Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:34 PM GMT

PDB ID	:	1U0F
Title	:	Crystal structure of mouse phosphoglucose isomerase in complex with glucose 6-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	:	1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

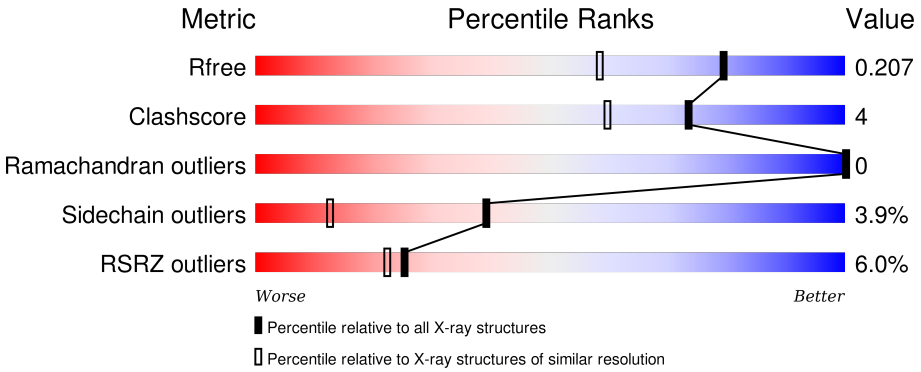
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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 >=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 <=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	4% 88% 10%
1	B	564	8% 87% 11%

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	A	900[A]	-	-	-	X
3	G6Q	A	901[B]	-	-	-	X
4	SO4	A	1002	-	-	-	X
4	SO4	B	1003	-	-	-	X
4	SO4	B	1007	-	-	-	X
4	SO4	B	1008	-	-	X	X
5	BME	B	1011	-	-	-	X
6	GOL	A	1021	-	-	-	X
6	GOL	A	1023	-	-	-	X
6	GOL	A	1026	-	-	X	X
6	GOL	A	1030	-	-	-	X
6	GOL	A	1031	-	-	-	X
6	GOL	A	1032	-	-	-	X
6	GOL	B	1028	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9903 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.

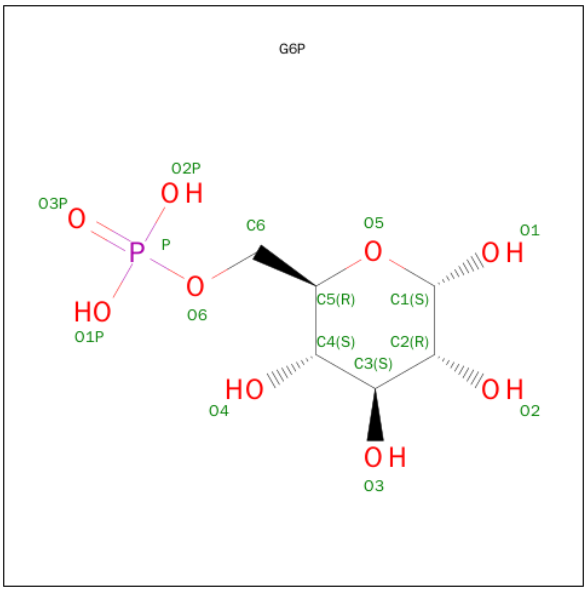
- Molecule 1 is a protein called Glucose-6-phosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	15	0
			4450	2843	769	819	19			
1	B	556	Total	C	N	O	S	0	13	0
			4446	2842	770	815	19			

There are 14 discrepancies between the modelled and reference sequences:

