Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:22 PM GMT

PDB ID	:	4EM5
Title	:	Trypanosoma cruzi Glucose-6-P Dehydrogenase in complex with G6P
Authors	:	Buschiazzo, A.; Botti, H.; Ortiz, C.; Comini, M.A.
Deposited on	:	2012-04-11
Resolution	:	3.35 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:

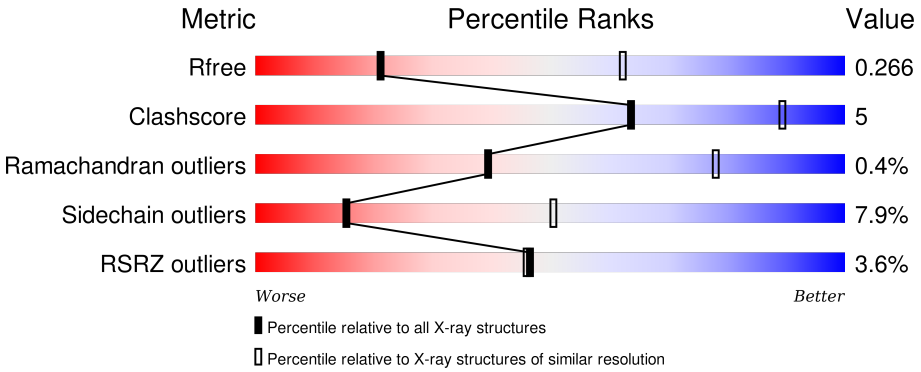
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.35 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	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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	541	4% 74% 14% • 10%
1	B	541	2% 74% 15% • 10%
1	C	541	4% 75% 14% • 9%
1	D	541	3% 74% 16% • 9%

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
3	SO4	A	603	-	-	X	-
3	SO4	B	603	-	-	-	X
3	SO4	B	604	-	-	X	-
3	SO4	C	607	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15722 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
1	A	485	Total	C	N	O	S	0	2	0
			3844	2436	686	707	15			
1	B	487	Total	C	N	O	S	0	0	0
			3849	2438	680	716	15			
1	C	494	Total	C	N	O	S	0	1	0
			3922	2483	698	725	16			
1	D	494	Total	C	N	O	S	0	0	0
			3916	2480	693	727	16			

There are 92 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

Continued on next page...

Continued from previous page...

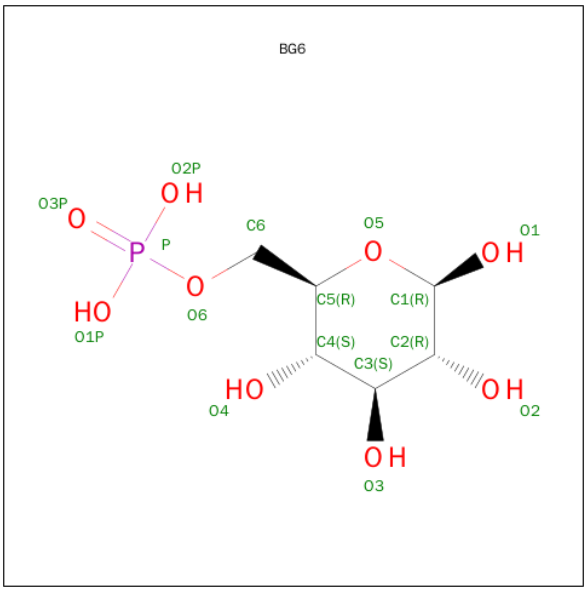
Chain	Residue	Modelled	Actual	Comment	Reference
A	36	ALA	-	EXPRESSION TAG	UNP Q1WBU6
A	37	SER	-	EXPRESSION TAG	UNP Q1WBU6
B	15	MET	-	EXPRESSION TAG	UNP Q1WBU6
B	16	GLY	-	EXPRESSION TAG	UNP Q1WBU6
B	17	SER	-	EXPRESSION TAG	UNP Q1WBU6
B	18	SER	-	EXPRESSION TAG	UNP Q1WBU6
B	19	HIS	-	EXPRESSION TAG	UNP Q1WBU6
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
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
C	30	PRO	-	EXPRESSION TAG	UNP Q1WBU6
C	31	ARG	-	EXPRESSION TAG	UNP Q1WBU6

Continued on next page...

Continued from previous page...

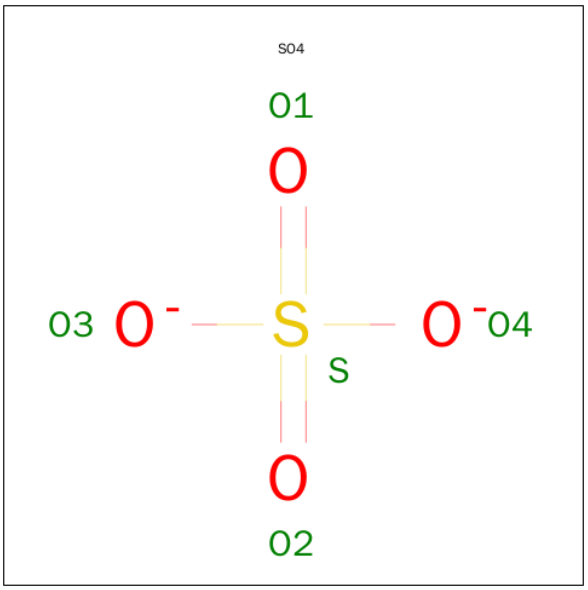
Chain	Residue	Modelled	Actual	Comment	Reference
C	32	GLY	-	EXPRESSION TAG	UNP Q1WBU6
C	33	SER	-	EXPRESSION TAG	UNP Q1WBU6
C	34	HIS	-	EXPRESSION TAG	UNP Q1WBU6
C	35	MET	-	EXPRESSION TAG	UNP Q1WBU6
C	36	ALA	-	EXPRESSION TAG	UNP Q1WBU6
C	37	SER	-	EXPRESSION TAG	UNP Q1WBU6
D	15	MET	-	EXPRESSION TAG	UNP Q1WBU6
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

- Molecule 2 is SUGAR (BETA-D-GLUCOSE-6-PHOSPHATE) (three-letter code: BG6) (formula: $C_6H_{13}O_9P$).



