Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 07:15 PM EDT

PDB ID	:	6D23
Title	:	GLUCOSE-6-P DEHYDROGENASE (APO FORM) FROM TRYPANOSOMA CRUZI
Authors	:	Botti, H.; Ortiz, C.; Comini, M.A.; Larrieux, N.; Buschiazzo, A.
Deposited on	:	2018-04-12
Resolution	:	2.85 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

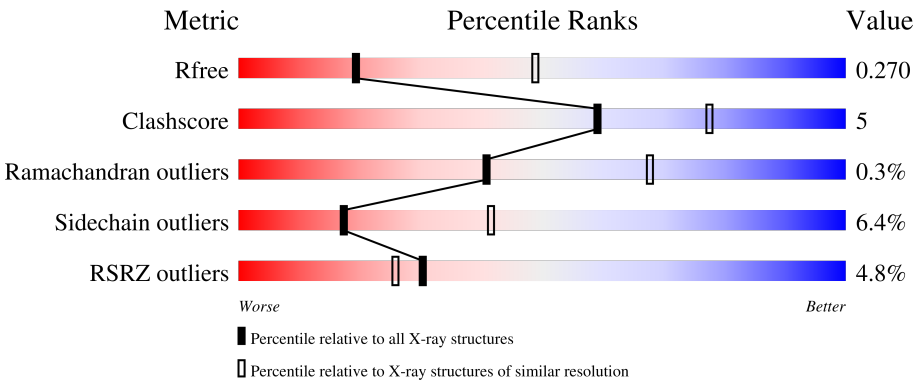
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	541	5% 75% 14% • 10%
1	B	541	4% 76% 13% • 9%
1	C	541	5% 78% 12% • 9%
1	D	541	4% 77% 14% • 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15846 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 1-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	3858	2446	684	713	15	0	3	0
1	B	490	3857	2445	675	722	15	0	1	0
1	C	494	3900	2472	686	726	16	0	3	0
1	D	494	3893	2468	684	725	16	0	2	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MET	-	expression tag	UNP Q1WBU6
A	16	GLY	-	expression tag	UNP Q1WBU6
A	17	SER	-	expression tag	UNP Q1WBU6
A	18	SER	-	expression tag	UNP Q1WBU6
A	19	HIS	-	expression tag	UNP Q1WBU6
A	20	HIS	-	expression tag	UNP Q1WBU6
A	21	HIS	-	expression tag	UNP Q1WBU6
A	22	HIS	-	expression tag	UNP Q1WBU6
A	23	HIS	-	expression tag	UNP Q1WBU6
A	24	HIS	-	expression tag	UNP Q1WBU6
A	25	SER	-	expression tag	UNP Q1WBU6
A	26	SER	-	expression tag	UNP Q1WBU6
A	27	GLY	-	expression tag	UNP Q1WBU6
A	28	LEU	-	expression tag	UNP Q1WBU6
A	29	VAL	-	expression tag	UNP Q1WBU6
A	30	PRO	-	expression tag	UNP Q1WBU6
A	31	ARG	-	expression tag	UNP Q1WBU6
A	32	GLY	-	expression tag	UNP Q1WBU6
A	33	SER	-	expression tag	UNP Q1WBU6
A	34	HIS	-	expression tag	UNP Q1WBU6
A	35	MET	-	expression tag	UNP Q1WBU6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	36	ALA	-	expression tag	UNP Q1WBU6
A	37	SER	-	expression tag	UNP Q1WBU6
A	290	GLU	ALA	conflict	UNP Q1WBU6
B	15	MET	-	expression tag	UNP Q1WBU6
B	16	GLY	-	expression tag	UNP Q1WBU6
B	17	SER	-	expression tag	UNP Q1WBU6
B	18	SER	-	expression tag	UNP Q1WBU6
B	19	HIS	-	expression tag	UNP Q1WBU6
B	20	HIS	-	expression tag	UNP Q1WBU6
B	21	HIS	-	expression tag	UNP Q1WBU6
B	22	HIS	-	expression tag	UNP Q1WBU6
B	23	HIS	-	expression tag	UNP Q1WBU6
B	24	HIS	-	expression tag	UNP Q1WBU6
B	25	SER	-	expression tag	UNP Q1WBU6
B	26	SER	-	expression tag	UNP Q1WBU6
B	27	GLY	-	expression tag	UNP Q1WBU6
B	28	LEU	-	expression tag	UNP Q1WBU6
B	29	VAL	-	expression tag	UNP Q1WBU6
B	30	PRO	-	expression tag	UNP Q1WBU6
B	31	ARG	-	expression tag	UNP Q1WBU6
B	32	GLY	-	expression tag	UNP Q1WBU6
B	33	SER	-	expression tag	UNP Q1WBU6
B	34	HIS	-	expression tag	UNP Q1WBU6
B	35	MET	-	expression tag	UNP Q1WBU6
B	36	ALA	-	expression tag	UNP Q1WBU6
B	37	SER	-	expression tag	UNP Q1WBU6
B	290	GLU	ALA	conflict	UNP Q1WBU6
C	15	MET	-	expression tag	UNP Q1WBU6
C	16	GLY	-	expression tag	UNP Q1WBU6
C	17	SER	-	expression tag	UNP Q1WBU6
C	18	SER	-	expression tag	UNP Q1WBU6
C	19	HIS	-	expression tag	UNP Q1WBU6
C	20	HIS	-	expression tag	UNP Q1WBU6
C	21	HIS	-	expression tag	UNP Q1WBU6
C	22	HIS	-	expression tag	UNP Q1WBU6
C	23	HIS	-	expression tag	UNP Q1WBU6
C	24	HIS	-	expression tag	UNP Q1WBU6
C	25	SER	-	expression tag	UNP Q1WBU6
C	26	SER	-	expression tag	UNP Q1WBU6
C	27	GLY	-	expression tag	UNP Q1WBU6
C	28	LEU	-	expression tag	UNP Q1WBU6
C	29	VAL	-	expression tag	UNP Q1WBU6

