



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2018 – 09:56 AM EST

PDB ID : 4BXC  
Title : Resolving the activation site of positive regulators in plant phosphoenolpyruvate carboxylase  
Authors : Schlieper, D.; Foerster, K.; Paulus, J.K.; Groth, G.  
Deposited on : 2013-07-10  
Resolution : 2.86 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030736

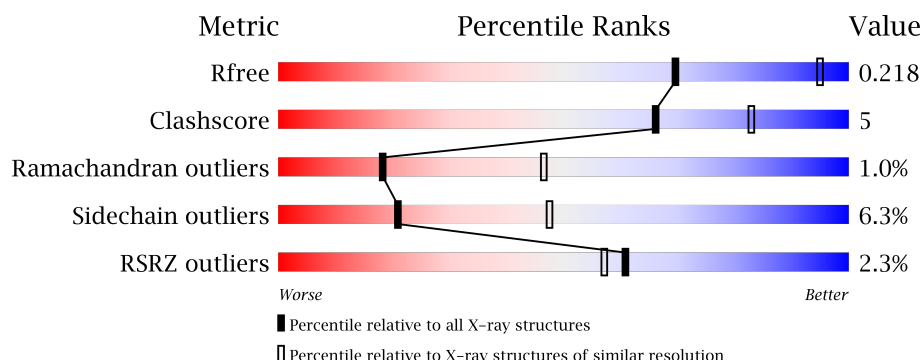
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.86 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))
$R_{free}$	100719	2469 (2.90-2.82)
Clashscore	112137	2749 (2.90-2.82)
Ramachandran outliers	110173	2687 (2.90-2.82)
Sidechain outliers	110143	2690 (2.90-2.82)
RSRZ outliers	101464	2487 (2.90-2.82)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	990	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>6%</div> </div> </div>
1	B	990	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>6%</div> </div> </div>

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	G6P	B	1967	-	-	-	X
3	SO4	A	1968	-	-	X	-
3	SO4	B	1968	-	-	X	-
4	EDO	B	1969	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14917 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 C4 PHOSPHOENOLPYRUVATE CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	929	Total	C	N	O	S	0	0	0
			7425	4711	1290	1390	34			
1	B	929	Total	C	N	O	S	0	0	0
			7421	4710	1285	1392	34			

There are 48 discrepancies between the modelled and reference sequences:

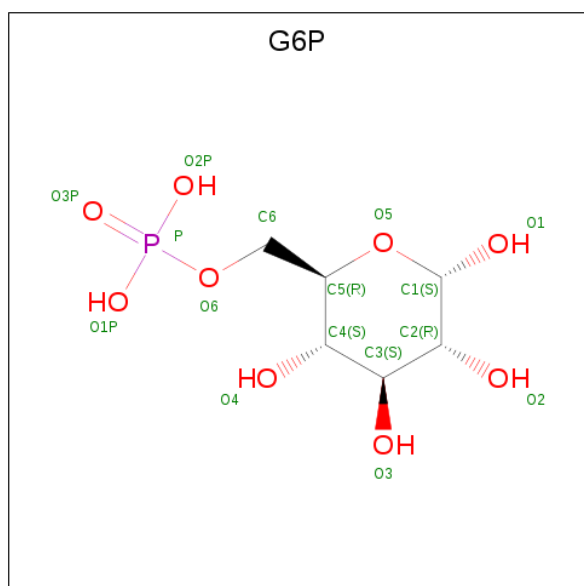
Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP P30694
A	-22	GLY	-	expression tag	UNP P30694
A	-21	HIS	-	expression tag	UNP P30694
A	-20	HIS	-	expression tag	UNP P30694
A	-19	HIS	-	expression tag	UNP P30694
A	-18	HIS	-	expression tag	UNP P30694
A	-17	HIS	-	expression tag	UNP P30694
A	-16	HIS	-	expression tag	UNP P30694
A	-15	HIS	-	expression tag	UNP P30694
A	-14	HIS	-	expression tag	UNP P30694
A	-13	HIS	-	expression tag	UNP P30694
A	-12	HIS	-	expression tag	UNP P30694
A	-11	SER	-	expression tag	UNP P30694
A	-10	SER	-	expression tag	UNP P30694
A	-9	GLY	-	expression tag	UNP P30694
A	-8	HIS	-	expression tag	UNP P30694
A	-7	GLU	-	expression tag	UNP P30694
A	-6	ASN	-	expression tag	UNP P30694
A	-5	LEU	-	expression tag	UNP P30694
A	-4	TYR	-	expression tag	UNP P30694
A	-3	PHE	-	expression tag	UNP P30694
A	-2	GLN	-	expression tag	UNP P30694
A	-1	GLY	-	expression tag	UNP P30694
A	0	HIS	-	expression tag	UNP P30694
B	-23	MET	-	expression tag	UNP P30694

