



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:31 PM GMT

PDB ID : 1U0G  
Title : Crystal structure of mouse phosphoglucose isomerase in complex with erythrose 4-phosphate  
Authors : Solomons, J.T.G.; Zimmerly, E.M.; Burns, S.; Krishnamurthy, N.; Swan, M.K.; Krings, S.; Muirhead, H.; Chirgwin, J.; Davies, C.  
Deposited on : 2004-07-13  
Resolution : 1.70 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

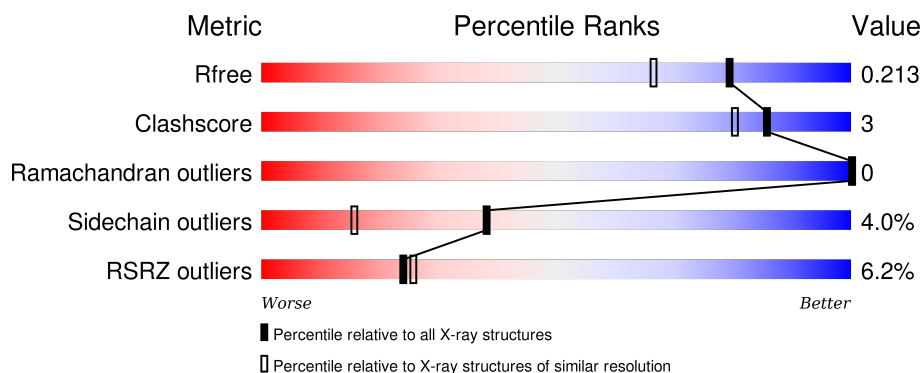
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	564	<div> <div>6%</div> <div>87%</div> <div>10% ..</div> </div>
1	B	564	<div> <div>6%</div> <div>90%</div> <div>9% .</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	SO4	B	955	-	-	-	X
3	E4P	B	902[B]	-	-	-	X
4	BME	A	963	-	-	-	X
4	BME	A	964	-	-	-	X
4	BME	B	966	-	-	-	X
5	GOL	A	971	-	-	-	X
5	GOL	A	973	-	-	-	X
5	GOL	A	975	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9783 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 Glucose-6-phosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	4	0
			4416	2823	764	811	18			
1	B	556	Total	C	N	O	S	0	6	0
			4418	2823	767	810	18			

There are 14 discrepancies between the modelled and reference sequences:

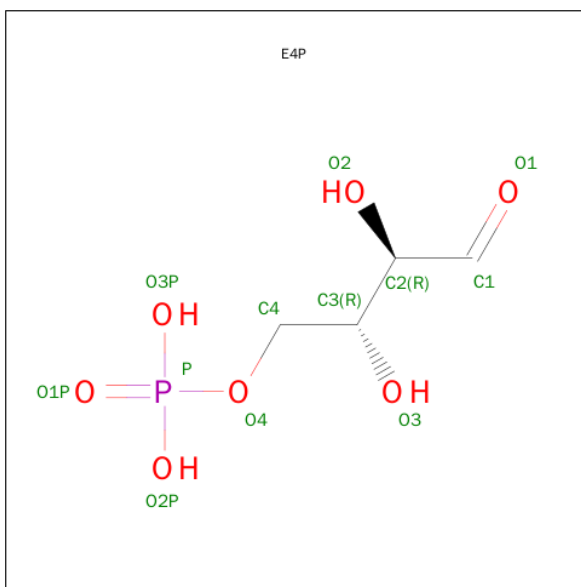
Chain	Residue	Modelled	Actual	Comment	Reference
A	263	LEU	PHE	SEE REMARK 999	UNP P06745
A	558	HIS	-	EXPRESSION TAG	UNP P06745
A	559	HIS	-	EXPRESSION TAG	UNP P06745
A	560	HIS	-	EXPRESSION TAG	UNP P06745
A	561	HIS	-	EXPRESSION TAG	UNP P06745
A	562	HIS	-	EXPRESSION TAG	UNP P06745
A	563	HIS	-	EXPRESSION TAG	UNP P06745
B	263	LEU	PHE	SEE REMARK 999	UNP P06745
B	558	HIS	-	EXPRESSION TAG	UNP P06745
B	559	HIS	-	EXPRESSION TAG	UNP P06745
B	560	HIS	-	EXPRESSION TAG	UNP P06745
B	561	HIS	-	EXPRESSION TAG	UNP P06745
B	562	HIS	-	EXPRESSION TAG	UNP P06745
B	563	HIS	-	EXPRESSION TAG	UNP P06745