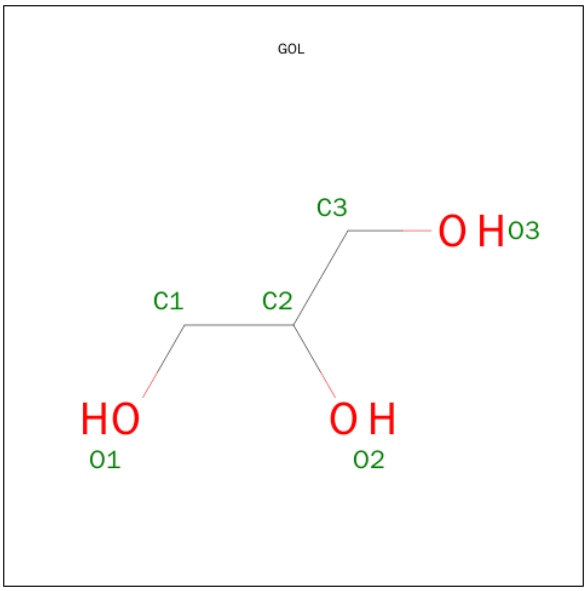
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O P 16 6 9 1	0	0
2	B	1	Total C O P 16 6 9 1	0	0
2	C	1	Total C O P 16 6 9 1	0	0
2	D	1	Total C O P 16 6 9 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

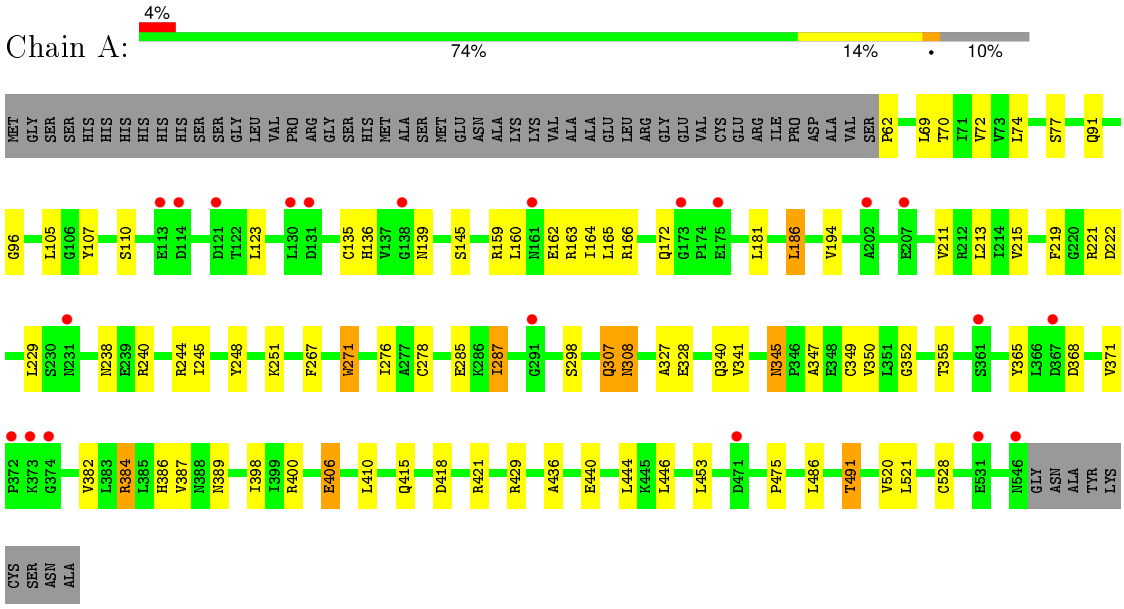
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total O 3 3	0	0
5	B	9	Total O 9 9	0	0
5	C	6	Total O 6 6	0	0
5	D	8	Total O 8 8	0	0

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.

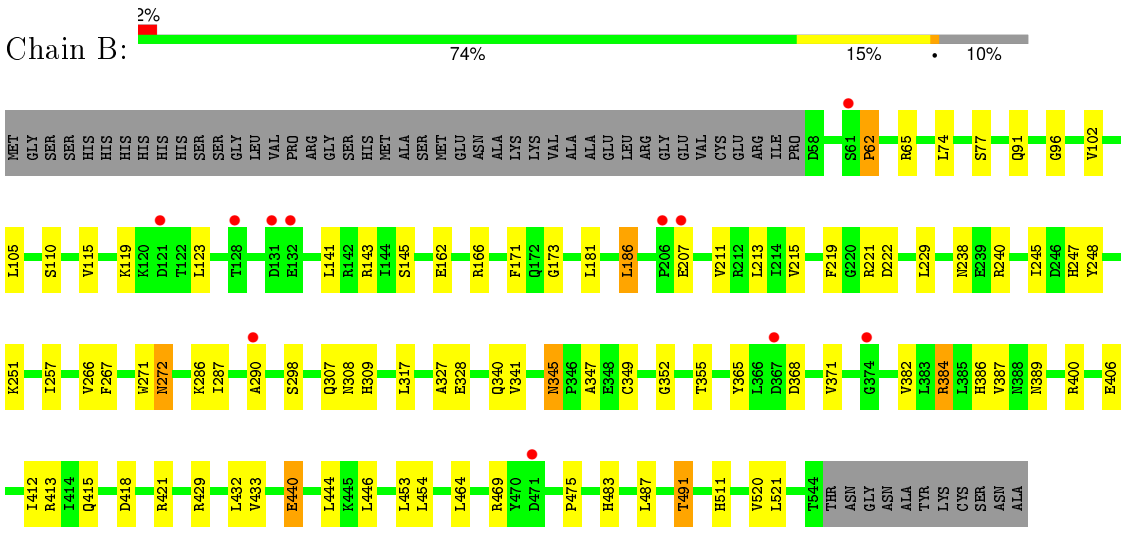
- Molecule 1: Glucose-6-phosphate 1-dehydrogenase

