Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 07:21 PM EDT

PDB ID	:	4MFD
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 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

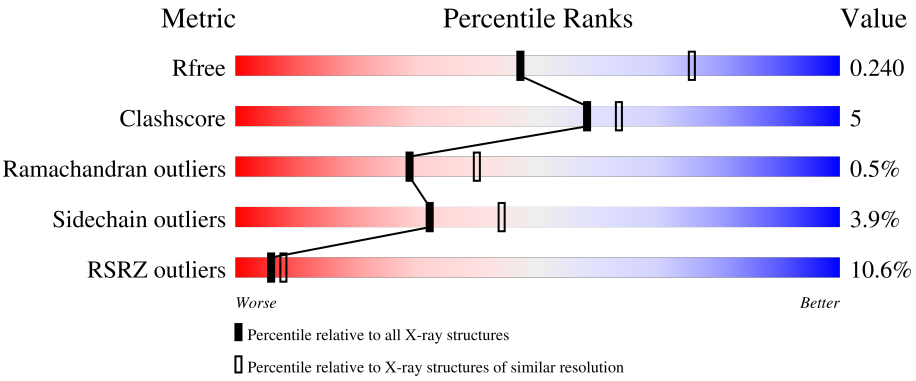
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 <=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	7% 81% 13% 6%
1	C	632	16% 80% 13% • 6%
1	D	632	14% 84% 9% • 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	-	-
5	CL	C	1104	-	-	X	-
6	GOL	B	1105	-	-	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
1	A	597	Total	C	N	O	S	0	1	0
			4557	2897	764	873	23			
1	B	597	Total	C	N	O	S	0	1	0
			4522	2878	759	862	23			
1	C	596	Total	C	N	O	S	0	1	0
			4368	2767	741	837	23			
1	D	597	Total	C	N	O	S	0	1	0
			4367	2752	746	846	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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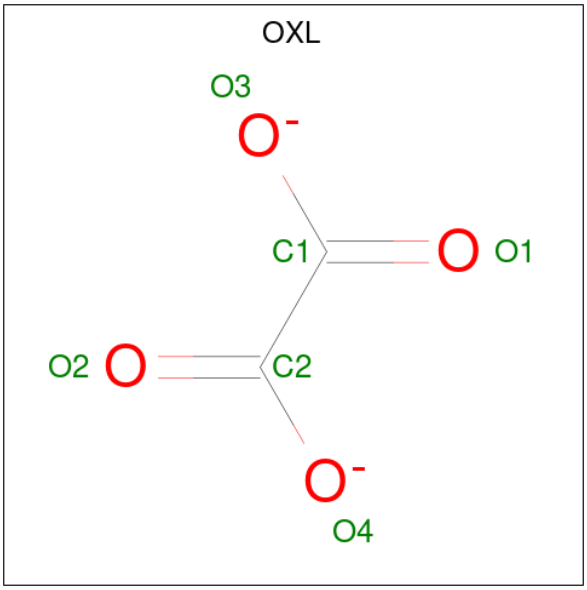
Chain	Residue	Modelled	Actual	Comment	Reference
D	454	SER	-	expression tag	UNP Q2K340
D	455	GLU	-	expression tag	UNP Q2K340
D	456	ASN	-	expression tag	UNP Q2K340
D	457	LEU	-	expression tag	UNP Q2K340
D	458	TYR	-	expression tag	UNP Q2K340
D	459	PHE	-	expression tag	UNP Q2K340
D	460	GLN	-	expression tag	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	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 (three-letter code: OXL) (formula: C_2O_4).



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

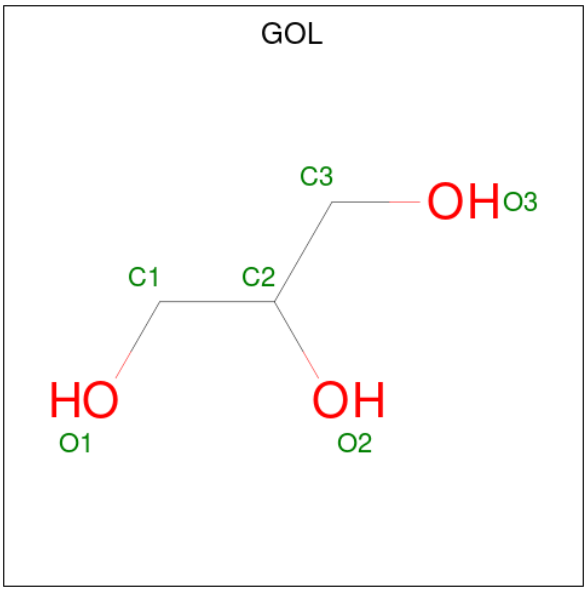
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 (three-letter code: 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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



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.

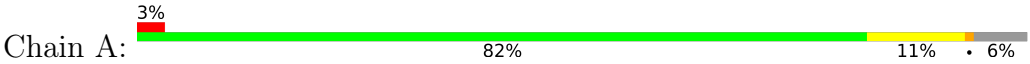
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	87	Total O 87 87	0	0
7	B	46	Total O 46 46	0	0
7	C	34	Total O 34 34	0	0
7	D	23	Total O 23 23	0	0

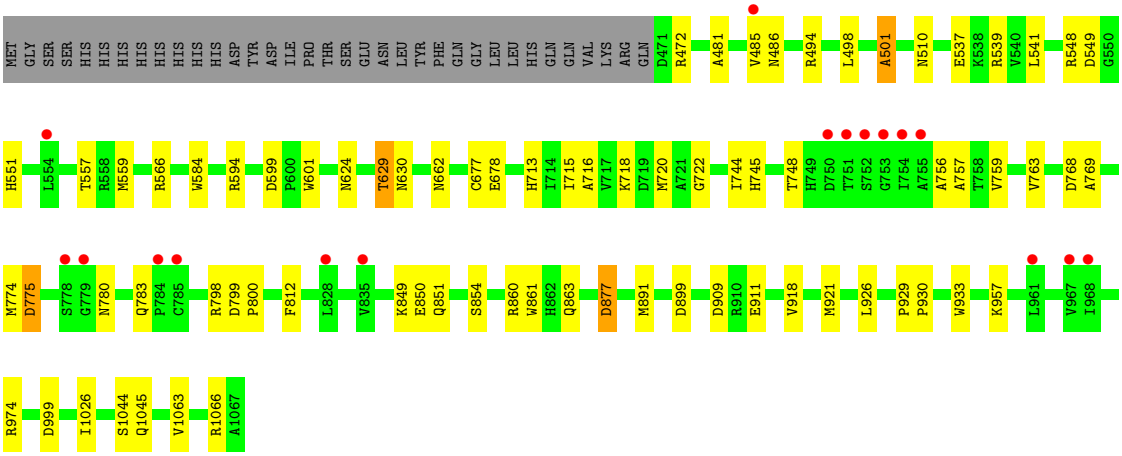
3 Residue-property plots (i)