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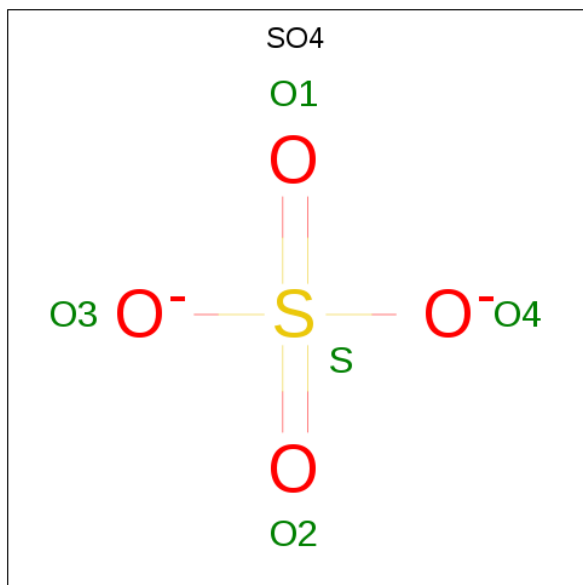
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	GLY	-	expression tag	UNP P30694
B	-21	HIS	-	expression tag	UNP P30694
B	-20	HIS	-	expression tag	UNP P30694
B	-19	HIS	-	expression tag	UNP P30694
B	-18	HIS	-	expression tag	UNP P30694
B	-17	HIS	-	expression tag	UNP P30694
B	-16	HIS	-	expression tag	UNP P30694
B	-15	HIS	-	expression tag	UNP P30694
B	-14	HIS	-	expression tag	UNP P30694
B	-13	HIS	-	expression tag	UNP P30694
B	-12	HIS	-	expression tag	UNP P30694
B	-11	SER	-	expression tag	UNP P30694
B	-10	SER	-	expression tag	UNP P30694
B	-9	GLY	-	expression tag	UNP P30694
B	-8	HIS	-	expression tag	UNP P30694
B	-7	GLU	-	expression tag	UNP P30694
B	-6	ASN	-	expression tag	UNP P30694
B	-5	LEU	-	expression tag	UNP P30694
B	-4	TYR	-	expression tag	UNP P30694
B	-3	PHE	-	expression tag	UNP P30694
B	-2	GLN	-	expression tag	UNP P30694
B	-1	GLY	-	expression tag	UNP P30694
B	0	HIS	-	expression tag	UNP P30694

- Molecule 2 is ALPHA-D-GLUCOSE-6-PHOSPHATE (three-letter code: G6P) (formula:  $C_6H_{13}O_9P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		

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



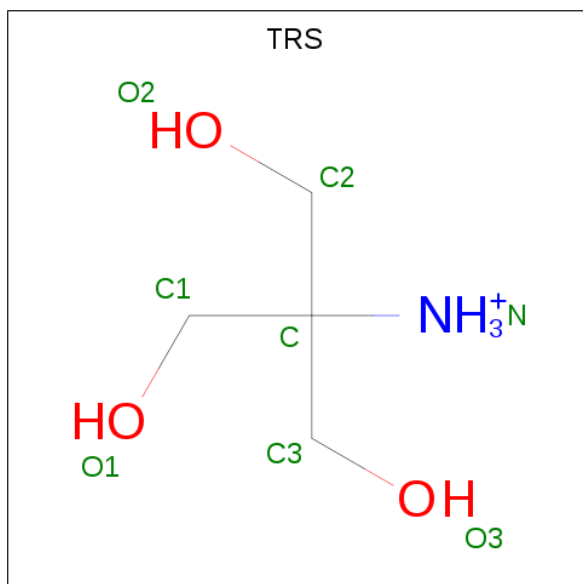
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