Chain A:



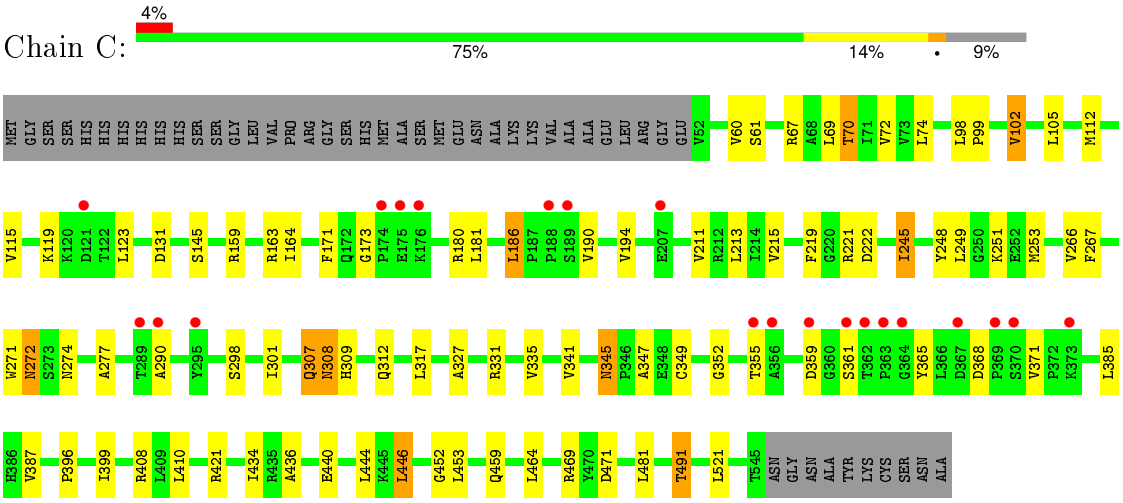
- Molecule 1: Glucose-6-phosphate 1-dehydrogenase

Chain B:



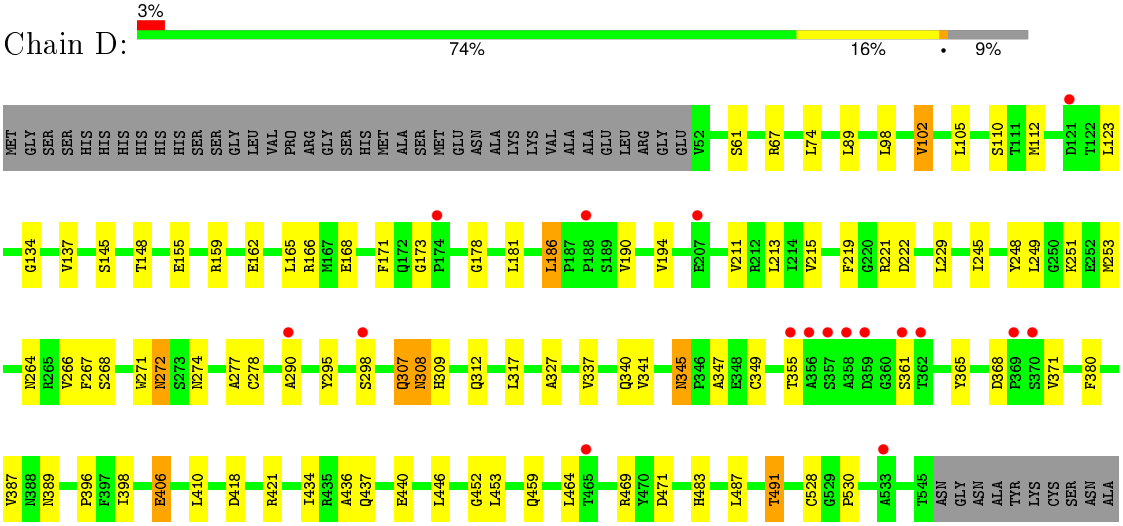
- Molecule 1: Glucose-6-phosphate 1-dehydrogenase

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	96.79Å 133.03Å 107.75Å 90.00° 100.27° 90.00°	Depositor
Resolution (Å)	34.78 – 3.35 34.16 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.78-3.35) 99.4 (34.16-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.217 , 0.246 0.235 , 0.266	Depositor DCC
R_{free} test set	796 reflections (2.11%)	DCC
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	1 of 38457 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	15722	wwPDB-VP
Average B, all atoms (Å^2)	36.0	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 26.87 % 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 2.4373e-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, 0.375 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, SO4, BG6

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	0/3929	0.71	0/5320
1	B	0.51	0/3929	0.72	0/5323
1	C	0.52	0/4006	0.72	0/5425
1	D	0.51	0/3997	0.72	0/5413
All	All	0.51	0/15861	0.72	0/21481

There are no bond length outliers.

There are no bond angle outliers.

