
1:C:478:THR:HA	1:C:1061:ILE:HG21	1.88	0.55
1:C:987:TYR:HB3	1:C:990:VAL:HB	1.89	0.55
1:D:494:ARG:NH1	1:D:494:ARG:HG2	2.10	0.55
1:A:549:ASP:HB3	1:A:783:GLN:HE22	1.70	0.55
1:B:519:LYS:HG2	1:B:612:PRO:O	2.07	0.55
1:B:486:ASN:ND2	1:B:1066:ARG:H	2.05	0.54
1:A:1045:GLN:HB3	1:A:1047:MET:HG2	1.88	0.54
1:A:1026:ILE:HG12	1:A:1026:ILE:O	2.08	0.54
1:C:624:ASN:HD21	1:C:630:ASN:ND2	2.06	0.54
1:C:1033:VAL:HG23	1:C:1055:ASN:OD1	2.07	0.54
1:A:488:HIS:CE1	1:A:490:GLU:HB2	2.42	0.53
1:D:683:TYR:CE1	1:D:724:LEU:HD13	2.43	0.53
1:B:791:GLU:HG2	1:D:836:TYR:CD2	2.44	0.53
1:D:694:LYS:HD3	1:D:695:TYR:CE2	2.44	0.53
1:C:694:LYS:NZ	1:C:931:SER:HB2	2.24	0.53
1:B:753:GLY:HA3	1:B:831:PRO:HB3	1.90	0.52
1:B:486:ASN:HD21	1:B:1066:ARG:H	1.55	0.52
1:D:621:ARG:HB2	1:D:625:GLY:O	2.09	0.52
1:D:651:PHE:HB2	1:D:670:ILE:HD13	1.91	0.52
1:C:633:ASP:OD1	1:C:951:ARG:NH1	2.44	0.51
1:D:1026:ILE:HG23	1:D:1027:GLU:HG3	1.93	0.51
1:B:618:MET:HB3	1:B:648:ILE:HD12	1.93	0.51
1:A:599:ASP:OD1	1:A:601:TRP:N	2.43	0.51
1:A:630:ASN:OD1	1:A:925:ASP:O	2.29	0.50
1:A:698:LYS:HG2	1:A:702:ASN:ND2	2.26	0.50
1:C:624:ASN:HD21	1:C:630:ASN:HD22	1.57	0.50
1:C:989:LYS:N	3:C:1102:CL:CL	2.81	0.50
1:A:590:ASP:HB2	1:A:987:TYR:CZ	2.47	0.49
1:B:753:GLY:HA2	6:B:1101:GOL:O1	2.11	0.49
1:A:590:ASP:OD1	1:A:594:ARG:NH2	2.45	0.49
1:A:1016:LEU:HD21	1:A:1022:LEU:HD22	1.94	0.49
1:A:537:GLU:HG3	1:A:539:ARG:HG2	1.94	0.49
1:A:730:LYS:CG	7:A:1270:HOH:O	2.60	0.49
1:D:548:ARG:HB3	1:D:582:GLU:OE1	2.13	0.49
1:D:809:ARG:CG	1:D:809:ARG:HH11	2.05	0.48
1:A:875:PHE:CZ	1:A:891[B]:MET:HE2	2.49	0.48
1:D:669:ALA:O	1:D:673:GLU:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:598:GLU:OE2	1:C:603:ARG:NH2	2.43	0.48
1:C:1021:GLU:CG	1:C:1035:VAL:HG22	2.41	0.48
1:A:551:HIS:CE1	1:A:559:MET:HB3	2.49	0.48
1:D:775:ASP:HB2	1:D:811:SER:OG	2.14	0.47
1:C:473:ALA:HB1	1:C:1054:LEU:HD21	1.96	0.47
1:B:471:ASP:OD2	1:B:475:LYS:HE3	2.15	0.47
1:B:541:LEU:HB3	1:B:579:LEU:HB2	1.95	0.47
1:A:486:ASN:ND2	1:A:1066:ARG:H	2.12	0.47
1:C:624:ASN:ND2	1:C:630:ASN:HD22	2.13	0.46
1:D:541:LEU:HB3	1:D:579:LEU:HB2	1.98	0.46
1:C:562:TYR:CE2	1:C:566:ARG:HD2	2.50	0.46
1:D:543:THR:HB	1:D:771:ASP:OD1	2.17	0.45
1:A:927:GLY:HA3	7:A:1224:HOH:O	2.15	0.45
1:D:987:TYR:HB3	1:D:990:VAL:HB	1.98	0.45
1:C:473:ALA:O	1:C:477:LEU:HG	2.17	0.45
