



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:16 PM GMT

PDB ID : 4E9I
Title : Glucose-6-P Dehydrogenase (apo form) from Trypanosoma cruzi
Authors : Botti, H.; Ortiz, C.; Comini, M.A.; Buschiazso, A.
Deposited on : 2012-03-21
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

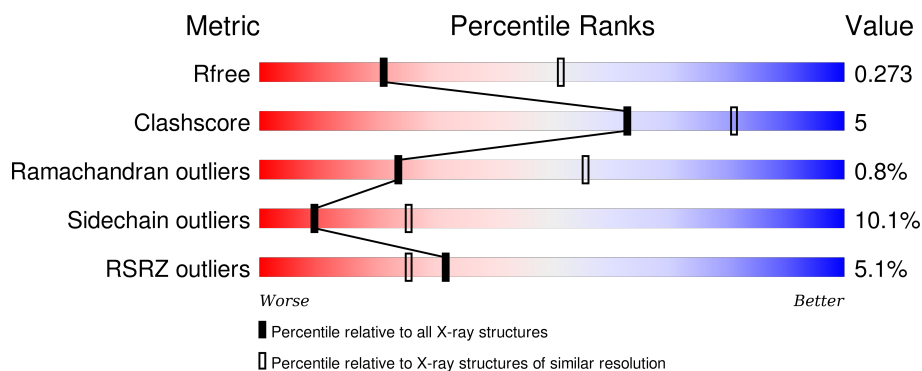
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	541	
1	B	541	
1	C	541	
1	D	541	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	603	-	-	-	X
3	GOL	A	609	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15769 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	488	Total	C	N	O	S	0	0	0
			3860	2445	682	718	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

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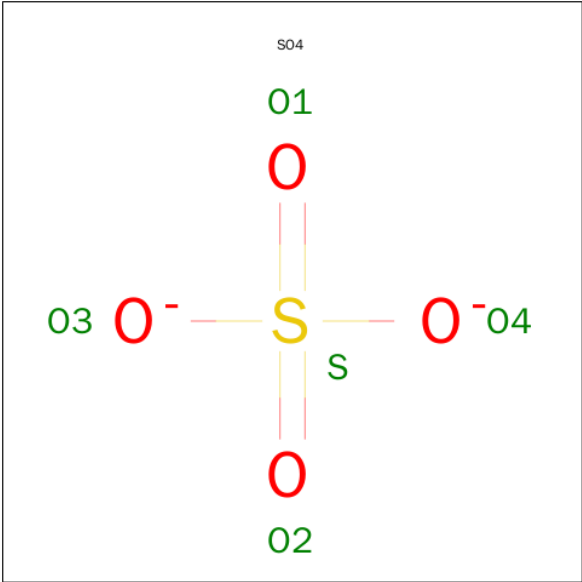
Chain	Residue	Modelled	Actual	Comment	Reference
A	36	ALA	-	EXPRESSION TAG	UNP Q1WBU6
A	37	SER	-	EXPRESSION TAG	UNP Q1WBU6
B	15	MET	-	EXPRESSION TAG	UNP Q1WBU6
B	16	GLY	-	EXPRESSION TAG	UNP Q1WBU6
B	17	SER	-	EXPRESSION TAG	UNP Q1WBU6
B	18	SER	-	EXPRESSION TAG	UNP Q1WBU6
B	19	HIS	-	EXPRESSION TAG	UNP Q1WBU6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

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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 SULFATE ION (three-letter code: SO4) (formula: O₄S).



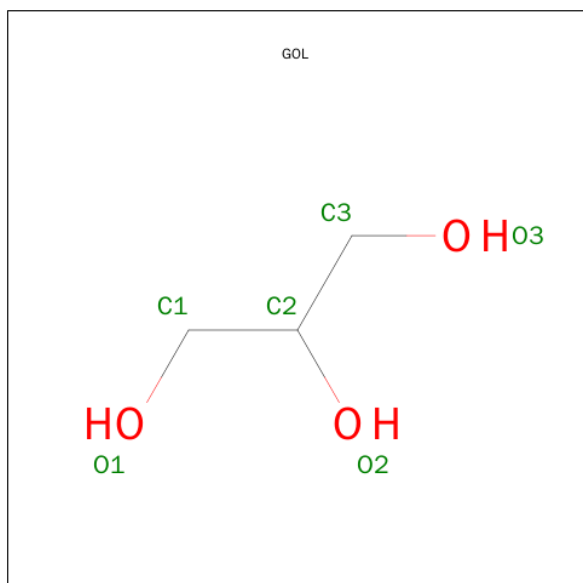
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total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

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

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



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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cl 1	0	0
4	D	2	Total 2	Cl 2	0	0
4	C	2	Total 2	Cl 2	0	0