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	3844	0	3831	42	0
1	B	3849	0	3821	42	0
1	C	3922	0	3914	45	0
1	D	3916	0	3905	45	0
2	A	16	0	11	0	0
2	B	16	0	11	1	0
2	C	16	0	11	0	0
2	D	16	0	11	2	0
3	A	20	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	35	0	0	3	0
3	C	30	0	0	3	0
3	D	10	0	0	0	0
4	C	6	0	8	0	0
5	A	3	0	0	0	0
5	B	9	0	0	1	0
5	C	6	0	0	1	0
5	D	8	0	0	0	0
All	All	15722	0	15523	161	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 (161) 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:238:ASN:HB3	1:B:240:ARG:HE	1.54	0.73
1:A:215:VAL:HG12	1:A:219:PHE:HE1	1.55	0.71
1:A:267:PHE:HE2	1:D:446:LEU:HD21	1.54	0.71
1:B:215:VAL:HG12	1:B:219:PHE:HE1	1.55	0.70
1:C:215:VAL:HG12	1:C:219:PHE:HE1	1.57	0.69
1:D:215:VAL:HG12	1:D:219:PHE:HE1	1.56	0.68
1:A:238:ASN:HB3	1:A:240:ARG:HE	1.60	0.67
1:C:368:ASP:HB3	1:C:371:VAL:HG12	1.78	0.65
1:A:368:ASP:HB3	1:A:371:VAL:HG12	1.78	0.65
1:D:368:ASP:HB3	1:D:371:VAL:HG12	1.78	0.65
1:B:368:ASP:HB3	1:B:371:VAL:HG12	1.79	0.65
1:A:406:GLU:HG2	1:A:528:CYS:SG	2.38	0.64
1:C:408:ARG:NH1	3:C:607:SO4:S	2.73	0.62
1:A:77:SER:HB2	3:A:603:SO4:O2	2.00	0.62
1:C:408:ARG:NH1	3:C:607:SO4:O4	2.31	0.62
1:D:345:ASN:HD21	1:D:347:ALA:HB3	1.65	0.61
1:B:475:PRO:HD3	1:C:452:GLY:HA2	1.82	0.60
1:B:341:VAL:HG22	1:B:387:VAL:HG22	1.84	0.59
1:D:380:PHE:CE1	1:D:530:PRO:HD2	2.38	0.59
1:B:102:VAL:O	1:B:143:ARG:HD3	2.03	0.59
1:B:62:PRO:HA	1:B:96:GLY:O	2.02	0.59
1:A:77:SER:HB2	3:A:603:SO4:S	2.43	0.58
1:B:257:ILE:N	5:B:705:HOH:O	2.36	0.58
1:D:248:TYR:HA	1:D:251:LYS:HD2	1.84	0.58
1:A:345:ASN:HD21	1:A:347:ALA:HB3	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:ASN:HD21	1:B:347:ALA:HB3	1.69	0.57
1:C:345:ASN:HD21	1:C:347:ALA:HB3	1.70	0.57
1:D:162:GLU:O	1:D:166:ARG:HG2	2.05	0.57
1:C:248:TYR:HA	1:C:251:LYS:HD2	1.86	0.56
1:C:327:ALA:HA	1:C:491:THR:HB	1.88	0.56
1:C:180:ARG:NH2	5:C:704:HOH:O	2.40	0.55
1:B:317:LEU:HD21	1:B:412:ILE:HG21	1.88	0.55
1:B:464:LEU:HD12	1:B:469:ARG:HG3	1.87	0.55
1:A:341:VAL:HG22	1:A:387:VAL:HG22	1.89	0.54
1:B:382:VAL:HG12	1:B:400:ARG:HG2	1.90	0.54
1:D:327:ALA:HA	1:D:491:THR:HB	1.89	0.54
1:C:186:LEU:HD13	1:C:190:VAL:HG23	1.89	0.54
1:B:327:ALA:HA	1:B:491:THR:HB	1.90	0.54
1:C:112:MET:HG2	1:C:115:VAL:HG22	1.90	0.54
1:C:253:MET:HE2	1:C:434:ILE:HG23	1.89	0.54
1:C:215:VAL:HG12	1:C:219:PHE:CE1	2.41	0.54
1:A:248:TYR:HA	1:A:251:LYS:HD2	1.90	0.54
1:B:215:VAL:HG12	1:B:219:PHE:CE1	2.40	0.54
1:C:171:PHE:CE2	1:C:173:GLY:HA3	2.43	0.54
1:A:327:ALA:HA	1:A:491:THR:HB	1.91	0.53
1:A:62:PRO:HA	1:A:96:GLY:O	2.08	0.53
1:D:215:VAL:HG12	1:D:219:PHE:CE1	2.41	0.53
1:B:415:GLN:HG2	1:B:429:ARG:HD3	1.91	0.53
1:B:77:SER:OG	1:B:110:SER:HB3	2.08	0.53
1:C:341:VAL:HG22	1:C:387:VAL:HG22	1.91	0.53
1:A:475:PRO:HD3	1:D:452:GLY:HA2	1.90	0.53
1:A:77:SER:OG	1:A:110:SER:HB3	2.09	0.52
1:A:162:GLU:O	1:A:166:ARG:HG2	2.09	0.52
1:A:70:THR:HG21	1:A:164:ILE:HG23	1.92	0.52
1:B:511:HIS:ND1	3:B:608:SO4:O3	2.41	0.52
1:D:148:THR:O	1:D:159:ARG:NH2	2.36	0.52
1:D:248:TYR:HE1	2:D:601:BG6:O3P	1.93	0.52
1:D:186:LEU:HD22	1:D:194:VAL:HG21	1.92	0.52
1:D:380:PHE:CD1	1:D:530:PRO:HD2	2.44	0.51
1:A:215:VAL:HG12	1:A:219:PHE:CE1	2.40	0.51
1:A:159:ARG:HD2	3:A:602:SO4:O1	2.11	0.51
1:D:341:VAL:HG22	1:D:387:VAL:HG22	1.92	0.51
1:D:74:LEU:HB3	1:D:186:LEU:HD23	1.92	0.50
1:B:266:VAL:HG21	1:C:444:LEU:HD11	1.93	0.50
1:B:171:PHE:CE2	1:B:173:GLY:HA3	2.47	0.50
1:D:221:ARG:NH1	1:D:298:SER:O	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLU:HG2	1:A:287:ILE:HD12	1.93	0.50
1:B:248:TYR:HA	1:B:251:LYS:HD2	1.93	0.50
1:A:350:VAL:HB	1:A:382:VAL:HG22	1.94	0.49
1:D:249:LEU:HD11	1:D:312:GLN:OE1	2.12	0.49
1:D:171:PHE:CE2	1:D:173:GLY:HA3	2.47	0.49
1:C:221:ARG:NH1	1:C:298:SER:O	2.45	0.49
1:A:136:HIS:HA	1:A:139:ASN:HD22	1.77	0.49
1:A:69:LEU:HD21	1:A:486:LEU:HD22	1.95	0.49
1:D:168:GLU:HG2	1:D:178:GLY:HA3	1.94	0.49
1:C:112:MET:HG2	1:C:115:VAL:CG2	2.42	0.49
1:D:67:ARG:HG2	1:D:178:GLY:HA2	1.95	0.49
1:D:278:CYS:SG	1:D:398:ILE:HD12	2.52	0.49
1:C:60:VAL:HG21	1:C:99:PRO:HA	1.94	0.49