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

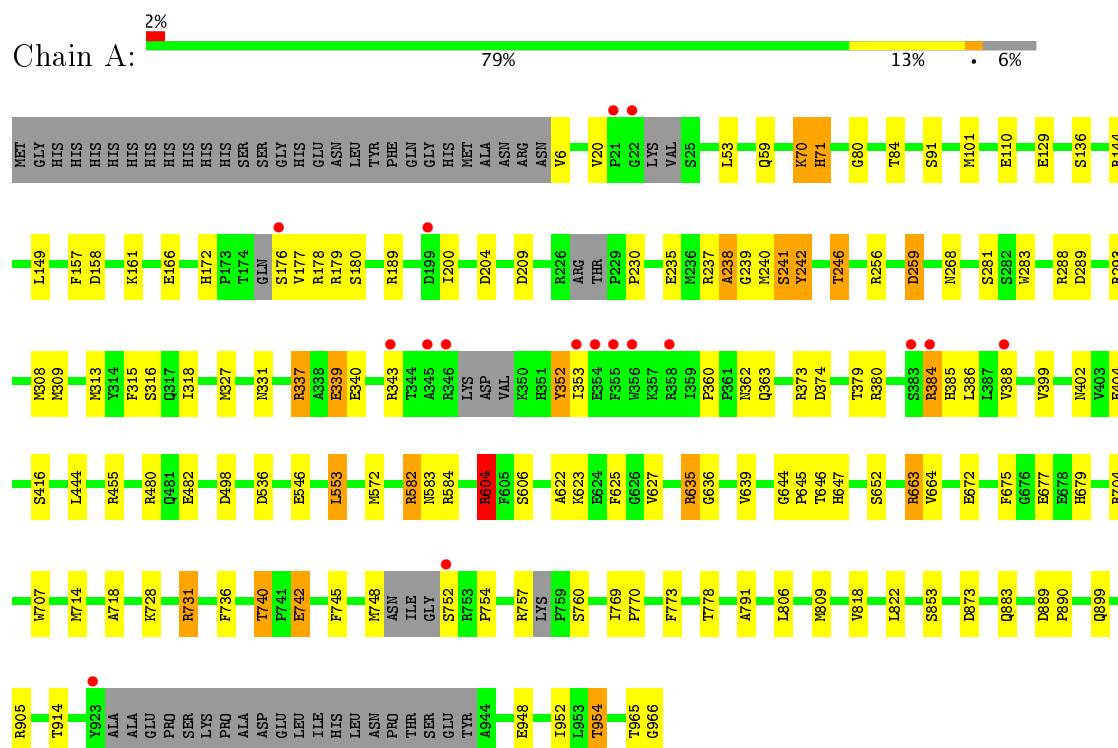
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total 12	O 12	0	0
6	B	1	Total 1	O 1	0	0

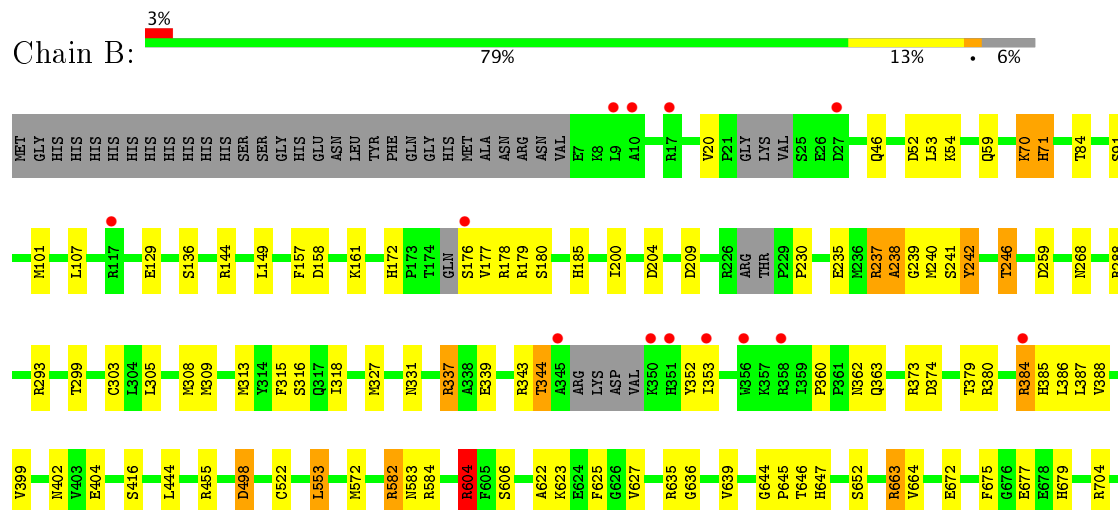
### 3 Residue-property plots

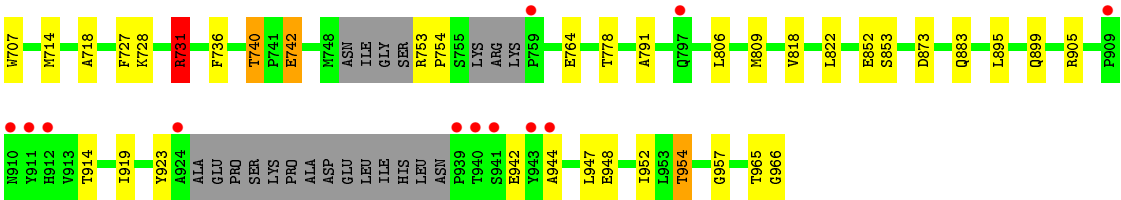
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: C4 PHOSPHOENOLPYRUVATE CARBOXYLASE