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



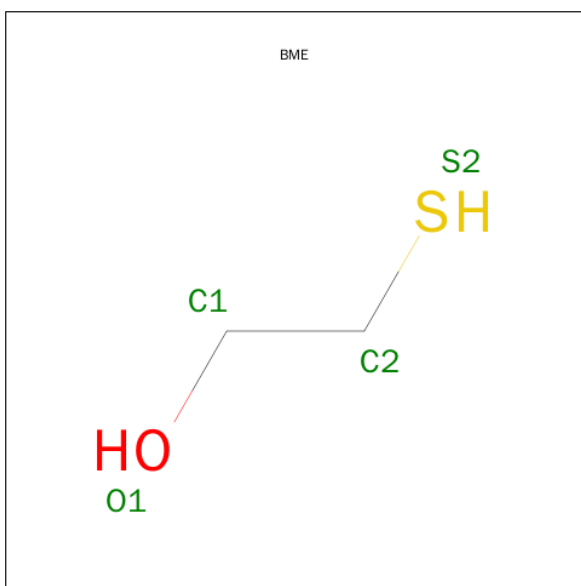
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ERYTHROSE-4-PHOSPHATE (three-letter code: E4P) (formula: C<sub>4</sub>H<sub>9</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	1
			13	4	8	1		
3	B	1	Total	C	O	P	0	1
			13	4	8	1		

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula:  $C_2H_6OS$ ).



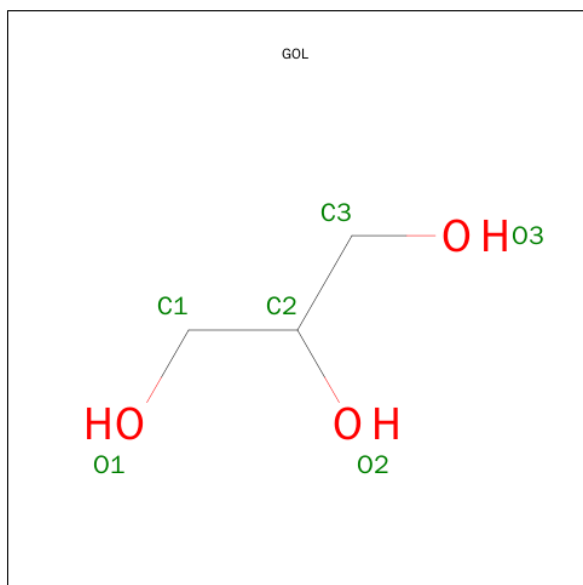
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	403	Total 403	O 403	0	0
6	B	429	Total 429	O 429	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.80 Å 115.60 Å 73.20 Å 90.00° 100.20° 90.00°	Depositor
Resolution (Å)	50.00 – 1.70 24.39 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-1.70) 96.0 (24.39-1.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 1.70 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.190 , 0.215 0.191 , 0.213	Depositor DCC
$R_{free}$ test set	5941 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.9	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 55.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 118664 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9783	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, E4P, SO4, BME

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	0.39	0/4545	0.66	10/6153 (0.2%)
1	B	0.39	0/4563	0.65	8/6174 (0.1%)
All	All	0.39	0/9108	0.66	18/12327 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	ASP	CB-CG-OD2	7.26	124.83	118.30
1	B	234	ASP	CB-CG-OD2	6.55	124.20	118.30
1	B	126	ASP	CB-CG-OD2	6.45	124.11	118.30
1	B	187	ASP	CB-CG-OD2	6.43	124.09	118.30
1	B	457	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	187	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	234	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	139[A]	ASP	CB-CG-OD2	5.85	123.57	118.30
1	A	139[B]	ASP	CB-CG-OD2	5.85	123.57	118.30
1	A	538	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	113	ASP	CB-CG-OD2	5.65	123.38	118.30
1	B	553	ASP	CB-CG-OD2	5.62	123.35	118.30
1	B	150	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	457	ASP	CB-CG-OD2	5.56	123.30	118.30
1	B	160	ASP	CB-CG-OD2	5.46	123.22	118.30
1	B	510	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	505	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	150	ASP	CB-CG-OD2	5.18	122.96	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	4416	0	4396	27	0
1	B	4418	0	4400	24	0
2	A	15	0	0	0	0
2	B	20	0	0	0	0
3	A	13	0	2	0	0
3	B	13	0	2	0	0
4	A	12	0	18	2	0
4	B	8	0	12	1	0
5	A	30	0	40	2	0
5	B	6	0	8	0	0
6	A	403	0	0	4	0
6	B	429	0	0	4	0
All	All	9783	0	8878	50	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 3.