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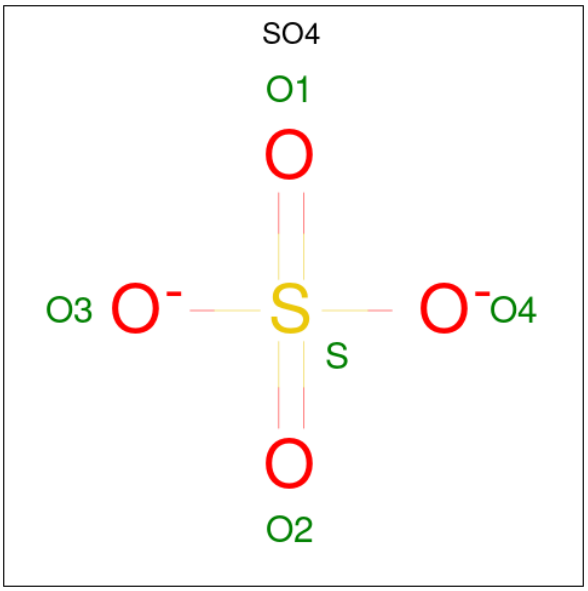
Chain	Residue	Modelled	Actual	Comment	Reference
C	30	PRO	-	expression tag	UNP Q1WBU6
C	31	ARG	-	expression tag	UNP Q1WBU6
C	32	GLY	-	expression tag	UNP Q1WBU6
C	33	SER	-	expression tag	UNP Q1WBU6
C	34	HIS	-	expression tag	UNP Q1WBU6
C	35	MET	-	expression tag	UNP Q1WBU6
C	36	ALA	-	expression tag	UNP Q1WBU6
C	37	SER	-	expression tag	UNP Q1WBU6
C	290	GLU	ALA	conflict	UNP Q1WBU6
D	15	MET	-	expression tag	UNP Q1WBU6
D	16	GLY	-	expression tag	UNP Q1WBU6
D	17	SER	-	expression tag	UNP Q1WBU6
D	18	SER	-	expression tag	UNP Q1WBU6
D	19	HIS	-	expression tag	UNP Q1WBU6
D	20	HIS	-	expression tag	UNP Q1WBU6
D	21	HIS	-	expression tag	UNP Q1WBU6
D	22	HIS	-	expression tag	UNP Q1WBU6
D	23	HIS	-	expression tag	UNP Q1WBU6
D	24	HIS	-	expression tag	UNP Q1WBU6
D	25	SER	-	expression tag	UNP Q1WBU6
D	26	SER	-	expression tag	UNP Q1WBU6
D	27	GLY	-	expression tag	UNP Q1WBU6
D	28	LEU	-	expression tag	UNP Q1WBU6
D	29	VAL	-	expression tag	UNP Q1WBU6
D	30	PRO	-	expression tag	UNP Q1WBU6
D	31	ARG	-	expression tag	UNP Q1WBU6
D	32	GLY	-	expression tag	UNP Q1WBU6
D	33	SER	-	expression tag	UNP Q1WBU6
D	34	HIS	-	expression tag	UNP Q1WBU6
D	35	MET	-	expression tag	UNP Q1WBU6
D	36	ALA	-	expression tag	UNP Q1WBU6
D	37	SER	-	expression tag	UNP Q1WBU6
D	290	GLU	ALA	conflict	UNP Q1WBU6

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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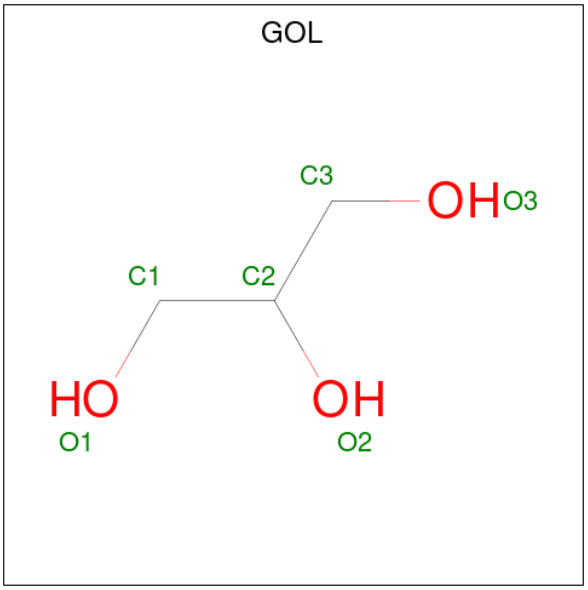
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	5	5	5	0	0
			Total	Cl		
4	B	4	4	4	0	0
			Total	Cl		
4	C	9	9	9	0	0
			Total	Cl		
4	D	5	5	5	0	0

- Molecule 5 is water.

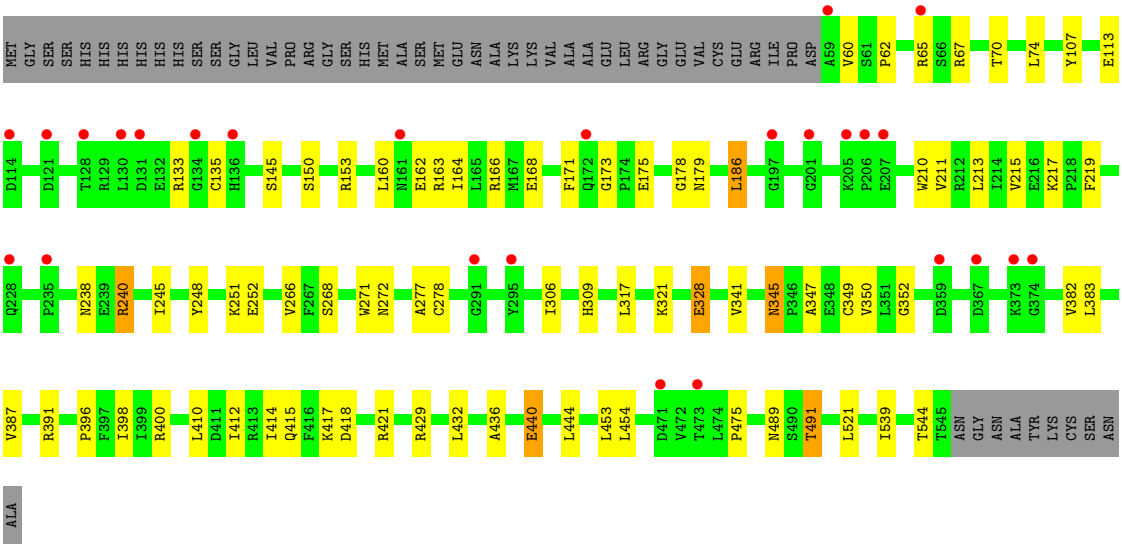
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	16	16	16	0	0
			Total	O		
5	B	8	8	8	0	0
			Total	O		
5	C	22	22	22	0	0
			Total	O		
5	D	29	29	29	0	0

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.