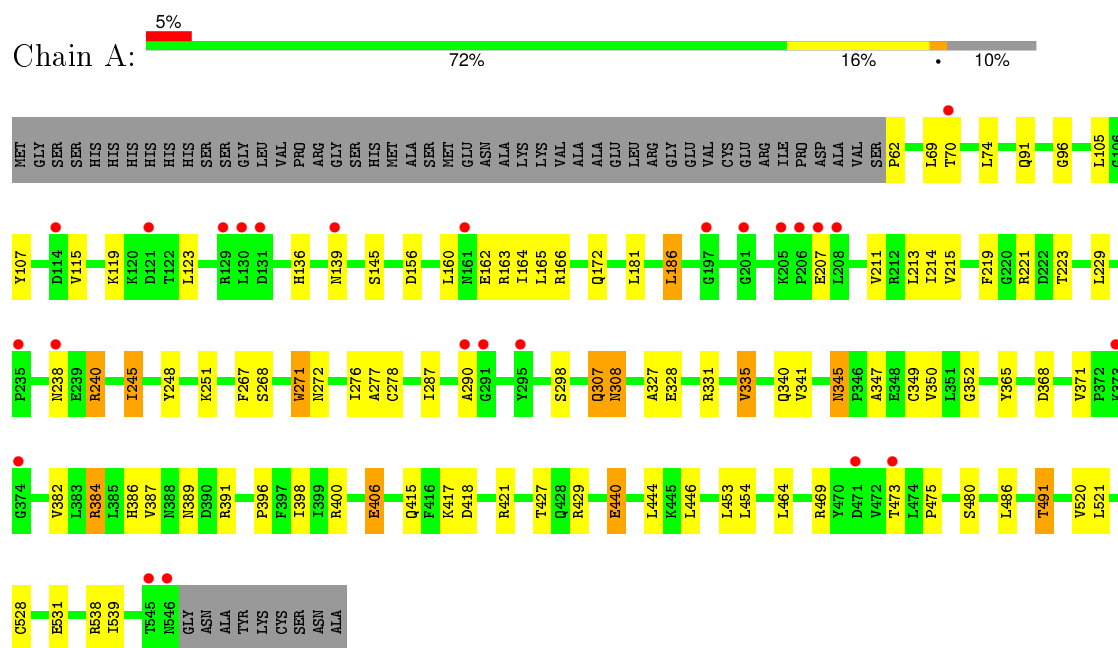
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total 9	O 9	0	0
5	B	9	Total 9	O 9	0	0
5	C	16	Total 16	O 16	0	0
5	D	20	Total 20	O 20	0	0

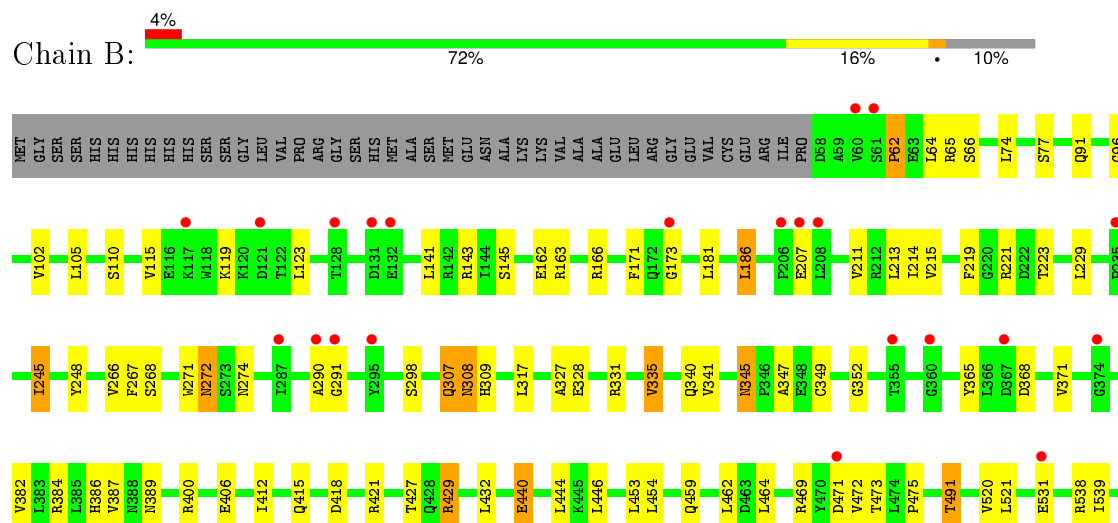
3 Residue-property plots

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



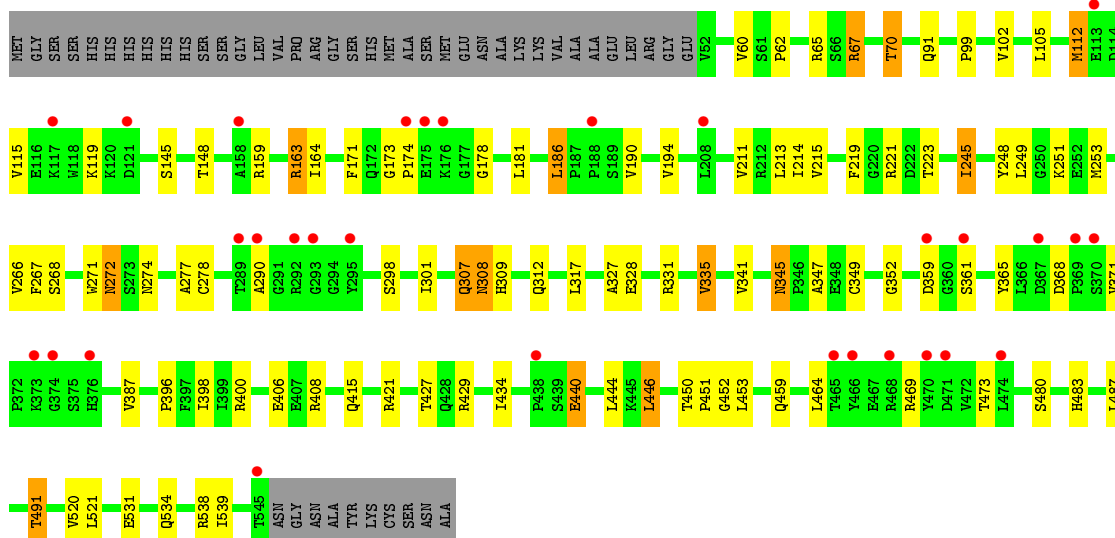
- Molecule 1: Glucose-6-phosphate 1-dehydrogenase