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.41 Å   121.23 Å   132.19 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	50.68 – 2.86 50.63 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.68-2.86) 99.7 (50.63-2.86)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.20 (at 2.86 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.184   ,   0.221 0.189   ,   0.218	Depositor DCC
$R_{free}$ test set	1253 reflections (2.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.6	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 36.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14917	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, EDO, G6P, 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	0.72	1/7578 (0.0%)	0.84	14/10246 (0.1%)
1	B	0.66	1/7576 (0.0%)	0.82	8/10248 (0.1%)
All	All	0.69	2/15154 (0.0%)	0.83	22/20494 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	546	GLU	CD-OE1	5.45	1.31	1.25
1	B	498	ASP	CB-CG	5.30	1.62	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	731	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	B	731	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	A	663	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	B	663	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	B	572	MET	CG-SD-CE	-6.41	89.95	100.20
1	A	572	MET	CG-SD-CE	-6.18	90.31	100.20
1	A	604	ARG	NE-CZ-NH1	6.03	123.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	663	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	A	373	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	B	663	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	259	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	B	604	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	288	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	259	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	B	852	GLU	CA-CB-CG	5.40	125.28	113.40
1	B	373	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	480	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	A	289	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	288	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	604	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	635	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	536	ASP	CB-CG-OD1	-5.00	113.80	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	353	ILE	Peptide
1	B	344	THR	Peptide
1	B	353	ILE	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	7425	0	7350	65	0
1	B	7421	0	7330	69	0
2	A	16	0	11	3	0
2	B	16	0	11	2	0
3	A	5	0	0	2	0
3	B	5	0	0	2	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
5	A	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	12	0	0	1	0
6	B	1	0	0	0	0
All	All	14917	0	14726	135	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 (135) 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:B:806:LEU:HA	1:B:809:MET:HE3	1.53	0.91
1:A:806:LEU:HA	1:A:809:MET:HE3	1.54	0.90
