



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 01:20 PM UTC

PDB ID : 6V3O / pdb_00006v3o
Title : Crystal structure of the T-state of maize C4-phosphoenolpyruvate carboxylase in complex with citrate
Authors : Carrizosa-Carbajal, E.I.; Munoz-Clares, R.A.; Gonzalez-Segura, L.
Deposited on : 2019-11-26
Resolution : 2.91 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

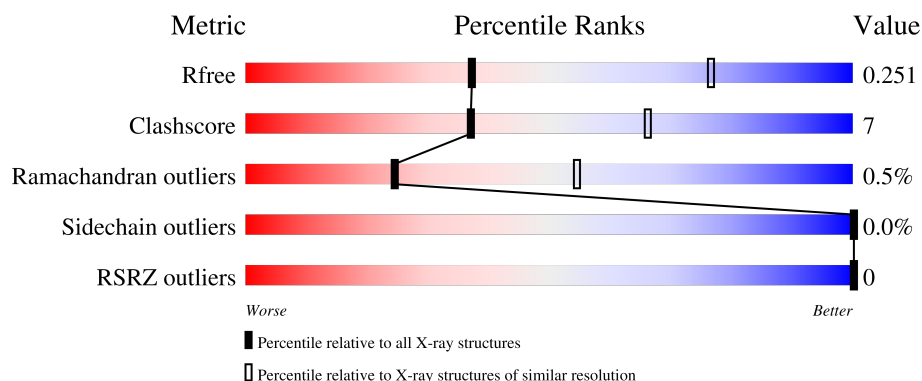
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

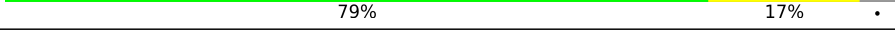
The reported resolution of this entry is 2.91 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	970	
1	B	970	
1	C	970	
1	D	970	
1	E	970	

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Mol	Chain	Length	Quality of chain
1	F	970	
1	G	970	
1	H	970	

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
2	SO4	A	1002	-	-	X	-
2	SO4	H	1002	-	-	X	-
3	FLC	C	1003	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 59688 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 Phosphoenolpyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	940	Total	C	N	O	S	0	0	0
			7488	4748	1307	1403	30			
1	B	942	Total	C	N	O	S	0	0	0
			7479	4737	1309	1403	30			
1	C	930	Total	C	N	O	S	0	0	0
			7390	4680	1294	1386	30			
1	D	927	Total	C	N	O	S	0	0	0
			7366	4665	1290	1381	30			
1	E	942	Total	C	N	O	S	0	0	0
			7502	4755	1310	1407	30			
1	F	944	Total	C	N	O	S	0	0	0
			7496	4748	1312	1406	30			
1	G	925	Total	C	N	O	S	0	0	0
			7359	4661	1289	1379	30			
1	H	930	Total	C	N	O	S	0	0	0
			7394	4684	1294	1386	30			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



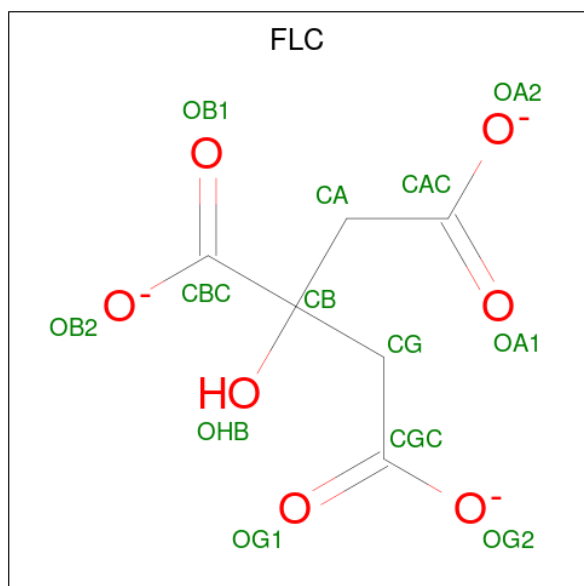
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0