T544
T545
ASN
GLY
ASN
ALA
TVR
LYS
CYS
SER
ASN
ALA

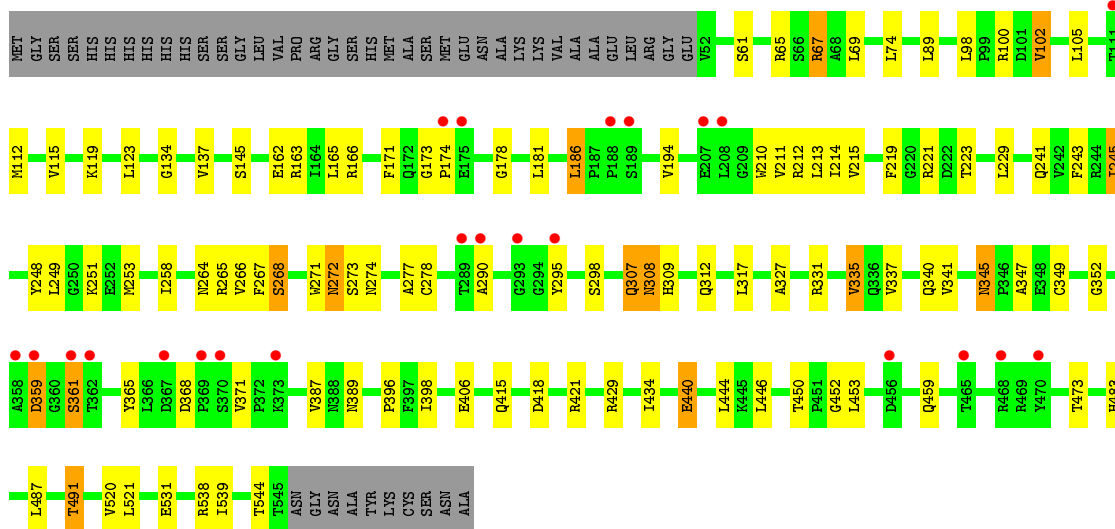
• Molecule 1: Glucose-6-phosphate 1-dehydrogenase

Chain C: 



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

Chain D: 