1:A:246:THR:HG21	1:A:675:PHE:O	1.72	0.88
1:B:246:THR:HG21	1:B:675:PHE:O	1.74	0.87
1:B:178:ARG:NH2	3:B:1968:SO4:O4	2.08	0.86
1:A:241:SER:OG	1:A:242:TYR:N	2.10	0.84
1:B:308:MET:SD	1:B:384:ARG:HD3	2.19	0.82
1:A:308:MET:SD	1:A:384:ARG:HD3	2.20	0.82
1:B:337:ARG:HH11	1:B:337:ARG:HG3	1.47	0.80
1:B:241:SER:OG	1:B:242:TYR:N	2.11	0.77
1:A:337:ARG:HG3	1:A:337:ARG:HH11	1.49	0.76
1:B:635:ARG:HG2	2:B:1967:G6P:H3	1.68	0.76
1:A:84:THR:O	1:A:905:ARG:NH2	2.23	0.72
1:B:84:THR:O	1:B:905:ARG:NH2	2.23	0.70
1:B:753:ARG:NH2	2:B:1967:G6P:O2P	2.28	0.67
1:B:157:PHE:CE2	1:B:161:LYS:HE3	2.31	0.65
1:A:677:GLU:OE2	1:A:679:HIS:HD2	1.79	0.65
1:A:178:ARG:NH2	3:A:1968:SO4:O2	2.30	0.63
1:A:157:PHE:CE2	1:A:161:LYS:HE3	2.33	0.62
1:B:20:VAL:HG11	1:B:883:GLN:HG3	1.84	0.60
1:B:59:GLN:OE1	1:B:59:GLN:HA	2.02	0.59
1:A:360:PRO:HD2	1:A:363:GLN:HE21	1.69	0.57
1:B:360:PRO:HD2	1:B:363:GLN:HE21	1.69	0.57
1:A:20:VAL:HG11	1:A:883:GLN:HG3	1.86	0.56
1:B:604:ARG:NH2	1:B:636:GLY:O	2.37	0.56
1:B:315:PHE:O	1:B:318:ILE:HG22	2.05	0.56
1:A:315:PHE:O	1:A:318:ILE:HG22	2.06	0.56
1:B:129:GLU:O	1:B:647:HIS:HB3	2.07	0.55
1:A:604:ARG:NH2	1:A:636:GLY:O	2.39	0.55
1:A:59:GLN:HA	1:A:59:GLN:OE1	2.08	0.54
1:A:129:GLU:O	1:A:647:HIS:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:GLN:HE21	1:A:954:THR:CG2	2.20	0.54
1:B:899:GLN:HE21	1:B:954:THR:CG2	2.19	0.54
1:B:553:LEU:N	1:B:553:LEU:HD23	2.23	0.53
1:A:136:SER:OG	1:A:144:ARG:NH2	2.41	0.53
1:A:20:VAL:HG13	1:A:20:VAL:O	2.07	0.53
1:B:20:VAL:O	1:B:20:VAL:HG13	2.09	0.52
1:A:70:LYS:O	1:A:71:HIS:HB2	2.10	0.52
1:B:582:ARG:NH1	1:B:625:PHE:O	2.44	0.51
1:A:582:ARG:NH1	1:A:625:PHE:O	2.43	0.51
1:B:70:LYS:O	1:B:71:HIS:HB2	2.10	0.51
1:A:553:LEU:N	1:A:553:LEU:HD23	2.26	0.51
1:B:136:SER:OG	1:B:144:ARG:NH2	2.41	0.50
1:B:172:HIS:HB3	1:B:176:SER:HB3	1.93	0.49
1:B:644:GLY:O	1:B:647:HIS:N	2.46	0.49
1:A:240:MET:HE2	1:A:309:MET:HB2	1.95	0.48
1:A:331:ASN:ND2	1:A:416:SER:HA	2.28	0.48
1:A:822:LEU:HD23	1:A:822:LEU:C	2.34	0.48
1:B:379:THR:HA	1:B:399:VAL:HG22	1.96	0.48
1:A:352:TYR:OH	1:A:374:ASP:OD1	2.32	0.48
1:A:644:GLY:O	1:A:647:HIS:N	2.47	0.48
1:B:331:ASN:ND2	1:B:416:SER:HA	2.29	0.48
1:B:553:LEU:HD23	1:B:553:LEU:H	1.79	0.48
1:B:822:LEU:HD23	1:B:822:LEU:C	2.34	0.48
1:A:379:THR:HA	1:A:399:VAL:HG22	1.96	0.47
1:B:235:GLU:O	1:B:238:ALA:HB3	2.15	0.47
1:B:923:TYR:CD1	1:B:923:TYR:N	2.81	0.47
1:A:748:MET:CB	1:A:752:SER:N	2.77	0.47
1:A:172:HIS:HB3	1:A:176:SER:HB3	1.97	0.47
1:B:240:MET:HG3	1:B:309:MET:SD	2.55	0.47
1:A:740:THR:HG22	1:A:742:GLU:HB3	1.97	0.46
1:B:740:THR:HG22	1:B:742:GLU:HB3	1.98	0.46
1:A:714:MET:HB3	1:A:791:ALA:HB1	1.98	0.46
1:B:379:THR:CA	1:B:399:VAL:HG22	2.46	0.46
1:A:736:PHE:O	1:A:740:THR:HB	2.16	0.46
1:A:965:THR:OG1	1:A:966:GLY:N	2.49	0.46
1:B:240:MET:HE2	1:B:309:MET:HB2	1.97	0.46
1:B:942:GLU:OE1	1:B:948:GLU:HG2	2.16	0.46
1:A:379:THR:CA	1:A:399:VAL:HG22	2.46	0.46
1:B:727:PHE:CE1	1:B:764:GLU:HG3	2.51	0.46
1:B:965:THR:OG1	1:B:966:GLY:N	2.49	0.46