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

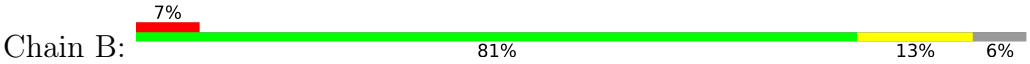
Chain A:

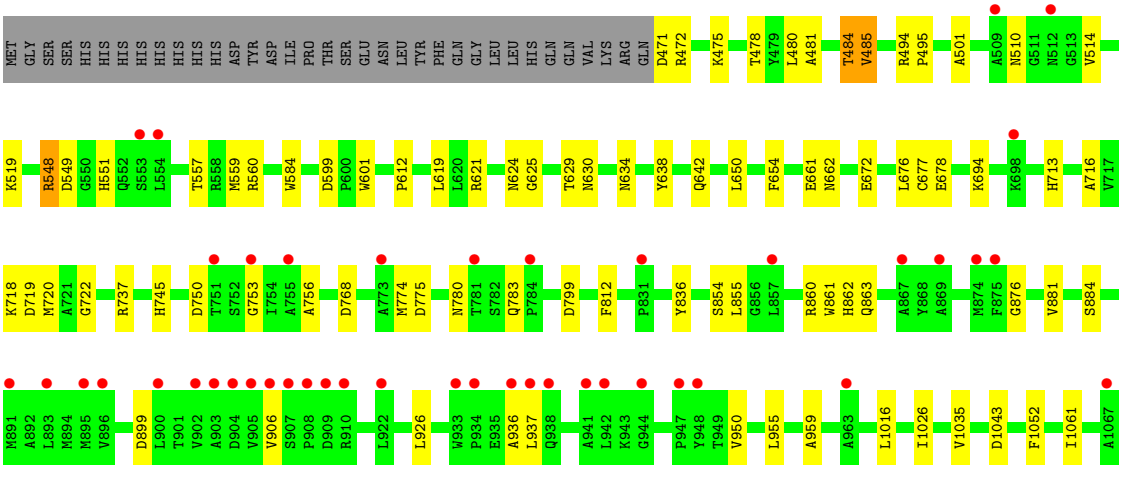




• Molecule 1: PYRUVATE CARBOXYLASE

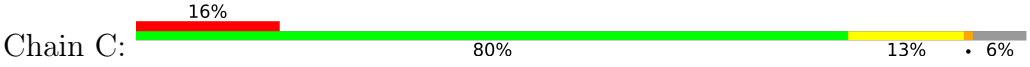
Chain B:

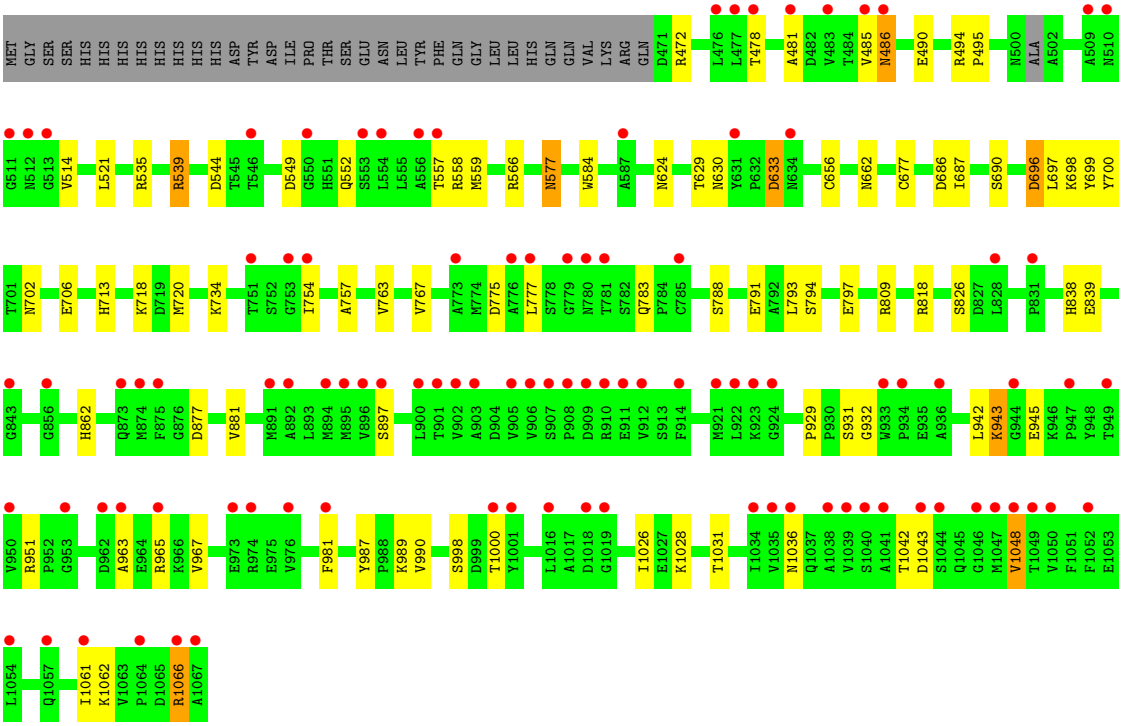




• Molecule 1: PYRUVATE CARBOXYLASE

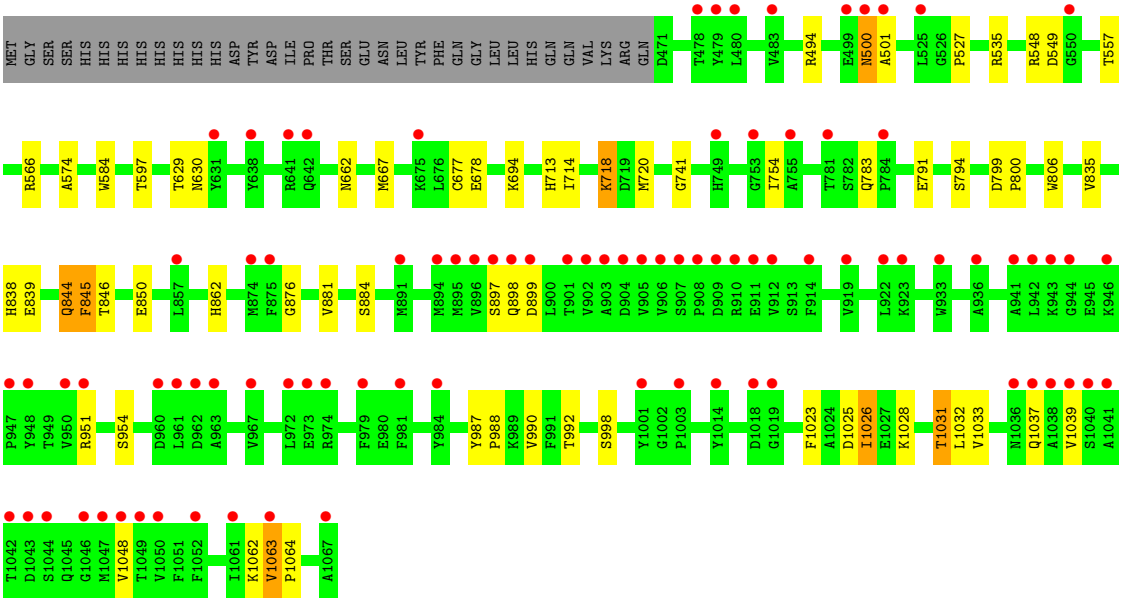
Chain C:





• 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	85.66Å 157.37Å 244.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.26 – 2.55 48.22 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.26-2.55) 99.4 (48.22-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.23 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.193 , 0.240 0.199 , 0.240	Depositor DCC
R_{free} test set	5409 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	56.4	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 48.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, OXL, KCX, GOL, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.88	2/4644 (0.0%)	0.93	9/6314 (0.1%)
1	B	0.68	0/4609	0.79	3/6274 (0.0%)
1	C	0.78	3/4453 (0.1%)	0.85	9/6079 (0.1%)
1	D	0.55	1/4453 (0.0%)	0.69	1/6078 (0.0%)
All	All	0.73	6/18159 (0.0%)	0.82	22/24745 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	791	GLU	CD-OE2	5.42	1.31	1.25
1	D	800	PRO	N-CD	5.25	1.55	1.47
1	C	788	SER	CB-OG	-5.13	1.35	1.42
1	C	1048	VAL	C-O	5.07	1.32	1.23
1	A	911	GLU	CD-OE2	5.06	1.31	1.25
1	A	877	ASP	N-CA	5.01	1.56	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	775	ASP	CB-CG-OD1	8.88	126.30	118.30
1	A	594	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	C	633	ASP	CB-CG-OD2	7.17	124.75	118.30
1	C	544	ASP	CB-CG-OD1	7.01	124.61	118.30
1	C	696	ASP	CB-CG-OD1	6.74	124.36	118.30
1	B	719	ASP	CB-CG-OD1	6.24	123.92	118.30
1	C	539	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	C	809	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	C	929	PRO	C-N-CD	5.96	140.91	128.40
1	C	791	GLU	OE1-CD-OE2	5.95	130.44	123.30
1	A	974	ARG	NE-CZ-NH1	5.94	123.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	594	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	A	798	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	C	539	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	D	799	ASP	C-N-CD	5.52	139.99	128.40
1	A	768	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	A	921	MET	CG-SD-CE	5.41	108.86	100.20
1	A	798	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	560	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	C	535	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	750	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	539	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	4557	0	4449	44	0
1	B	4522	0	4382	45	0
1	C	4368	0	4069	53	0
1	D	4367	0	4013	33	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	4	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	16929	167	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.