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.85Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.207 , 0.250 0.222 , 0.273	Depositor DCC
R_{free} test set	1257 reflections (2.07%)	DCC
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 , 59.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 62009 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15769	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.74	0/5320
1	B	0.51	0/3940	0.76	1/5337 (0.0%)
1	C	0.52	0/4006	0.76	0/5425
1	D	0.51	0/3997	0.76	0/5413
All	All	0.51	0/15872	0.76	1/21495 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	SER	C-N-CA	5.12	134.49	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	3844	0	3831	45	0
1	B	3860	0	3839	41	0
1	C	3922	0	3914	47	0
1	D	3916	0	3905	46	0
2	A	40	0	0	0	0
2	B	35	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	25	0	0	1	0
2	D	20	0	0	0	0
3	A	12	0	16	2	0
3	B	6	0	8	0	0
3	C	18	0	24	2	0
3	D	12	0	16	2	0
4	A	1	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	9	0	0	0	0
5	B	9	0	0	0	0
5	C	16	0	0	1	0
5	D	20	0	0	0	0
All	All	15769	0	15553	166	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 (166) 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	0.78
1:B:215:VAL:HG12	1:B:219:PHE:HE1	1.47	0.77
1:C:215:VAL:HG12	1:C:219:PHE:HE1	1.48	0.77
1:A:215:VAL:HG12	1:A:219:PHE:HE1	1.49	0.76
1:A:406:GLU:HG2	1:A:528:CYS:SG	2.31	0.71
1:A:368:ASP:HB3	1:A:371:VAL:HG12	1.74	0.70
1:C:368:ASP:HB3	1:C:371:VAL:HG12	1.74	0.69
1:A:391[B]:ARG:HE	3:A:610:GOL:H12	1.58	0.69
1:D:368:ASP:HB3	1:D:371:VAL:HG12	1.74	0.68
1:B:368:ASP:HB3	1:B:371:VAL:HG12	1.75	0.68
1:B:475:PRO:HD3	1:C:452:GLY:HA2	1.74	0.68
1:A:70:THR:HG21	1:A:164:ILE:HG23	1.78	0.65
1:B:102:VAL:O	1:B:143:ARG:HD3	1.96	0.65
1:C:345:ASN:HD21	1:C:347:ALA:HB3	1.63	0.64
1:C:215:VAL:HG12	1:C:219:PHE:CE1	2.33	0.63
1:D:345:ASN:HD21	1:D:347:ALA:HB3	1.64	0.62
1:C:249:LEU:HD11	1:C:312:GLN:OE1	2.00	0.62
1:A:391[A]:ARG:HH22	3:A:610:GOL:H31	1.63	0.61
1:B:215:VAL:HG12	1:B:219:PHE:CE1	2.33	0.61
1:A:345:ASN:HD21	1:A:347:ALA:HB3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:ASN:HD21	1:B:347:ALA:HB3	1.65	0.61
1:D:215:VAL:HG12	1:D:219:PHE:CE1	2.32	0.61
1:B:62:PRO:HA	1:B:96:GLY:O	2.01	0.61
1:A:267:PHE:HE2	1:D:446:LEU:HD21	1.66	0.61
1:A:136:HIS:HA	1:A:139:ASN:HD22	1.68	0.59
1:C:171:PHE:CE2	1:C:173:GLY:HA3	2.39	0.58
1:B:341:VAL:HG22	1:B:387:VAL:HG22	1.86	0.57
1:A:215:VAL:HG12	1:A:219:PHE:CE1	2.35	0.57
1:B:464:LEU:HD12	1:B:469:ARG:HG3	1.86	0.57
1:C:186:LEU:HD22	1:C:194:VAL:HG21	1.87	0.56
1:D:272:ASN:HD22	1:D:274:ASN:H	1.53	0.56
1:A:475:PRO:HD3	1:D:452:GLY:HA2	1.87	0.55
1:C:272:ASN:HD22	1:C:274:ASN:H	1.54	0.55
1:B:74:LEU:HB3	1:B:186:LEU:HD21	1.86	0.55
1:D:249:LEU:HD11	1:D:312:GLN:OE1	2.06	0.55
1:A:214:ILE:HG23	1:A:245:ILE:HG13	1.89	0.54
1:C:214:ILE:HG23	1:C:245:ILE:HG13	1.89	0.54
1:D:67:ARG:HG2	1:D:178:GLY:HA2	1.90	0.54
1:A:341:VAL:HG22	1:A:387:VAL:HG22	1.89	0.54
1:B:162:GLU:O	1:B:166:ARG:HG2	2.08	0.53
1:D:74:LEU:HB3	1:D:186:LEU:HD23	1.90	0.53
1:B:214:ILE:HG23	1:B:245:ILE:HG13	1.90	0.53
1:C:62:PRO:HA	1:C:65:ARG:HG3	1.91	0.53
1:B:317:LEU:HD21	1:B:412:ILE:HG21	1.91	0.53
1:D:162:GLU:O	1:D:166:ARG:HG2	2.09	0.53
1:D:98:LEU:HB3	1:D:102:VAL:HG21	1.90	0.53
1:D:253:MET:HE3	1:D:434:ILE:HG23	1.90	0.52
1:D:278:CYS:SG	1:D:398:ILE:HD12	2.49	0.52
1:A:238:ASN:HB3	1:A:240:ARG:HE	1.75	0.52
1:D:214:ILE:HG23	1:D:245:ILE:HG13	1.90	0.52
1:C:253:MET:HE3	1:C:434:ILE:HG23	1.91	0.52
1:D:258:ILE:HG21	3:D:605:GOL:H12	1.90	0.52
1:D:272:ASN:C	1:D:272:ASN:HD22	2.13	0.52
1:C:341:VAL:HG22	1:C:387:VAL:HG22	1.92	0.51
1:D:134:GLY:O	1:D:137:VAL:HG12	2.10	0.51
1:B:384:ARG:NH1	1:B:386:HIS:HE1	2.08	0.51
1:D:171:PHE:CE2	1:D:173:GLY:HA3	2.45	0.51
1:B:171:PHE:CE2	1:B:173:GLY:HA3	2.46	0.51
1:A:272:ASN:HB2	1:A:391[B]:ARG:HG3	1.91	0.51
1:B:272:ASN:HD22	1:B:274:ASN:H	1.59	0.51
1:A:69:LEU:HD21	1:A:486:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HB3	1:A:186:LEU:HD21	1.93	0.49
1:C:60:VAL:HG21	1:C:99:PRO:HA	1.93	0.49
1:D:221:ARG:NH1	1:D:298:SER:O	2.46	0.49
1:A:415:GLN:HG2	1:A:429:ARG:HD3	1.93	0.49
1:C:70:THR:HG21	1:C:164:ILE:HG23	1.94	0.49
1:C:221:ARG:NH1	1:C:298:SER:O	2.45	0.49
1:A:162:GLU:O	1:A:166:ARG:HG2	2.13	0.49
1:C:272:ASN:C	1:C:272:ASN:HD22	2.15	0.49
1:D:341:VAL:HG22	1:D:387:VAL:HG22	1.93	0.49
1:A:350:VAL:HB	1:A:382:VAL:HG22	1.95	0.49
1:C:307:GLN:HE21	1:C:308:ASN:HD22	1.60	0.49
1:D:307:GLN:HE21	1:D:308:ASN:HD22	1.60	0.49