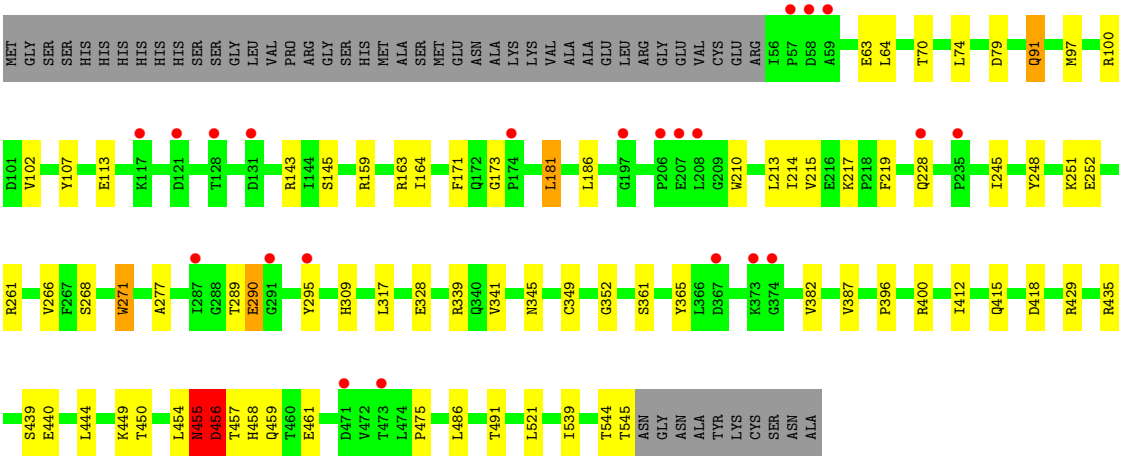
• Molecule 1: Glucose-6-phosphate 1-dehydrogenase

Chain A:



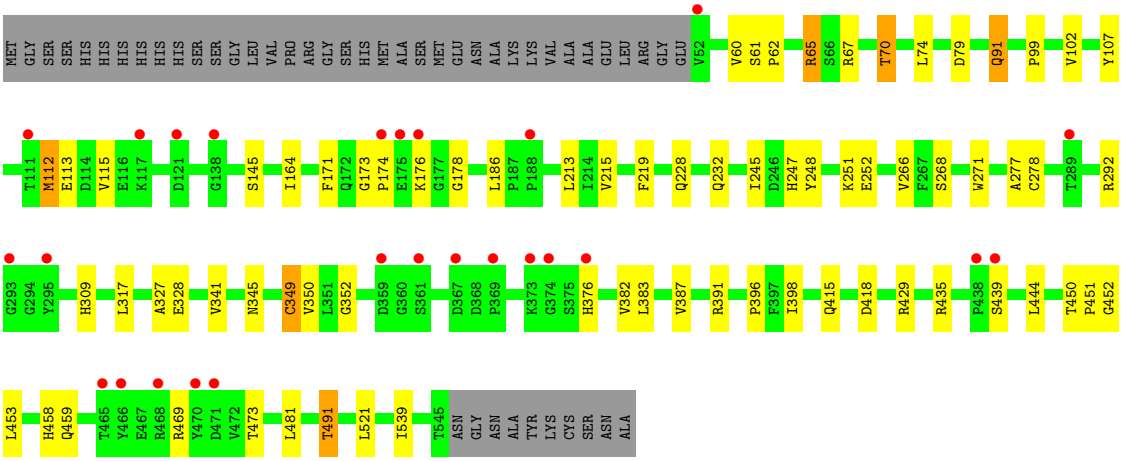
• Molecule 1: Glucose-6-phosphate 1-dehydrogenase

Chain B:



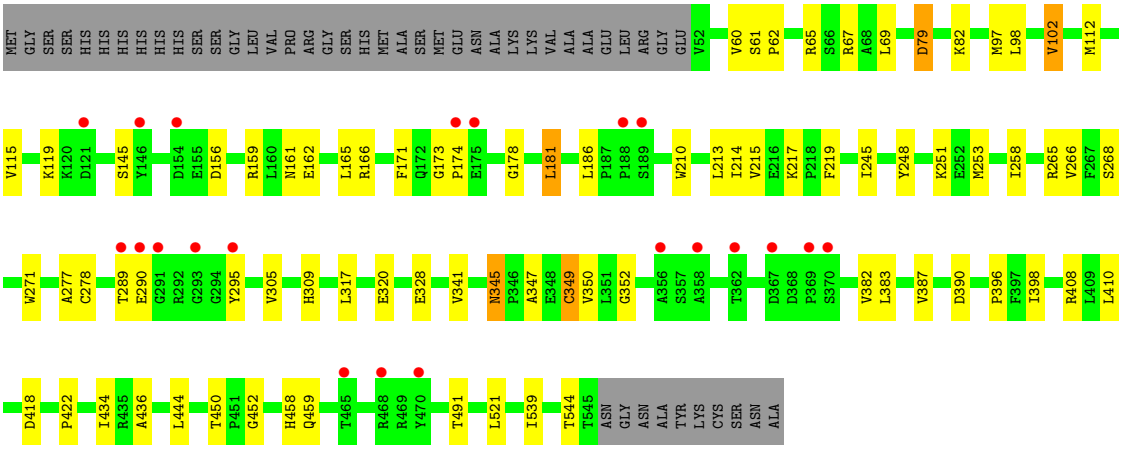
• Molecule 1: Glucose-6-phosphate 1-dehydrogenase

Chain C:



• Molecule 1: Glucose-6-phosphate 1-dehydrogenase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.61Å 132.96Å 107.83Å 90.00° 100.11° 90.00°	Depositor
Resolution (Å)	29.63 – 2.85 29.63 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.63-2.85) 99.0 (29.63-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.85Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.204 , 0.249 0.219 , 0.270	Depositor DCC
R_{free} test set	1257 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å^2)	39.4	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 61.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	15846	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6399e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, CL, 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	0.50	0/3945	0.72	0/5344
1	B	0.51	0/3938	0.74	2/5342 (0.0%)
1	C	0.53	0/3988	0.74	0/5407
1	D	0.52	0/3977	0.72	0/5393
All	All	0.52	0/15848	0.73	2/21486 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	455[A]	ASN	C-N-CA	5.98	136.64	121.70
1	B	455[B]	ASN	C-N-CA	5.98	136.64	121.70

There are no chirality outliers.

There are no planarity outliers.