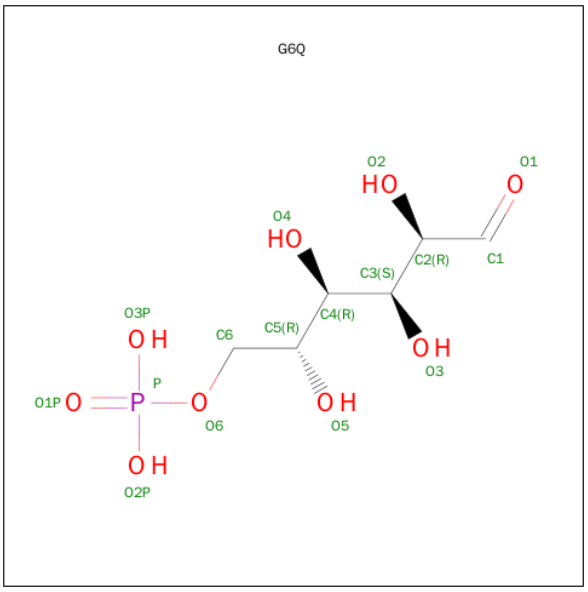
Chain	Residue	Modelled	Actual	Comment	Reference
A	263	LEU	PHE	SEE REMARK 999	UNP P06745
A	558	HIS	-	EXPRESSION TAG	UNP P06745
A	559	HIS	-	EXPRESSION TAG	UNP P06745
A	560	HIS	-	EXPRESSION TAG	UNP P06745
A	561	HIS	-	EXPRESSION TAG	UNP P06745
A	562	HIS	-	EXPRESSION TAG	UNP P06745
A	563	HIS	-	EXPRESSION 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 SUGAR (ALPHA-D-GLUCOSE-6-PHOSPHATE) (three-letter code: G6P) (formula: $C_6H_{13}O_9P$).



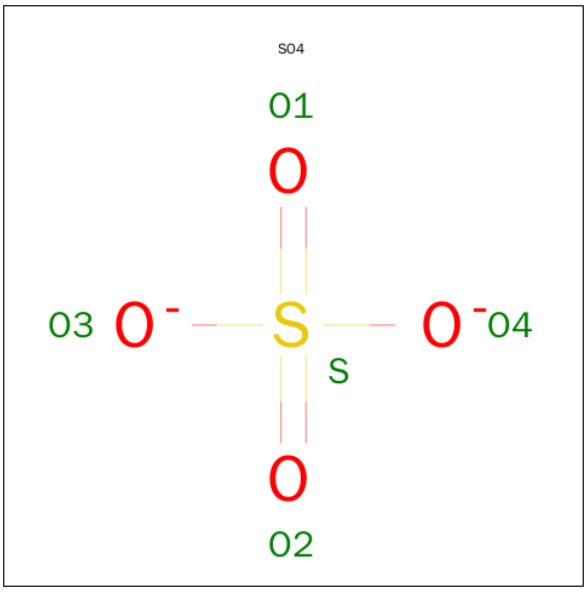
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	17	6	10	1	0	1

- Molecule 3 is SUGAR (GLUCOSE-6-PHOSPHATE) (three-letter code: G6Q) (formula: $C_6H_{13}O_9P$).



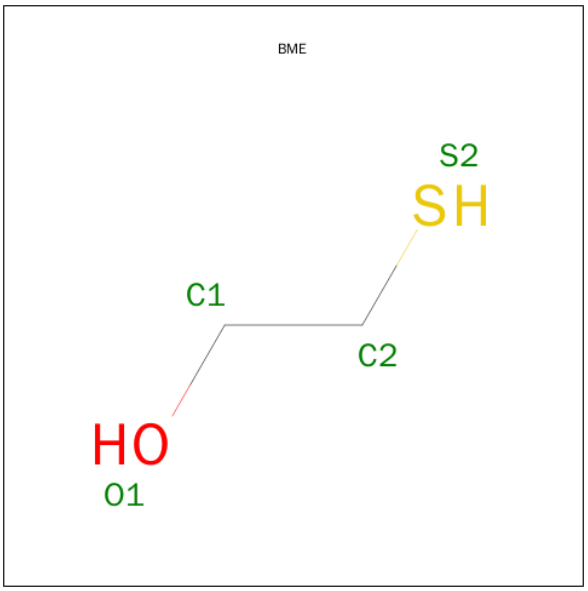
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	16	6	9	1	0	1