1:C:245:ILE:HD13	1:C:481:LEU:HD13	1.95	0.48
1:A:267:PHE:CE2	1:D:446:LEU:HD21	2.42	0.47
1:B:267:PHE:HE2	1:C:446:LEU:HD21	1.78	0.47
1:C:186:LEU:HD22	1:C:194:VAL:HG21	1.95	0.47
1:D:248:TYR:CD2	1:D:309:HIS:HB3	2.49	0.47
1:C:272:ASN:C	1:C:272:ASN:HD22	2.18	0.47
1:D:264:ASN:O	1:D:268:SER:HB2	2.15	0.47
1:D:272:ASN:C	1:D:272:ASN:HD22	2.18	0.47
1:A:415:GLN:HG2	1:A:429:ARG:HD3	1.96	0.47
1:B:221:ARG:NH1	1:B:298:SER:O	2.48	0.46
1:B:444:LEU:HD11	1:C:266:VAL:HG21	1.98	0.46
1:B:446:LEU:HD21	1:C:267:PHE:HE2	1.79	0.46
1:C:249:LEU:HD11	1:C:312:GLN:OE1	2.16	0.46
1:C:159:ARG:NH1	3:C:605:SO4:O2	2.48	0.46
1:A:221:ARG:NH1	1:A:298:SER:O	2.49	0.46
1:B:162:GLU:O	1:B:166:ARG:HG2	2.16	0.46
1:C:464:LEU:HA	1:C:469:ARG:HH21	1.81	0.46
1:A:444:LEU:HD11	1:D:266:VAL:HG21	1.98	0.45
1:B:119:LYS:HB3	1:B:141:LEU:HD22	1.98	0.45
1:D:437:GLN:NE2	2:D:601:BG6:O2P	2.49	0.45
1:C:253:MET:CE	1:C:434:ILE:HG23	2.46	0.45
1:D:253:MET:HE2	1:D:434:ILE:HG23	1.97	0.45
1:D:406:GLU:HG2	1:D:528:CYS:SG	2.57	0.45
1:D:277:ALA:O	1:D:396:PRO:HD2	2.15	0.45
1:C:98:LEU:HB3	1:C:102:VAL:HG21	1.98	0.45
1:B:77:SER:HB2	3:B:604:SO4:S	2.57	0.44
1:D:98:LEU:HB3	1:D:102:VAL:HG21	1.99	0.44
1:A:384:ARG:NH1	1:A:386:HIS:CE1	2.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:MET:CE	1:D:434:ILE:HG23	2.48	0.44
1:D:483:HIS:CE1	1:D:487:LEU:HD11	2.53	0.44
1:C:277:ALA:O	1:C:396:PRO:HD2	2.18	0.44
1:B:272:ASN:C	1:B:272:ASN:HD22	2.21	0.43
1:C:248:TYR:CD2	1:C:309:HIS:HB3	2.54	0.43
1:A:444:LEU:HD21	1:D:266:VAL:HG11	2.01	0.43
1:D:464:LEU:HA	1:D:469:ARG:HH21	1.82	0.43
1:B:115:VAL:HG12	1:B:119:LYS:HE2	2.00	0.43
1:C:272:ASN:HD22	1:C:274:ASN:H	1.67	0.43
1:D:307:GLN:HE21	1:D:308:ASN:HD22	1.66	0.43
1:A:382:VAL:HG12	1:A:400:ARG:HG2	2.01	0.43
1:D:134:GLY:O	1:D:137:VAL:HG12	2.19	0.43
1:D:186:LEU:HD13	1:D:190:VAL:HG23	2.01	0.42
1:A:186:LEU:HD22	1:A:194:VAL:HG21	2.01	0.42
1:A:278:CYS:SG	1:A:398:ILE:HD12	2.59	0.42
1:A:219:PHE:HD1	1:A:244[B]:ARG:HH11	1.66	0.42
1:C:385:LEU:HD12	1:C:399:ILE:HD12	2.01	0.42
1:B:267:PHE:CE2	1:C:446:LEU:HD21	2.55	0.42
1:B:74:LEU:HB3	1:B:186:LEU:HD21	2.01	0.42
1:A:446:LEU:HD13	1:D:267:PHE:HE2	1.85	0.42
1:C:365:TYR:CE2	1:C:371:VAL:HG21	2.55	0.42
1:B:444:LEU:HD21	1:C:266:VAL:HG11	2.01	0.42
1:B:365:TYR:CE2	1:B:371:VAL:HG21	2.55	0.42
1:B:413:ARG:HD3	1:B:433:VAL:HG22	2.02	0.42
1:D:410:LEU:HD23	1:D:436:ALA:HB3	2.02	0.42
1:B:340:GLN:NE2	1:B:389:ASN:HD22	2.17	0.42
1:A:352:GLY:HA2	1:A:521:LEU:O	2.19	0.42
1:A:410:LEU:HD23	1:A:436:ALA:HB3	2.01	0.42
1:C:410:LEU:HD23	1:C:436:ALA:HB3	2.02	0.42
1:C:70:THR:HG21	1:C:164:ILE:HG23	2.01	0.42
1:C:115:VAL:HG12	1:C:119:LYS:HE2	2.02	0.42
1:C:352:GLY:HA2	1:C:521:LEU:O	2.20	0.42
1:D:248:TYR:CE2	1:D:309:HIS:HB3	2.55	0.41
1:C:307:GLN:HE21	1:C:308:ASN:HD22	1.67	0.41
1:D:272:ASN:HD22	1:D:274:ASN:H	1.68	0.41
1:A:77:SER:HB2	3:A:603:SO4:O4	2.21	0.41
1:B:444:LEU:HG	1:B:446:LEU:CD1	2.51	0.41
1:D:365:TYR:CE2	1:D:371:VAL:HG21	2.55	0.41
1:B:483:HIS:CD2	1:B:487:LEU:HD11	2.56	0.41
1:C:69:LEU:HD23	1:C:102:VAL:HG13	2.03	0.41
1:D:340:GLN:NE2	1:D:389:ASN:HD22	2.18	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:TYR:CD2	1:A:160:LEU:HD13	2.55	0.41
1:B:77:SER:HB2	3:B:604:SO4:O3	2.21	0.40
1:B:248:TYR:CD2	1:B:309:HIS:HB3	2.57	0.40
1:C:72:VAL:HG12	1:C:74:LEU:HD22	2.03	0.40
1:A:340:GLN:NE2	1:A:389:ASN:HD22	2.19	0.40
1:A:365:TYR:CE2	1:A:371:VAL:HG21	2.56	0.40
1:A:271:TRP:HA	1:A:276:ILE:HD11	2.04	0.40
1:A:72:VAL:HG12	1:A:74:LEU:HD22	2.03	0.40
1:B:247:HIS:CE1	2:B:601:BG6:HC61	2.56	0.40
1:B:352:GLY:HA2	1:B:521:LEU:O	2.20	0.40
1:C:331:ARG:O	1:C:335:VAL:HG13	2.22	0.40
1:B:384:ARG:NH1	1:B:386:HIS:CE1	2.90	0.40
1:A:307:GLN:HE21	1:A:308:ASN:HD22	1.69	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	485/541 (90%)	459 (95%)	26 (5%)	0	100	100
1	B	485/541 (90%)	453 (93%)	29 (6%)	3 (1%)	30	70
1	C	493/541 (91%)	467 (95%)	24 (5%)	2 (0%)	39	78
1	D	492/541 (91%)	469 (95%)	21 (4%)	2 (0%)	39	78
All	All	1955/2164 (90%)	1848 (94%)	100 (5%)	7 (0%)	39	78