1:B:736:PHE:O	1:B:740:THR:HB	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLU:O	1:A:238:ALA:HB3	2.16	0.45
1:A:718:ALA:HB2	1:A:791:ALA:HB2	1.99	0.45
1:A:385:HIS:O	1:A:386:LEU:C	2.55	0.44
1:B:714:MET:HB3	1:B:791:ALA:HB1	1.98	0.44
1:B:242:TYR:OH	1:B:672:GLU:OE1	2.33	0.44
1:A:704:ARG:HD3	1:A:707:TRP:CZ2	2.52	0.44
1:B:385:HIS:O	1:B:386:LEU:C	2.55	0.44
1:B:704:ARG:HD3	1:B:707:TRP:CZ2	2.51	0.44
1:B:337:ARG:CG	1:B:337:ARG:HH11	2.24	0.44
1:A:240:MET:HG3	1:A:309:MET:SD	2.58	0.44
1:B:352:TYR:OH	1:B:374:ASP:OD1	2.35	0.44
1:A:806:LEU:HD23	1:A:809:MET:HE3	2.00	0.44
1:B:180:SER:N	3:B:1968:SO4:O2	2.38	0.44
1:A:242:TYR:OH	1:A:672:GLU:OE1	2.35	0.43
1:A:283:TRP:CZ3	2:A:1967:G6P:H4	2.53	0.43
1:A:553:LEU:H	1:A:553:LEU:HD23	1.81	0.43
1:B:622:ALA:HB1	1:B:627:VAL:O	2.18	0.43
1:A:899:GLN:HB2	1:A:954:THR:CG2	2.49	0.43
1:B:242:TYR:OH	1:B:672:GLU:HA	2.19	0.43
1:B:303:CYS:SG	1:B:522:CYS:HB3	2.58	0.43
1:B:899:GLN:HB2	1:B:954:THR:HG23	2.00	0.43
1:A:622:ALA:HB1	1:A:627:VAL:O	2.19	0.43
1:B:899:GLN:HE21	1:B:954:THR:HG22	1.83	0.43
1:B:309:MET:O	1:B:313:MET:HG3	2.18	0.43
1:A:635:ARG:HD3	2:A:1967:G6P:H5	2.01	0.43
1:A:745:PHE:CD2	1:A:773:PHE:CE1	3.07	0.43
1:B:731:ARG:HG2	1:B:731:ARG:HH11	1.84	0.43
1:A:644:GLY:N	1:A:645:PRO:CD	2.82	0.42
1:A:899:GLN:HB2	1:A:954:THR:HG23	2.00	0.42
1:B:899:GLN:HB2	1:B:954:THR:CG2	2.49	0.42
1:A:242:TYR:OH	1:A:672:GLU:HA	2.19	0.42
1:A:110:GLU:OE1	1:A:189:ARG:NH1	2.51	0.42
1:B:718:ALA:HB2	1:B:791:ALA:HB2	2.00	0.42
1:B:736:PHE:CE1	1:B:740:THR:HG21	2.55	0.42
1:A:769:ILE:HB	1:A:770:PRO:HD3	2.02	0.41
1:A:180:SER:HB3	3:A:1968:SO4:O1	2.20	0.41
1:B:172:HIS:HB3	1:B:176:SER:CB	2.50	0.41
2:A:1967:G6P:O5	2:A:1967:G6P:P	2.78	0.41
1:A:309:MET:O	1:A:313:MET:HG3	2.20	0.41
1:A:166:GLU:OE2	1:A:281:SER:OG	2.32	0.41
1:A:889:ASP:O	1:A:890:PRO:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:948:GLU:O	1:B:952:ILE:HG12	2.20	0.41
1:A:80:GLY:O	1:A:84:THR:HG22	2.20	0.41
1:A:899:GLN:HE21	1:A:954:THR:HG22	1.84	0.41
1:B:944:ALA:CB	1:B:947:LEU:HD12	2.50	0.41
1:A:482:GLU:HG2	6:A:2006:HOH:O	2.20	0.41
1:B:644:GLY:O	1:B:645:PRO:C	2.59	0.41
1:B:288:ARG:NH2	1:B:299:THR:OG1	2.41	0.41
1:B:895:LEU:HD13	1:B:957:GLY:HA3	2.03	0.41
1:B:52:ASP:HB3	1:B:919:ILE:HG23	2.03	0.41
1:B:107:LEU:HD21	1:B:185:HIS:HB3	2.04	0.40
1:B:240:MET:CE	1:B:309:MET:HB2	2.52	0.40
1:B:644:GLY:N	1:B:645:PRO:CD	2.85	0.40
1:A:256:ARG:O	1:A:259:ASP:HB2	2.21	0.40
1:A:806:LEU:HA	1:A:809:MET:CE	2.37	0.40
1:A:948:GLU:O	1:A:952:ILE:HG12	2.20	0.40
1:B:305:LEU:HG	1:B:387:LEU:HD21	2.03	0.40
1:B:46:GLN:HE21	1:B:54:LYS:HE3	1.86	0.40
1:B:677:GLU:OE1	1:B:679:HIS:N	2.54	0.40
1:A:455:ARG:HD3	1:A:455:ARG:HA	1.87	0.40
1:A:339:GLU:O	1:A:340:GLU:C	2.60	0.40
1:A:740:THR:CG2	1:A:742:GLU:H	2.35	0.40
1:B:455:ARG:HA	1:B:455:ARG:HD3	1.90	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	913/990 (92%)	862 (94%)	42 (5%)	9 (1%)	18	46
1	B	913/990 (92%)	867 (95%)	37 (4%)	9 (1%)	18	46
All	All	1826/1980 (92%)	1729 (95%)	79 (4%)	18 (1%)	18	46