1:B:836:TYR:CD2	1:D:791:GLU:HG2	2.51	0.45
1:D:589:PHE:CD2	1:D:626:VAL:HG11	2.52	0.45
1:D:551:HIS:CE1	1:D:559:MET:HB3	2.52	0.45
1:B:624:ASN:ND2	1:B:630:ASN:OD1	2.50	0.45
1:B:551:HIS:CE1	1:B:559:MET:HB3	2.51	0.45
1:A:1025:ASP:OD2	1:A:1031:THR:OG1	2.25	0.44
1:C:624:ASN:ND2	1:C:630:ASN:ND2	2.65	0.44
1:B:677:CYS:N	1:B:713:HIS:HD2	2.02	0.44
1:D:803:ASP:HA	1:D:804:PRO:HD3	1.91	0.44
1:B:483:VAL:O	1:B:487:GLY:N	2.50	0.44
1:D:849:LYS:HD2	1:D:861:TRP:CE2	2.53	0.44
1:D:1016:LEU:HD21	1:D:1022:LEU:HD22	1.98	0.44
1:C:723:LEU:HD11	1:C:839:GLU:HG2	1.99	0.44
1:C:551:HIS:ND1	1:C:557:THR:HA	2.32	0.43
1:C:1023:PHE:HA	1:C:1032:LEU:O	2.18	0.43
1:C:541:LEU:O	1:C:769:ALA:HA	2.18	0.43
1:A:566:ARG:HG3	1:A:566:ARG:HH11	1.84	0.43
1:A:774:MET:O	1:A:775:ASP:C	2.57	0.43
1:B:938:GLN:HG2	1:B:942:LEU:HD22	2.01	0.43
1:D:621:ARG:HD2	5:D:1104:PYR:O1	2.19	0.43
1:C:835:VAL:HA	1:C:838:HIS:CE1	2.54	0.43
1:B:779:GLY:CA	6:B:1101:GOL:H12	2.48	0.43
1:D:914:PHE:HB3	1:D:915:PRO:HD2	2.01	0.43
1:C:1017:ALA:O	1:C:1020:GLU:HB3	2.19	0.43
1:C:694:LYS:HZ1	1:C:931:SER:HB2	1.82	0.42
1:C:838:HIS:O	1:C:839:GLU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:968:ILE:HG13	1:C:968:ILE:O	2.19	0.42
1:D:1027:GLU:HB2	1:D:1028:LYS:H	1.64	0.42
1:C:929:PRO:HD3	1:C:933:TRP:CZ2	2.53	0.42
1:C:634:ASN:OD1	1:C:634:ASN:N	2.51	0.42
1:B:567:ILE:HD13	1:B:813:TYR:CG	2.54	0.42
1:C:897:SER:C	1:C:899:ASP:H	2.23	0.42
1:A:633:ASP:OD1	1:A:951:ARG:NH1	2.49	0.42
1:A:929:PRO:HD3	1:A:933:TRP:CZ2	2.54	0.42
1:A:663:MET:O	1:A:667:MET:HG3	2.20	0.42
1:D:548:ARG:HE	1:D:582:GLU:CD	2.23	0.42
1:C:656:CYS:SG	1:C:883:PRO:HD2	2.59	0.42
1:C:929:PRO:HD3	1:C:933:TRP:CE2	2.55	0.41
1:C:750:ASP:C	1:C:780:ASN:O	2.59	0.41
1:A:874:MET:HG2	1:A:937:LEU:HD22	2.02	0.41
1:D:678:GLU:HA	1:D:714:ILE:O	2.20	0.41
1:B:567:ILE:HD13	1:B:813:TYR:CD2	2.55	0.41
1:B:756:ALA:CB	1:D:754:ILE:HG22	2.51	0.41
1:A:541:LEU:O	1:A:769:ALA:HA	2.21	0.41
1:A:812[B]:PHE:CE1	1:C:862:HIS:CD2	3.09	0.41
1:A:894:MET:HE3	1:A:894:MET:HB2	1.79	0.41
1:A:757:ALA:HA	1:C:757:ALA:HB2	2.03	0.41
1:D:891:MET:CE	1:D:891:MET:HA	2.50	0.41
1:C:942:LEU:O	1:C:943:LYS:C	2.59	0.41
1:B:987:TYR:HB3	1:B:990:VAL:HB	2.02	0.41
1:B:839:GLU:OE1	1:B:880:LYS:NZ	2.54	0.41
1:D:494:ARG:CG	1:D:494:ARG:NH1	2.83	0.40
1:D:844:GLN:O	1:D:845:PHE:C	2.59	0.40