- Molecule 3 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



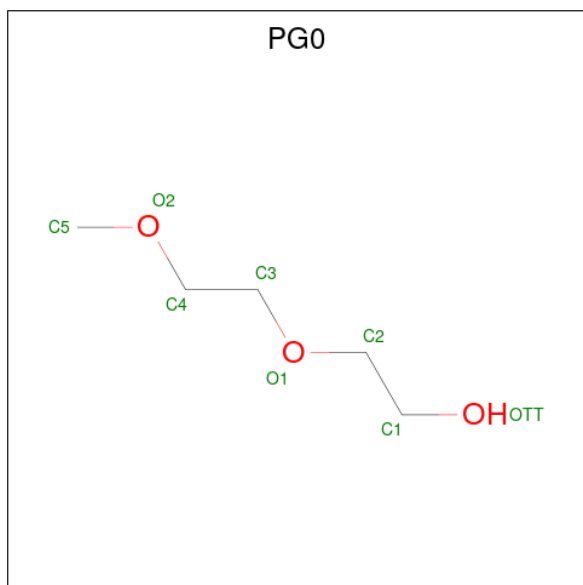
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0
3	B	1	Total C O 13 6 7	0	0
3	B	1	Total C O 13 6 7	0	0

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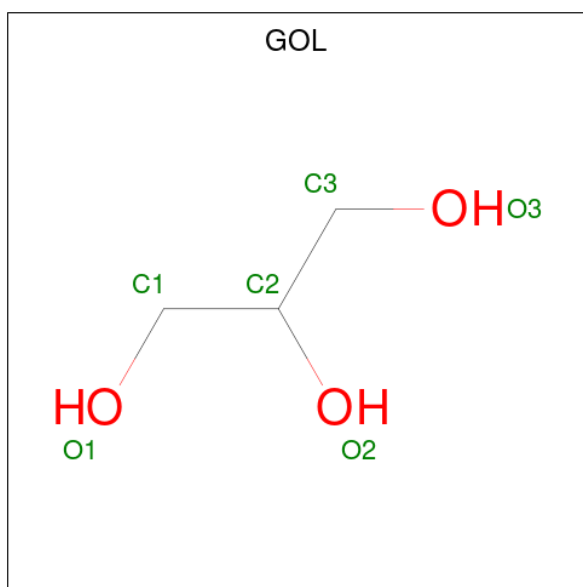
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			13	6	7		
3	E	1	Total	C	O	0	0
			13	6	7		
3	F	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: C₅H₁₂O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			8	5	3		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		

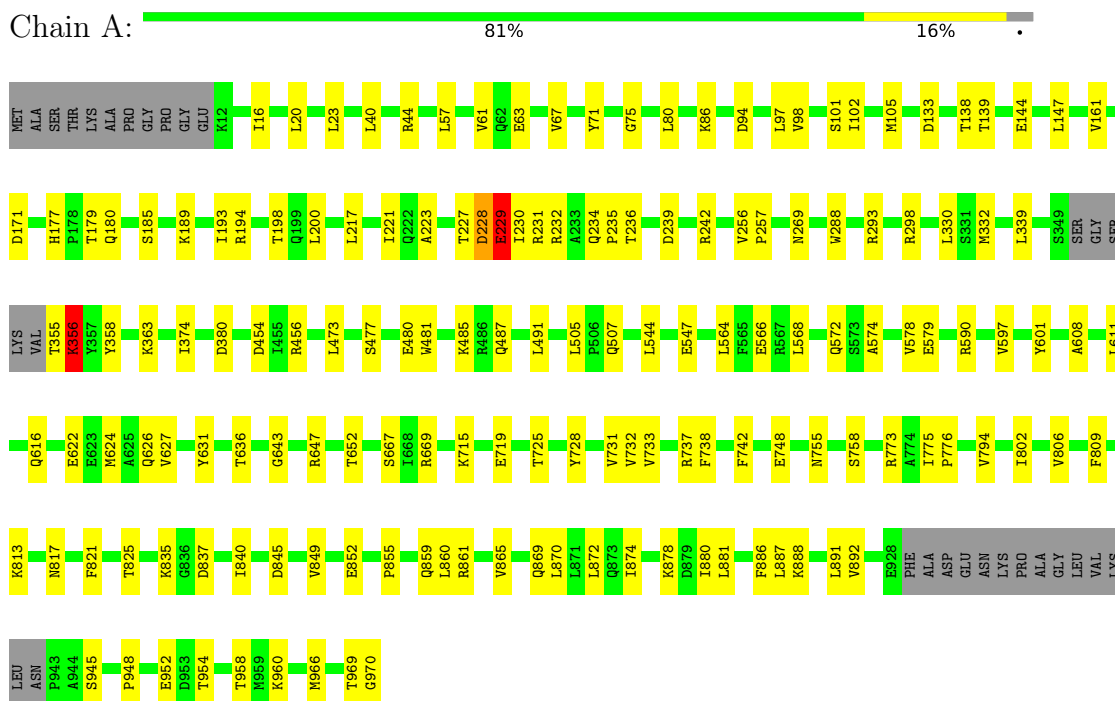
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	C	1	Total	O	0	0
			1	1		
6	F	1	Total	O	0	0
			1	1		
6	G	2	Total	O	0	0
			2	2		
6	H	1	Total	O	0	0
			1	1		