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	PRO
1	B	230	PRO
1	A	71	HIS
1	A	237	ARG
1	A	239	GLY
1	B	71	HIS
1	B	237	ARG
1	B	239	GLY
1	B	344	THR
1	A	362	ASN
1	A	444	LEU
1	B	444	LEU
1	A	238	ALA
1	A	241	SER
1	B	238	ALA
1	B	362	ASN
1	B	754	PRO
1	A	754	PRO

### 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	800/866 (92%)	748 (94%)	52 (6%)	20	46
1	B	799/866 (92%)	750 (94%)	49 (6%)	22	49
All	All	1599/1732 (92%)	1498 (94%)	101 (6%)	21	47

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	53	LEU
1	A	70	LYS
1	A	91	SER
1	A	101	MET

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Mol	Chain	Res	Type
1	A	149	LEU
1	A	158	ASP
1	A	177	VAL
1	A	179	ARG
1	A	200	ILE
1	A	204	ASP
1	A	209	ASP
1	A	242	TYR
1	A	246	THR
1	A	268	ASN
1	A	293	ARG
1	A	316	SER
1	A	327	MET
1	A	337	ARG
1	A	339	GLU
1	A	343	ARG
1	A	352	TYR
1	A	380	ARG
1	A	384	ARG
1	A	388	VAL
1	A	402	ASN
1	A	404	GLU
1	A	498	ASP
1	A	553	LEU
1	A	582	ARG
1	A	583	ASN
1	A	584	ARG
1	A	604	ARG
1	A	606	SER
1	A	623	LYS
1	A	639	VAL
1	A	646	THR
1	A	652	SER
1	A	663	ARG
1	A	664	VAL
1	A	728	LYS
1	A	731	ARG
1	A	740	THR
1	A	742	GLU
1	A	757	ARG
1	A	760	SER
1	A	778	THR

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Mol	Chain	Res	Type
1	A	818	VAL
1	A	853	SER
1	A	873	ASP
1	A	914	THR
1	A	954	THR
1	B	53	LEU
1	B	70	LYS
1	B	91	SER
1	B	101	MET
1	B	149	LEU
1	B	158	ASP
1	B	177	VAL
1	B	179	ARG
1	B	200	ILE
1	B	204	ASP
1	B	209	ASP
1	B	237	ARG
1	B	242	TYR
1	B	246	THR
1	B	268	ASN
1	B	293	ARG
1	B	316	SER
1	B	327	MET
1	B	337	ARG
1	B	339	GLU
1	B	343	ARG
1	B	380	ARG
1	B	384	ARG
1	B	388	VAL
1	B	402	ASN
1	B	404	GLU
1	B	498	ASP
1	B	553	LEU
1	B	582	ARG
1	B	583	ASN
1	B	584	ARG
1	B	604	ARG
1	B	606	SER
1	B	623	LYS
1	B	639	VAL
1	B	646	THR
1	B	652	SER

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Mol	Chain	Res	Type
1	B	663	ARG
1	B	664	VAL
1	B	728	LYS
1	B	731	ARG
1	B	740	THR
1	B	742	GLU
1	B	778	THR
1	B	818	VAL
1	B	853	SER
1	B	873	ASP
1	B	914	THR
1	B	954	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	213	HIS
1	A	244	HIS
1	A	268	ASN
1	A	363	GLN
1	A	583	ASN
1	A	615	GLN
1	A	653	GLN
1	A	679	HIS
1	A	794	HIS
1	A	802	ASN
1	A	899	GLN
1	A	963	GLN
1	B	46	GLN
1	B	213	HIS
1	B	244	HIS
1	B	268	ASN
1	B	363	GLN
1	B	583	ASN
1	B	615	GLN
1	B	653	GLN
1	B	794	HIS
1	B	802	ASN
1	B	899	GLN
1	B	910	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