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	3858	0	3834	45	0
1	B	3857	0	3804	39	0
1	C	3900	0	3855	34	0
1	D	3893	0	3848	39	0
2	A	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	30	0	0	1	0
2	C	20	0	0	0	0
2	D	40	0	0	0	0
3	A	30	0	40	7	0
3	B	30	0	40	4	0
3	C	36	0	48	0	0
3	D	24	0	32	5	0
4	A	5	0	0	0	0
4	B	4	0	0	0	0
4	C	9	0	0	0	0
4	D	5	0	0	1	0
5	A	16	0	0	0	0
5	B	8	0	0	0	0
5	C	22	0	0	1	0
5	D	29	0	0	0	0
All	All	15846	0	15501	146	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 (146) 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:215:VAL:HG12	1:D:219:PHE:HE1	1.46	0.79
1:C:215:VAL:HG12	1:C:219:PHE:HE1	1.48	0.78
1:B:215:VAL:HG12	1:B:219:PHE:HE1	1.47	0.78
1:A:215:VAL:HG12	1:A:219:PHE:HE1	1.49	0.77
1:B:251:LYS:HG2	3:B:608:GOL:H12	1.74	0.68
1:A:321:LYS:HB2	3:A:609:GOL:H31	1.76	0.67
1:B:435:ARG:HH21	1:B:439:SER:HB3	1.59	0.66
1:B:461:GLU:HB2	1:C:469:ARG:HH12	1.61	0.65
1:B:261:ARG:HD3	1:B:271:TRP:CE2	2.32	0.64
1:B:91:GLN:HA	1:B:91:GLN:HE21	1.62	0.63
1:C:349:CYS:HB2	1:C:383:LEU:HD23	1.81	0.63
1:D:345:ASN:HD21	1:D:347:ALA:HB3	1.64	0.61
1:A:345:ASN:HD21	1:A:347:ALA:HB3	1.65	0.61
1:C:215:VAL:HG12	1:C:219:PHE:CE1	2.35	0.61
1:B:215:VAL:HG12	1:B:219:PHE:CE1	2.35	0.60
1:D:215:VAL:HG12	1:D:219:PHE:CE1	2.34	0.60
1:B:252:GLU:OE2	1:C:451:PRO:HA	2.00	0.60
1:A:60:VAL:HG13	1:A:65:ARG:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:THR:HG21	1:C:164:ILE:HG23	1.84	0.59
3:A:608:GOL:H32	3:A:609:GOL:H2	1.85	0.59
1:D:349:CYS:HB2	1:D:383:LEU:HD23	1.83	0.59
1:B:415:GLN:HG2	1:B:429:ARG:HD3	1.85	0.58
1:A:252:GLU:N	3:A:610:GOL:H11	2.19	0.58
1:A:215:VAL:HG12	1:A:219:PHE:CE1	2.36	0.58
1:B:475:PRO:HD3	1:C:452:GLY:HA2	1.86	0.57
1:B:341:VAL:HG22	1:B:387:VAL:HG22	1.87	0.56
1:D:181:LEU:HD21	1:D:214:ILE:HG13	1.86	0.56
1:B:449:LYS:HD2	1:B:455[B]:ASN:OD1	2.06	0.56
1:A:70:THR:HG21	1:A:164:ILE:HG23	1.88	0.55
1:C:91:GLN:HE21	1:C:91:GLN:HA	1.70	0.55
1:C:60:VAL:HG21	1:C:99:PRO:HA	1.89	0.55
1:A:415:GLN:HG2	1:A:429:ARG:HD3	1.89	0.55
1:A:162:GLU:O	1:A:166:ARG:HG2	2.07	0.54
1:C:473:THR:HA	5:C:718:HOH:O	2.07	0.54
1:A:341:VAL:HG22	1:A:387:VAL:HG22	1.89	0.54
1:A:321:LYS:CB	3:A:609:GOL:H31	2.37	0.54
1:A:168:GLU:HG2	1:A:178:GLY:HA3	1.90	0.54
1:C:278:CYS:SG	1:C:398:ILE:HD12	2.49	0.53
1:C:341:VAL:HG22	1:C:387:VAL:HG22	1.91	0.53
1:D:248:TYR:HA	1:D:251:LYS:HD2	1.89	0.53
1:B:352:GLY:HA2	1:B:521:LEU:O	2.09	0.53
1:D:62:PRO:HA	1:D:65:ARG:HG3	1.89	0.52
1:A:238:ASN:HB3	1:A:240:ARG:HE	1.75	0.52
1:C:352:GLY:HA2	1:C:521:LEU:O	2.10	0.52
1:A:352:GLY:HA2	1:A:521:LEU:O	2.09	0.52
1:D:352:GLY:HA2	1:D:521:LEU:O	2.09	0.52
1:D:410:LEU:HD23	1:D:436:ALA:HB3	1.92	0.52
1:C:248:TYR:HA	1:C:251:LYS:HD2	1.91	0.51
1:A:248:TYR:HA	1:A:251:LYS:HD2	1.93	0.51
1:B:444:LEU:HD11	1:C:266:VAL:HG21	1.93	0.51
1:D:341:VAL:HG22	1:D:387:VAL:HG22	1.92	0.51
1:C:171:PHE:CE2	1:C:173:GLY:HA3	2.46	0.51
1:A:440:GLU:CG	3:A:610:GOL:H12	2.41	0.50
1:A:440:GLU:HG2	3:A:610:GOL:H12	1.93	0.50
1:D:258:ILE:HG21	3:D:609:GOL:H12	1.93	0.50
1:A:278:CYS:SG	1:A:398:ILE:HD12	2.51	0.50
1:A:306:ILE:HD13	1:A:383:LEU:CD1	2.41	0.50
1:D:305:VAL:HG22	3:D:612:GOL:C3	2.41	0.50
1:B:248:TYR:HA	1:B:251:LYS:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:THR:HG23	3:B:607:GOL:H11	1.93	0.50
1:A:306:ILE:HD13	1:A:383:LEU:HD11	1.94	0.50
1:A:62:PRO:HA	1:A:65:ARG:HD3	1.94	0.50
1:B:266:VAL:HG21	1:C:444:LEU:HD11	1.92	0.50
1:A:67:ARG:HD3	1:A:175:GLU:HB3	1.93	0.49
1:C:435:ARG:HH21	1:C:439:SER:HB2	1.77	0.49
1:B:289:THR:HG21	1:B:365:TYR:HE1	1.77	0.48
1:D:79:ASP:HA	1:D:82:LYS:HE2	1.95	0.48
1:B:317:LEU:HD21	1:B:412:ILE:HG21	1.94	0.48
1:D:171:PHE:CE2	1:D:173:GLY:HA3	2.48	0.48
1:D:156:ASP:HA	1:D:159:ARG:HD3	1.96	0.48
1:D:248:TYR:CD2	1:D:309:HIS:HB3	2.49	0.48