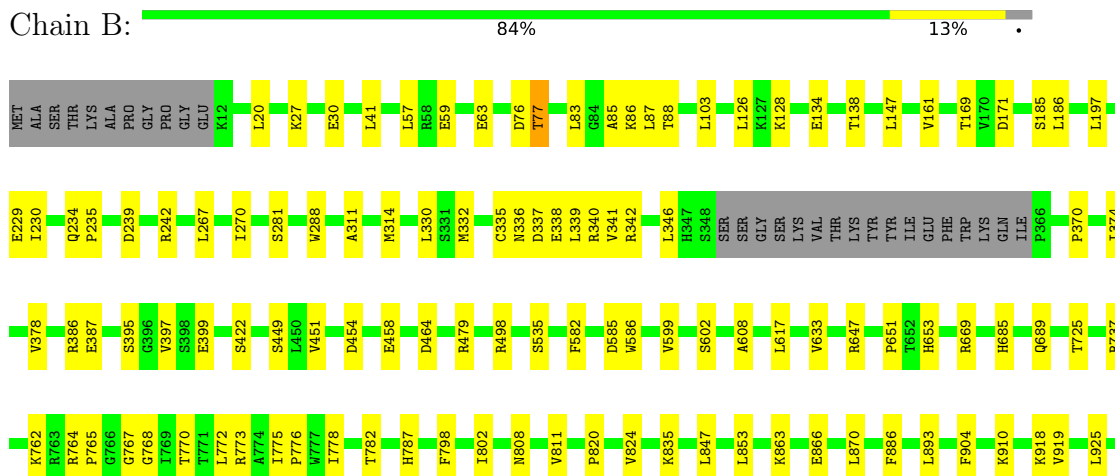
3 Residue-property plots

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: Phosphoenolpyruvate carboxylase



• Molecule 1: Phosphoenolpyruvate carboxylase



E928
F929
A930
D931
K934
P935
V939
P943
M966
T969
G970

• Molecule 1: Phosphoenolpyruvate carboxylase

Chain C:  81% 14%

MET ALA SER THR LYS PRO GLY PRO GLY LYS H13 I16 D17 L20 R21 D38 L41 V42 L52 H53 L57 R58 E59 F60 V61 Q62 E63 E66 V67 K74 G75 D76 L83 G84 A85 T88 Q89 D94 L97 V98 I102 L103 H104 M105
L108 K148 V151 S152 K156 S157 P158 E159 E160 V161 F162 K166 H177 H178 T179 S181 S185 A223 R226 T227 D228 E229 T230 R231 R232 N241 K258 T283 W288 R293 P332 C335 R340 V341 R342 E345 L346 S349 SER GLY SER
LYS VAL THR LYS TVR ILE GLU PHE TRP LYS ALA GLN I365 F370 P370 V373 I374 K381 T385 I400 S401 A402 S405 F406 T407 F412 L413 E414 P415 C419 V420 K421 L439 W443 F444 T445 D454 L455 R456 W481 K485 R498 R556 Q557 Q572
H596 R610 Q616 E622 Q626 F638 H639 G642 R647 G648 G649 T652 T671 V672 Q673 V676 C680 E686 T690 M703 W713 T775 P776 T782 H787 Q810 W811 L812 L813 E814 H815 E851 K854 L893 T908
I912 K918 V919 T920 P921 K927 GLU PHE ASP GLU ASN LYS L941 S945 P948 P949 G950 L951 E952 R953 T954 L955 L956 T957 T958 K959 G961 N968 T969 G970

