



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 25, 2024 – 04:57 AM EDT

PDB ID : 6QU5
Title : Crystal Structure of Phosphofructokinase from Trypanosoma brucei in complex with an allosteric inhibitor etcb12
Authors : McNae, I.W.; Dornan, J.; Walkinshaw, M.D.
Deposited on : 2019-02-26
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ 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 ⓘ](#)) 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	:	2.37.1
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)	:	2.37.1

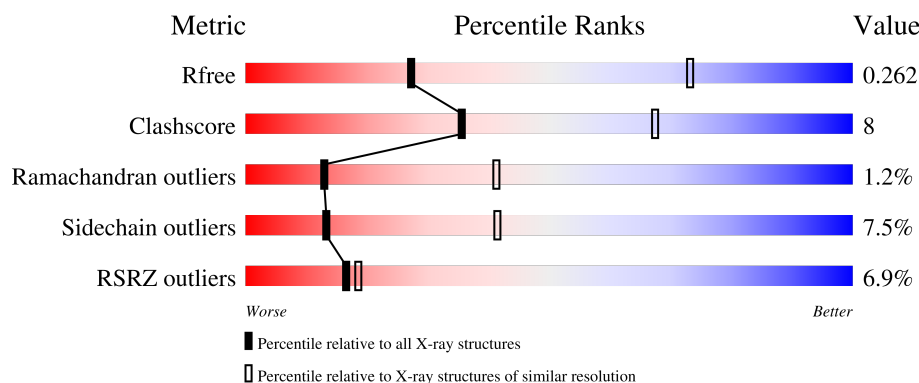
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 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 $\leq 5\%$. 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	507	<div> <div>0%</div> <div> <div>71%</div> <div>15%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	507	<div> <div>4%</div> <div> <div>72%</div> <div>16%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	507	<div> <div>5%</div> <div> <div>71%</div> <div>16%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	507	<div> <div>6%</div> <div> <div>72%</div> <div>16%</div> <div>•</div> <div>11%</div> </div> </div>
1	E	507	<div> <div>2%</div> <div> <div>70%</div> <div>17%</div> <div>•</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	507	
1	G	507	
1	H	507	

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
4	JJ8	B	503	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28255 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 ATP-dependent 6-phosphofructokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3487	2187	639	644	17			
1	B	459	Total	C	N	O	S	0	0	0
			3539	2218	648	656	17			
1	C	461	Total	C	N	O	S	0	0	0
			3552	2226	651	658	17			
1	D	453	Total	C	N	O	S	0	0	0
			3493	2189	642	645	17			
1	E	456	Total	C	N	O	S	0	0	0
			3519	2205	648	649	17			
1	F	456	Total	C	N	O	S	0	0	0
			3514	2202	645	650	17			
1	G	455	Total	C	N	O	S	0	0	0
			3511	2201	646	647	17			
1	H	453	Total	C	N	O	S	0	0	0
			3496	2193	641	645	17			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP O15648
A	-18	GLY	-	expression tag	UNP O15648
A	-17	SER	-	expression tag	UNP O15648
A	-16	SER	-	expression tag	UNP O15648
A	-15	HIS	-	expression tag	UNP O15648
A	-14	HIS	-	expression tag	UNP O15648
A	-13	HIS	-	expression tag	UNP O15648
A	-12	HIS	-	expression tag	UNP O15648
A	-11	HIS	-	expression tag	UNP O15648
A	-10	HIS	-	expression tag	UNP O15648
A	-9	SER	-	expression tag	UNP O15648
A	-8	SER	-	expression tag	UNP O15648
A	-7	GLY	-	expression tag	UNP O15648