1:C:74:LEU:HD13	1:C:107:TYR:HB3	1.96	0.47
1:B:248:TYR:CD2	1:B:309:HIS:HB3	2.49	0.47
3:B:614:GOL:H11	1:D:390:ASP:HB3	1.97	0.47
1:A:248:TYR:CD2	1:A:309:HIS:HB3	2.50	0.47
1:C:248:TYR:CD2	1:C:309:HIS:HB3	2.49	0.47
1:D:305:VAL:HG22	3:D:612:GOL:H32	1.96	0.47
1:B:100:ARG:O	1:B:143:ARG:HD2	2.15	0.47
1:C:415:GLN:HG2	1:C:429:ARG:HD3	1.96	0.47
1:A:317:LEU:HD21	1:A:412:ILE:HG21	1.95	0.46
1:A:171:PHE:CE2	1:A:173:GLY:HA3	2.51	0.46
1:A:272:ASN:CB	1:A:391[B]:ARG:HG3	2.45	0.46
1:B:171:PHE:CE2	1:B:173:GLY:HA3	2.51	0.46
1:B:181:LEU:HD11	1:B:214:ILE:HD12	1.98	0.46
1:D:162:GLU:HA	1:D:165:LEU:HD12	1.97	0.46
1:C:112:MET:HG2	1:C:115:VAL:HG22	1.97	0.45
1:D:408:ARG:NH1	4:D:615:CL:CL	2.87	0.45
1:A:179:ASN:HD22	1:A:210:TRP:H	1.63	0.45
1:A:489:ASN:OD1	1:A:491:THR:HG23	2.16	0.45
1:B:215:VAL:CG1	1:B:219:PHE:HE1	2.25	0.45
1:B:544:THR:HG22	1:B:545:THR:H	1.82	0.45
1:D:60:VAL:HG13	1:D:65:ARG:HG2	1.99	0.45
1:D:210:TRP:CB	3:D:610:GOL:H2	2.47	0.45
1:D:215:VAL:CG1	1:D:219:PHE:HE1	2.25	0.45
1:D:277:ALA:O	1:D:396:PRO:HD2	2.16	0.45
1:D:210:TRP:HB3	3:D:610:GOL:H2	1.99	0.45
1:C:62:PRO:HA	1:C:65:ARG:HG3	1.99	0.44
1:C:450:THR:HG22	1:C:458:HIS:HB3	1.99	0.44
1:A:475:PRO:HD3	1:D:452:GLY:HA2	1.98	0.44
1:C:67:ARG:HG2	1:C:178:GLY:HA2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:ARG:HG2	1:D:178:GLY:HA2	2.00	0.44
1:D:450:THR:HG22	1:D:458:HIS:HB3	2.00	0.44
1:B:382:VAL:HG12	1:B:400:ARG:HG2	2.00	0.43
3:A:607:GOL:H11	1:C:391:ARG:HA	1.98	0.43
1:A:382:VAL:HG12	1:A:400:ARG:HG2	1.99	0.43
1:B:70:THR:HG21	1:B:164:ILE:HG23	2.00	0.43
1:B:289:THR:HG21	1:B:365:TYR:CE1	2.53	0.43
1:C:327:ALA:HA	1:C:491:THR:HG23	2.00	0.43
1:D:278:CYS:SG	1:D:398:ILE:HD12	2.59	0.43
1:B:444:LEU:HD21	1:C:266:VAL:HG11	2.01	0.43
1:C:277:ALA:O	1:C:396:PRO:HD2	2.18	0.43
1:D:115:VAL:O	1:D:119:LYS:HG3	2.18	0.43
1:A:266:VAL:HG11	1:D:444:LEU:HD21	2.01	0.43
1:B:159:ARG:HD2	2:B:604:SO4:O1	2.18	0.43
1:A:272:ASN:HB3	1:A:391[B]:ARG:HG3	2.01	0.42
1:B:102:VAL:O	1:B:143:ARG:HD3	2.19	0.42
1:A:238:ASN:HD22	1:A:240:ARG:NH2	2.18	0.42
1:A:74:LEU:HB3	1:A:186:LEU:HD21	2.01	0.42
1:A:410:LEU:HD23	1:A:436:ALA:HB3	2.01	0.42
1:D:98:LEU:HB3	1:D:102:VAL:HG21	2.00	0.42
1:D:253:MET:HE3	1:D:434:ILE:HG23	2.01	0.42
1:A:350:VAL:HB	1:A:382:VAL:HG22	2.01	0.42
1:B:277:ALA:O	1:B:396:PRO:HD2	2.19	0.42
1:A:414:ILE:HD13	1:A:432:LEU:HD23	2.01	0.41
1:B:64:LEU:HD21	1:B:486:LEU:HB3	2.02	0.41
1:A:453:LEU:HD23	1:D:97:MET:SD	2.60	0.41
1:B:181:LEU:HD21	1:B:214:ILE:HG13	2.00	0.41
1:A:277:ALA:O	1:A:396:PRO:HD2	2.20	0.41
1:B:450:THR:OG1	1:B:456:ASP:HB3	2.20	0.41
1:C:247:HIS:HA	1:C:481:LEU:HD11	2.02	0.41
1:A:150:SER:OG	1:A:153:ARG:HB2	2.20	0.41
1:C:292:ARG:HA	1:C:292:ARG:HD3	1.94	0.41
1:D:69:LEU:HD23	1:D:102:VAL:HG13	2.02	0.41
1:D:161:ASN:O	1:D:165:LEU:HG	2.20	0.41
1:A:107:TYR:CD2	1:A:160:LEU:HD13	2.55	0.41
1:A:417:LYS:HB2	1:D:265:ARG:HD2	2.02	0.41
1:A:444:LEU:HD11	1:D:266:VAL:HG21	2.02	0.41
1:B:450:THR:HG22	1:B:458:HIS:HB3	2.03	0.40
1:D:350:VAL:HB	1:D:382:VAL:HG13	2.03	0.40
1:C:350:VAL:HB	1:C:382:VAL:HG13	2.03	0.40
1:A:215:VAL:CG1	1:A:219:PHE:HE1	2.26	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328[A]:GLU:OE1	1:A:328[A]:GLU:HA	2.20	0.40
1:B:74:LEU:HD13	1:B:107:TYR:HB3	2.04	0.40
1:B:210:TRP:HA	3:B:609:GOL:H2	2.02	0.40
1:B:475:PRO:CD	1:C:452:GLY:HA2	2.51	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	488/541 (90%)	462 (95%)	25 (5%)	1 (0%)	47	75
1	B	489/541 (90%)	456 (93%)	30 (6%)	3 (1%)	25	53
1	C	495/541 (92%)	469 (95%)	25 (5%)	1 (0%)	47	75
1	D	494/541 (91%)	469 (95%)	24 (5%)	1 (0%)	47	75
All	All	1966/2164 (91%)	1856 (94%)	104 (5%)	6 (0%)	41	68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	440	GLU
1	B	290	GLU
1	B	440	GLU
1	B	456	ASP
1	C	174	PRO
1	D	174	PRO