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	62	PRO
1	D	290	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	290	ALA
1	C	290	ALA
1	C	361	SER
1	B	440	GLU
1	D	361	SER

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	410/461 (89%)	379 (92%)	31 (8%)	16	53
1	B	412/461 (89%)	379 (92%)	33 (8%)	15	50
1	C	422/461 (92%)	390 (92%)	32 (8%)	16	53
1	D	422/461 (92%)	387 (92%)	35 (8%)	14	48
All	All	1666/1844 (90%)	1535 (92%)	131 (8%)	15	50

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	105	LEU
1	A	123	LEU
1	A	135	CYS
1	A	145	SER
1	A	163	ARG
1	A	165	LEU
1	A	172	GLN
1	A	181	LEU
1	A	186	LEU
1	A	211	VAL
1	A	213	LEU
1	A	222	ASP
1	A	229	LEU
1	A	245	ILE
1	A	271	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	287	ILE
1	A	307	GLN
1	A	308	ASN
1	A	328	GLU
1	A	345	ASN
1	A	349	CYS
1	A	355	THR
1	A	384	ARG
1	A	406	GLU
1	A	418	ASP
1	A	421	ARG
1	A	440	GLU
1	A	453	LEU
1	A	491	THR
1	A	520	VAL
1	B	65	ARG
1	B	91	GLN
1	B	105	LEU
1	B	123	LEU
1	B	145	SER
1	B	181	LEU
1	B	186	LEU
1	B	207	GLU
1	B	211	VAL
1	B	213	LEU
1	B	222	ASP
1	B	229	LEU
1	B	245	ILE
1	B	271	TRP
1	B	272	ASN
1	B	286	LYS
1	B	287	ILE
1	B	307	GLN
1	B	308	ASN
1	B	328	GLU
1	B	345	ASN
1	B	349	CYS
1	B	355	THR
1	B	384	ARG
1	B	406	GLU
1	B	418	ASP
1	B	421	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	432	LEU
1	B	440	GLU
1	B	453	LEU
1	B	454	LEU
1	B	491	THR
1	B	520	VAL
1	C	61	SER
1	C	67	ARG
1	C	70	THR
1	C	102	VAL
1	C	105	LEU
1	C	123	LEU
1	C	131	ASP
1	C	145	SER
1	C	163	ARG
1	C	181	LEU
1	C	186	LEU
1	C	211	VAL
1	C	213	LEU
1	C	222	ASP
1	C	245	ILE
1	C	271	TRP
1	C	272	ASN
1	C	301	ILE
1	C	307	GLN
1	C	308	ASN
1	C	317	LEU
1	C	345	ASN
1	C	349	CYS
1	C	355	THR
1	C	359	ASP
1	C	421	ARG
1	C	440	GLU
1	C	446	LEU
1	C	453	LEU
1	C	459	GLN
1	C	471	ASP
1	C	491	THR
1	D	61	SER
1	D	89	LEU
1	D	102	VAL
1	D	105	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	110	SER
1	D	112	MET
1	D	123	LEU
1	D	145	SER
1	D	155	GLU
1	D	165	LEU
1	D	181	LEU
1	D	186	LEU
1	D	211	VAL
1	D	213	LEU
1	D	222	ASP
1	D	229	LEU
1	D	245	ILE
1	D	271	TRP
1	D	272	ASN
1	D	295	TYR
1	D	307	GLN
1	D	308	ASN
1	D	317	LEU
1	D	337	VAL
1	D	345	ASN
1	D	349	CYS
1	D	355	THR
1	D	406	GLU
1	D	418	ASP
1	D	421	ARG
1	D	440	GLU
1	D	453	LEU
1	D	459	GLN
1	D	471	ASP
1	D	491	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	247	HIS
1	A	307	GLN
1	A	340	GLN
1	A	345	ASN
1	B	232	GLN
1	B	247	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	272	ASN
1	B	307	GLN
1	B	340	GLN
1	B	345	ASN
1	B	483	HIS
1	C	91	GLN
1	C	247	HIS
1	C	272	ASN
1	C	307	GLN
1	C	340	GLN
1	C	345	ASN
1	C	428	GLN
1	D	272	ASN
1	D	307	GLN
1	D	340	GLN
1	D	345	ASN
1	D	483	HIS