7 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	G6P	A	1967	-	16,16,16	1.64	4 (25%)	24,24,24	2.79	9 (37%)
3	SO4	A	1968	-	4,4,4	0.39	0	6,6,6	0.66	0
4	EDO	A	1969	-	3,3,3	0.71	0	2,2,2	0.20	0
5	TRS	A	1970	-	7,7,7	1.05	0	9,9,9	1.07	1 (11%)
2	G6P	B	1967	-	16,16,16	1.09	1 (6%)	24,24,24	1.87	7 (29%)
3	SO4	B	1968	-	4,4,4	0.50	0	6,6,6	0.91	0
4	EDO	B	1969	-	3,3,3	0.75	0	2,2,2	0.31	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
2	G6P	A	1967	-	-	0/6/26/26	0/1/1/1
3	SO4	A	1968	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	1969	-	-	0/1/1/1	0/0/0/0
5	TRS	A	1970	-	-	0/9/9/9	0/0/0/0
2	G6P	B	1967	-	-	0/6/26/26	0/1/1/1
3	SO4	B	1968	-	-	0/0/0/0	0/0/0/0
4	EDO	B	1969	-	-	0/1/1/1	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1967	G6P	O1-C1	2.12	1.46	1.39
2	B	1967	G6P	O1-C1	2.49	1.48	1.39
2	A	1967	G6P	C4-C3	2.65	1.59	1.52
2	A	1967	G6P	C3-C2	2.69	1.59	1.52
2	A	1967	G6P	O3-C3	3.84	1.51	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1967	G6P	O2-C2-C1	-5.74	97.82	109.75
2	B	1967	G6P	O2-C2-C1	-3.57	102.34	109.75
2	B	1967	G6P	O2P-P-O6	-2.23	100.80	106.73
5	A	1970	TRS	C1-C-N	-2.21	103.02	107.73
2	B	1967	G6P	O5-C1-C2	-2.04	106.65	110.04
2	A	1967	G6P	O1-C1-C2	2.02	115.13	109.42
2	B	1967	G6P	O1-C1-O5	2.11	116.45	110.20
2	A	1967	G6P	C3-C4-C5	2.23	114.16	110.22
2	A	1967	G6P	O2-C2-C3	2.35	115.47	110.36
2	A	1967	G6P	O4-C4-C3	2.44	115.67	110.36
2	B	1967	G6P	O5-C5-C4	2.55	114.36	109.66
2	B	1967	G6P	C1-C2-C3	3.83	117.57	110.65
2	B	1967	G6P	C1-O5-C5	4.08	120.75	113.39
2	A	1967	G6P	P-O6-C6	4.69	131.22	118.30
2	A	1967	G6P	O5-C5-C4	4.82	118.54	109.66
2	A	1967	G6P	C1-O5-C5	5.55	123.40	113.39
2	A	1967	G6P	C1-C2-C3	6.45	122.31	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1967	G6P	3	0
3	A	1968	SO4	2	0
2	B	1967	G6P	2	0
3	B	1968	SO4	2	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 ⓘ

### 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<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	929/990 (93%)	-0.30	17 (1%) 69 66	36, 60, 113, 172	0
1	B	929/990 (93%)	-0.13	25 (2%) 55 50	43, 71, 125, 170	0
All	All	1858/1980 (93%)	-0.22	42 (2%) 61 57	36, 66, 119, 172	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	939	PRO	6.7
1	B	941	SER	5.3
1	B	940	THR	5.2
1	B	351	HIS	5.1
1	A	176	SER	5.1
1	B	9	LEU	4.6
1	A	752	SER	4.4
1	B	943	TYR	4.4
1	A	346	ARG	4.3
1	A	21	PRO	3.4
1	A	358	ARG	3.3
1	A	356	TRP	3.3
1	B	759	PRO	3.2
1	A	199	ASP	3.1
1	A	345	ALA	3.1
1	B	924	ALA	3.1
1	A	353	ILE	3.1
1	A	343	ARG	3.0
1	A	355	PHE	2.8
1	B	911	TYR	2.8
1	B	27	ASP	2.7
1	A	22	GLY	2.7
1	B	910	ASN	2.7
1	B	353	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	944	ALA	2.6
1	B	350	LYS	2.5
1	B	345	ALA	2.5
1	B	356	TRP	2.4
1	B	176	SER	2.4
1	B	358	ARG	2.3
1	B	17	ARG	2.3
1	B	117	ARG	2.3
1	B	384	ARG	2.3
1	A	388	VAL	2.2
1	A	384	ARG	2.2
1	A	383	SER	2.2
1	B	909	PRO	2.2
1	B	10	ALA	2.1
1	A	354	GLU	2.1
1	A	923	TYR	2.1
1	B	912	HIS	2.1
1	B	797	GLN	2.1

## 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 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<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	B	1969	4/4	0.85	0.66	7.23	74,74,77,82	0
2	G6P	B	1967	16/16	0.83	0.29	2.10	98,106,157,158	0
2	G6P	A	1967	16/16	0.87	0.24	1.55	58,95,126,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	TRS	A	1970	8/8	0.92	0.19	1.03	64,79,84,86	0
3	SO4	B	1968	5/5	0.95	0.12	-1.37	69,76,97,97	0
3	SO4	A	1968	5/5	0.97	0.12	-1.37	72,87,93,102	0
4	EDO	A	1969	4/4	0.90	0.12	-	63,74,77,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.