1:B:540:VAL:HG21	1:B:763:VAL:HG22	2.02	0.40
1:D:881:VAL:O	1:D:884:SER:N	2.55	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	596/632 (94%)	577 (97%)	16 (3%)	3 (0%)	34	54
1	B	592/632 (94%)	563 (95%)	26 (4%)	3 (0%)	34	54
1	C	582/632 (92%)	541 (93%)	33 (6%)	8 (1%)	14	23
1	D	581/632 (92%)	540 (93%)	36 (6%)	5 (1%)	21	36
All	All	2351/2528 (93%)	2221 (94%)	111 (5%)	19 (1%)	24	40

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1041	ALA
1	D	500	ASN
1	D	510	ASN
1	D	1028	LYS
1	A	1029	GLY
1	B	501	ALA
1	B	935	GLU
1	C	943	LYS
1	C	1019	GLY
1	D	501	ALA
1	A	500	ASN
1	A	513	GLY
1	C	498	LEU
1	C	499	GLU
1	C	897	SER
1	D	621	ARG
1	C	877	ASP
1	C	945	GLU
1	B	906	VAL

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	462/519 (89%)	441 (96%)	21 (4%)	34	56
1	B	447/519 (86%)	433 (97%)	14 (3%)	47	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	422/519 (81%)	406 (96%)	16 (4%)	40 65
1	D	412/519 (79%)	393 (95%)	19 (5%)	33 55
All	All	1743/2076 (84%)	1673 (96%)	70 (4%)	38 62

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	494	ARG
1	A	510	ASN
1	A	538	LYS
1	A	557	THR
1	A	566	ARG
1	A	584	TRP
1	A	590	ASP
1	A	597	THR
1	A	672	GLU
1	A	698	LYS
1	A	720	MET
1	A	725	LYS
1	A	854	SER
1	A	860	ARG
1	A	899	ASP
1	A	911	GLU
1	A	926	LEU
1	A	943	LYS
1	A	999	ASP
1	A	1026	ILE
1	A	1045	GLN
1	B	476	LEU
1	B	534	MET
1	B	557	THR
1	B	566	ARG
1	B	584	TRP
1	B	717	VAL
1	B	720	MET
1	B	775	ASP
1	B	794	SER
1	B	855	LEU
1	B	882	THR
1	B	899	ASP
1	B	926	LEU

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Mol	Chain	Res	Type
1	B	989	LYS
1	C	553	SER
1	C	577	ASN
1	C	584	TRP
1	C	629	THR
1	C	630	ASN
1	C	720	MET
1	C	775	ASP
1	C	794	SER
1	C	847	ASN
1	C	866	GLN
1	C	873	GLN
1	C	909	ASP
1	C	998	SER
1	C	1018	ASP
1	C	1021	GLU
1	C	1033	VAL
1	D	471	ASP
1	D	494	ARG
1	D	557	THR
1	D	584	TRP
1	D	597	THR
1	D	626	VAL
1	D	720	MET
1	D	797	GLU
1	D	809	ARG
1	D	829	LYS
1	D	850	GLU
1	D	882	THR
1	D	891	MET
1	D	897	SER
1	D	926	LEU
1	D	974	ARG
1	D	998	SER
1	D	999	ASP
1	D	1027	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	486	ASN
1	A	577	ASN

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Mol	Chain	Res	Type
1	A	630	ASN
1	A	713	HIS
1	A	783	GLN
1	B	486	ASN
1	B	577	ASN
1	B	713	HIS
1	B	783	GLN
1	B	820	GLN
1	B	1045	GLN
1	C	486	ASN