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	412/462 (89%)	389 (94%)	23 (6%)	21	47
1	B	412/462 (89%)	382 (93%)	30 (7%)	14	35
1	C	417/462 (90%)	388 (93%)	29 (7%)	15	37
1	D	416/462 (90%)	388 (93%)	28 (7%)	16	39
All	All	1657/1848 (90%)	1547 (93%)	110 (7%)	17	40

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	GLU
1	A	133	ARG
1	A	135	CYS
1	A	145	SER
1	A	163	ARG
1	A	186	LEU
1	A	211	VAL
1	A	213	LEU
1	A	217	LYS
1	A	240	ARG
1	A	245	ILE
1	A	268	SER
1	A	271	TRP
1	A	328[A]	GLU
1	A	328[B]	GLU
1	A	345	ASN
1	A	349	CYS
1	A	418	ASP
1	A	421	ARG
1	A	454	LEU
1	A	491	THR
1	A	539	ILE
1	A	544	THR
1	B	63	GLU
1	B	79	ASP
1	B	91	GLN
1	B	97	MET
1	B	113	GLU

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Mol	Chain	Res	Type
1	B	145	SER
1	B	163	ARG
1	B	181	LEU
1	B	186	LEU
1	B	213	LEU
1	B	217	LYS
1	B	228	GLN
1	B	245	ILE
1	B	268	SER
1	B	271	TRP
1	B	290	GLU
1	B	295	TYR
1	B	328	GLU
1	B	339	ARG
1	B	345	ASN
1	B	349	CYS
1	B	361	SER
1	B	418	ASP
1	B	454	LEU
1	B	455[A]	ASN
1	B	455[B]	ASN
1	B	456	ASP
1	B	459	GLN
1	B	491	THR
1	B	539	ILE
1	C	61	SER
1	C	65	ARG
1	C	70	THR
1	C	79	ASP
1	C	91	GLN
1	C	102	VAL
1	C	112	MET
1	C	113	GLU
1	C	145	SER
1	C	176	LYS
1	C	186	LEU
1	C	213	LEU
1	C	228[A]	GLN
1	C	228[B]	GLN
1	C	245	ILE
1	C	252	GLU
1	C	268	SER

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Mol	Chain	Res	Type
1	C	271	TRP
1	C	317	LEU
1	C	328	GLU
1	C	345	ASN
1	C	349	CYS
1	C	376	HIS
1	C	418[A]	ASP
1	C	418[B]	ASP
1	C	453	LEU
1	C	459	GLN
1	C	491	THR
1	C	539	ILE
1	D	61	SER
1	D	79	ASP
1	D	102	VAL
1	D	112	MET
1	D	145	SER
1	D	166	ARG
1	D	181	LEU
1	D	186	LEU
1	D	213	LEU
1	D	217	LYS
1	D	245	ILE
1	D	268	SER
1	D	271	TRP
1	D	289	THR
1	D	290	GLU
1	D	295	TYR
1	D	317	LEU
1	D	320	GLU
1	D	328	GLU
1	D	345	ASN
1	D	349	CYS
1	D	418[A]	ASP
1	D	418[B]	ASP
1	D	422	PRO
1	D	459	GLN
1	D	491	THR
1	D	539	ILE
1	D	544	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	238	ASN
1	A	345	ASN
1	B	91	GLN
1	B	386	HIS
1	C	91	GLN
1	C	255	GLN
1	D	345	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 67 ligands modelled in this entry, 23 are monoatomic - leaving 44 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	$\#\|Z\| > 2$
3	GOL	B	609	-	5,5,5	0.14	0	5,5,5	0.29	0
3	GOL	B	614	-	5,5,5	0.18	0	5,5,5	0.24	0
3	GOL	A	607	-	5,5,5	0.20	0	5,5,5	0.81	0
3	GOL	C	608	-	5,5,5	0.11	0	5,5,5	0.40	0
2	SO4	D	606	-	4,4,4	0.17	0	6,6,6	0.15	0
3	GOL	D	612	-	5,5,5	0.13	0	5,5,5	0.22	0
2	SO4	D	605	-	4,4,4	0.17	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	D	602	-	4,4,4	0.19	0	6,6,6	0.23	0
2	SO4	A	605	-	4,4,4	0.13	0	6,6,6	0.17	0
2	SO4	D	603	-	4,4,4	0.23	0	6,6,6	0.29	0