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



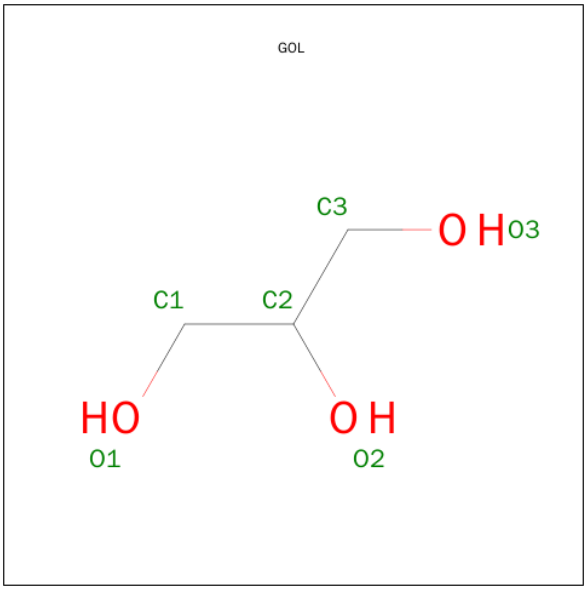
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 7 is water.

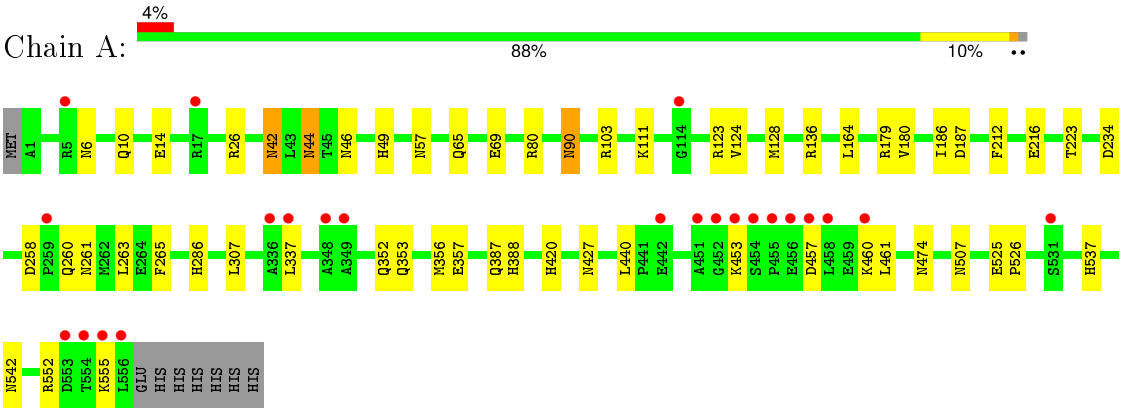
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	441	Total O 441 441	0	1
7	B	417	Total O 417 417	0	1

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

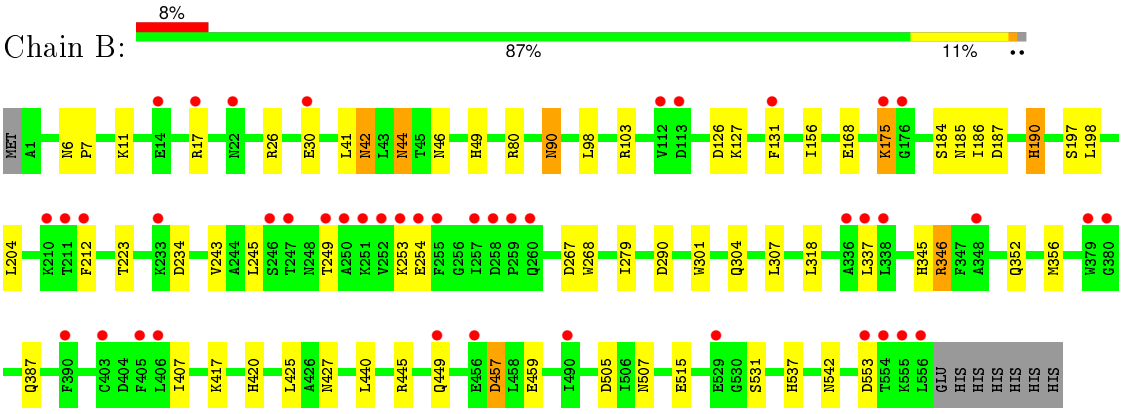
- Molecule 1: Glucose-6-phosphate isomerase