1	C	624	ASN
1	C	630	ASN
1	C	702	ASN
1	C	713	HIS
1	C	783	GLN
1	D	470	GLN
1	D	486	ASN
1	D	577	ASN
1	D	624	ASN
1	D	713	HIS
1	D	783	GLN

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	A	718	1,2	7,11,12	0.87	0	7,12,14	1.96	1 (14%)
1	KCX	B	718	1,2	7,11,12	0.49	0	7,12,14	3.98	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	KCX	C	718	1,2	7,11,12	0.75	0	7,12,14	1.08	1 (14%)
1	KCX	D	718	1,2	7,11,12	0.52	0	7,12,14	2.92	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	718	KCX	CE-NZ-CX	2.03	125.79	123.49
1	A	718	KCX	CE-NZ-CX	4.63	128.73	123.49
1	D	718	KCX	CE-NZ-CX	7.17	131.61	123.49
1	B	718	KCX	CE-NZ-CX	9.92	134.72	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 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	$\#\|Z\| > 2$
5	PYR	A	1104	-	2,5,5	0.36	0	2,6,6	0.63	0
6	GOL	B	1101	-	5,5,5	0.31	0	5,5,5	1.18	0
5	PYR	B	1105	-	2,5,5	0.28	0	2,6,6	0.61	0
6	GOL	C	1101	-	5,5,5	0.38	0	5,5,5	1.51	0
5	PYR	C	1105	-	2,5,5	0.05	0	2,6,6	0.81	0
5	PYR	D	1104	-	2,5,5	0.42	0	2,6,6	0.27	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
5	PYR	A	1104	-	-	0/0/4/4	0/0/0/0
6	GOL	B	1101	-	-	0/4/4/4	0/0/0/0
5	PYR	B	1105	-	-	0/0/4/4	0/0/0/0
6	GOL	C	1101	-	-	0/4/4/4	0/0/0/0
5	PYR	C	1105	-	-	0/0/4/4	0/0/0/0
5	PYR	D	1104	-	-	0/0/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1101	GOL	5	0
5	D	1104	PYR	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	596/632 (94%)	0.07	16 (2%) 58 63	31, 48, 72, 130	19 (3%)
1	B	595/632 (94%)	0.31	53 (8%) 12 13	42, 63, 108, 149	17 (2%)
1	C	590/632 (93%)	0.81	93 (15%) 3 3	34, 81, 162, 211	14 (2%)
1	D	589/632 (93%)	0.50	56 (9%) 10 11	49, 81, 123, 140	14 (2%)
All	All	2370/2528 (93%)	0.42	218 (9%) 11 12	31, 65, 130, 211	64 (2%)

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	968	ILE	7.3
1	C	963	ALA	6.5
1	D	501	ALA	6.4
1	B	891[A]	MET	5.8
1	C	914	PHE	5.6
1	C	1046	GLY	5.4
1	D	948	TYR	5.4
1	C	900	LEU	5.1
1	C	906	VAL	5.1
1	C	1067	ALA	5.1
1	B	900	LEU	5.1
1	C	894	MET	4.9
1	C	981	PHE	4.9
1	D	950	VAL	4.9
1	B	908	PRO	4.9
1	B	944	GLY	4.9
1	C	942	LEU	4.8
1	C	941	ALA	4.7
1	C	896	VAL	4.5
1	C	902	VAL	4.4
1	C	922	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	1067	ALA	4.3
1	C	966	LYS	4.1
1	A	968	ILE	4.1
1	D	1044	SER	4.1
1	D	947	PRO	4.1
1	D	961	LEU	4.0
