



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 3, 2023 – 09:30 AM EDT

PDB ID : 6U2T  
Title : Crystal structure of the T-state of maize C4-phosphoenolpyruvate carboxylase in complex with malate  
Authors : Carrizosa-Carbajal, E.I.; Munoz-Clares, R.A.; Gonzalez-Segura, L.  
Deposited on : 2019-08-20  
Resolution : 2.80 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](mailto: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 : 4.02b-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

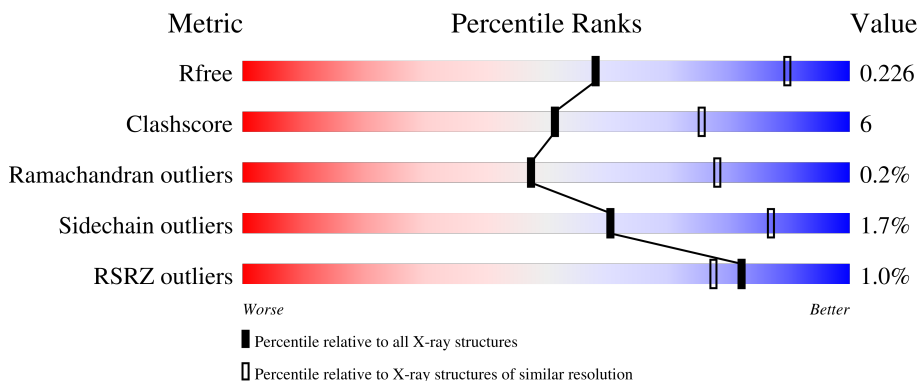
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	 2% 76% 18% • 5%
1	B	970	 % 82% 12% 6%
1	C	970	 % 82% 12% • 5%
1	D	970	 % 83% 12% 5%

## 2 Entry composition [i](#)

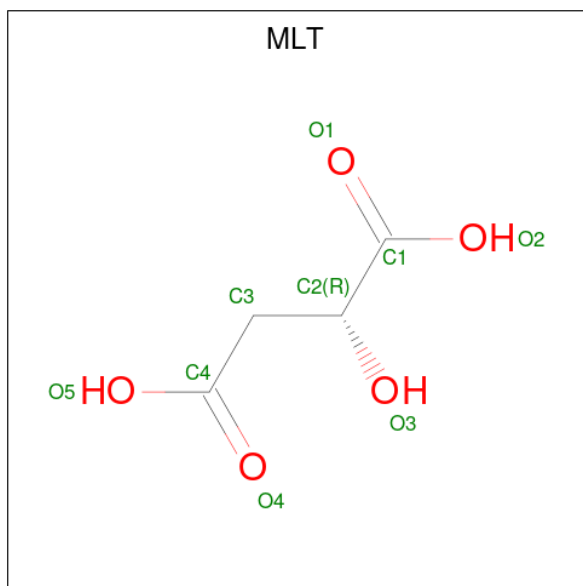
There are 5 unique types of molecules in this entry. The entry contains 29386 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	919	Total 7305	C 4630	N 1276	O 1369	S 30	0	0	0
1	B	915	Total 7296	C 4624	N 1274	O 1368	S 30	0	3	0
1	C	918	Total 7297	C 4625	N 1276	O 1366	S 30	0	0	0
1	D	919	Total 7334	C 4646	N 1282	O 1376	S 30	0	3	0

- Molecule 2 is D-MALATE (three-letter code: MLT) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>5</sub>).



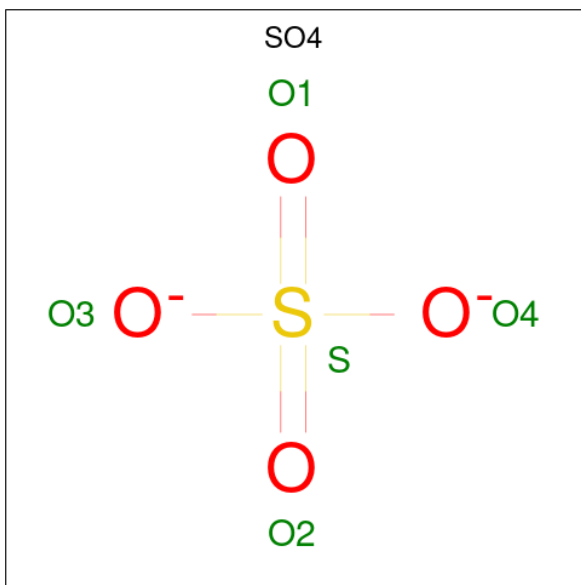
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 9	C 4	O 5	0	0
2	B	1	Total 9	C 4	O 5	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			9	4	5		
2	D	1	Total	C	O	0	0
			9	4	5		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