All (50) 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)
4:A:964:BME:H21	1:B:369:ARG:HD2	1.69	0.73
1:B:128:MET:HG2	1:B:263:LEU:HD13	1.78	0.65
1:B:291:HIS:HE1	6:B:1176:HOH:O	1.84	0.61
1:B:151:ILE:CG2	1:B:206:ILE:HD12	2.32	0.59
1:A:387:GLN:HE22	1:A:427:ASN:HB3	1.66	0.58
1:B:80:ARG:HD2	1:B:307:LEU:HA	1.84	0.57
1:B:387:GLN:HE22	1:B:427:ASN:HB3	1.70	0.57
1:A:442:GLU:CD	1:A:442:GLU:H	2.07	0.56
1:B:186:ILE:HB	1:B:216:GLU:HG3	1.89	0.55
1:B:554:THR:HG21	6:B:1257:HOH:O	2.07	0.53
1:A:186:ILE:HB	1:A:216:GLU:HG3	1.91	0.53
1:B:112:VAL:O	1:B:115:LYS:HG3	2.08	0.53
1:A:80:ARG:HD2	1:A:307:LEU:HA	1.91	0.52
1:A:550:GLN:NE2	6:A:1206:HOH:O	2.43	0.51
5:A:975:GOL:H12	6:A:1221:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ILE:HD13	1:A:425:LEU:HD23	1.93	0.50
1:B:89:ILE:HG22	4:B:966:BME:H11	1.94	0.50
1:B:151:ILE:CG2	1:B:206:ILE:CD1	2.90	0.49
1:A:80:ARG:HG3	1:A:306:PHE:CE2	2.47	0.49
1:A:362:TYR:CD2	1:B:396:GLN:HG2	2.47	0.49
1:B:468:GLU:HG2	6:B:1160:HOH:O	2.13	0.48
1:A:25:LEU:HB3	1:A:436:MET:HG2	1.97	0.47
1:A:125:LEU:HB3	5:A:973:GOL:H31	1.97	0.46
1:A:253:LYS:HG3	1:A:259:PRO:HD3	1.98	0.46
1:B:41:LEU:HD11	1:B:318:LEU:HD12	1.96	0.46
1:A:522:LYS:HG3	6:A:1315:HOH:O	2.16	0.46
1:A:62:GLU:HG3	6:A:1235:HOH:O	2.16	0.45
1:A:234:ASP:OD2	1:A:236:SER:HB2	2.17	0.44
1:A:536:SER:HB3	1:A:537:HIS:CD2	2.52	0.44
1:B:239:ALA:HA	6:B:1001:HOH:O	2.18	0.44
1:B:151:ILE:HG23	1:B:206:ILE:CD1	2.47	0.44
1:A:71:ALA:HB2	1:A:321:LEU:HD21	1.99	0.44
1:A:260:GLN:HE21	1:A:260:GLN:HB2	1.64	0.44
1:B:287:VAL:O	1:B:291:HIS:HD2	2.01	0.44
1:A:41:LEU:HD11	1:A:318:LEU:HD12	1.99	0.43
1:A:129:LYS:O	1:A:133:GLN:HG3	2.19	0.43
1:B:80:ARG:HG3	1:B:306:PHE:CE2	2.53	0.43
1:A:172:PRO:HG3	1:A:343:TYR:CE1	2.53	0.43
1:B:345:HIS:HA	1:B:382:PRO:HG3	2.00	0.43
1:A:387:GLN:HA	1:A:391:TYR:CG	2.54	0.42
1:A:446:LYS:HD2	1:A:449:GLN:HE22	1.85	0.42
1:A:550:GLN:HB3	1:A:550:GLN:HE21	1.71	0.42
1:A:362:TYR:CE2	1:B:396:GLN:HG2	2.55	0.42
1:B:407:ILE:HD13	1:B:425:LEU:HD23	2.01	0.42
1:B:405:PHE:HB3	1:B:428:PHE:CE1	2.55	0.42
1:B:555:LYS:HA	1:B:555:LYS:HD2	1.94	0.41
1:A:466:VAL:HG11	4:A:964:BME:H12	2.03	0.41
1:A:206:ILE:HD11	1:A:285:LEU:HD12	2.03	0.41
1:A:72:LYS:HE2	1:A:311:LEU:HD12	2.03	0.41
1:B:186:ILE:HB	1:B:216:GLU:CG	2.50	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	558/564 (99%)	545 (98%)	13 (2%)	0	100	100
1	B	560/564 (99%)	544 (97%)	16 (3%)	0	100	100
All	All	1118/1128 (99%)	1089 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	478/482 (99%)	454 (95%)	24 (5%)	30	11
1	B	480/482 (100%)	464 (97%)	16 (3%)	45	22
All	All	958/964 (99%)	918 (96%)	40 (4%)	38	14