1	D	525	LEU	4.0
1	C	937	LEU	4.0
1	B	941	ALA	4.0
1	D	933	TRP	4.0
1	C	1048	VAL	3.9
1	C	919	VAL	3.9
1	D	981	PHE	3.9
1	D	502	ALA	3.9
1	C	970	LYS	3.9
1	B	893	LEU	3.9
1	B	942	LEU	3.8
1	D	875	PHE	3.8
1	C	620	LEU	3.8
1	B	936	ALA	3.7
1	C	976	VAL	3.7
1	B	902	VAL	3.6
1	C	874	MET	3.6
1	C	891	MET	3.6
1	C	955	LEU	3.6
1	B	906	VAL	3.6
1	C	619	LEU	3.6
1	C	965	ARG	3.5
1	C	621	ARG	3.5
1	A	972	LEU	3.5
1	C	652	ARG	3.5
1	B	857	LEU	3.4
1	D	972	LEU	3.4
1	C	967	VAL	3.4
1	C	947	PRO	3.3
1	D	1067	ALA	3.3
1	D	946	LYS	3.3
1	D	974	ARG	3.3
1	C	653	VAL	3.2
1	A	779	GLY	3.2
1	C	984	TYR	3.2
1	C	931	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	907	SER	3.2
1	B	896	VAL	3.2
1	C	903	ALA	3.2
1	C	1047	MET	3.2
1	C	908	PRO	3.1
1	C	934	PRO	3.1
1	C	905	VAL	3.1
1	D	967	VAL	3.1
1	C	911	GLU	3.1
1	D	963	ALA	3.1
1	C	897	SER	3.1
1	C	909	ASP	3.1
1	B	485	VAL	3.1
1	D	945	GLU	3.1
1	C	893	LEU	3.0
1	C	782	SER	3.0
1	A	785	CYS	3.0
1	C	753	GLY	3.0
1	D	976	VAL	3.0
1	C	915	PRO	3.0
1	C	964	GLU	3.0
1	D	936	ALA	3.0
1	D	984	TYR	2.9
1	C	873	GLN	2.9
1	D	900	LEU	2.9
1	C	910	ARG	2.9
1	C	779	GLY	2.9
1	D	966	LYS	2.9
1	B	785	CYS	2.9
1	C	936	ALA	2.9
1	B	901	THR	2.8
1	C	781	THR	2.8
1	A	750	ASP	2.8
1	B	945	GLU	2.8
1	D	965	ARG	2.8
1	B	486	ASN	2.8
1	C	972	LEU	2.8
1	D	1014	TYR	2.8
1	C	938	GLN	2.8
1	A	756	ALA	2.8
1	D	934	PRO	2.7
1	C	907	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	499	GLU	2.7
1	A	1029	GLY	2.7
1	D	1047	MET	2.7
1	D	1036	ASN	2.7
1	A	778	SER	2.6
1	A	1028	LYS	2.6
1	D	902	VAL	2.6
1	D	720	MET	2.6
1	B	904	ASP	2.6
1	D	903	ALA	2.6
1	C	831	PRO	2.6
1	C	1066	ARG	2.6
1	C	1001	TYR	2.6
1	B	934	PRO	2.6
1	B	501	ALA	2.6
1	B	755	ALA	2.6
1	D	1051	PHE	2.6
1	B	874	MET	2.6
1	C	747	HIS	2.6
1	C	973	GLU	2.5
1	C	754	ILE	2.5
1	C	933	TRP	2.5
1	B	919	VAL	2.5
1	C	944	GLY	2.5
1	B	910	ARG	2.5
1	C	508	TYR	2.5
1	C	546	THR	2.5
1	D	882	THR	2.5
1	D	772	ALA	2.5
1	D	749	HIS	2.5
1	A	755	ALA	2.5
1	C	693	PRO	2.4
1	C	748	THR	2.4
1	D	991	PHE	2.4
1	B	963	ALA	2.4
1	B	965	ARG	2.4
1	B	961	LEU	2.4
1	D	781	THR	2.4
1	B	754	ILE	2.4
1	D	704	ALA	2.4
1	B	510	ASN	2.4
1	C	785	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	975	GLU	2.4
1	C	587	ALA	2.4
1	A	782	SER	2.3
1	D	968	ILE	2.3
1	C	1064	PRO	2.3
1	B	914	PHE	2.3
1	C	586	GLY	2.3
1	C	757	ALA	2.3
1	D	914	PHE	2.3
1	D	500	ASN	2.3