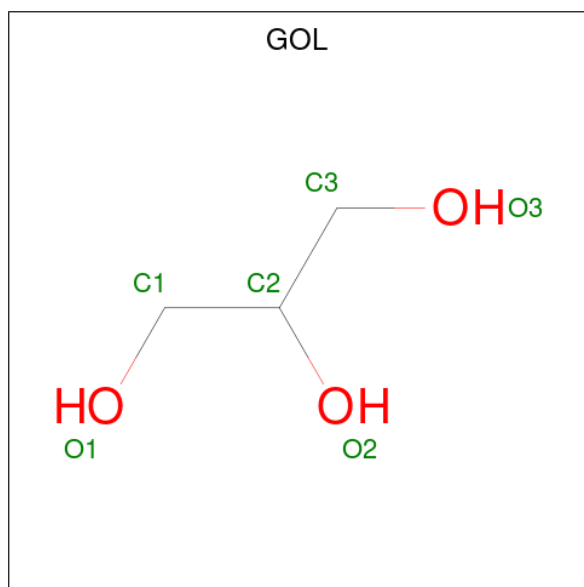
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total O 3 3	0	0
5	B	12	Total O 12 12	0	0
5	C	21	Total O 21 21	0	0
5	D	21	Total O 21 21	0	0

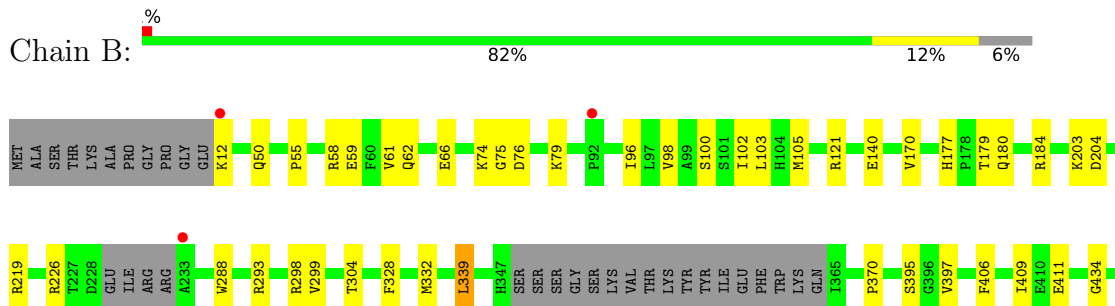
### 3 Residue-property plots [i](#)

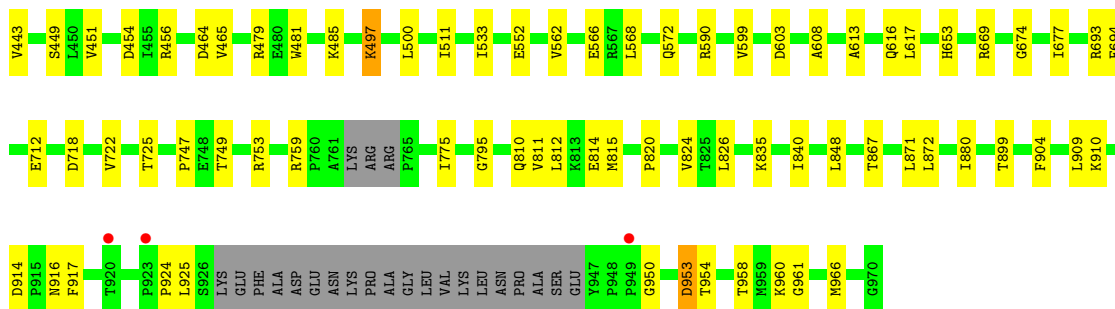
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Phosphoenolpyruvate carboxylase