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	62	GLU
1	A	103	ARG
1	A	127	LYS
1	A	212	PHE
1	A	236	SER
1	A	253	LYS
1	A	260	GLN

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Mol	Chain	Res	Type
1	A	337	LEU
1	A	442	GLU
1	A	446	LYS
1	A	454	SER
1	A	456	GLU
1	A	461	LEU
1	A	478	PHE
1	A	519	GLN
1	A	523	LYS
1	A	527	GLU
1	A	531	SER
1	A	536	SER
1	A	550	GLN
1	A	554	THR
1	A	555	LYS
1	A	556	LEU
1	B	103	ARG
1	B	115	LYS
1	B	175	LYS
1	B	197	SER
1	B	198	LEU
1	B	212	PHE
1	B	240	LYS
1	B	254	GLU
1	B	416	ARG
1	B	445	ARG
1	B	465[A]	LYS
1	B	465[B]	LYS
1	B	522[A]	LYS
1	B	522[B]	LYS
1	B	553	ASP
1	B	556	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	16	HIS
1	A	37	ASN
1	A	38	ASN
1	A	65	GLN
1	A	82	ASN

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Mol	Chain	Res	Type
1	A	104	ASN
1	A	260	GLN
1	A	387	GLN
1	A	449	GLN
1	A	550	GLN
1	A	551	GLN
1	B	16	HIS
1	B	22	ASN
1	B	65	GLN
1	B	82	ASN
1	B	291	HIS
1	B	387	GLN
1	B	551	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](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