All (167) 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
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
1:A:677:CYS:H	1:A:713:HIS:HD2	1.26	0.84
1:D:1026:ILE:HD12	1:D:1026:ILE:O	1.78	0.82
1:A:481:ALA:O	1:A:485:VAL:HG12	1.80	0.81
1:A:630:ASN:HD21	1:A:662:ASN:HD21	1.32	0.77
1:C:486:ASN:OD1	1:C:1066:ARG:CG	2.26	0.73
1:A:485:VAL:HG11	1:A:1063:VAL:HG21	1.70	0.73
1:A:472:ARG:HB3	1:A:1026:ILE:CD1	2.21	0.71
1:C:481:ALA:O	1:C:485:VAL:HG22	1.92	0.69
1:B:549:ASP:HB3	1:B:783:GLN:HE22	1.58	0.68
1:A:485:VAL:HG11	1:A:1063:VAL:CG2	2.25	0.67
1:A:624:ASN:HD22	1:A:629:THR:C	1.99	0.66
1:A:549:ASP:HB3	1:A:783:GLN:HE22	1.60	0.65
1:A:780:ASN:HA	7:A:1270:HOH:O	1.97	0.64
1:C:677:CYS:H	1:C:713:HIS:HD2	1.44	0.64
1:B:484:THR:HG23	1:B:1016:LEU:H	1.62	0.63
1:C:989:LYS:N	5:C:1104:CL:CL	2.68	0.63
1:D:838:HIS:O	1:D:839:GLU:HB2	1.97	0.62
1:C:486:ASN:HD22	1:C:486:ASN:N	1.97	0.62
1:B:630:ASN:HD21	1:B:662:ASN:HD21	1.48	0.62
1:B:677:CYS:H	1:B:713:HIS:HD2	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:GLU:O	1:C:494:ARG:NH2	2.32	0.62
1:C:942:LEU:O	1:C:943:LYS:C	2.37	0.61
1:A:799:ASP:OD1	1:A:800:PRO:HD2	2.00	0.60
1:C:559:MET:O	7:C:1225:HOH:O	2.16	0.60
1:C:633:ASP:OD1	1:C:951:ARG:NH1	2.34	0.60
1:B:780:ASN:N	6:B:1105:GOL:O1	2.29	0.60
1:C:485:VAL:HG23	1:C:486:ASN:HD22	1.65	0.59
1:C:485:VAL:C	1:C:486:ASN:HD22	2.05	0.59
1:D:630:ASN:HD21	1:D:662:ASN:HD21	1.48	0.59
1:C:577:ASN:HB2	7:C:1230:HOH:O	2.03	0.59
1:D:500:ASN:HD22	1:D:500:ASN:N	1.97	0.59
1:C:677:CYS:H	1:C:713:HIS:CD2	2.20	0.59
1:A:677:CYS:H	1:A:713:HIS:CD2	2.13	0.58
1:A:757:ALA:HA	1:C:757:ALA:HB2	1.85	0.58
1:A:851:GLN:O	1:A:854:SER:HB3	2.04	0.57
1:A:1045:GLN:OE1	1:A:1045:GLN:HA	2.05	0.57
1:B:619:LEU:HD11	1:B:654:PHE:CD2	2.39	0.57
1:C:624:ASN:ND2	1:C:630:ASN:OD1	2.38	0.57
1:B:481:ALA:O	1:B:485:VAL:HG13	2.05	0.56
1:D:500:ASN:H	1:D:500:ASN:ND2	1.97	0.56
1:B:599:ASP:OD1	1:B:601:TRP:N	2.38	0.56
1:A:757:ALA:CA	1:C:757:ALA:HB2	2.36	0.55
1:A:930:PRO:HD3	7:A:1242:HOH:O	2.06	0.54
1:A:891[B]:MET:HE1	1:A:918:VAL:HG11	1.90	0.54
1:A:485:VAL:CG1	1:A:1063:VAL:HG21	2.35	0.54
1:C:549:ASP:HB3	1:C:783:GLN:HE22	1.73	0.54
1:B:753:GLY:HA2	6:B:1105:GOL:H12	1.88	0.54
1:A:485:VAL:O	1:A:485:VAL:HG22	2.08	0.54
1:A:860:ARG:O	1:A:861:TRP:C	2.44	0.53
1:D:549:ASP:HB3	1:D:783:GLN:HE22	1.72	0.53
1:B:860:ARG:O	1:B:863:GLN:N	2.39	0.53
1:B:471:ASP:OD2	1:B:475:LYS:HE3	2.09	0.53
1:A:722:GLY:HA2	1:A:748:THR:OG1	2.10	0.52
1:B:881:VAL:O	1:B:884:SER:N	2.42	0.52
1:C:763:VAL:HA	1:C:767:VAL:HG12	1.91	0.52
1:D:835:VAL:HA	1:D:838:HIS:CE1	2.44	0.52
1:D:1026:ILE:HD12	1:D:1026:ILE:C	2.26	0.52
1:D:1063:VAL:HB	1:D:1064:PRO:HD2	1.92	0.51
1:D:597:THR:HG22	1:D:597:THR:O	2.09	0.51
1:D:881:VAL:H	1:D:884:SER:HG	1.57	0.51
1:A:677:CYS:N	1:A:713:HIS:HD2	2.01	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:777:LEU:HD21	1:C:818:ARG:HD2	1.93	0.50
1:A:486:ASN:HD21	1:A:1066:ARG:H	1.58	0.50
1:C:697:LEU:O	1:C:698:LYS:C	2.50	0.50
1:C:777:LEU:CD2	1:C:818:ARG:HD2	2.42	0.50
1:B:836:TYR:CD2	1:D:791:GLU:HG2	2.47	0.50
1:C:699:TYR:HE2	1:C:700:TYR:CE1	2.30	0.50
1:C:942:LEU:O	1:C:945:GLU:N	2.45	0.50
1:B:950:VAL:CG2	1:B:955:LEU:HD11	2.42	0.49
1:A:849:LYS:HE2	7:A:1276:HOH:O	2.12	0.49
1:C:630:ASN:HD21	1:C:662:ASN:HD21	1.59	0.49
1:B:780:ASN:H	6:B:1105:GOL:HO1	1.58	0.49
1:A:548:ARG:HD2	1:A:548:ARG:C	2.33	0.49
1:A:1045:GLN:OE1	1:A:1045:GLN:CA	2.61	0.49
1:B:494:ARG:HB3	1:B:495:PRO:CD	2.42	0.49
1:C:539:ARG:HG3	1:C:539:ARG:O	2.12	0.49
1:D:1025:ASP:OD2	1:D:1031:THR:HG22	2.12	0.49
1:C:1048:VAL:O	1:C:1062:LYS:HA	2.13	0.49
1:D:845:PHE:C	1:D:845:PHE:CD2	2.86	0.48
1:C:1043:ASP:OD1	1:C:1043:ASP:C	2.51	0.48
1:A:498:LEU:O	1:A:501:ALA:HB2	2.14	0.48
1:C:656:CYS:HA	1:C:881:VAL:CG1	2.43	0.48
1:B:722:GLY:HA3	7:B:1224:HOH:O	2.13	0.47