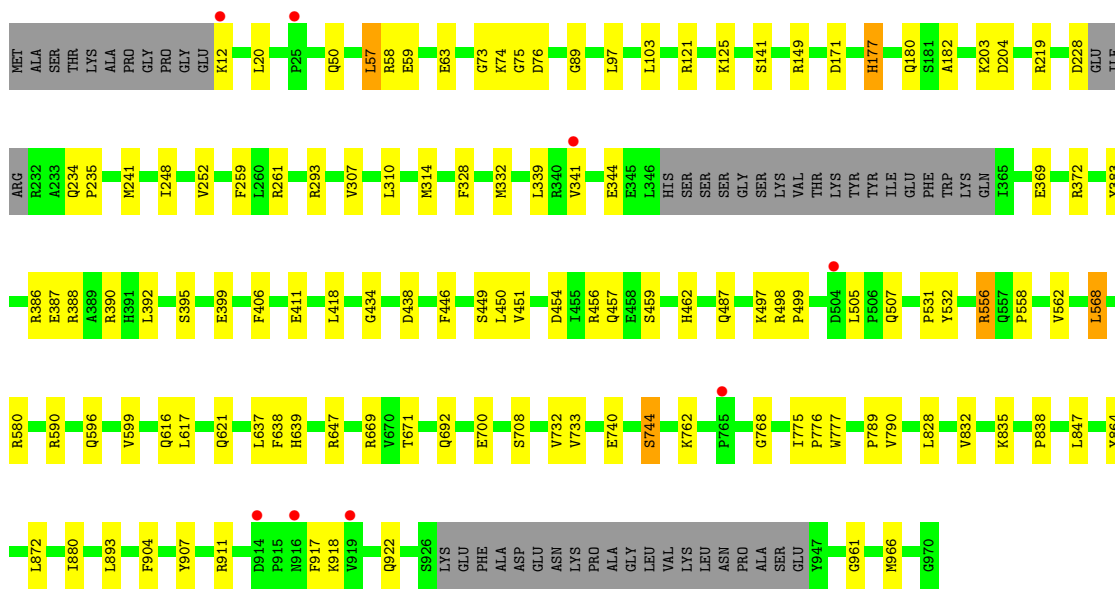
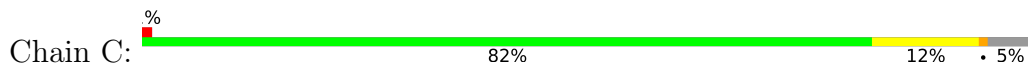


- Molecule 1: Phosphoenolpyruvate carboxylase

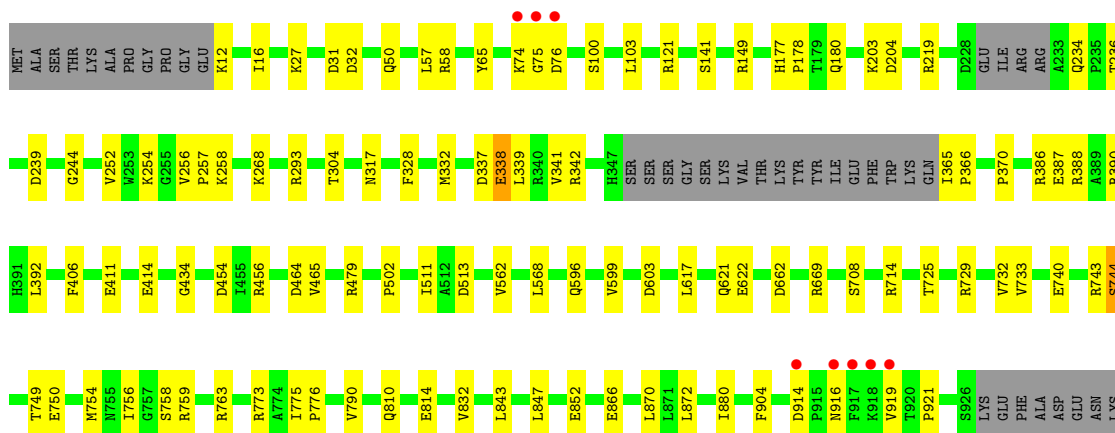
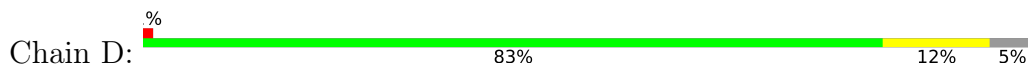