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

24 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	BG6	A	601	-	16,16,16	0.68	0	23,24,24	1.52	5 (21%)
3	SO4	A	602	-	4,4,4	0.37	0	6,6,6	0.29	0
3	SO4	A	603	-	4,4,4	0.06	0	6,6,6	0.27	0
3	SO4	A	604	-	4,4,4	0.34	0	6,6,6	0.37	0
3	SO4	A	605	-	4,4,4	0.30	0	6,6,6	0.23	0
2	BG6	B	601	-	16,16,16	0.91	0	23,24,24	1.60	7 (30%)
3	SO4	B	602	-	4,4,4	0.61	0	6,6,6	0.30	0
3	SO4	B	603	-	4,4,4	0.63	0	6,6,6	0.27	0
3	SO4	B	604	-	4,4,4	0.19	0	6,6,6	0.45	0
3	SO4	B	605	-	4,4,4	0.23	0	6,6,6	0.31	0
3	SO4	B	606	-	4,4,4	0.55	0	6,6,6	0.76	0
3	SO4	B	607	-	4,4,4	0.35	0	6,6,6	0.22	0
3	SO4	B	608	-	4,4,4	0.29	0	6,6,6	0.26	0
2	BG6	C	601	-	16,16,16	0.87	0	23,24,24	1.58	5 (21%)
3	SO4	C	602	-	4,4,4	0.36	0	6,6,6	0.42	0
3	SO4	C	603	-	4,4,4	0.27	0	6,6,6	0.19	0
3	SO4	C	604	-	4,4,4	0.17	0	6,6,6	0.14	0
3	SO4	C	605	-	4,4,4	0.17	0	6,6,6	0.22	0
3	SO4	C	606	-	4,4,4	0.29	0	6,6,6	0.25	0
3	SO4	C	607	-	4,4,4	0.22	0	6,6,6	0.23	0
4	GOL	C	608	-	5,5,5	0.20	0	5,5,5	0.70	0
2	BG6	D	601	-	16,16,16	0.59	0	23,24,24	1.31	3 (13%)
3	SO4	D	602	-	4,4,4	0.25	0	6,6,6	0.33	0
3	SO4	D	603	-	4,4,4	0.39	0	6,6,6	0.37	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	BG6	A	601	-	-	0/6/26/26	0/1/1/1
3	SO4	A	602	-	-	0/0/0/0	0/0/0/0
3	SO4	A	603	-	-	0/0/0/0	0/0/0/0
3	SO4	A	604	-	-	0/0/0/0	0/0/0/0
3	SO4	A	605	-	-	0/0/0/0	0/0/0/0
2	BG6	B	601	-	-	0/6/26/26	0/1/1/1
3	SO4	B	602	-	-	0/0/0/0	0/0/0/0
3	SO4	B	603	-	-	0/0/0/0	0/0/0/0
3	SO4	B	604	-	-	0/0/0/0	0/0/0/0
3	SO4	B	605	-	-	0/0/0/0	0/0/0/0
3	SO4	B	606	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	B	607	-	-	0/0/0/0	0/0/0/0
3	SO4	B	608	-	-	0/0/0/0	0/0/0/0
2	BG6	C	601	-	-	0/6/26/26	0/1/1/1
3	SO4	C	602	-	-	0/0/0/0	0/0/0/0
3	SO4	C	603	-	-	0/0/0/0	0/0/0/0
3	SO4	C	604	-	-	0/0/0/0	0/0/0/0
3	SO4	C	605	-	-	0/0/0/0	0/0/0/0
3	SO4	C	606	-	-	0/0/0/0	0/0/0/0
3	SO4	C	607	-	-	0/0/0/0	0/0/0/0
4	GOL	C	608	-	-	0/4/4/4	0/0/0/0
2	BG6	D	601	-	-	0/6/26/26	0/1/1/1
3	SO4	D	602	-	-	0/0/0/0	0/0/0/0
3	SO4	D	603	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	BG6	C1-C2-C3	-2.86	106.18	110.43
2	A	601	BG6	O2P-P-O6	-2.80	98.49	106.56
2	C	601	BG6	C4-C3-C2	-2.49	106.14	110.79
2	B	601	BG6	O5-C5-C4	2.02	113.48	109.68
2	B	601	BG6	O3-C3-C4	2.02	114.89	110.34
2	C	601	BG6	O2-C2-C1	2.13	114.50	109.82
2	D	601	BG6	O2P-P-O1P	2.15	115.57	107.38
2	D	601	BG6	O5-C5-C6	2.18	111.06	106.61
2	B	601	BG6	C6-C5-C4	2.26	117.16	112.03
2	B	601	BG6	C4-C3-C2	2.31	115.10	110.79
2	C	601	BG6	O4-C4-C5	2.37	115.52	109.24
2	A	601	BG6	O6-P-O3P	2.45	113.37	107.14
2	A	601	BG6	O5-C1-C2	2.47	113.73	109.80
2	A	601	BG6	O2P-P-O1P	2.50	116.89	107.38
2	B	601	BG6	O5-C5-C6	2.50	111.73	106.61
2	B	601	BG6	C1-C2-C3	2.74	114.50	110.43
2	C	601	BG6	O5-C1-C2	3.03	114.63	109.80
2	A	601	BG6	C1-O5-C5	3.17	119.33	113.47
2	B	601	BG6	O5-C1-C2	3.37	115.17	109.80
2	C	601	BG6	C1-O5-C5	3.88	120.64	113.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	SO4	1	0
3	A	603	SO4	3	0
2	B	601	BG6	1	0
3	B	604	SO4	2	0
3	B	608	SO4	1	0
3	C	605	SO4	1	0