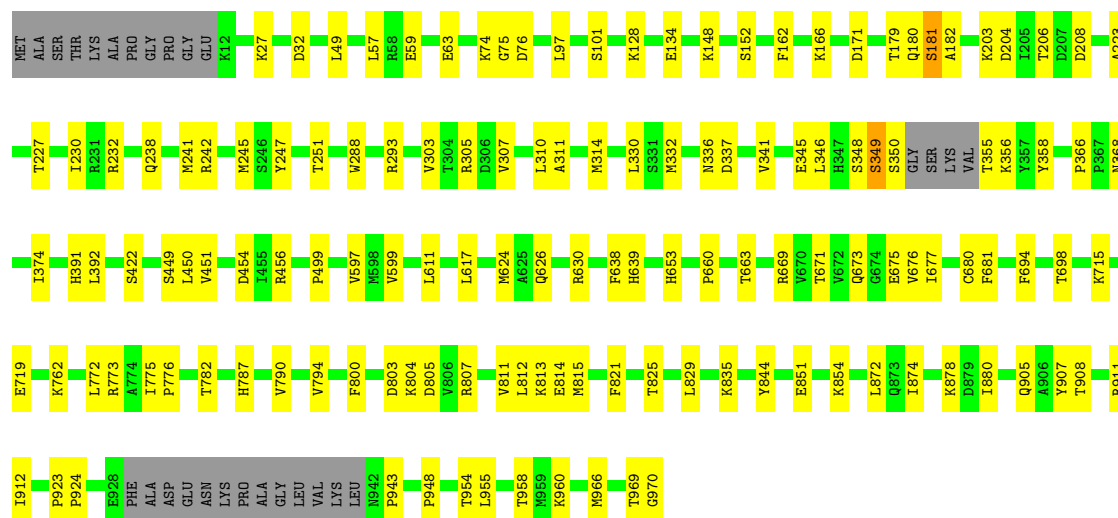
• Molecule 1: Phosphoenolpyruvate carboxylase

Chain D:  79% 17%

MET ALA SER THR LYS PRO GLY PRO GLY K12 Q19 Q91 V24 S29 F30 D31 Y37 R44 H53 R58 Q62 E66 V67 E72 K74 G75 D76 K79 L80 L83 G84 A85 K86 L87 T88 D94 L97 V98 I102 M105 K125
T138 L147 V151 K156 S157 P158 E159 E160 V161 H177 Q180 S181 L186 K189 N201 D214 T227 R231 R232 A233 Q234 M241 R242 Y243 S246 V256 P257 W288 R293 S331 M332 H347 S348 S349 SER GLY SER LYS VAL THR LYS
TYR TTR ILE GLU PHE TRP LYS GLN I365 F366 P367 R372 K381 T385 R388 H391 S398 E399 I400 S401 S404 F406 F407 I431 D454 I455 R456 S459 V465 L473 W481 K485 L494 P502 L505 P506 Q507 T508 I511 P525
S528 P531 S535 L568 Q572 V597 M598 V599 S602 A613 L617 E623 V627 L635 F638 H639 R647 G648 G649 P651 P660 T663 R669 V670 T671 G674 E675 I677 M703 W720 E726 E727 Q727 T728 F729 S730 R743 S744
T749 M754 I775 P776 T782 R785 F786 H787 L792 F798 V811 L812 M815 M831 K835 V849 A850 E851 E852 L853 K854 L870 L871 L872 Q873 I874 I880 F886 L887 K888 L891 V892 L893 R894 R895 I898 T899 V903 N916 F917 K918
V919 T920 P923 P924 L925 S926 K927 GLU PHE ASP GLU ASN LYS PRO PRO GLY LEU VAL LYS LEU ASN ALA S945 P948 E952 I956 M959 T969 G970

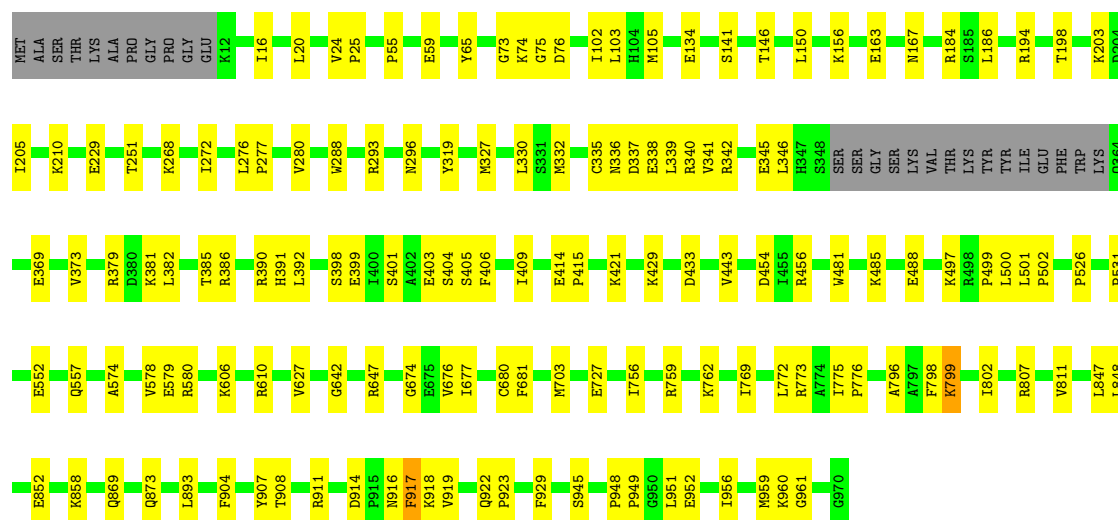
• Molecule 1: Phosphoenolpyruvate carboxylase