1:B:478:THR:HA	1:B:1061:ILE:HG21	1.96	0.47
1:B:694:LYS:NZ	1:B:876:GLY:O	2.47	0.47
1:C:698:LYS:O	1:C:702:ASN:N	2.48	0.47
1:D:535:ARG:HD3	1:D:741:GLY:O	2.15	0.47
1:C:963:ALA:O	1:C:967:VAL:HG23	2.14	0.47
1:C:990:VAL:HG23	5:C:1104:CL:CL	2.52	0.47
1:B:812:PHE:HE1	1:D:862:HIS:CD2	2.33	0.47
1:A:929:PRO:HD3	1:A:933:TRP:CZ2	2.50	0.46
1:A:849:LYS:HA	1:A:861:TRP:CZ3	2.50	0.46
1:B:650:LEU:HA	1:B:676:LEU:HB2	1.98	0.46
1:D:1023:PHE:CE1	1:D:1033:VAL:HG22	2.51	0.46
1:C:838:HIS:O	1:C:839:GLU:HB2	2.15	0.46
1:C:1036:ASN:OD1	1:C:1036:ASN:C	2.53	0.46
1:C:677:CYS:N	1:C:713:HIS:HD2	2.13	0.45
1:D:951:ARG:O	1:D:954:SER:OG	2.23	0.45
1:A:860:ARG:HG2	1:A:863:GLN:NE2	2.32	0.45
1:C:494:ARG:HB3	1:C:495:PRO:CD	2.47	0.45
1:D:718:KCX:CX	7:D:1223:HOH:O	2.64	0.45
1:C:699:TYR:CE2	1:C:700:TYR:CE1	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:HIS:CE1	1:B:559:MET:HB3	2.52	0.45
1:B:737:ARG:NH2	1:B:768:ASP:OD1	2.50	0.45
1:B:1035:VAL:O	1:B:1052:PHE:HA	2.17	0.45
1:D:678:GLU:HA	1:D:714:ILE:O	2.17	0.45
1:B:634:ASN:HD21	1:B:959:ALA:N	2.15	0.44
1:B:677:CYS:H	1:B:713:HIS:CD2	2.32	0.44
1:A:551:HIS:CE1	1:A:559:MET:HB3	2.53	0.44
1:A:812:PHE:HE1	1:C:862:HIS:CD2	2.35	0.44
1:C:472:ARG:CD	1:C:1026:ILE:HD11	2.48	0.44
1:B:519:LYS:HG2	1:B:612:PRO:O	2.18	0.44
1:A:812:PHE:CE1	1:C:862:HIS:CD2	3.06	0.43
1:A:716:ALA:HA	1:A:745:HIS:O	2.18	0.43
1:D:548:ARG:HD2	1:D:548:ARG:C	2.39	0.43
1:D:1026:ILE:HG22	1:D:1032:LEU:HG	1.99	0.43
1:A:486:ASN:ND2	1:A:1066:ARG:H	2.17	0.43
1:B:799:ASP:OD1	1:B:799:ASP:C	2.57	0.43
1:B:1043:ASP:OD1	1:B:1043:ASP:C	2.57	0.43
1:D:527:PRO:HB2	1:D:713:HIS:CD2	2.54	0.43
1:D:694:LYS:NZ	1:D:876:GLY:O	2.52	0.43
1:C:478:THR:HA	1:C:1061:ILE:HG21	2.01	0.43
1:D:844:GLN:O	1:D:846:THR:N	2.52	0.43
1:D:1048:VAL:O	1:D:1062:LYS:HA	2.19	0.43
1:A:678:GLU:OE1	1:A:745:HIS:ND1	2.45	0.42
1:D:574:ALA:HB1	1:D:806:TRP:CG	2.54	0.42
1:D:988:PRO:O	1:D:992:THR:OG1	2.35	0.42
1:A:599:ASP:OD1	1:A:601:TRP:N	2.48	0.42
1:B:936:ALA:O	1:B:937:LEU:C	2.54	0.42
1:C:552:GLN:HG3	1:C:557:THR:OG1	2.20	0.42
1:C:696:ASP:O	1:C:699:TYR:HB3	2.20	0.42
1:A:756:ALA:CB	1:C:754:ILE:HG22	2.49	0.42
1:B:624:ASN:HD22	1:B:629:THR:C	2.23	0.42
1:A:541:LEU:O	1:A:769:ALA:HA	2.19	0.42
1:B:630:ASN:ND2	1:B:662:ASN:HD21	2.13	0.42
1:B:753:GLY:HA2	6:B:1105:GOL:C1	2.50	0.42
1:B:774:MET:O	1:B:775:ASP:C	2.58	0.42
1:A:715:ILE:HB	1:A:744:ILE:HD13	2.02	0.42
1:C:486:ASN:ND2	1:C:486:ASN:N	2.66	0.42
1:A:774:MET:O	1:A:775:ASP:C	2.57	0.42
1:B:494:ARG:CB	1:B:495:PRO:CD	2.98	0.41
1:A:929:PRO:HD3	1:A:933:TRP:CE2	2.55	0.41
1:C:987:TYR:HB3	1:C:990:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:667:MET:HG2	1:D:677:CYS:SG	2.61	0.41
1:B:716:ALA:HA	1:B:745:HIS:O	2.20	0.41
1:A:759:VAL:O	1:A:763:VAL:HG23	2.20	0.41
1:B:472:ARG:CB	1:B:1026:ILE:HD11	2.51	0.41
1:C:472:ARG:HG2	1:C:1026:ILE:HD11	2.03	0.41
1:B:650:LEU:C	1:B:650:LEU:HD23	2.41	0.41
1:B:678:GLU:OE1	1:B:745:HIS:ND1	2.48	0.41
1:A:549:ASP:HB3	1:A:783:GLN:NE2	2.31	0.41
1:B:621:ARG:HB2	1:B:625:GLY:O	2.20	0.41
1:C:793:LEU:HD23	1:C:793:LEU:HA	1.80	0.41
1:D:898:GLN:O	1:D:899:ASP:C	2.59	0.41
1:B:548:ARG:C	1:B:548:ARG:HD2	2.42	0.40
1:B:756:ALA:CB	1:D:754:ILE:HG22	2.51	0.40
1:C:965:ARG:HA	1:C:981:PHE:CE1	2.56	0.40
1:D:987:TYR:HB3	1:D:990:VAL:HB	2.03	0.40
1:B:638:TYR:O	1:B:642:GLN:HG2	2.21	0.40
1:B:860:ARG:O	1:B:862:HIS:N	2.54	0.40
1:C:485:VAL:CG2	1:C:486:ASN:ND2	2.72	0.40
1:C:686:ASP:OD1	1:C:686:ASP:C	2.59	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	595/632 (94%)	577 (97%)	16 (3%)	2 (0%)	41	51
1	B	595/632 (94%)	570 (96%)	22 (4%)	3 (0%)	29	40
1	C	592/632 (94%)	557 (94%)	32 (5%)	3 (0%)	29	40
1	D	595/632 (94%)	566 (95%)	25 (4%)	4 (1%)	22	30
All	All	2377/2528 (94%)	2270 (96%)	95 (4%)	12 (0%)	29	40