1:D:359:ASP:OD1	1:D:361:SER:HB3	2.13	0.48
1:A:446:LEU:HD13	1:D:267:PHE:HE2	1.78	0.48
1:D:212:ARG:HD3	1:D:243:PHE:CE1	2.49	0.48
1:C:115:VAL:HG12	1:C:119:LYS:HE2	1.96	0.48
1:D:444:LEU:HG	1:D:446:LEU:HD13	1.96	0.48
1:C:186:LEU:HD13	1:C:190:VAL:HG23	1.94	0.48
1:D:248:TYR:CD2	1:D:309:HIS:HB3	2.48	0.48
1:A:278:CYS:SG	1:A:398:ILE:HD12	2.54	0.48
1:D:248:TYR:HA	1:D:251:LYS:HD2	1.95	0.47
1:D:277:ALA:O	1:D:396:PRO:HD2	2.13	0.47
1:A:272:ASN:CB	1:A:391[B]:ARG:HG3	2.44	0.47
1:A:307:GLN:HE21	1:A:308:ASN:HD22	1.63	0.47
1:B:415:GLN:HG2	1:B:429:ARG:HD3	1.95	0.47
1:B:115:VAL:HG12	1:B:119:LYS:HE2	1.97	0.47
1:B:307:GLN:HE21	1:B:308:ASN:HD22	1.63	0.46
1:C:112:MET:HG2	1:C:115:VAL:HG22	1.97	0.46
1:D:186:LEU:HD22	1:D:194:VAL:HG21	1.97	0.46
1:B:272:ASN:HD22	1:B:272:ASN:C	2.18	0.46
1:D:327:ALA:HA	1:D:491:THR:HB	1.96	0.46
1:A:382:VAL:HG12	1:A:400:ARG:HG2	1.98	0.46
1:A:327:ALA:HA	1:A:491:THR:HB	1.98	0.46
1:C:248:TYR:HA	1:C:251:LYS:HD2	1.98	0.46
1:B:444:LEU:HG	1:B:446:LEU:HD13	1.97	0.46
1:B:384:ARG:HH11	1:B:386:HIS:CE1	2.34	0.46
1:B:266:VAL:HG21	1:C:444:LEU:HD11	1.98	0.46
1:B:221:ARG:NH1	1:B:298:SER:O	2.49	0.46
1:D:264:ASN:O	1:D:268:SER:HB2	2.16	0.46
1:C:67:ARG:HG2	1:C:178:GLY:HA2	1.97	0.45
1:C:327:ALA:HA	1:C:491:THR:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:ALA:O	1:C:396:PRO:HD2	2.17	0.45
1:C:253:MET:CE	1:C:434:ILE:HG23	2.46	0.45
1:B:327:ALA:HA	1:B:491:THR:HB	1.99	0.44
1:B:215:VAL:CG1	1:B:219:PHE:HE1	2.26	0.44
1:C:365:TYR:CE2	1:C:371:VAL:HG21	2.52	0.44
1:C:331:ARG:O	1:C:335:VAL:HG13	2.17	0.44
1:A:384:ARG:NH1	1:A:386:HIS:HE1	2.15	0.44
1:A:248:TYR:HA	1:A:251:LYS:HD2	1.98	0.44
1:A:221:ARG:NH1	1:A:298:SER:O	2.50	0.44
1:D:210:TRP:HB2	3:D:606:GOL:H2	1.99	0.44
1:C:163:ARG:NH1	2:C:602:SO4:S	2.90	0.44
1:A:464:LEU:HD12	1:A:469:ARG:NE	2.33	0.44
1:C:248:TYR:CD2	1:C:309:HIS:HB3	2.53	0.44
1:D:331:ARG:O	1:D:335:VAL:HG13	2.17	0.44
1:A:365:TYR:CE2	1:A:371:VAL:HG21	2.53	0.44
1:A:115:VAL:HG12	1:A:119:LYS:HE2	2.00	0.44
1:C:278:CYS:SG	1:C:398:ILE:HD12	2.58	0.44
1:B:384:ARG:HH11	1:B:386:HIS:HE1	1.66	0.43
1:B:446:LEU:HD21	1:C:267:PHE:HE2	1.83	0.43
1:C:112:MET:HG2	1:C:115:VAL:CG2	2.48	0.43
1:D:248:TYR:CE2	1:D:309:HIS:HB3	2.53	0.43
1:A:107:TYR:OH	1:A:156:ASP:HB3	2.17	0.43
1:D:365:TYR:CE2	1:D:371:VAL:HG21	2.53	0.43
1:D:115:VAL:HG12	1:D:119:LYS:HE2	1.99	0.43
1:B:365:TYR:CE2	1:B:371:VAL:HG21	2.53	0.43
1:B:340:GLN:NE2	1:B:389:ASN:HD22	2.16	0.43
1:D:352:GLY:HA2	1:D:521:LEU:O	2.19	0.43
1:C:186:LEU:CD2	1:C:194:VAL:HG21	2.48	0.42
1:D:253:MET:CE	1:D:434:ILE:HG23	2.48	0.42
1:A:464:LEU:HA	1:A:469:ARG:HH21	1.85	0.42
1:A:352:GLY:HA2	1:A:521:LEU:O	2.19	0.42
1:C:483:HIS:CE1	1:C:487:LEU:HD11	2.54	0.42
1:B:382:VAL:HG12	1:B:400:ARG:HG2	2.02	0.42
1:B:77:SER:OG	1:B:110:SER:HB3	2.20	0.42
1:C:534:GLN:HE22	3:C:607:GOL:H12	1.84	0.42
1:D:340:GLN:NE2	1:D:389:ASN:HD22	2.18	0.42
1:D:415:GLN:HG2	1:D:429:ARG:HD3	2.01	0.41
1:B:352:GLY:HA2	1:B:521:LEU:O	2.19	0.41
1:B:119:LYS:HB3	1:B:141:LEU:HD22	2.02	0.41
1:C:400:ARG:HH22	3:C:607:GOL:H11	1.86	0.41
1:C:352:GLY:HA2	1:C:521:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ARG:O	1:A:335:VAL:HG13	2.19	0.41
1:B:544:THR:HG22	1:B:545:THR:H	1.86	0.41
1:A:271:TRP:HA	1:A:276:ILE:HD11	2.03	0.41
1:B:267:PHE:HE2	1:C:446:LEU:HD21	1.84	0.41
1:B:248:TYR:CD2	1:B:309:HIS:HB3	2.56	0.41
1:A:444:LEU:HD21	1:D:266:VAL:HG11	2.03	0.41
1:B:462:LEU:HD23	1:C:464:LEU:HB2	2.03	0.41
1:C:464:LEU:HA	1:C:469:ARG:HH21	1.86	0.41
1:A:464:LEU:HD12	1:A:469:ARG:HE	1.86	0.41
1:A:107:TYR:CD2	1:A:160:LEU:HD13	2.56	0.41
1:A:340:GLN:NE2	1:A:389:ASN:HD22	2.18	0.41
1:C:415:GLN:HG2	1:C:429:ARG:HD3	2.02	0.41
1:D:69:LEU:HD23	1:D:102:VAL:HG13	2.02	0.41
1:B:444:LEU:HD11	1:C:266:VAL:HG21	2.03	0.41
1:A:62:PRO:HA	1:A:96:GLY:O	2.21	0.40
1:A:277:ALA:O	1:A:396:PRO:HD2	2.20	0.40
1:A:417:LYS:HB2	1:D:265:ARG:HD2	2.03	0.40
1:A:444:LEU:HD11	1:D:266:VAL:HG21	2.03	0.40
1:C:148:THR:O	1:C:159:ARG:NH2	2.42	0.40
1:C:408:ARG:NH1	5:C:711:HOH:O	2.54	0.40
1:B:331:ARG:O	1:B:335:VAL:HG13	2.20	0.40
1:B:472:VAL:HG11	1:C:451:PRO:HB2	2.03	0.40
1:D:483:HIS:CE1	1:D:487:LEU:HD11	2.57	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%)	461 (95%)	22 (4%)	2 (0%)	39 71
1	B	486/541 (90%)	452 (93%)	29 (6%)	5 (1%)	19 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	493/541 (91%)	467 (95%)	22 (4%)	4 (1%)	24	56
1	D	492/541 (91%)	467 (95%)	20 (4%)	5 (1%)	19	49
All	All	1956/2164 (90%)	1847 (94%)	93 (5%)	16 (1%)	24	56