3	C	607	SO4	2	0
2	D	601	BG6	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^{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	485/541 (89%)	0.13	21 (4%)	39	38	10, 36, 71, 95	0
1	B	487/541 (90%)	0.03	11 (2%)	64	64	11, 33, 67, 91	0
1	C	494/541 (91%)	0.09	21 (4%)	39	38	6, 34, 67, 83	0
1	D	494/541 (91%)	0.05	17 (3%)	49	49	6, 35, 66, 95	0
All	All	1960/2164 (90%)	0.07	70 (3%)	46	46	6, 35, 68, 95	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	471	ASP	4.6
1	B	128	THR	4.1
1	C	359	ASP	3.9
1	B	374	GLY	3.8
1	A	546	ASN	3.6
1	C	369	PRO	3.5
1	B	206	PRO	3.4
1	D	359	ASP	3.2
1	D	370	SER	3.1
1	C	174	PRO	3.1
1	C	175	GLU	3.1
1	B	131	ASP	3.1
1	C	290	ALA	3.0
1	D	362	THR	3.0
1	A	373	LYS	3.0
1	C	361	SER	3.0
1	A	374	GLY	3.0
1	B	207	GLU	3.0
1	D	121	ASP	2.9
1	D	290	ALA	2.9
1	A	367	ASP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	295	TYR	2.8
1	A	114	ASP	2.8
1	C	289	THR	2.8
1	C	188	PRO	2.7
1	B	121	ASP	2.7
1	B	61	SER	2.7
1	C	370	SER	2.7
1	C	367	ASP	2.7
1	C	207	GLU	2.6
1	A	471	ASP	2.6
1	D	356	ALA	2.6
1	D	358	ALA	2.6
1	A	207	GLU	2.6
1	C	355	THR	2.6
1	D	298	SER	2.6
1	D	361	SER	2.6
1	C	363	PRO	2.5
1	C	176	LYS	2.5
1	C	356	ALA	2.4
1	C	121	ASP	2.4
1	A	161	ASN	2.4
1	D	207	GLU	2.4
1	A	121	ASP	2.4
1	A	361	SER	2.4
1	A	131	ASP	2.4
1	A	202	ALA	2.3
1	B	132	GLU	2.3
1	D	355	THR	2.3
1	D	465	THR	2.3
1	A	113	GLU	2.3
1	C	364	GLY	2.3
1	D	188	PRO	2.3
1	A	231	ASN	2.2
1	A	175	GLU	2.2
1	D	174	PRO	2.2
1	B	367	ASP	2.2
1	D	369	PRO	2.2
1	D	533	ALA	2.2
1	C	189	SER	2.1
1	B	290	ALA	2.1
1	C	362	THR	2.1
1	C	373	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	357	SER	2.1
1	A	138	GLY	2.1
1	A	173	GLY	2.1
1	A	130	LEU	2.1
1	A	531	GLU	2.1
1	A	291	GLY	2.0
1	A	372	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^{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
3	SO4	B	603	5/5	0.91	0.21	3.18	65,67,67,68	0
4	GOL	C	608	6/6	0.90	0.23	1.25	3,21,25,25	0
2	BG6	B	601	16/16	0.84	0.26	0.97	42,51,55,55	0
2	BG6	C	601	16/16	0.87	0.23	0.96	59,66,72,74	0
3	SO4	B	607	5/5	0.93	0.30	0.68	50,51,51,53	0
2	BG6	A	601	16/16	0.90	0.23	-0.01	57,63,66,67	0
2	BG6	D	601	16/16	0.90	0.21	-0.47	61,63,68,71	0
3	SO4	A	604	5/5	0.96	0.18	-0.58	43,47,48,51	0
3	SO4	C	605	5/5	0.96	0.21	-0.70	60,60,61,63	0
3	SO4	B	604	5/5	0.98	0.13	-1.72	28,32,33,36	0
3	SO4	D	602	5/5	0.98	0.09	-2.21	40,42,43,45	0
3	SO4	C	602	5/5	0.98	0.10	-2.40	39,39,42,42	0
3	SO4	A	603	5/5	0.97	0.12	-2.66	39,39,41,43	0
3	SO4	B	605	5/5	0.91	0.19	-	66,68,69,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	B	606	5/5	0.94	0.17	-	28,33,34,36	0
3	SO4	C	607	5/5	0.85	0.28	-	72,75,76,76	0
3	SO4	D	603	5/5	0.79	0.33	-	82,83,84,86	0
3	SO4	C	603	5/5	0.84	0.28	-	75,77,77,78	0
3	SO4	B	602	5/5	0.92	0.13	-	57,60,61,65	0
3	SO4	A	602	5/5	0.90	0.17	-	70,75,75,77	0
3	SO4	C	606	5/5	0.80	0.27	-	80,81,84,85	0
3	SO4	A	605	5/5	0.91	0.25	-	74,76,77,78	0
3	SO4	C	604	5/5	0.94	0.14	-	65,67,67,68	0
3	SO4	B	608	5/5	0.97	0.23	-	64,65,66,66	0

6.5 Other polymers

There are no such residues in this entry.