All (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
1	C	877	ASP
1	C	943	LYS
1	C	1028	LYS
1	A	877	ASP
1	B	861	TRP
1	D	844	GLN
1	B	906	VAL

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%)	452 (97%)	15 (3%)	39	53
1	B	456/519 (88%)	442 (97%)	14 (3%)	40	54
1	C	417/519 (80%)	394 (94%)	23 (6%)	21	29
1	D	411/519 (79%)	395 (96%)	16 (4%)	32	44
All	All	1751/2076 (84%)	1683 (96%)	68 (4%)	32	44

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	537	GLU
1	A	557	THR
1	A	566	ARG
1	A	584	TRP
1	A	629	THR
1	A	720	MET

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Mol	Chain	Res	Type
1	A	850	GLU
1	A	899	ASP
1	A	909	ASP
1	A	926	LEU
1	A	957	LYS
1	A	999	ASP
1	A	1044	SER
1	B	484	THR
1	B	485	VAL
1	B	510	ASN
1	B	514	VAL
1	B	548	ARG
1	B	557	THR
1	B	584	TRP
1	B	661	GLU
1	B	672	GLU
1	B	720	MET
1	B	854	SER
1	B	855	LEU
1	B	899	ASP
1	B	926	LEU
1	C	486	ASN
1	C	514	VAL
1	C	521	LEU
1	C	558	ARG
1	C	566	ARG
1	C	577	ASN
1	C	584	TRP
1	C	629	THR
1	C	687	ILE
1	C	690	SER
1	C	706	GLU
1	C	720	MET
1	C	734	LYS
1	C	775	ASP
1	C	794	SER
1	C	797	GLU
1	C	826	SER
1	C	897	SER
1	C	998	SER
1	C	1000	THR
1	C	1031	THR

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Mol	Chain	Res	Type
1	C	1042	THR
1	C	1066	ARG
1	D	494	ARG
1	D	500	ASN
1	D	557	THR
1	D	566	ARG
1	D	584	TRP
1	D	629	THR
1	D	720	MET
1	D	794	SER
1	D	850	GLU
1	D	897	SER
1	D	998	SER
1	D	1026	ILE
1	D	1031	THR
1	D	1037	GLN
1	D	1039	VAL
1	D	1063	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) 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	863	GLN
1	B	512	ASN
1	B	577	ASN
1	B	624	ASN
1	B	630	ASN
1	B	713	HIS
1	B	783	GLN
1	B	820	GLN
1	C	486	ASN
1	C	577	ASN
1	C	624	ASN
1	C	630	ASN
1	C	642	GLN

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Mol	Chain	Res	Type
1	C	702	ASN
1	C	713	HIS
1	C	783	GLN
1	C	1057	GLN
1	D	486	ASN
1	D	500	ASN
1	D	577	ASN
1	D	624	ASN
1	D	630	ASN
1	D	713	HIS
1	D	783	GLN
1	D	863	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	D	718	1,2	9,11,12	0.64	0	5,12,14	2.21	2 (40%)
1	KCX	B	718	1,2	9,11,12	0.83	0	5,12,14	2.95	2 (40%)
1	KCX	C	718	1,2	9,11,12	0.85	0	5,12,14	2.02	2 (40%)
1	KCX	A	718	1,2	9,11,12	1.71	1 (11%)	5,12,14	2.92	3 (60%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	718	KCX	CX-NZ	4.05	1.42	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	718	KCX	CE-NZ-CX	5.25	130.31	121.89
1	B	718	KCX	OQ1-CX-NZ	4.44	131.84	124.96
1	B	718	KCX	CE-NZ-CX	4.31	128.80	121.89
1	D	718	KCX	CE-NZ-CX	3.92	128.18	121.89
1	C	718	KCX	CE-NZ-CX	2.90	126.54	121.89
1	A	718	KCX	CD-CE-NZ	2.83	120.30	112.21
1	C	718	KCX	OQ1-CX-NZ	-2.48	121.11	124.96
1	D	718	KCX	OQ1-CX-NZ	-2.34	121.33	124.96
1	A	718	KCX	CD-CG-CB	2.34	121.90	113.62

There are no chirality outliers.

All (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
1	C	718	KCX	O-C-CA-CB
1	D	718	KCX	O-C-CA-CB
1	B	718	KCX	CG-CD-CE-NZ
1	C	718	KCX	CE-CD-CG-CB
1	C	718	KCX	N-CA-CB-CG
1	D	718	KCX	CE-CD-CG-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 monosaccharides 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	1.80	2 (40%)	6,6,6	1.43	1 (16%)
6	GOL	B	1105	-	5,5,5	0.38	0	5,5,5	1.13	1 (20%)
6	GOL	A	1105	-	5,5,5	0.41	0	5,5,5	0.93	0
3	OXL	D	1102	-	5,5,5	1.74	1 (20%)	6,6,6	1.28	0
3	OXL	B	1102	-	5,5,5	2.14	1 (20%)	6,6,6	0.65	0
3	OXL	A	1102	-	5,5,5	1.83	2 (40%)	6,6,6	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	C	1102	-	-	4/4/4/4	-
6	GOL	B	1105	-	-	2/4/4/4	-
6	GOL	A	1105	-	-	0/4/4/4	-
3	OXL	D	1102	-	-	4/4/4/4	-
3	OXL	B	1102	-	-	4/4/4/4	-
3	OXL	A	1102	-	-	4/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1102	OXL	C2-C1	-3.57	1.44	1.54
3	C	1102	OXL	C2-C1	-2.54	1.47	1.54
3	C	1102	OXL	O1-C1	2.46	1.29	1.22
3	A	1102	OXL	C2-C1	-2.39	1.47	1.54
3	A	1102	OXL	O4-C2	-2.15	1.24	1.30
3	D	1102	OXL	O1-C1	2.15	1.28	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1102	OXL	O4-C2-C1	2.38	120.22	113.16
6	B	1105	GOL	C3-C2-C1	-2.20	103.17	111.70

There are no chirality outliers.