Chain E:  83% 14%



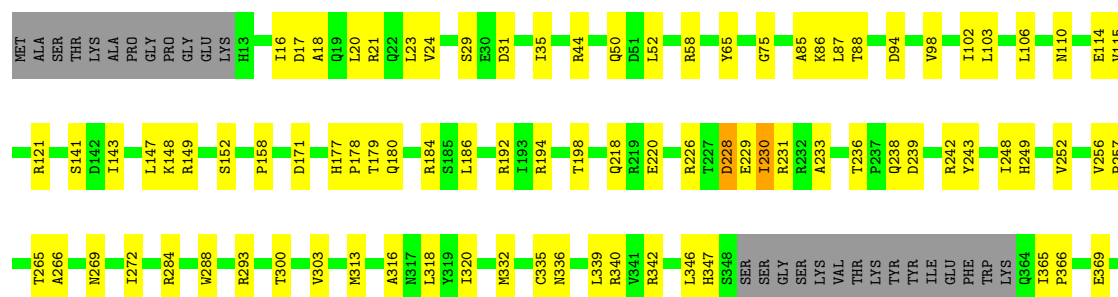
• Molecule 1: Phosphoenolpyruvate carboxylase

Chain F: 82% 15% •



• Molecule 1: Phosphoenolpyruvate carboxylase

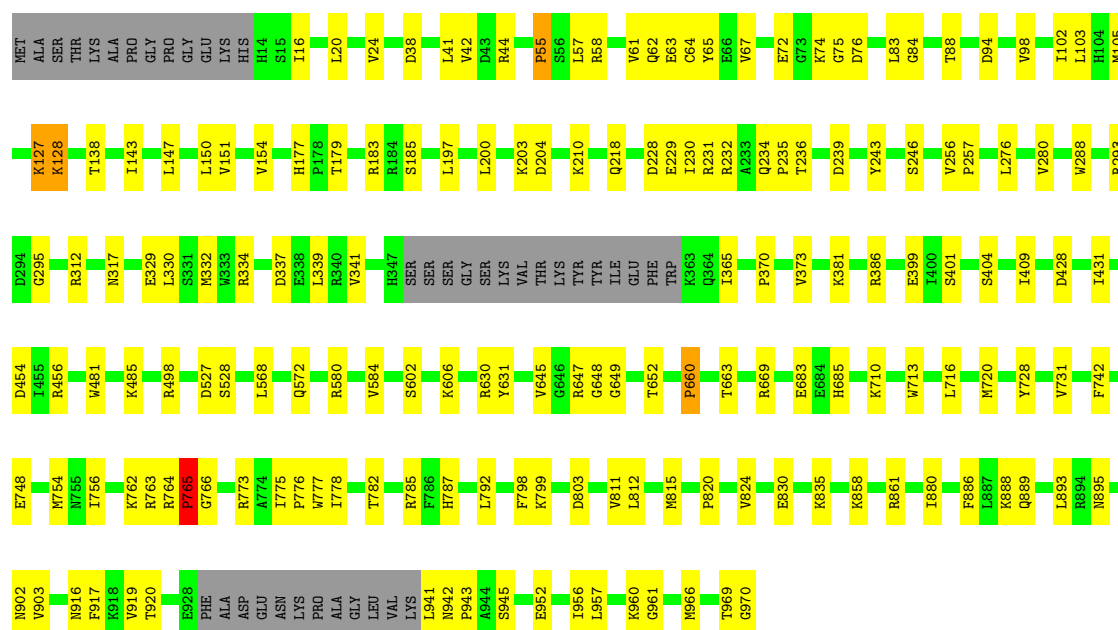
Chain G: 74% 21% 5%





• Molecule 1: Phosphoenolpyruvate carboxylase

Chain H: 78% 17% •



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	140.69Å 217.98Å 173.57Å 90.00° 91.05° 90.00°	Depositor
Resolution (Å)	49.20 – 2.91 49.20 – 2.91	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.20-2.91) 93.7 (49.20-2.91)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.218 , 0.249 0.220 , 0.251	Depositor DCC
R_{free} test set	11281 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.198 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	59688	wwPDB-VP
Average B, all atoms (Å ²)	60.0	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG0, FLC, GOL, SO4