Chain A:



- Molecule 1: Glucose-6-phosphate isomerase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.40Å 116.80Å 73.90Å 90.00° 101.60° 90.00°	Depositor
Resolution (Å)	45.00 – 1.60 45.45 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.6 (45.00-1.60) 94.5 (45.45-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.21 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.178 , 0.207 0.179 , 0.207	Depositor DCC
R_{free} test set	7207 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	18.1	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 50.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 143580 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9903	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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, G6P, G6Q, 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	0.51	0/4631	0.70	3/6269 (0.0%)
1	B	0.48	0/4617	0.70	9/6247 (0.1%)
All	All	0.49	0/9248	0.70	12/12516 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	290	ASP	CB-CG-OD2	7.79	125.31	118.30
1	B	267	ASP	CB-CG-OD2	7.74	125.27	118.30
1	B	187	ASP	CB-CG-OD2	6.56	124.20	118.30
1	A	187	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	234	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	457	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	234	ASP	CB-CG-OD2	6.10	123.79	118.30
1	B	457	ASP	CB-CG-OD2	6.10	123.79	118.30
1	B	126	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	505	ASP	CB-CG-OD2	5.27	123.05	118.30
1	B	346	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	553	ASP	CB-CG-OD2	5.01	122.81	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	4450	0	4434	36	0
1	B	4446	0	4438	36	0
2	A	17	0	12	0	0
3	A	16	0	11	2	0
4	A	10	0	0	0	0
4	B	30	0	0	2	0
5	B	4	0	6	0	0
6	A	54	0	72	13	0
6	B	18	0	24	2	0
7	A	441	0	0	5	0
7	B	417	0	0	9	0
All	All	9903	0	8997	75	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 4.