All (18) 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
3	B	1102	OXL	O3-C1-C2-O4
3	D	1102	OXL	O1-C1-C2-O2
3	D	1102	OXL	O1-C1-C2-O4
3	D	1102	OXL	O3-C1-C2-O2
3	D	1102	OXL	O3-C1-C2-O4
3	C	1102	OXL	O1-C1-C2-O4
3	A	1102	OXL	O1-C1-C2-O2
3	C	1102	OXL	O1-C1-C2-O2
3	C	1102	OXL	O3-C1-C2-O4
3	A	1102	OXL	O3-C1-C2-O2
3	C	1102	OXL	O3-C1-C2-O2
6	B	1105	GOL	O2-C2-C3-O3
6	B	1105	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1105	GOL	4	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%)	0.01	17 (2%) 51 59	29, 50, 82, 122	9 (1%)
1	B	596/632 (94%)	0.28	44 (7%) 14 18	44, 64, 109, 153	7 (1%)
1	C	595/632 (94%)	0.84	102 (17%) 1 1	35, 96, 183, 235	4 (0%)
1	D	596/632 (94%)	0.69	90 (15%) 2 2	51, 93, 142, 166	6 (1%)
All	All	2383/2528 (94%)	0.46	253 (10%) 6 8	29, 70, 150, 235	26 (1%)