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	0.23	1/7646 (0.0%)	0.43	1/10351 (0.0%)
1	B	0.22	0/7635	0.43	0/10339
1	C	0.24	1/7543 (0.0%)	0.43	1/10213 (0.0%)
1	D	0.27	1/7518 (0.0%)	0.46	1/10179 (0.0%)
1	E	0.24	1/7660 (0.0%)	0.45	3/10371 (0.0%)
1	F	0.25	1/7652 (0.0%)	0.44	1/10363 (0.0%)
1	G	0.21	0/7511	0.44	0/10168
1	H	0.50	3/7546 (0.0%)	0.46	3/10217 (0.0%)
All	All	0.28	8/60711 (0.0%)	0.44	10/82201 (0.0%)

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	A	0	1
1	B	0	2
All	All	0	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	765	PRO	N-CD	-37.72	0.94	1.47
1	D	948	PRO	CA-C	-14.27	1.44	1.51
1	C	948	PRO	CA-C	10.46	1.57	1.51
1	E	948	PRO	CA-C	10.38	1.57	1.51
1	F	799	LYS	CE-NZ	9.80	1.78	1.49

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	948	PRO	O-C-N	-10.82	116.33	121.31
1	F	799	LYS	CA-CB-CG	-8.94	96.21	114.10
1	E	948	PRO	O-C-N	8.46	125.20	121.31
1	C	948	PRO	O-C-N	8.26	125.11	121.31
1	H	765	PRO	CB-CG-CD	-7.36	82.55	106.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	229	GLU	Peptide
1	B	928	GLU	Peptide
1	B	931	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7488	0	7474	111	0
1	B	7479	0	7472	80	0
1	C	7390	0	7387	108	0
1	D	7366	0	7360	107	0
1	E	7502	0	7484	89	0
1	F	7496	0	7490	103	1
1	G	7359	0	7356	142	1
1	H	7394	0	7397	124	0
2	A	15	0	0	3	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	15	0	0	0	0
2	E	15	0	0	0	0
2	F	15	0	0	1	0
2	G	15	0	0	0	0
2	H	15	0	0	2	0
3	A	13	0	5	1	0
3	B	26	0	10	4	0
3	C	13	0	5	4	0
3	E	13	0	5	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	13	0	5	3	0
4	D	8	0	12	1	0
5	G	6	0	8	0	0
5	H	6	0	8	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
6	G	2	0	0	0	0
6	H	1	0	0	0	0
All	All	59688	0	59478	845	1

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 7.

The worst 5 of 845 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:H:765:PRO:CD	1:H:765:PRO:CG	1.76	1.57
1:F:799:LYS:NZ	1:F:799:LYS:CE	1.78	1.43
1:A:355:THR:O	1:A:356:LYS:HE2	1.48	1.09
1:F:911:ARG:HH21	1:F:919:VAL:HG11	1.21	1.06
1:H:762:LYS:HD3	1:H:765:PRO:HA	1.38	1.04

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:VAL:O	1:G:810:GLN:NE2[1_655]	2.09	0.11

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	934/970 (96%)	897 (96%)	31 (3%)	6 (1%)	21	51
1	B	938/970 (97%)	905 (96%)	31 (3%)	2 (0%)	43	72
1	C	924/970 (95%)	897 (97%)	24 (3%)	3 (0%)	36	65
1	D	921/970 (95%)	886 (96%)	31 (3%)	4 (0%)	30	59
1	E	936/970 (96%)	905 (97%)	27 (3%)	4 (0%)	30	59
1	F	940/970 (97%)	904 (96%)	31 (3%)	5 (0%)	24	54
1	G	919/970 (95%)	879 (96%)	34 (4%)	6 (1%)	18	48
1	H	924/970 (95%)	883 (96%)	34 (4%)	7 (1%)	16	44
All	All	7436/7760 (96%)	7156 (96%)	243 (3%)	37 (0%)	24	54