All (75) 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:A:136:ARG:HE	6:A:1026:GOL:H32	1.07	1.09
1:B:449[A]:GLN:NE2	7:B:1383:HOH:O	1.92	1.00
6:B:1029:GOL:H32	7:B:1264:HOH:O	1.77	0.85
1:B:449[B]:GLN:NE2	7:B:1337:HOH:O	2.11	0.83
1:A:136:ARG:NE	6:A:1026:GOL:H32	1.92	0.80
1:B:301:TRP:O	1:B:304[B]:GLN:HG3	1.81	0.79
1:B:531:SER:H	6:B:1029:GOL:H12	1.51	0.74
1:B:449[B]:GLN:NE2	7:B:1383:HOH:O	2.21	0.74
1:B:537:HIS:H	1:B:542:ASN:HD21	1.36	0.73
1:A:537:HIS:H	1:A:542:ASN:HD21	1.38	0.70
4:B:1008:SO4:O2	7:B:1266:HOH:O	2.08	0.69
4:B:1008:SO4:O4	7:B:1342:HOH:O	2.13	0.67
1:A:42:ASN:HD21	1:A:49:HIS:HD2	1.40	0.67
1:A:136:ARG:HH21	6:A:1026:GOL:H12	1.60	0.65
1:B:185:ASN:H	1:B:190:HIS:HD2	1.42	0.65
1:B:445:ARG:O	1:B:449[B]:GLN:HG3	1.98	0.64
1:A:136:ARG:HE	6:A:1026:GOL:C3	1.99	0.63
1:A:179:ARG:HG2	6:A:1030:GOL:H11	1.84	0.59
1:B:345:HIS:HD2	7:B:1139:HOH:O	1.85	0.59
1:A:42:ASN:ND2	1:A:49:HIS:HD2	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:GLU:OE2	1:B:345:HIS:HE1	1.87	0.58
1:A:387:GLN:HE22	1:A:427:ASN:HB3	1.68	0.58
1:A:57:ASN:HD21	1:A:474:ASN:ND2	2.02	0.57
6:A:1026:GOL:O2	7:A:1207:HOH:O	2.16	0.57
1:B:175:LYS:HB2	7:B:1150:HOH:O	2.05	0.56
1:A:42:ASN:HD21	1:A:49:HIS:CD2	2.22	0.56
1:A:261:ASN:ND2	6:A:1027:GOL:O1	2.39	0.55
1:A:388:HIS:CE1	1:B:156:ILE:HD12	2.43	0.54
1:A:223:THR:OG1	1:B:420:HIS:HE1	1.91	0.53
1:A:420:HIS:HE1	1:B:223:THR:OG1	1.91	0.52
1:A:6:ASN:O	1:A:10[B]:GLN:HG3	2.09	0.52
7:A:1323:HOH:O	1:B:457:ASP:HB3	2.09	0.52
1:B:184:SER:H	1:B:190:HIS:CD2	2.28	0.52
6:A:1032:GOL:H32	7:A:1323:HOH:O	2.10	0.51
1:B:131:PHE:CZ	1:B:243:VAL:HG11	2.45	0.51
1:A:42:ASN:C	1:A:42:ASN:HD22	2.13	0.51
1:A:186:ILE:HB	1:A:216:GLU:HG3	1.94	0.49
1:A:90:ASN:ND2	1:A:507:ASN:HD21	2.10	0.49
1:A:186:ILE:O	1:B:420:HIS:HD2	1.96	0.48
1:A:525:GLU:HB2	1:A:526:PRO:HD3	1.96	0.48
1:A:357:GLU:OE2	3:A:901[B]:G6Q:H2	2.13	0.48
1:B:44:ASN:ND2	1:B:46:ASN:H	2.12	0.47
1:A:164[B]:LEU:HD11	6:A:1025:GOL:H31	1.94	0.47
1:B:80:ARG:HD2	1:B:307:LEU:HA	1.95	0.47
1:B:245:LEU:HD13	1:B:279:ILE:HA	1.96	0.47
1:B:42:ASN:ND2	1:B:49:HIS:HD2	2.12	0.47
1:A:353:GLN:OE1	3:A:901[B]:G6Q:H1	2.15	0.47
1:B:352:GLN:O	1:B:356:MET:HB2	2.14	0.47
1:B:42:ASN:HD21	1:B:49:HIS:CD2	2.33	0.46
1:A:258:ASP:OD2	1:A:260:GLN:HG2	2.16	0.46
1:A:65:GLN:O	1:A:69:GLU:HG2	2.16	0.46
1:B:387:GLN:HE22	1:B:427:ASN:HB3	1.79	0.46
1:B:346:ARG:HD3	7:B:1273:HOH:O	2.16	0.46
1:A:44:ASN:ND2	1:A:46:ASN:H	2.14	0.46
1:B:42:ASN:HD22	1:B:42:ASN:C	2.20	0.46
1:A:164[B]:LEU:CD1	6:A:1025:GOL:H31	2.47	0.45
1:A:420:HIS:HD2	1:B:186:ILE:O	1.99	0.45
1:B:42:ASN:HD21	1:B:49:HIS:HD2	1.62	0.45
1:B:407:ILE:HD13	1:B:425:LEU:HD23	1.98	0.45
1:A:111:LYS:HE2	7:A:1423:HOH:O	2.17	0.45
1:A:128:MET:HG2	1:A:263:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1032:GOL:C3	7:A:1323:HOH:O	2.65	0.44
1:B:98:LEU:HB2	1:B:268:TRP:CE3	2.53	0.44
1:A:180[B]:VAL:HG22	1:A:286:HIS:CE1	2.53	0.43
1:A:90:ASN:HD22	1:A:507:ASN:HD21	1.66	0.43
1:A:352:GLN:O	1:A:356:MET:HB2	2.18	0.43
1:A:124:VAL:O	1:A:128:MET:HG3	2.19	0.42
1:B:41:LEU:HD11	1:B:318:LEU:HD12	2.01	0.42
1:B:6:ASN:HA	1:B:7:PRO:HD3	1.93	0.42
1:B:90:ASN:HD22	1:B:507:ASN:HD21	1.69	0.41
1:A:80:ARG:HD2	1:A:307:LEU:HA	2.02	0.41
1:B:249:THR:HG22	1:B:253:LYS:HE2	2.03	0.41
1:B:44:ASN:C	1:B:44:ASN:HD22	2.24	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	569/564 (101%)	557 (98%)	12 (2%)	0	100	100
1	B	567/564 (100%)	550 (97%)	17 (3%)	0	100	100
All	All	1136/1128 (101%)	1107 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	489/482 (102%)	473 (97%)	16 (3%)	45 17
1	B	487/482 (101%)	465 (96%)	22 (4%)	34 10
All	All	976/964 (101%)	938 (96%)	38 (4%)	39 13