3	GOL	B	607	-	5,5,5	0.21	0	5,5,5	0.44	0
2	SO4	A	603	-	4,4,4	0.10	0	6,6,6	0.36	0
2	SO4	B	605	-	4,4,4	0.15	0	6,6,6	0.33	0
2	SO4	A	604	-	4,4,4	0.23	0	6,6,6	0.13	0
3	GOL	A	608	-	5,5,5	0.14	0	5,5,5	0.37	0
3	GOL	C	602	-	5,5,5	0.17	0	5,5,5	0.34	0
2	SO4	A	602	-	4,4,4	0.29	0	6,6,6	0.32	0
2	SO4	C	604	-	4,4,4	0.26	0	6,6,6	0.47	0
2	SO4	C	605	-	4,4,4	0.23	0	6,6,6	0.22	0
3	GOL	B	615	-	5,5,5	0.23	0	5,5,5	0.23	0
2	SO4	D	601	-	4,4,4	0.25	0	6,6,6	0.39	0
2	SO4	A	601	-	4,4,4	0.21	0	6,6,6	0.42	0
2	SO4	C	606	-	4,4,4	0.42	0	6,6,6	0.41	0
2	SO4	C	607	-	4,4,4	0.13	0	6,6,6	0.13	0
3	GOL	C	609	-	5,5,5	0.15	0	5,5,5	0.31	0
3	GOL	C	611	-	5,5,5	0.13	0	5,5,5	0.24	0
2	SO4	B	603	-	4,4,4	0.15	0	6,6,6	0.16	0
2	SO4	D	607	-	4,4,4	0.16	0	6,6,6	0.24	0
3	GOL	C	601	-	5,5,5	0.14	0	5,5,5	0.25	0
3	GOL	C	610	-	5,5,5	0.29	0	5,5,5	0.33	0
2	SO4	D	604	-	4,4,4	0.11	0	6,6,6	0.22	0
3	GOL	B	608	-	5,5,5	0.20	0	5,5,5	0.31	0
2	SO4	B	602	-	4,4,4	0.26	0	6,6,6	0.31	0
3	GOL	D	611	-	5,5,5	0.22	0	5,5,5	0.24	0
3	GOL	A	609	-	5,5,5	0.12	0	5,5,5	0.26	0
3	GOL	D	609	-	5,5,5	0.20	0	5,5,5	0.49	0
2	SO4	A	606	-	4,4,4	0.20	0	6,6,6	0.24	0
2	SO4	B	604	-	4,4,4	0.40	0	6,6,6	0.29	0
2	SO4	B	601	-	4,4,4	0.15	0	6,6,6	0.55	0
3	GOL	A	611	-	5,5,5	0.10	0	5,5,5	0.39	0
3	GOL	A	610	-	5,5,5	0.13	0	5,5,5	0.96	0
2	SO4	B	606	-	4,4,4	0.16	0	6,6,6	0.17	0
3	GOL	D	610	-	5,5,5	0.20	0	5,5,5	0.57	0
2	SO4	D	608	-	4,4,4	0.25	0	6,6,6	0.15	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	GOL	B	609	-	-	0/4/4/4	-
3	GOL	B	614	-	-	2/4/4/4	-
3	GOL	A	607	-	-	0/4/4/4	-
3	GOL	C	608	-	-	1/4/4/4	-
3	GOL	D	612	-	-	2/4/4/4	-
3	GOL	B	607	-	-	1/4/4/4	-
3	GOL	A	608	-	-	2/4/4/4	-
3	GOL	C	602	-	-	0/4/4/4	-
3	GOL	B	615	-	-	2/4/4/4	-
3	GOL	C	609	-	-	1/4/4/4	-
3	GOL	C	611	-	-	0/4/4/4	-
3	GOL	C	601	-	-	0/4/4/4	-
3	GOL	C	610	-	-	0/4/4/4	-
3	GOL	B	608	-	-	2/4/4/4	-
3	GOL	D	611	-	-	4/4/4/4	-
3	GOL	D	609	-	-	0/4/4/4	-
3	GOL	A	609	-	-	2/4/4/4	-
3	GOL	A	611	-	-	0/4/4/4	-
3	GOL	A	610	-	-	2/4/4/4	-
3	GOL	D	610	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	609	GOL	O1-C1-C2-C3
3	B	608	GOL	C1-C2-C3-O3
3	B	615	GOL	O1-C1-C2-C3
3	D	610	GOL	C1-C2-C3-O3
3	D	611	GOL	O1-C1-C2-O2
3	D	611	GOL	C1-C2-C3-O3
3	D	612	GOL	C1-C2-C3-O3
3	A	609	GOL	O1-C1-C2-O2
3	A	608	GOL	C1-C2-C3-O3
3	A	610	GOL	C1-C2-C3-O3
3	D	611	GOL	O1-C1-C2-C3
3	D	610	GOL	O2-C2-C3-O3
3	D	612	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	608	GOL	O2-C2-C3-O3
3	A	610	GOL	O2-C2-C3-O3
3	B	615	GOL	O1-C1-C2-O2
3	C	608	GOL	C1-C2-C3-O3
3	A	608	GOL	O2-C2-C3-O3
3	D	611	GOL	O2-C2-C3-O3
3	B	614	GOL	O1-C1-C2-C3
3	B	614	GOL	O1-C1-C2-O2
3	B	607	GOL	C1-C2-C3-O3
3	C	609	GOL	C1-C2-C3-O3