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	62	PRO
1	C	290	ALA
1	A	290	ALA
1	A	440	GLU
1	B	440	GLU
1	C	361	SER
1	D	290	ALA
1	B	290	ALA
1	C	440	GLU
1	D	361	SER
1	D	440	GLU
1	D	273	SER
1	B	429	ARG
1	B	291	GLY
1	C	174	PRO
1	D	174	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	410/461 (89%)	370 (90%)	40 (10%)	10	27
1	B	414/461 (90%)	373 (90%)	41 (10%)	10	27
1	C	422/461 (92%)	381 (90%)	41 (10%)	10	27
1	D	422/461 (92%)	376 (89%)	46 (11%)	8	21
All	All	1668/1844 (90%)	1500 (90%)	168 (10%)	9	25

All (168) 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	145	SER
1	A	163	ARG
1	A	165	LEU
1	A	172	GLN
1	A	181	LEU
1	A	186	LEU
1	A	207	GLU
1	A	211	VAL
1	A	213	LEU
1	A	223	THR
1	A	229	LEU
1	A	240	ARG
1	A	245	ILE
1	A	268	SER
1	A	271	TRP
1	A	287	ILE
1	A	307	GLN
1	A	308	ASN
1	A	328	GLU
1	A	335	VAL
1	A	345	ASN
1	A	349	CYS
1	A	384	ARG
1	A	406	GLU
1	A	418	ASP
1	A	421	ARG
1	A	427	THR
1	A	440	GLU
1	A	453	LEU
1	A	454	LEU
1	A	473	THR
1	A	480	SER
1	A	491	THR
1	A	520	VAL
1	A	531	GLU
1	A	538	ARG
1	A	539	ILE
1	B	64	LEU
1	B	65	ARG

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Mol	Chain	Res	Type
1	B	91	GLN
1	B	105	LEU
1	B	123	LEU
1	B	145	SER
1	B	163	ARG
1	B	181	LEU
1	B	186	LEU
1	B	207	GLU
1	B	211	VAL
1	B	213	LEU
1	B	223	THR
1	B	229	LEU
1	B	245	ILE
1	B	268	SER
1	B	271	TRP
1	B	272	ASN
1	B	307	GLN
1	B	308	ASN
1	B	328	GLU
1	B	335	VAL
1	B	345	ASN
1	B	349	CYS
1	B	406	GLU
1	B	418	ASP
1	B	421	ARG
1	B	427	THR
1	B	432	LEU
1	B	440	GLU
1	B	453	LEU
1	B	454	LEU
1	B	459	GLN
1	B	471	ASP
1	B	473	THR
1	B	491	THR
1	B	520	VAL
1	B	531	GLU
1	B	538	ARG
1	B	539	ILE
1	B	545	THR
1	C	67	ARG
1	C	70	THR
1	C	91	GLN

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Mol	Chain	Res	Type
1	C	102	VAL
1	C	105	LEU
1	C	112	MET
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	223	THR
1	C	245	ILE
1	C	268	SER
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	328	GLU
1	C	335	VAL
1	C	345	ASN
1	C	349	CYS
1	C	359	ASP
1	C	406	GLU
1	C	421	ARG
1	C	427	THR
1	C	440	GLU
1	C	446	LEU
1	C	450	THR
1	C	453	LEU
1	C	459	GLN
1	C	473	THR
1	C	480	SER
1	C	491	THR
1	C	520	VAL
1	C	531	GLU
1	C	538	ARG
1	C	539	ILE
1	D	61	SER
1	D	65	ARG
1	D	67	ARG
1	D	89	LEU

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Mol	Chain	Res	Type
1	D	100	ARG
1	D	102	VAL
1	D	105	LEU
1	D	112	MET
1	D	123	LEU
1	D	145	SER
1	D	163	ARG
1	D	165	LEU
1	D	181	LEU
1	D	186	LEU
1	D	211	VAL
1	D	213	LEU
1	D	223	THR
1	D	229	LEU
1	D	241	GLN
1	D	245	ILE
1	D	268	SER
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	335	VAL
1	D	337	VAL
1	D	345	ASN
1	D	349	CYS
1	D	359	ASP
1	D	406	GLU
1	D	418	ASP
1	D	421	ARG
1	D	440	GLU
1	D	450	THR
1	D	453	LEU
1	D	459	GLN
1	D	473	THR
1	D	491	THR
1	D	520	VAL
1	D	531	GLU
1	D	538	ARG
1	D	539	ILE
1	D	544	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	204	GLN
1	A	307	GLN
1	A	340	GLN
1	A	345	ASN
1	B	204	GLN
1	B	238	ASN
1	B	272	ASN
1	B	307	GLN
1	B	340	GLN
1	B	345	ASN
1	B	386	HIS
1	B	428	GLN
1	C	91	GLN
1	C	172	GLN
1	C	204	GLN
1	C	272	ASN
1	C	307	GLN
1	C	340	GLN
1	C	345	ASN
1	C	483	HIS
1	C	534	GLN
1	D	172	GLN
1	D	272	ASN
1	D	307	GLN
1	D	340	GLN
1	D	345	ASN
1	D	428	GLN