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	26	ARG
1	A	42	ASN
1	A	44	ASN
1	A	90	ASN
1	A	103	ARG
1	A	123	ARG
1	A	212	PHE
1	A	265	PHE
1	A	337	LEU
1	A	440	LEU
1	A	453	LYS
1	A	460	LYS
1	A	461	LEU
1	A	552	ARG
1	A	555	LYS
1	B	11	LYS
1	B	17	ARG
1	B	26	ARG
1	B	30	GLU
1	B	42	ASN
1	B	44	ASN
1	B	90	ASN
1	B	103	ARG
1	B	127	LYS
1	B	175	LYS
1	B	190	HIS
1	B	197	SER
1	B	198	LEU
1	B	204	LEU
1	B	212	PHE
1	B	254	GLU
1	B	337	LEU
1	B	417	LYS

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Mol	Chain	Res	Type
1	B	440	LEU
1	B	459	GLU
1	B	515[A]	GLU
1	B	515[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	37	ASN
1	A	38	ASN
1	A	42	ASN
1	A	44	ASN
1	A	49	HIS
1	A	65	GLN
1	A	82	ASN
1	A	90	ASN
1	A	104	ASN
1	A	153	ASN
1	A	215	GLN
1	A	261	ASN
1	A	304	GLN
1	A	353	GLN
1	A	387	GLN
1	A	420	HIS
1	A	449	GLN
1	A	474	ASN
1	A	542	ASN
1	B	8	GLN
1	B	10	GLN
1	B	22	ASN
1	B	42	ASN
1	B	44	ASN
1	B	49	HIS
1	B	82	ASN
1	B	90	ASN
1	B	153	ASN
1	B	190	HIS
1	B	215	GLN
1	B	345	HIS
1	B	353	GLN
1	B	373	GLN

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Mol	Chain	Res	Type
1	B	385	ASN
1	B	387	GLN
1	B	420	HIS
1	B	542	ASN

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)