There are no ring outliers.

12 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	609	GOL	1	0
3	B	614	GOL	1	0
3	A	607	GOL	1	0
3	D	612	GOL	2	0
3	B	607	GOL	1	0
3	A	608	GOL	1	0
3	B	608	GOL	1	0
3	A	609	GOL	3	0
3	D	609	GOL	1	0
2	B	604	SO4	1	0
3	A	610	GOL	3	0
3	D	610	GOL	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	487/541 (90%)	0.16	26 (5%)	26	22	12, 44, 82, 106	0
1	B	490/541 (90%)	0.02	22 (4%)	33	28	14, 41, 78, 99	0
1	C	494/541 (91%)	0.08	26 (5%)	26	22	13, 42, 78, 98	0
1	D	494/541 (91%)	0.01	21 (4%)	35	30	14, 41, 75, 99	0
All	All	1965/2164 (90%)	0.07	95 (4%)	30	26	12, 42, 79, 106	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	358	ALA	5.0
1	C	295	TYR	4.9
1	D	293	GLY	4.7
1	B	291	GLY	4.4
1	B	206	PRO	4.4
1	B	131	ASP	4.3
1	A	131	ASP	4.3
1	A	206	PRO	4.0
1	C	470	TYR	4.0
1	B	58	ASP	4.0
1	C	369	PRO	4.0
1	B	207	GLU	3.9
1	C	289	THR	3.9
1	D	295	TYR	3.8
1	B	367	ASP	3.8
1	A	471	ASP	3.8
1	A	473	THR	3.8
1	B	117	LYS	3.7
1	D	465	THR	3.6
1	A	197	GLY	3.6
1	C	465	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	290	GLU	3.3
1	D	174	PRO	3.3
1	C	361	SER	3.2
1	A	291	GLY	3.2
1	A	59	ALA	3.2
1	A	207	GLU	3.2
1	A	295	TYR	3.1
1	A	65	ARG	3.0
1	D	189	SER	3.0
1	A	121	ASP	2.9
1	D	289	THR	2.9
1	D	468	ARG	2.9
1	B	128	THR	2.9
1	C	175	GLU	2.9
1	C	466	TYR	2.9
1	B	208	LEU	2.8
1	C	374	GLY	2.8
1	A	373	LYS	2.8
1	C	188	PRO	2.8
1	D	370	SER	2.7
1	D	291	GLY	2.7
1	A	228	GLN	2.7
1	D	362	THR	2.7
1	A	172	GLN	2.7
1	C	367	ASP	2.7
1	A	205	LYS	2.7
1	D	188	PRO	2.6
1	C	176	LYS	2.6
1	D	175	GLU	2.6
1	A	128	THR	2.6
1	C	359	ASP	2.6
1	D	470	TYR	2.6
1	B	235	PRO	2.6
1	C	471	ASP	2.6
1	C	468	ARG	2.6
1	A	374	GLY	2.5
1	D	369	PRO	2.5
1	C	52	VAL	2.5
1	B	121	ASP	2.5
1	C	373	LYS	2.5
1	A	201	GLY	2.5
1	B	374	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	130	LEU	2.5
1	B	373	LYS	2.4
1	B	197	GLY	2.4
1	B	57	PRO	2.4
1	A	235	PRO	2.4
1	A	359	ASP	2.4
1	B	471	ASP	2.4
1	C	293	GLY	2.3
1	C	121	ASP	2.3
1	C	439	SER	2.3
1	B	295	TYR	2.3
1	A	161	ASN	2.3
1	B	174	PRO	2.3
1	A	136	HIS	2.2
1	D	367	ASP	2.2
1	A	114	ASP	2.2
1	A	134	GLY	2.2
1	A	367	ASP	2.2
1	C	111	THR	2.1
1	C	376	HIS	2.1
1	B	287	ILE	2.1
1	B	228	GLN	2.1
1	D	154	ASP	2.1
1	D	356	ALA	2.1
1	C	138	GLY	2.1
1	B	473	THR	2.0
1	C	117	LYS	2.0
1	B	59	ALA	2.0
1	C	174	PRO	2.0
1	C	438	PRO	2.0
1	D	121	ASP	2.0
1	D	146	TYR	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 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	609	6/6	0.56	0.34	72,78,82,84	0
3	GOL	C	611	6/6	0.68	0.29	56,60,61,64	0
4	CL	D	616	1/1	0.68	0.20	82,82,82,82	0
4	CL	D	615	1/1	0.69	0.10	77,77,77,77	0
4	CL	A	615	1/1	0.73	0.13	68,68,68,68	0
3	GOL	D	610	6/6	0.74	0.29	37,53,55,55	0
4	CL	B	611	1/1	0.74	0.18	94,94,94,94	0
4	CL	C	614	1/1	0.75	0.12	68,68,68,68	0
3	GOL	A	607	6/6	0.76	0.34	38,43,46,46	0
3	GOL	A	610	6/6	0.76	0.38	51,54,55,56	0
4	CL	A	614	1/1	0.77	0.27	74,74,74,74	0
4	CL	C	603	1/1	0.78	0.27	79,79,79,79	0
2	SO4	B	603	5/5	0.78	0.32	121,121,122,123	0
3	GOL	D	612	6/6	0.79	0.30	59,62,63,64	0
3	GOL	B	607	6/6	0.79	0.18	43,45,47,47	0
3	GOL	D	609	6/6	0.79	0.30	51,56,58,59	0
3	GOL	B	615	6/6	0.79	0.28	40,48,49,49	0
3	GOL	C	610	6/6	0.81	0.20	46,51,52,52	0
4	CL	C	615	1/1	0.81	0.16	68,68,68,68	0
3	GOL	A	611	6/6	0.81	0.20	53,56,61,62	0
3	GOL	B	608	6/6	0.81	0.22	50,56,58,59	0
3	GOL	D	611	6/6	0.82	0.20	31,34,39,45	0
3	GOL	A	608	6/6	0.82	0.28	55,57,58,59	0
3	GOL	A	609	6/6	0.82	0.30	55,60,60,61	0
4	CL	C	613	1/1	0.82	0.10	64,64,64,64	0
2	SO4	D	604	5/5	0.83	0.25	90,92,92,94	0
3	GOL	C	601	6/6	0.83	0.29	73,75,77,77	0
3	GOL	C	609	6/6	0.83	0.23	42,46,49,49	0
2	SO4	C	607	5/5	0.86	0.23	105,105,106,107	0
2	SO4	D	605	5/5	0.87	0.29	123,123,123,123	0
2	SO4	D	603	5/5	0.88	0.22	72,72,74,77	0
4	CL	A	616	1/1	0.88	0.08	59,59,59,59	0
2	SO4	D	607	5/5	0.88	0.25	107,108,108,109	0
4	CL	B	612	1/1	0.88	0.10	67,67,67,67	0
2	SO4	D	608	5/5	0.88	0.21	104,105,106,108	0
4	CL	D	617	1/1	0.88	0.09	66,66,66,66	0
4	CL	C	618	1/1	0.89	0.09	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	C	602	6/6	0.90	0.25	42,42,43,44	0
2	SO4	D	602	5/5	0.90	0.18	79,80,83,83	0
2	SO4	A	605	5/5	0.90	0.21	106,107,107,108	0
2	SO4	C	606	5/5	0.91	0.18	69,75,75,76	0
4	CL	C	616	1/1	0.91	0.08	80,80,80,80	0
2	SO4	B	606	5/5	0.91	0.56	106,107,107,109	0
2	SO4	A	603	5/5	0.92	0.20	69,72,72,74	0
4	CL	C	617	1/1	0.92	0.12	67,67,67,67	0
3	GOL	C	608	6/6	0.93	0.18	44,45,45,47	0
4	CL	B	610	1/1	0.93	0.07	60,60,60,60	0
4	CL	C	612	1/1	0.94	0.08	48,48,48,48	0
4	CL	A	613	1/1	0.94	0.09	41,41,41,41	0
4	CL	D	613	1/1	0.94	0.13	67,67,67,67	0
4	CL	D	614	1/1	0.94	0.10	69,69,69,69	0
3	GOL	B	614	6/6	0.94	0.16	23,29,33,37	0
2	SO4	B	604	5/5	0.94	0.11	59,62,64,65	0
2	SO4	D	606	5/5	0.94	0.52	130,131,131,132	0
2	SO4	A	604	5/5	0.95	0.19	67,68,68,70	0
2	SO4	C	605	5/5	0.95	0.31	70,71,72,72	0
4	CL	C	619	1/1	0.95	0.15	67,67,67,67	0
4	CL	B	613	1/1	0.95	0.06	47,47,47,47	0
2	SO4	A	602	5/5	0.96	0.14	68,69,69,71	0
4	CL	A	612	1/1	0.96	0.06	58,58,58,58	0
2	SO4	B	602	5/5	0.96	0.14	68,68,70,70	0
2	SO4	D	601	5/5	0.97	0.13	40,43,45,46	0
2	SO4	B	601	5/5	0.97	0.10	49,50,52,57	0
2	SO4	A	601	5/5	0.97	0.11	55,56,57,62	0
2	SO4	A	606	5/5	0.98	0.12	44,45,48,52	0
2	SO4	C	604	5/5	0.98	0.11	42,43,44,46	0
2	SO4	B	605	5/5	0.99	0.12	43,44,49,50	0

6.5 Other polymers (i)

There are no such residues in this entry.