1	B	753	GLY	2.3
1	A	751	THR	2.3
1	B	751	THR	2.3
1	D	906	VAL	2.3
1	B	784	PRO	2.3
1	B	873	GLN	2.2
1	B	487	GLY	2.2
1	B	875	PHE	2.2
1	C	904	ASP	2.2
1	C	1021	GLU	2.2
1	A	784	PRO	2.2
1	C	1063	VAL	2.2
1	B	509	ALA	2.2
1	C	618	MET	2.2
1	D	941	ALA	2.2
1	C	962	ASP	2.2
1	D	782	SER	2.2
1	C	830	GLY	2.2
1	D	530	PHE	2.2
1	C	901	THR	2.2
1	B	756	ALA	2.2
1	C	945	GLU	2.2
1	C	950	VAL	2.2
1	C	1050	VAL	2.2
1	C	959	ALA	2.2
1	B	781	THR	2.2
1	D	949	THR	2.2
1	B	970	LYS	2.2
1	A	509	ALA	2.2
1	D	676	LEU	2.2
1	D	707	LEU	2.2
1	B	894	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	948	TYR	2.1
1	D	713	HIS	2.1
1	B	895	MET	2.1
1	C	780	ASN	2.1
1	C	939	LYS	2.1
1	C	892	ALA	2.1
1	B	984	TYR	2.1
1	A	753	GLY	2.1
1	C	784	PRO	2.1
1	D	975	GLU	2.1
1	B	514	VAL	2.1
1	B	903	ALA	2.1
1	C	1061	ILE	2.1
1	D	754	ILE	2.1
1	C	487	GLY	2.1
1	D	784	PRO	2.1
1	C	755	ALA	2.1
1	A	780	ASN	2.1
1	D	753	GLY	2.1
1	C	865	ALA	2.0
1	C	974	ARG	2.0
1	C	943	LYS	2.0
1	B	693	PRO	2.0
1	B	750	ASP	2.0
1	D	935	GLU	2.0
1	B	892	ALA	2.0
1	D	747	HIS	2.0
1	B	782	SER	2.0
1	C	961	LEU	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	B	718	12/13	0.98	0.23	-	55,57,60,61	0
1	KCX	A	718	12/13	0.98	0.22	-	37,40,46,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	KCX	D	718	12/13	0.96	0.28	-	62,66,73,74	0
1	KCX	C	718	12/13	0.97	0.28	-	54,59,66,70	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
5	PYR	C	1105	6/6	0.96	0.78	7.72	30,32,35,38	6
5	PYR	D	1104	6/6	0.88	0.44	5.28	46,51,60,60	3
5	PYR	B	1105	6/6	0.98	0.39	5.21	34,41,44,48	3
4	MG	D	1102	1/1	0.79	0.26	1.32	57,57,57,57	0
6	GOL	C	1101	6/6	0.97	0.35	1.26	45,47,51,51	0
5	PYR	A	1104	6/6	0.99	0.22	1.16	44,51,52,54	0
4	MG	A	1103	1/1	0.99	0.17	0.75	45,45,45,45	0
4	MG	C	1103	1/1	0.92	0.16	0.06	41,41,41,41	0
6	GOL	B	1101	6/6	0.96	0.24	-0.46	49,56,59,64	0
4	MG	B	1103	1/1	0.84	0.06	-2.55	52,52,52,52	0
2	ZN	A	1101	1/1	0.99	0.13	-2.74	43,43,43,43	0
2	ZN	B	1104	1/1	0.99	0.14	-3.08	51,51,51,51	0
2	ZN	C	1104	1/1	0.99	0.15	-3.83	54,54,54,54	0
2	ZN	D	1103	1/1	0.98	0.17	-5.72	60,60,60,60	0
3	CL	D	1101	1/1	0.95	0.11	-	79,79,79,79	0
3	CL	A	1102	1/1	0.99	0.09	-	53,53,53,53	0
3	CL	B	1102	1/1	0.90	0.09	-	66,66,66,66	0
3	CL	C	1102	1/1	0.98	0.10	-	76,76,76,76	0

6.5 Other polymers (i)

There are no such residues in this entry.