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	806	VAL
1	C	75	GLY
1	C	181	SER
1	D	75	GLY
1	D	231	ARG

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	809/832 (97%)	808 (100%)	1 (0%)	88	97
1	B	808/832 (97%)	808 (100%)	0	100	100
1	C	800/832 (96%)	800 (100%)	0	100	100
1	D	797/832 (96%)	797 (100%)	0	100	100
1	E	811/832 (98%)	811 (100%)	0	100	100
1	F	810/832 (97%)	810 (100%)	0	100	100
1	G	796/832 (96%)	796 (100%)	0	100	100
1	H	800/832 (96%)	800 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	6431/6656 (97%)	6430 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	356	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	621	GLN
1	H	167	ASN
1	F	817	ASN
1	G	621	GLN
1	H	616	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

31 ligands 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
2	SO4	D	1003	-	4,4,4	0.26	0	6,6,6	0.08	0
2	SO4	D	1004	-	4,4,4	0.26	0	6,6,6	0.22	0
2	SO4	C	1002	-	4,4,4	0.25	0	6,6,6	0.23	0
2	SO4	E	1002	-	4,4,4	0.22	0	6,6,6	0.16	0
2	SO4	C	1001	-	4,4,4	0.25	0	6,6,6	0.20	0
3	FLC	F	1004	-	12,12,12	1.32	0	17,17,17	1.36	2 (11%)
3	FLC	A	1004	-	12,12,12	1.13	0	17,17,17	1.46	1 (5%)
2	SO4	A	1003	-	4,4,4	0.30	0	6,6,6	0.18	0
3	FLC	B	1003	-	12,12,12	1.07	0	17,17,17	1.34	1 (5%)
2	SO4	F	1001	-	4,4,4	0.24	0	6,6,6	0.23	0
2	SO4	F	1003	-	4,4,4	0.30	0	6,6,6	0.16	0
3	FLC	B	1004	-	12,12,12	1.16	0	17,17,17	1.51	2 (11%)
5	GOL	H	1001	-	5,5,5	0.90	0	5,5,5	1.03	0
2	SO4	A	1002	-	4,4,4	0.26	0	6,6,6	0.20	0
2	SO4	A	1001	-	4,4,4	0.30	0	6,6,6	0.21	0
2	SO4	B	1001	-	4,4,4	0.22	0	6,6,6	0.22	0
2	SO4	H	1002	-	4,4,4	0.30	0	6,6,6	0.24	0
3	FLC	E	1004	-	12,12,12	1.15	0	17,17,17	1.26	1 (5%)
2	SO4	G	1004	-	4,4,4	0.23	0	6,6,6	0.22	0
2	SO4	E	1003	-	4,4,4	0.23	0	6,6,6	0.20	0
4	PG0	D	1001	-	7,7,7	0.48	0	6,6,6	0.39	0
2	SO4	B	1002	-	4,4,4	0.23	0	6,6,6	0.24	0
2	SO4	E	1001	-	4,4,4	0.25	0	6,6,6	0.11	0
2	SO4	H	1004	-	4,4,4	0.26	0	6,6,6	0.18	0
2	SO4	F	1002	-	4,4,4	0.29	0	6,6,6	0.14	0
5	GOL	G	1001	-	5,5,5	0.92	0	5,5,5	1.07	0
3	FLC	C	1003	-	12,12,12	1.14	0	17,17,17	1.33	2 (11%)
2	SO4	D	1002	-	4,4,4	0.28	0	6,6,6	0.29	0
2	SO4	H	1003	-	4,4,4	0.23	0	6,6,6	0.18	0
2	SO4	G	1002	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	G	1003	-	4,4,4	0.26	0	6,6,6	0.19	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FLC	B	1004	-	-	7/16/16/16	-
3	FLC	E	1004	-	-	15/16/16/16	-
5	GOL	H	1001	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG0	D	1001	-	-	3/5/5/5	-
5	GOL	G	1001	-	-	2/4/4/4	-
3	FLC	C	1003	-	-	9/16/16/16	-
3	FLC	F	1004	-	-	7/16/16/16	-
3	FLC	A	1004	-	-	7/16/16/16	-
3	FLC	B	1003	-	-	10/16/16/16	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1004	FLC	OB2-CBC-CB	3.96	120.73	113.14
3	B	1004	FLC	OB2-CBC-CB	3.70	120.24	113.14
3	B	1003	FLC	OB2-CBC-CB	3.48	119.82	113.14
3	E	1004	FLC	OB2-CBC-CB	3.21	119.30	113.14
3	F	1004	FLC	OB2-CBC-CB	3.07	119.04	113.14

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1004	FLC	CG-CB-CBC-OB1
3	A	1004	FLC	CG-CB-CBC-OB2
3	A	1004	FLC	OHB-CB-CBC-OB1
3	A	1004	FLC	OHB-CB-CBC-OB2
3	A	1004	FLC	CA-CB-CG-CGC

There are no ring outliers.