• Molecule 1: Phosphoenolpyruvate carboxylase



• Molecule 1: Phosphoenolpyruvate carboxylase



PRO	E946
ALA	E952
GLY	D9E3
LEU	T954
VAL	T958
LYS	G961
LEU	T969
ASN	G970
PRO	
ALA	
SER	



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.94Å 140.93Å 376.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.36 – 2.80 48.36 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.5 (48.36-2.80) 94.5 (48.36-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.183 , 0.226 0.184 , 0.226	Depositor DCC
$R_{free}$ test set	6538 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.8	Xtrriage
Anisotropy	0.121	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	29386	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.29	0/7456	0.46	1/10094 (0.0%)
1	B	0.27	0/7446	0.45	0/10079
1	C	0.27	0/7447	0.45	1/10081 (0.0%)
1	D	0.27	0/7485	0.45	1/10132 (0.0%)
All	All	0.27	0/29834	0.45	3/40386 (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	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	910	LYS	CD-CE-NZ	-7.74	93.89	111.70
1	C	57	LEU	CB-CG-CD2	-6.40	100.12	111.00
1	D	763	ARG	C-N-CA	5.68	135.90	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	298	ARG	Peptide

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	244	GLY	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7305	0	7299	127	0
1	B	7296	0	7283	67	0
1	C	7297	0	7299	77	0
1	D	7334	0	7321	69	0
2	A	9	0	4	0	0
2	B	9	0	4	0	0
2	C	9	0	4	0	0
2	D	9	0	4	0	0
3	A	10	0	0	1	0
3	B	15	0	0	0	0
3	C	15	0	0	0	0
3	D	15	0	0	1	0
4	D	6	0	8	0	0
5	A	3	0	0	0	0
5	B	12	0	0	0	0
5	C	21	0	0	0	0
5	D	21	0	0	0	0
All	All	29386	0	29226	329	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 6.

The worst 5 of 329 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:759:ARG:HH22	1:D:775:ILE:HD13	1.25	0.97
1:A:910:LYS:NZ	1:A:917:PHE:CD2	2.50	0.80
1:C:89:GLY:HA3	1:C:922:GLN:HE21	1.48	0.79
1:C:203:LYS:HD3	1:C:204:ASP:H	1.50	0.76
1:A:910:LYS:NZ	1:A:917:PHE:CG	2.53	0.76

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	911/970 (94%)	890 (98%)	19 (2%)	2 (0%)	47 78
1	B	908/970 (94%)	882 (97%)	24 (3%)	2 (0%)	47 78
1	C	910/970 (94%)	894 (98%)	15 (2%)	1 (0%)	51 81
1	D	914/970 (94%)	892 (98%)	21 (2%)	1 (0%)	51 81
All	All	3643/3880 (94%)	3558 (98%)	79 (2%)	6 (0%)	47 78

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	LYS
1	B	299	VAL
1	A	75	GLY
1	B	75	GLY
1	C	75	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	790/832 (95%)	773 (98%)	17 (2%)	52 83
1	B	789/832 (95%)	775 (98%)	14 (2%)	59 86
1	C	789/832 (95%)	779 (99%)	10 (1%)	69 91

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	793/832 (95%)	777 (98%)	16 (2%)	55	84
All	All	3161/3328 (95%)	3104 (98%)	57 (2%)	60	86

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	848	LEU
1	D	744	SER
1	C	395	SER
1	D	708	SER
1	D	338[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	188	GLN
1	C	462	HIS
1	D	787	HIS
1	C	967	GLN
1	D	177	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