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

Of 37 ligands modelled in this entry, 5 are monoatomic - leaving 32 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	$\# Z > 2$
2	SO4	A	601	-	4,4,4	0.33	0	6,6,6	0.23	0
2	SO4	A	602	-	4,4,4	0.20	0	6,6,6	0.23	0
2	SO4	A	603	-	4,4,4	0.19	0	6,6,6	0.39	0
2	SO4	A	604	-	4,4,4	0.28	0	6,6,6	0.13	0
2	SO4	A	605	-	4,4,4	0.22	0	6,6,6	0.33	0
2	SO4	A	606	-	4,4,4	0.12	0	6,6,6	0.10	0
2	SO4	A	607	-	4,4,4	0.24	0	6,6,6	0.21	0
2	SO4	A	608	-	4,4,4	0.21	0	6,6,6	0.17	0
3	GOL	A	609	-	5,5,5	0.22	0	5,5,5	0.56	0
3	GOL	A	610	-	5,5,5	0.19	0	5,5,5	0.29	0
2	SO4	B	601	-	4,4,4	0.45	0	6,6,6	0.50	0
2	SO4	B	602	-	4,4,4	0.27	0	6,6,6	0.57	0
2	SO4	B	603	-	4,4,4	0.16	0	6,6,6	0.20	0
2	SO4	B	604	-	4,4,4	0.37	0	6,6,6	0.23	0
2	SO4	B	605	-	4,4,4	0.24	0	6,6,6	0.11	0
2	SO4	B	606	-	4,4,4	0.21	0	6,6,6	0.27	0
2	SO4	B	607	-	4,4,4	0.22	0	6,6,6	0.18	0
3	GOL	B	608	-	5,5,5	0.19	0	5,5,5	0.31	0
2	SO4	C	601	-	4,4,4	0.38	0	6,6,6	0.41	0
2	SO4	C	602	-	4,4,4	0.23	0	6,6,6	0.15	0
2	SO4	C	603	-	4,4,4	0.37	0	6,6,6	0.31	0
2	SO4	C	604	-	4,4,4	0.39	0	6,6,6	0.17	0
2	SO4	C	605	-	4,4,4	0.14	0	6,6,6	0.11	0
3	GOL	C	606	-	5,5,5	0.13	0	5,5,5	0.50	0
3	GOL	C	607	-	5,5,5	0.15	0	5,5,5	0.47	0
3	GOL	C	608	-	5,5,5	0.23	0	5,5,5	0.40	0
2	SO4	D	601	-	4,4,4	0.19	0	6,6,6	0.32	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	0.11	0	6,6,6	0.31	0
2	SO4	D	603	-	4,4,4	0.28	0	6,6,6	0.40	0
2	SO4	D	604	-	4,4,4	0.22	0	6,6,6	0.11	0
3	GOL	D	605	-	5,5,5	0.14	0	5,5,5	0.40	0
3	GOL	D	606	-	5,5,5	0.21	0	5,5,5	0.54	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	SO4	A	601	-	-	0/0/0/0	0/0/0/0
2	SO4	A	602	-	-	0/0/0/0	0/0/0/0
2	SO4	A	603	-	-	0/0/0/0	0/0/0/0
2	SO4	A	604	-	-	0/0/0/0	0/0/0/0
2	SO4	A	605	-	-	0/0/0/0	0/0/0/0
2	SO4	A	606	-	-	0/0/0/0	0/0/0/0
2	SO4	A	607	-	-	0/0/0/0	0/0/0/0
2	SO4	A	608	-	-	0/0/0/0	0/0/0/0
3	GOL	A	609	-	-	0/4/4/4	0/0/0/0
3	GOL	A	610	-	-	0/4/4/4	0/0/0/0
2	SO4	B	601	-	-	0/0/0/0	0/0/0/0
2	SO4	B	602	-	-	0/0/0/0	0/0/0/0
2	SO4	B	603	-	-	0/0/0/0	0/0/0/0
2	SO4	B	604	-	-	0/0/0/0	0/0/0/0
2	SO4	B	605	-	-	0/0/0/0	0/0/0/0
2	SO4	B	606	-	-	0/0/0/0	0/0/0/0
2	SO4	B	607	-	-	0/0/0/0	0/0/0/0
3	GOL	B	608	-	-	0/4/4/4	0/0/0/0
2	SO4	C	601	-	-	0/0/0/0	0/0/0/0
2	SO4	C	602	-	-	0/0/0/0	0/0/0/0
2	SO4	C	603	-	-	0/0/0/0	0/0/0/0
2	SO4	C	604	-	-	0/0/0/0	0/0/0/0
2	SO4	C	605	-	-	0/0/0/0	0/0/0/0
3	GOL	C	606	-	-	0/4/4/4	0/0/0/0
3	GOL	C	607	-	-	0/4/4/4	0/0/0/0
3	GOL	C	608	-	-	0/4/4/4	0/0/0/0
2	SO4	D	601	-	-	0/0/0/0	0/0/0/0
2	SO4	D	602	-	-	0/0/0/0	0/0/0/0
2	SO4	D	603	-	-	0/0/0/0	0/0/0/0
2	SO4	D	604	-	-	0/0/0/0	0/0/0/0
3	GOL	D	605	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	606	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	610	GOL	2	0
2	C	602	SO4	1	0
3	C	607	GOL	2	0
3	D	605	GOL	1	0
3	D	606	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	485/541 (89%)	0.20	25 (5%)	31	24	15, 45, 85, 106	0
1	B	488/541 (90%)	0.08	22 (4%)	37	31	15, 40, 82, 97	0
1	C	494/541 (91%)	0.12	30 (6%)	25	18	12, 42, 80, 94	0
1	D	494/541 (91%)	0.03	23 (4%)	35	29	12, 41, 76, 92	0
All	All	1961/2164 (90%)	0.11	100 (5%)	32	25	12, 42, 81, 106	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	546	ASN	5.2
1	B	206	PRO	5.1
1	C	295	TYR	4.6
1	C	470	TYR	4.4
1	C	369	PRO	4.4
1	D	290	ALA	4.4
1	A	471	ASP	4.2
1	B	131	ASP	4.2
1	A	131	ASP	4.1
1	B	367	ASP	4.0
1	A	206	PRO	4.0
1	B	61	SER	3.9