Of 24 ligands modelled in this entry, 1 is modelled with single atom - leaving 23 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	A	1001	-	4,4,4	0.14	0	6,6,6	0.16	0
4	SO4	A	1002	-	4,4,4	0.22	0	6,6,6	0.07	0
6	GOL	A	1021	-	5,5,5	0.30	0	5,5,5	0.46	0
6	GOL	A	1023	-	5,5,5	0.41	0	5,5,5	0.44	0
6	GOL	A	1024	-	5,5,5	0.31	0	5,5,5	0.54	0
6	GOL	A	1025	-	5,5,5	0.34	0	5,5,5	0.24	0
6	GOL	A	1026	-	5,5,5	0.33	0	5,5,5	0.43	0
6	GOL	A	1027	-	5,5,5	0.37	0	5,5,5	0.39	0
6	GOL	A	1030	-	5,5,5	0.41	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GOL	A	1031	-	5,5,5	0.53	0	5,5,5	0.59	0
6	GOL	A	1032	-	5,5,5	0.37	0	5,5,5	0.32	0
2	G6P	A	900[A]	-	16,16,16	0.98	1 (6%)	23,24,24	3.11	9 (39%)
3	G6Q	A	901[B]	-	15,15,15	1.46	2 (13%)	18,21,21	1.52	3 (16%)
4	SO4	B	1003	-	4,4,4	0.19	0	6,6,6	0.07	0
4	SO4	B	1004	-	4,4,4	0.18	0	6,6,6	0.14	0
4	SO4	B	1005	-	4,4,4	0.20	0	6,6,6	0.11	0
4	SO4	B	1006	-	4,4,4	0.14	0	6,6,6	0.13	0
4	SO4	B	1007	-	4,4,4	0.19	0	6,6,6	0.10	0
4	SO4	B	1008	-	4,4,4	0.16	0	6,6,6	0.16	0
5	BME	B	1011	-	3,3,3	0.31	0	2,2,2	0.09	0
6	GOL	B	1022	-	5,5,5	0.32	0	5,5,5	0.30	0
6	GOL	B	1028	-	5,5,5	0.29	0	5,5,5	0.35	0
6	GOL	B	1029	-	5,5,5	0.30	0	5,5,5	0.42	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
4	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
6	GOL	A	1021	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1023	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1024	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1025	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1026	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1027	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1030	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1031	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1032	-	-	0/4/4/4	0/0/0/0
2	G6P	A	900[A]	-	-	0/6/26/26	0/1/1/1
3	G6Q	A	901[B]	-	-	0/18/20/20	0/0/0/0
4	SO4	B	1003	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1005	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1006	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1007	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1008	-	-	0/0/0/0	0/0/0/0
5	BME	B	1011	-	-	0/1/1/1	0/0/0/0
6	GOL	B	1022	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	1028	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1029	-	-	0/4/4/4	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901[B]	G6Q	C2-C1	2.25	1.54	1.50
2	A	900[A]	G6P	P-O3P	2.42	1.59	1.51
3	A	901[B]	G6Q	O1-C1	4.82	1.42	1.19