22 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	E4P	A	901[A]	-	11,11,11	1.82	2 (18%)	10,15,15	1.47	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	E4P	A	901[B]	-	11,11,11	1.87	2 (18%)	10,15,15	1.44	2 (20%)
2	SO4	A	951	-	4,4,4	0.26	0	6,6,6	0.15	0
2	SO4	A	954	-	4,4,4	0.22	0	6,6,6	0.09	0
2	SO4	A	956	-	4,4,4	0.26	0	6,6,6	0.06	0
4	BME	A	962	-	3,3,3	0.23	0	2,2,2	0.27	0
4	BME	A	963	-	3,3,3	0.25	0	2,2,2	0.27	0
4	BME	A	964	-	3,3,3	0.22	0	2,2,2	0.55	0
5	GOL	A	971	-	5,5,5	0.31	0	5,5,5	0.55	0
5	GOL	A	973	-	5,5,5	0.28	0	5,5,5	0.18	0
5	GOL	A	974	-	5,5,5	0.38	0	5,5,5	0.25	0
5	GOL	A	975	-	5,5,5	0.37	0	5,5,5	0.41	0
5	GOL	A	976	-	5,5,5	0.34	0	5,5,5	0.35	0
3	E4P	B	902[A]	-	11,11,11	1.73	2 (18%)	10,15,15	1.36	2 (20%)
3	E4P	B	902[B]	-	11,11,11	1.77	2 (18%)	10,15,15	1.29	2 (20%)
2	SO4	B	952	-	4,4,4	0.21	0	6,6,6	0.14	0
2	SO4	B	953	-	4,4,4	0.25	0	6,6,6	0.15	0
2	SO4	B	955	-	4,4,4	0.28	0	6,6,6	0.12	0
2	SO4	B	957	-	4,4,4	0.23	0	6,6,6	0.09	0
4	BME	B	961	-	3,3,3	0.27	0	2,2,2	0.13	0
4	BME	B	966	-	3,3,3	0.20	0	2,2,2	0.33	0
5	GOL	B	972	-	5,5,5	0.35	0	5,5,5	0.36	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	E4P	A	901[A]	-	-	0/10/12/12	0/0/0/0
3	E4P	A	901[B]	-	-	0/10/12/12	0/0/0/0
2	SO4	A	951	-	-	0/0/0/0	0/0/0/0
2	SO4	A	954	-	-	0/0/0/0	0/0/0/0
2	SO4	A	956	-	-	0/0/0/0	0/0/0/0
4	BME	A	962	-	-	0/1/1/1	0/0/0/0
4	BME	A	963	-	-	0/1/1/1	0/0/0/0
4	BME	A	964	-	-	0/1/1/1	0/0/0/0
5	GOL	A	971	-	-	0/4/4/4	0/0/0/0
5	GOL	A	973	-	-	0/4/4/4	0/0/0/0
5	GOL	A	974	-	-	0/4/4/4	0/0/0/0
5	GOL	A	975	-	-	0/4/4/4	0/0/0/0
5	GOL	A	976	-	-	0/4/4/4	0/0/0/0
3	E4P	B	902[A]	-	-	0/10/12/12	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	E4P	B	902[B]	-	-	0/10/12/12	0/0/0/0
2	SO4	B	952	-	-	0/0/0/0	0/0/0/0
2	SO4	B	953	-	-	0/0/0/0	0/0/0/0
2	SO4	B	955	-	-	0/0/0/0	0/0/0/0
2	SO4	B	957	-	-	0/0/0/0	0/0/0/0
4	BME	B	961	-	-	0/1/1/1	0/0/0/0
4	BME	B	966	-	-	0/1/1/1	0/0/0/0
5	GOL	B	972	-	-	0/4/4/4	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901[A]	E4P	P-O4	-2.36	1.52	1.60
3	A	901[B]	E4P	P-O4	-2.36	1.52	1.60
3	B	902[A]	E4P	P-O4	-2.29	1.52	1.60
3	B	902[B]	E4P	P-O4	-2.29	1.52	1.60
3	B	902[A]	E4P	O1-C1	4.78	1.41	1.19
3	B	902[B]	E4P	O1-C1	4.94	1.42	1.19
3	A	901[A]	E4P	O1-C1	4.95	1.42	1.19
3	A	901[B]	E4P	O1-C1	5.14	1.43	1.19

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901[A]	E4P	O1-C1-C2	-3.40	115.69	125.60
3	A	901[B]	E4P	O1-C1-C2	-3.28	116.03	125.60
3	B	902[A]	E4P	O1-C1-C2	-2.96	116.97	125.60
3	B	902[B]	E4P	O1-C1-C2	-2.67	117.81	125.60
3	B	902[A]	E4P	O2-C2-C1	-2.51	104.23	110.22
3	B	902[B]	E4P	O2-C2-C1	-2.51	104.23	110.22
3	A	901[A]	E4P	O2-C2-C1	-2.39	104.51	110.22
3	A	901[B]	E4P	O2-C2-C1	-2.39	104.51	110.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	964	BME	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	973	GOL	1	0
5	A	975	GOL	1	0
4	B	966	BME	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 ⓘ