11 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1004	FLC	3	0
3	A	1004	FLC	1	0
3	B	1003	FLC	2	0
2	F	1003	SO4	1	0
3	B	1004	FLC	2	0
2	A	1002	SO4	2	0
2	A	1001	SO4	1	0
2	H	1002	SO4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1004	FLC	2	0
4	D	1001	PG0	1	0
3	C	1003	FLC	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	940/970 (96%)	-1.63	0 100 100	41, 58, 79, 98	0
1	B	942/970 (97%)	-1.65	0 100 100	40, 55, 77, 104	0
1	C	930/970 (95%)	-1.63	0 100 100	37, 55, 84, 105	0
1	D	927/970 (95%)	-1.62	0 100 100	41, 61, 86, 109	0
1	E	942/970 (97%)	-1.65	0 100 100	42, 58, 76, 99	0
1	F	944/970 (97%)	-1.64	0 100 100	43, 56, 78, 107	0
1	G	925/970 (95%)	-1.58	0 100 100	42, 66, 91, 111	0
1	H	930/970 (95%)	-1.60	0 100 100	40, 58, 89, 106	0
All	All	7480/7760 (96%)	-1.63	0 100 100	37, 58, 84, 111	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	1003	5/5	0.97	0.05	94,94,94,94	0
5	GOL	H	1001	6/6	0.97	0.09	55,65,70,71	0
2	SO4	E	1002	5/5	0.98	0.06	79,79,79,79	0
2	SO4	F	1002	5/5	0.98	0.05	82,82,82,82	0
2	SO4	F	1003	5/5	0.98	0.05	84,84,84,84	0
5	GOL	G	1001	6/6	0.98	0.07	63,63,64,64	0
2	SO4	C	1002	5/5	0.98	0.04	91,91,91,91	0
2	SO4	D	1002	5/5	0.99	0.05	71,71,71,71	0
2	SO4	A	1002	5/5	0.99	0.04	74,74,74,74	0
2	SO4	D	1004	5/5	0.99	0.02	73,73,73,73	0
2	SO4	E	1001	5/5	0.99	0.03	74,74,74,74	0
2	SO4	A	1003	5/5	0.99	0.04	63,63,63,63	0
2	SO4	E	1003	5/5	0.99	0.03	70,70,70,70	0
2	SO4	F	1001	5/5	0.99	0.03	73,73,73,73	0
2	SO4	B	1001	5/5	0.99	0.03	74,74,74,74	0
2	SO4	B	1002	5/5	0.99	0.03	77,77,77,77	0
2	SO4	G	1002	5/5	0.99	0.03	80,80,80,80	0
2	SO4	G	1003	5/5	0.99	0.03	82,82,82,82	0
2	SO4	G	1004	5/5	0.99	0.03	93,93,93,93	0
2	SO4	H	1002	5/5	0.99	0.04	92,92,92,92	0
2	SO4	H	1003	5/5	0.99	0.04	79,79,79,79	0
2	SO4	H	1004	5/5	0.99	0.06	82,82,82,82	0
3	FLC	B	1003	13/13	0.99	0.03	54,54,54,54	0
3	FLC	C	1003	13/13	0.99	0.03	58,58,58,58	0
3	FLC	E	1004	13/13	0.99	0.03	62,62,62,62	0
3	FLC	F	1004	13/13	0.99	0.03	59,59,59,59	0
4	PG0	D	1001	8/8	0.99	0.06	54,59,66,69	0
2	SO4	C	1001	5/5	0.99	0.05	66,66,66,66	0
2	SO4	A	1001	5/5	0.99	0.05	73,73,73,73	0
3	FLC	A	1004	13/13	1.00	0.02	62,62,62,62	0
3	FLC	B	1004	13/13	1.00	0.02	53,53,53,53	0

6.5 Other polymers ⓘ

There are no such residues in this entry.