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP O15648
A	-5	VAL	-	expression tag	UNP O15648
A	-4	PRO	-	expression tag	UNP O15648
A	-3	ARG	-	expression tag	UNP O15648
A	-2	GLY	-	expression tag	UNP O15648
A	-1	SER	-	expression tag	UNP O15648
A	0	HIS	-	expression tag	UNP O15648
B	-19	MET	-	initiating methionine	UNP O15648
B	-18	GLY	-	expression tag	UNP O15648
B	-17	SER	-	expression tag	UNP O15648
B	-16	SER	-	expression tag	UNP O15648
B	-15	HIS	-	expression tag	UNP O15648
B	-14	HIS	-	expression tag	UNP O15648
B	-13	HIS	-	expression tag	UNP O15648
B	-12	HIS	-	expression tag	UNP O15648
B	-11	HIS	-	expression tag	UNP O15648
B	-10	HIS	-	expression tag	UNP O15648
B	-9	SER	-	expression tag	UNP O15648
B	-8	SER	-	expression tag	UNP O15648
B	-7	GLY	-	expression tag	UNP O15648
B	-6	LEU	-	expression tag	UNP O15648
B	-5	VAL	-	expression tag	UNP O15648
B	-4	PRO	-	expression tag	UNP O15648
B	-3	ARG	-	expression tag	UNP O15648
B	-2	GLY	-	expression tag	UNP O15648
B	-1	SER	-	expression tag	UNP O15648
B	0	HIS	-	expression tag	UNP O15648
C	-19	MET	-	initiating methionine	UNP O15648
C	-18	GLY	-	expression tag	UNP O15648
C	-17	SER	-	expression tag	UNP O15648
C	-16	SER	-	expression tag	UNP O15648
C	-15	HIS	-	expression tag	UNP O15648
C	-14	HIS	-	expression tag	UNP O15648
C	-13	HIS	-	expression tag	UNP O15648
C	-12	HIS	-	expression tag	UNP O15648
C	-11	HIS	-	expression tag	UNP O15648
C	-10	HIS	-	expression tag	UNP O15648
C	-9	SER	-	expression tag	UNP O15648
C	-8	SER	-	expression tag	UNP O15648
C	-7	GLY	-	expression tag	UNP O15648
C	-6	LEU	-	expression tag	UNP O15648
C	-5	VAL	-	expression tag	UNP O15648

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP O15648
C	-3	ARG	-	expression tag	UNP O15648
C	-2	GLY	-	expression tag	UNP O15648
C	-1	SER	-	expression tag	UNP O15648
C	0	HIS	-	expression tag	UNP O15648
D	-19	MET	-	initiating methionine	UNP O15648
D	-18	GLY	-	expression tag	UNP O15648
D	-17	SER	-	expression tag	UNP O15648
D	-16	SER	-	expression tag	UNP O15648
D	-15	HIS	-	expression tag	UNP O15648
D	-14	HIS	-	expression tag	UNP O15648
D	-13	HIS	-	expression tag	UNP O15648
D	-12	HIS	-	expression tag	UNP O15648
D	-11	HIS	-	expression tag	UNP O15648
D	-10	HIS	-	expression tag	UNP O15648
D	-9	SER	-	expression tag	UNP O15648
D	-8	SER	-	expression tag	UNP O15648
D	-7	GLY	-	expression tag	UNP O15648
D	-6	LEU	-	expression tag	UNP O15648
D	-5	VAL	-	expression tag	UNP O15648
D	-4	PRO	-	expression tag	UNP O15648
D	-3	ARG	-	expression tag	UNP O15648
D	-2	GLY	-	expression tag	UNP O15648
D	-1	SER	-	expression tag	UNP O15648
D	0	HIS	-	expression tag	UNP O15648
E	-19	MET	-	initiating methionine	UNP O15648
E	-18	GLY	-	expression tag	UNP O15648
E	-17	SER	-	expression tag	UNP O15648
E	-16	SER	-	expression tag	UNP O15648
E	-15	HIS	-	expression tag	UNP O15648
E	-14	HIS	-	expression tag	UNP O15648
E	-13	HIS	-	expression tag	UNP O15648
E	-12	HIS	-	expression tag	UNP O15648
E	-11	HIS	-	expression tag	UNP O15648
E	-10	HIS	-	expression tag	UNP O15648
E	-9	SER	-	expression tag	UNP O15648
E	-8	SER	-	expression tag	UNP O15648
E	-7	GLY	-	expression tag	UNP O15648
E	-6	LEU	-	expression tag	UNP O15648
E	-5	VAL	-	expression tag	UNP O15648
E	-4	PRO	-	expression tag	UNP O15648
E	-3	ARG	-	expression tag	UNP O15648