### 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	556/564 (98%)	0.41	33 (5%) 26 27	12, 17, 28, 37	1 (0%)
1	B	556/564 (98%)	0.42	36 (6%) 22 24	11, 17, 28, 38	0
All	All	1112/1128 (98%)	0.42	69 (6%) 24 26	11, 17, 28, 38	1 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	556	LEU	6.7
1	A	451	ALA	6.4
1	A	452	GLY	6.3
1	B	555	LYS	5.8
1	A	555	LYS	5.7
1	B	553	ASP	5.2
1	A	531	SER	5.1
1	B	235	PRO	4.7
1	B	456	GLU	4.7
1	A	456	GLU	4.2
1	B	531	SER	4.1
1	A	454	SER	4.0
1	A	553	ASP	3.9
1	A	556	LEU	3.8
1	A	260	GLN	3.7
1	B	238	VAL	3.6
1	B	554	THR	3.6
1	A	455	PRO	3.5
1	A	17	ARG	3.4
1	A	535	THR	3.4
1	B	258	ASP	3.4
1	B	176	GLY	3.4
1	B	237	ALA	3.1
1	B	254	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	176	GLY	3.0
1	B	250	ALA	3.0
1	A	529	GLU	3.0
1	A	457	ASP	3.0
1	A	532	SER	3.0
1	B	253	LYS	3.0
1	B	455	PRO	2.9
1	B	290	ASP	2.9
1	B	532	SER	2.9
1	A	442	GLU	2.8
1	A	450	ALA	2.8
1	B	21	ALA	2.8
1	A	554	THR	2.8
1	B	233	LYS	2.6
1	A	536	SER	2.6
1	A	102	LEU	2.6
1	B	113	ASP	2.6
1	B	206	ILE	2.6
1	A	5	ARG	2.5
1	B	369	ARG	2.5
1	B	454	SER	2.5
1	B	248	ASN	2.4
1	B	30	GLU	2.4
1	A	14	GLU	2.4
1	B	417	LYS	2.4
1	A	362	TYR	2.3
1	B	22	ASN	2.3
1	B	239	ALA	2.3
1	A	61	LYS	2.3
1	A	254	GLU	2.3
1	A	417	LYS	2.3
1	A	46	ASN	2.3
1	B	17	ARG	2.3
1	B	234	ASP	2.3
1	B	457	ASP	2.3
1	B	5	ARG	2.2
1	B	257	ILE	2.2
1	B	175	LYS	2.1
1	A	115	LYS	2.1
1	B	236	SER	2.1
1	A	253	LYS	2.1
1	B	461	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	123	ARG	2.0
1	A	407	ILE	2.0
1	A	259	PRO	2.0

## 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	BME	B	966	4/4	0.82	0.36	13.53	45,46,46,48	0
5	GOL	A	973	6/6	0.81	0.29	6.55	26,29,30,31	0
3	E4P	B	902[B]	12/12	0.94	0.11	6.34	12,14,16,16	1
2	SO4	B	955	5/5	0.91	0.22	5.61	32,32,32,33	5
5	GOL	A	971	6/6	0.78	0.24	4.07	25,26,28,29	0
5	GOL	A	975	6/6	0.78	0.20	3.54	38,39,39,42	0
4	BME	A	964	4/4	0.73	0.30	2.95	40,40,40,42	0
4	BME	A	963	4/4	0.94	0.23	2.13	35,36,36,39	0
3	E4P	B	902[A]	12/12	0.94	0.11	1.41	7,14,16,16	1
4	BME	B	961	4/4	0.82	0.17	1.29	32,33,34,37	0
3	E4P	A	901[A]	12/12	0.95	0.10	0.80	3,12,16,16	1
5	GOL	A	974	6/6	0.78	0.17	0.79	29,33,34,35	0
5	GOL	B	972	6/6	0.87	0.16	0.68	21,24,26,29	0
3	E4P	A	901[B]	12/12	0.95	0.10	0.31	10,12,16,16	1
2	SO4	A	951	5/5	0.89	0.12	0.17	27,27,27,27	5
5	GOL	A	976	6/6	0.80	0.15	0.14	35,36,36,38	0
2	SO4	A	954	5/5	0.91	0.22	-	33,33,33,34	5
2	SO4	B	952	5/5	0.90	0.21	-	26,26,27,27	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	957	5/5	0.91	0.40	-	27,27,27,27	5
2	SO4	A	956	5/5	0.93	0.19	-	32,32,32,33	5
4	BME	A	962	4/4	0.65	0.28	-	47,47,47,49	0
2	SO4	B	953	5/5	0.92	0.23	-	31,31,31,31	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.