All (253) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	896	VAL	8.3
1	C	934	PRO	8.1
1	D	875	PHE	6.2
1	C	907	SER	5.9
1	C	933	TRP	5.8
1	D	906	VAL	5.6
1	D	914	PHE	5.4
1	D	981	PHE	5.3
1	D	944	GLY	5.2
1	D	961	LEU	5.2
1	B	937	LEU	5.1
1	B	909	ASP	5.0
1	D	907	SER	5.0
1	C	905	VAL	5.0
1	A	968	ILE	4.9
1	C	1050	VAL	4.9
1	C	912	VAL	4.8
1	D	1036	ASN	4.8
1	B	906	VAL	4.7
1	D	972	LEU	4.6
1	C	509	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	906	VAL	4.3
1	D	1067	ALA	4.3
1	D	947	PRO	4.3
1	C	1001	TYR	4.3
1	B	933	TRP	4.2
1	C	894	MET	4.2
1	B	902	VAL	4.2
1	D	1019	GLY	4.2
1	C	914	PHE	4.2
1	D	903	ALA	4.2
1	B	908	PRO	4.1
1	B	874	MET	4.1
1	D	896	VAL	4.0
1	C	903	ALA	4.0
1	D	1044	SER	4.0
1	D	895	MET	3.9
1	B	867	ALA	3.9
1	C	900	LEU	3.9
1	D	898	GLN	3.9
1	D	1046	GLY	3.8
1	C	512	ASN	3.8
1	C	891[A]	MET	3.8
1	C	947	PRO	3.8
1	B	891[A]	MET	3.7
1	D	974	ARG	3.7
1	C	485	VAL	3.7
1	C	874	MET	3.7
1	D	1052	PHE	3.7
1	D	902	VAL	3.7
1	C	779	GLY	3.7
1	B	895	MET	3.7
1	B	900	LEU	3.7
1	D	479	TYR	3.6
1	C	922	LEU	3.6
1	D	984	TYR	3.6
1	C	981	PHE	3.6
1	C	1067	ALA	3.6
1	C	1039	VAL	3.6
1	D	1001	TYR	3.6
1	D	891[A]	MET	3.6
1	D	933	TRP	3.6
1	D	1050	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	1040	SER	3.5
1	A	485	VAL	3.5
1	B	893	LEU	3.5
1	C	950	VAL	3.5
1	D	941	ALA	3.5
1	C	1036	ASN	3.4
1	C	1048	VAL	3.4
1	C	1046	GLY	3.4
1	B	963	ALA	3.4
1	D	478	THR	3.4
1	D	973	GLU	3.4
1	D	1014	TYR	3.3
1	D	894	MET	3.3
1	D	923	LYS	3.3
1	B	907	SER	3.3
1	D	905	VAL	3.3
1	C	1044	SER	3.3
1	D	908	PRO	3.2
1	C	476	LEU	3.2
1	C	892	ALA	3.2
1	B	904	ASP	3.2
1	C	897	SER	3.2
1	D	501	ALA	3.2
1	D	1040	SER	3.2
1	B	934	PRO	3.2
1	D	525	LEU	3.1
1	D	950	VAL	3.1
1	B	905	VAL	3.1
1	B	942	LEU	3.1
1	B	948	TYR	3.1
1	A	785	CYS	3.1
1	C	953	GLY	3.1
1	C	973	GLU	3.1
1	C	908	PRO	3.1
1	D	1041	ALA	3.1
1	D	904	ASP	3.1
1	D	948	TYR	3.1
1	A	835	VAL	3.0
1	D	911	GLU	3.0
1	C	781	THR	3.0
1	C	910	ARG	3.0
1	C	511	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	874	MET	3.0
1	C	1052	PHE	2.9
1	D	1061	ILE	2.9
1	C	510	ASN	2.9
1	D	1042	THR	2.9
1	A	750	ASP	2.9
1	D	960	ASP	2.9
1	C	944	GLY	2.9
1	B	896	VAL	2.9
1	C	1047	MET	2.9
1	C	483	VAL	2.8
1	D	1039	VAL	2.8
1	B	751	THR	2.8
1	C	875	PHE	2.8
1	B	784	PRO	2.8
1	C	923	LYS	2.8
1	D	631	TYR	2.8
1	B	875	PHE	2.8
1	D	979	PHE	2.8
1	B	781	THR	2.7
1	B	941	ALA	2.7
1	A	784	PRO	2.7
1	B	755	ALA	2.7
1	C	963	ALA	2.7
1	D	936	ALA	2.7
1	C	1057	GLN	2.7
1	C	831	PRO	2.7
1	C	481	ALA	2.7
1	C	1041	ALA	2.7
1	C	1066	ARG	2.7
1	D	912	VAL	2.7
1	A	778	SER	2.7
1	D	1063	VAL	2.7
1	A	752	SER	2.7
1	C	556	ALA	2.7
1	D	897	SER	2.7
1	C	634	ASN	2.7
1	A	755	ALA	2.6
1	C	546	THR	2.6
1	C	477	LEU	2.6
1	C	974	ARG	2.6
1	C	753	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	1043	ASP	2.6
1	B	698	LYS	2.6
1	D	1037	GLN	2.6
1	D	942	LEU	2.6
1	C	780	ASN	2.6
1	D	951	ARG	2.6
1	C	1000	THR	2.5
1	D	943	LYS	2.5
1	C	486	ASN	2.5
1	C	1018	ASP	2.5
1	B	869	ALA	2.5
1	D	1048	VAL	2.5
1	C	936	ALA	2.5
1	C	909	ASP	2.5
1	C	873	GLN	2.5
1	B	1067	ALA	2.5
1	B	512	ASN	2.5
1	C	754	ILE	2.5
1	C	911	GLU	2.5
1	C	976	VAL	2.4
1	D	483	VAL	2.4
1	D	499	GLU	2.4
1	A	779	GLY	2.4
1	D	638	TYR	2.4
1	C	587	ALA	2.4
1	D	1049	THR	2.4
1	A	753	GLY	2.4
1	D	901	THR	2.4
1	B	753	GLY	2.4
1	D	909	ASP	2.4
1	C	921	MET	2.4
1	A	751	THR	2.4
1	D	946	LYS	2.4
1	C	751	THR	2.4
1	C	1019	GLY	2.3
1	C	895	MET	2.3
1	D	963	ALA	2.3
1	D	962	ASP	2.3
1	D	1038	ALA	2.3
1	C	1016	LEU	2.3
1	C	1064	PRO	2.3
1	D	899	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	910	ARG	2.3
1	D	753	GLY	2.3
1	B	903	ALA	2.3
1	C	828	LEU	2.3
1	D	749	HIS	2.3
1	A	828	LEU	2.3
1	D	922	LEU	2.3
1	D	641	ARG	2.2
1	D	1003	PRO	2.2
1	B	554	LEU	2.2
1	D	857	LEU	2.2
1	B	553	SER	2.2
1	C	1035	VAL	2.2
1	D	967	VAL	2.2
1	C	965	ARG	2.2
1	C	901	THR	2.2
1	C	785	CYS	2.2
1	C	1034	ILE	2.2
1	D	1047	MET	2.2
1	C	1038	ALA	2.2
1	A	554	LEU	2.2
1	B	773	ALA	2.2
1	C	773	ALA	2.2
1	D	781	THR	2.2
1	B	831	PRO	2.2
1	B	936	ALA	2.1
1	C	478	THR	2.1
1	C	513	GLY	2.1
1	A	961	LEU	2.1
1	C	553	SER	2.1
1	C	924	GLY	2.1
1	B	922	LEU	2.1
1	C	1054	LEU	2.1
1	C	843	GLY	2.1
1	D	919	VAL	2.1
1	B	944	GLY	2.1
1	D	755	ALA	2.1
1	C	949	THR	2.1
1	C	1049	THR	2.1
1	C	554	LEU	2.1
1	D	910	ARG	2.1
1	D	675	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	856	GLY	2.1
1	A	967	VAL	2.1
1	C	776	ALA	2.1
1	C	1061	ILE	2.1
1	B	509	ALA	2.1
1	D	784	PRO	2.1
1	C	631	TYR	2.1
1	D	1018	ASP	2.1
1	D	1043	ASP	2.1
1	D	480	LEU	2.1
1	D	550	GLY	2.1
1	D	642	GLN	2.1
1	B	947	PRO	2.0
1	C	777	LEU	2.0
1	D	500	ASN	2.0
1	C	962	ASP	2.0
1	C	557	THR	2.0
1	C	902	VAL	2.0
1	C	550	GLY	2.0
1	A	754	ILE	2.0
1	B	857	LEU	2.0
1	B	938	GLN	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. 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	B-factors(Å^2)	Q<0.9
1	KCX	C	718	12/13	0.93	0.23	65,73,85,90	0
1	KCX	D	718	12/13	0.97	0.22	71,75,79,80	0
1	KCX	A	718	12/13	0.98	0.22	33,37,42,44	0
1	KCX	B	718	12/13	0.99	0.22	49,54,55,59	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 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	B-factors(Å^2)	Q<0.9
4	MG	C	1103	1/1	0.81	0.23	44,44,44,44	0
4	MG	B	1103	1/1	0.82	0.07	51,51,51,51	0
4	MG	A	1103	1/1	0.83	0.10	49,49,49,49	0
4	MG	D	1103	1/1	0.86	0.18	66,66,66,66	0
5	CL	C	1104	1/1	0.86	0.09	78,78,78,78	0
5	CL	B	1104	1/1	0.87	0.18	67,67,67,67	0
3	OXL	C	1102	6/6	0.90	0.21	63,74,78,80	0
3	OXL	D	1102	6/6	0.91	0.16	66,72,74,76	0
2	ZN	D	1101	1/1	0.94	0.12	56,56,56,56	1
6	GOL	B	1105	6/6	0.94	0.28	55,59,66,73	0
5	CL	D	1104	1/1	0.95	0.09	104,104,104,104	0
2	ZN	C	1101	1/1	0.96	0.17	58,58,58,58	1
6	GOL	A	1105	6/6	0.96	0.37	49,53,54,57	0
3	OXL	B	1102	6/6	0.96	0.14	47,54,57,63	0
5	CL	A	1104	1/1	0.97	0.06	56,56,56,56	0
3	OXL	A	1102	6/6	0.98	0.16	40,48,53,55	0
2	ZN	B	1101	1/1	0.98	0.16	42,42,42,42	1
2	ZN	A	1101	1/1	0.99	0.15	37,37,37,37	1

6.5 Other polymers (i)

There are no such residues in this entry.