16 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
3	SO4	D	1003	-	4,4,4	0.13	0	6,6,6	0.09	0
3	SO4	B	1002	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	A	1003	-	4,4,4	0.15	0	6,6,6	0.12	0
3	SO4	A	1002	-	4,4,4	0.13	0	6,6,6	0.21	0
2	MLT	A	1001	-	8,8,8	1.06	0	10,10,10	1.56	1 (10%)
3	SO4	C	1003	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	C	1002	-	4,4,4	0.16	0	6,6,6	0.05	0
3	SO4	C	1004	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	D	1004	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	B	1004	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	D	1002	-	4,4,4	0.16	0	6,6,6	0.46	0
2	MLT	C	1001	-	8,8,8	1.04	0	10,10,10	1.66	2 (20%)
4	GOL	D	1005	-	5,5,5	0.90	0	5,5,5	0.99	0
2	MLT	D	1001	-	8,8,8	1.06	0	10,10,10	1.60	2 (20%)
3	SO4	B	1003	-	4,4,4	0.14	0	6,6,6	0.07	0
2	MLT	B	1001	-	8,8,8	1.06	0	10,10,10	1.77	3 (30%)

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
2	MLT	A	1001	-	-	4/8/8/8	-
2	MLT	C	1001	-	-	4/8/8/8	-
4	GOL	D	1005	-	-	2/4/4/4	-
2	MLT	D	1001	-	-	4/8/8/8	-
2	MLT	B	1001	-	-	3/8/8/8	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	MLT	O2-C1-C2	3.55	120.52	112.72

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	MLT	O2-C1-C2	3.48	120.37	112.72
2	D	1001	MLT	O2-C1-C2	3.39	120.16	112.72
2	A	1001	MLT	O2-C1-C2	3.36	120.10	112.72
2	B	1001	MLT	C2-C3-C4	-2.22	106.64	112.13

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	MLT	O1-C1-C2-O3
2	A	1001	MLT	O2-C1-C2-O3
2	A	1001	MLT	O2-C1-C2-C3
2	B	1001	MLT	O1-C1-C2-O3
2	B	1001	MLT	O2-C1-C2-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	SO4	1	0
3	D	1002	SO4	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	919/970 (94%)	-0.02	16 (1%) 70 63	37, 62, 91, 118	0
1	B	915/970 (94%)	-0.23	6 (0%) 87 84	29, 48, 81, 107	0
1	C	918/970 (94%)	-0.16	8 (0%) 84 80	30, 47, 77, 119	0
1	D	919/970 (94%)	-0.21	8 (0%) 84 80	29, 46, 82, 119	0
All	All	3671/3880 (94%)	-0.15	38 (1%) 82 77	29, 51, 85, 119	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	916	ASN	4.3
1	C	916	ASN	4.1
1	A	765	PRO	4.1
1	A	919	VAL	3.7
1	D	919	VAL	3.6

### 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 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<sup>th</sup> 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
3	SO4	B	1003	5/5	0.79	0.23	102,116,129,130	0
3	SO4	B	1004	5/5	0.86	0.23	104,105,113,118	0
3	SO4	D	1003	5/5	0.89	0.20	92,101,106,121	0
3	SO4	D	1002	5/5	0.90	0.24	77,87,95,97	0
3	SO4	A	1002	5/5	0.91	0.22	94,97,101,104	0
3	SO4	C	1003	5/5	0.91	0.19	83,89,95,103	0
3	SO4	C	1004	5/5	0.92	0.19	101,106,113,115	0
3	SO4	B	1002	5/5	0.93	0.20	89,91,96,99	0
3	SO4	C	1002	5/5	0.93	0.14	98,100,112,126	0
3	SO4	A	1003	5/5	0.93	0.17	124,124,129,132	0
2	MLT	C	1001	9/9	0.94	0.22	43,48,52,61	0
4	GOL	D	1005	6/6	0.94	0.20	68,71,82,93	0
2	MLT	D	1001	9/9	0.95	0.24	40,43,50,51	0
2	MLT	B	1001	9/9	0.95	0.22	41,49,53,53	0
2	MLT	A	1001	9/9	0.95	0.20	51,61,62,68	0
3	SO4	D	1004	5/5	0.96	0.14	80,91,95,100	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.