1	D	293	GLY	3.8
1	C	290	ALA	3.8
1	B	128	THR	3.7
1	C	466	TYR	3.7
1	B	207	GLU	3.6
1	B	471	ASP	3.6
1	C	293	GLY	3.5
1	C	468	ARG	3.4
1	A	207	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	174	PRO	3.4
1	B	290	ALA	3.4
1	C	465	THR	3.4
1	A	129	ARG	3.3
1	A	197	GLY	3.3
1	D	358	ALA	3.2
1	B	291	GLY	3.2
1	D	359	ASP	3.2
1	C	175	GLU	3.1
1	B	208	LEU	3.1
1	D	465	THR	3.1
1	B	60	VAL	3.1
1	A	161	ASN	3.1
1	A	201	GLY	3.0
1	A	291	GLY	3.0
1	C	471	ASP	2.9
1	D	111	THR	2.9
1	A	295	TYR	2.8
1	B	132	GLU	2.8
1	A	114	ASP	2.8
1	A	235	PRO	2.8
1	B	117	LYS	2.7
1	B	295	TYR	2.7
1	D	208	LEU	2.7
1	D	175	GLU	2.7
1	D	370	SER	2.7
1	A	130	LEU	2.6
1	A	208	LEU	2.6
1	D	295	TYR	2.6
1	C	208	LEU	2.6
1	A	473	THR	2.6
1	C	370	SER	2.6
1	A	374	GLY	2.6
1	D	188	PRO	2.6
1	B	360	GLY	2.6
1	C	373	LYS	2.6
1	A	205	LYS	2.5
1	B	374	GLY	2.5
1	C	438	PRO	2.5
1	C	367	ASP	2.5
1	C	188	PRO	2.5
1	B	121	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	235	PRO	2.5
1	C	117	LYS	2.5
1	A	121	ASP	2.5
1	C	545	THR	2.5
1	D	369	PRO	2.5
1	D	367	ASP	2.4
1	C	113	GLU	2.4
1	C	289	THR	2.3
1	D	468	ARG	2.3
1	C	158	ALA	2.3
1	D	361	SER	2.3
1	C	359	ASP	2.2
1	D	362	THR	2.2
1	D	373	LYS	2.2
1	C	361	SER	2.2
1	C	374	GLY	2.2
1	A	373	LYS	2.2
1	D	189	SER	2.2
1	D	456	ASP	2.2
1	C	474	LEU	2.2
1	B	287	ILE	2.2
1	A	545	THR	2.2
1	B	173	GLY	2.1
1	C	176	LYS	2.1
1	A	238	ASN	2.1
1	C	121	ASP	2.1
1	C	376	HIS	2.1
1	A	290	ALA	2.1
1	C	292	ARG	2.1
1	B	355	THR	2.1
1	D	289	THR	2.1
1	A	139	ASN	2.1
1	B	531	GLU	2.1
1	D	207	GLU	2.1
1	C	174	PRO	2.1
1	D	470	TYR	2.0
1	A	70	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	A	609	6/6	0.89	0.23	3.35	36,37,39,40	0
2	SO4	B	603	5/5	0.84	0.28	2.08	104,105,106,108	0
3	GOL	D	605	6/6	0.82	0.23	1.96	62,66,67,67	0
2	SO4	C	602	5/5	0.94	0.27	1.88	73,73,75,76	0
3	GOL	D	606	6/6	0.74	0.24	1.41	41,52,53,54	0
2	SO4	C	604	5/5	0.79	0.21	1.34	91,92,94,94	0
3	GOL	A	610	6/6	0.86	0.24	1.12	45,47,49,52	0
3	GOL	B	608	6/6	0.91	0.20	1.01	41,41,42,43	0
2	SO4	C	603	5/5	0.89	0.20	0.83	72,77,77,78	0
2	SO4	D	604	5/5	0.88	0.22	0.75	104,104,105,105	0
2	SO4	A	605	5/5	0.90	0.34	0.53	82,82,83,84	0
3	GOL	C	606	6/6	0.91	0.20	0.09	41,41,45,46	0
2	SO4	A	606	5/5	0.90	0.19	-0.35	109,110,110,111	0
2	SO4	D	602	5/5	0.92	0.17	-0.41	76,78,80,81	0
2	SO4	A	602	5/5	0.94	0.16	-0.46	67,67,69,70	0
3	GOL	C	607	6/6	0.95	0.16	-0.67	44,46,49,51	0
2	SO4	B	607	5/5	0.99	0.13	-0.75	42,44,47,49	0
2	SO4	A	601	5/5	0.98	0.12	-0.99	55,55,57,62	0
2	SO4	B	602	5/5	0.96	0.14	-1.01	66,68,68,70	0
2	SO4	A	608	5/5	0.99	0.12	-1.70	42,42,47,48	0
2	SO4	D	601	5/5	0.97	0.13	-1.73	40,43,44,45	0
2	SO4	C	601	5/5	0.98	0.09	-2.22	42,42,44,45	0
4	CL	C	609	1/1	0.92	0.09	-2.26	49,49,49,49	0
3	GOL	C	608	6/6	0.88	0.21	-	35,37,41,41	0
4	CL	A	611	1/1	0.95	0.07	-	52,52,52,52	0
2	SO4	D	603	5/5	0.93	0.16	-	74,74,75,77	0
2	SO4	A	604	5/5	0.92	0.20	-	73,73,75,75	0
2	SO4	A	607	5/5	0.86	0.25	-	99,99,101,102	0
2	SO4	B	606	5/5	0.97	0.25	-	61,64,65,66	0
4	CL	D	607	1/1	0.74	0.22	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	A	603	5/5	0.93	0.19	-	70,73,74,74	0
4	CL	C	610	1/1	0.75	0.14	-	66,66,66,66	0
2	SO4	C	605	5/5	0.81	0.23	-	109,109,110,110	0
2	SO4	B	605	5/5	0.93	0.23	-	79,79,80,80	0
4	CL	D	608	1/1	0.94	0.15	-	65,65,65,65	0
2	SO4	B	604	5/5	0.93	0.12	-	69,72,72,73	0
2	SO4	B	601	5/5	0.97	0.10	-	45,46,49,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.