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	900[A]	G6P	O2-C2-C3	-4.07	101.17	110.34
3	A	901[B]	G6Q	O1-C1-C2	-3.91	114.20	125.60
2	A	900[A]	G6P	O2-C2-C1	-3.08	103.03	109.82
3	A	901[B]	G6Q	O3P-P-O1P	2.06	117.20	110.58
3	A	901[B]	G6Q	C3-C2-C1	2.08	114.74	111.68
2	A	900[A]	G6P	O5-C5-C6	2.94	112.62	106.61
2	A	900[A]	G6P	C4-C3-C2	3.26	116.89	110.79
2	A	900[A]	G6P	C1-O5-C5	4.31	121.45	113.47
2	A	900[A]	G6P	C3-C4-C5	4.65	118.30	110.20
2	A	900[A]	G6P	O5-C1-C2	6.00	119.36	109.80
2	A	900[A]	G6P	O5-C5-C4	6.25	121.42	109.68
2	A	900[A]	G6P	C1-C2-C3	7.01	120.85	110.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1025	GOL	2	0
6	A	1026	GOL	5	0
6	A	1027	GOL	1	0
6	A	1030	GOL	3	0
6	A	1032	GOL	2	0
3	A	901[B]	G6Q	2	0
4	B	1008	SO4	2	0
6	B	1029	GOL	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	556/564 (98%)	-0.02	23 (4%)	41	37	13, 19, 34, 50	0
1	B	556/564 (98%)	0.27	44 (7%)	15	13	13, 23, 37, 45	0
All	All	1112/1128 (98%)	0.12	67 (6%)	25	22	13, 21, 36, 50	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	555	LYS	5.5
1	B	253	LYS	5.3
1	A	556	LEU	4.7
1	B	254	GLU	4.7
1	B	131	PHE	4.7
1	A	456	GLU	4.7
1	B	556	LEU	4.6
1	A	553	ASP	4.5
1	B	211	THR	4.2
1	B	553	ASP	4.0
1	A	455	PRO	3.9
1	A	452	GLY	3.8
1	B	456	GLU	3.7
1	B	247	THR	3.7
1	B	246	SER	3.6
1	B	337	LEU	3.6
1	B	250	ALA	3.5
1	A	554	THR	3.4
1	B	555	LYS	3.4
1	B	255	PHE	3.3
1	B	348	ALA	3.3
1	B	249	THR	3.2
1	A	5	ARG	3.2
1	B	257	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	451	ALA	3.1
1	B	176	GLY	3.1
1	A	457	ASP	3.0
1	B	251	LYS	3.0
1	A	17	ARG	3.0
1	B	338	LEU	2.9
1	B	554	THR	2.9
1	A	460	LYS	2.9
1	B	260	GLN	2.7
1	B	22	ASN	2.7
1	B	210	LYS	2.7
1	A	442	GLU	2.7
1	B	175	LYS	2.7
1	A	114	GLY	2.6
1	B	212	PHE	2.6
1	A	454	SER	2.6
1	B	17	ARG	2.5
1	A	259	PRO	2.5
1	B	30	GLU	2.5
1	B	449[A]	GLN	2.4
1	A	453	LYS	2.4
1	B	529	GLU	2.4
1	B	113	ASP	2.4
1	B	379	TRP	2.4
1	B	112	VAL	2.3
1	B	252	VAL	2.3
1	A	531	SER	2.3
1	A	348	ALA	2.3
1	A	458	LEU	2.3
1	B	390	PHE	2.3
1	B	405	PHE	2.3
1	B	258	ASP	2.2
1	B	336	ALA	2.1
1	B	259	PRO	2.1
1	A	349	ALA	2.1
1	B	490	ILE	2.1
1	B	380	GLY	2.1
1	A	337	LEU	2.1
1	B	406	LEU	2.1
1	B	14	GLU	2.1
1	A	336	ALA	2.0
1	B	403	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	233	LYS	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	A	1002	5/5	0.93	0.24	25.40	75,75,76,76	0
6	GOL	A	1030	6/6	0.66	0.25	18.66	29,34,38,39	0
4	SO4	B	1003	5/5	0.84	0.26	17.52	65,65,65,66	0
4	SO4	B	1008	5/5	0.94	0.35	11.34	58,58,58,58	0
6	GOL	A	1032	6/6	0.56	0.41	10.76	41,43,45,47	0
4	SO4	B	1007	5/5	0.92	0.29	5.10	64,65,65,65	0
6	GOL	A	1023	6/6	0.86	0.22	4.83	34,35,36,38	0
3	G6Q	A	901[B]	16/16	0.94	0.15	4.61	8,17,20,22	16
6	GOL	B	1028	6/6	0.79	0.27	3.97	40,41,42,43	0
5	BME	B	1011	4/4	0.86	0.13	3.93	40,41,42,43	0
6	GOL	A	1031	6/6	0.83	0.20	3.58	27,35,37,38	0
2	G6P	A	900[A]	16/16	0.94	0.14	3.37	26,30,32,32	16
6	GOL	A	1021	6/6	0.90	0.15	2.47	29,29,32,33	0
6	GOL	A	1026	6/6	0.76	0.23	2.46	38,39,41,41	0
6	GOL	A	1027	6/6	0.80	0.18	1.75	38,39,40,40	0
6	GOL	A	1024	6/6	0.82	0.18	1.45	33,35,36,37	0
6	GOL	A	1025	6/6	0.88	0.14	0.89	40,41,42,43	0
4	SO4	A	1001	5/5	0.93	0.17	0.76	41,41,42,43	0
6	GOL	B	1022	6/6	0.91	0.13	0.32	32,33,34,35	0
4	SO4	B	1004	5/5	0.97	0.15	-0.13	36,37,38,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	B	1006	5/5	0.93	0.23	-	55,55,56,56	0
4	SO4	B	1005	5/5	0.76	0.32	-	79,79,79,79	0
2	G6P	A	900[B]	1/16	0.94	0.14	-	29,29,29,29	1
6	GOL	B	1029	6/6	0.77	0.21	-	39,40,41,43	0

6.5 Other polymers (i)

There are no such residues in this entry.