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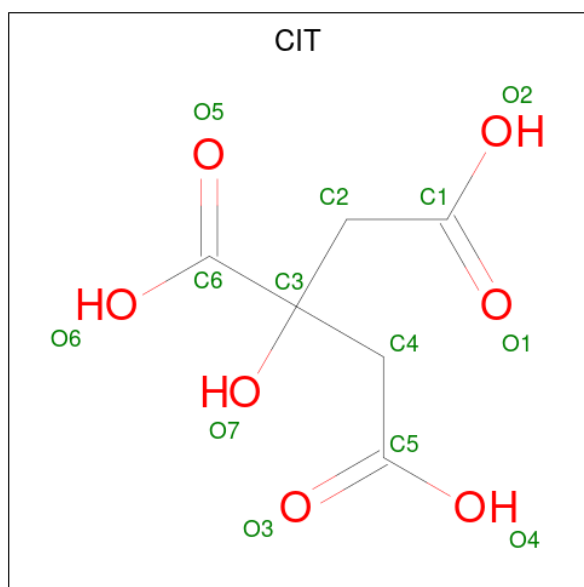
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E	-2	GLY	-	expression tag	UNP O15648
E	-1	SER	-	expression tag	UNP O15648
E	0	HIS	-	expression tag	UNP O15648
F	-19	MET	-	initiating methionine	UNP O15648
F	-18	GLY	-	expression tag	UNP O15648
F	-17	SER	-	expression tag	UNP O15648
F	-16	SER	-	expression tag	UNP O15648
F	-15	HIS	-	expression tag	UNP O15648
F	-14	HIS	-	expression tag	UNP O15648
F	-13	HIS	-	expression tag	UNP O15648
F	-12	HIS	-	expression tag	UNP O15648
F	-11	HIS	-	expression tag	UNP O15648
F	-10	HIS	-	expression tag	UNP O15648
F	-9	SER	-	expression tag	UNP O15648
F	-8	SER	-	expression tag	UNP O15648
F	-7	GLY	-	expression tag	UNP O15648
F	-6	LEU	-	expression tag	UNP O15648
F	-5	VAL	-	expression tag	UNP O15648
F	-4	PRO	-	expression tag	UNP O15648
F	-3	ARG	-	expression tag	UNP O15648
F	-2	GLY	-	expression tag	UNP O15648
F	-1	SER	-	expression tag	UNP O15648
F	0	HIS	-	expression tag	UNP O15648
G	-19	MET	-	initiating methionine	UNP O15648
G	-18	GLY	-	expression tag	UNP O15648
G	-17	SER	-	expression tag	UNP O15648
G	-16	SER	-	expression tag	UNP O15648
G	-15	HIS	-	expression tag	UNP O15648
G	-14	HIS	-	expression tag	UNP O15648
G	-13	HIS	-	expression tag	UNP O15648
G	-12	HIS	-	expression tag	UNP O15648
G	-11	HIS	-	expression tag	UNP O15648
G	-10	HIS	-	expression tag	UNP O15648
G	-9	SER	-	expression tag	UNP O15648
G	-8	SER	-	expression tag	UNP O15648
G	-7	GLY	-	expression tag	UNP O15648
G	-6	LEU	-	expression tag	UNP O15648
G	-5	VAL	-	expression tag	UNP O15648
G	-4	PRO	-	expression tag	UNP O15648
G	-3	ARG	-	expression tag	UNP O15648
G	-2	GLY	-	expression tag	UNP O15648
G	-1	SER	-	expression tag	UNP O15648

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP O15648
H	-19	MET	-	initiating methionine	UNP O15648
H	-18	GLY	-	expression tag	UNP O15648
H	-17	SER	-	expression tag	UNP O15648
H	-16	SER	-	expression tag	UNP O15648
H	-15	HIS	-	expression tag	UNP O15648
H	-14	HIS	-	expression tag	UNP O15648
H	-13	HIS	-	expression tag	UNP O15648
H	-12	HIS	-	expression tag	UNP O15648
H	-11	HIS	-	expression tag	UNP O15648
H	-10	HIS	-	expression tag	UNP O15648
H	-9	SER	-	expression tag	UNP O15648
H	-8	SER	-	expression tag	UNP O15648
H	-7	GLY	-	expression tag	UNP O15648
H	-6	LEU	-	expression tag	UNP O15648
H	-5	VAL	-	expression tag	UNP O15648
H	-4	PRO	-	expression tag	UNP O15648
H	-3	ARG	-	expression tag	UNP O15648
H	-2	GLY	-	expression tag	UNP O15648
H	-1	SER	-	expression tag	UNP O15648
H	0	HIS	-	expression tag	UNP O15648

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



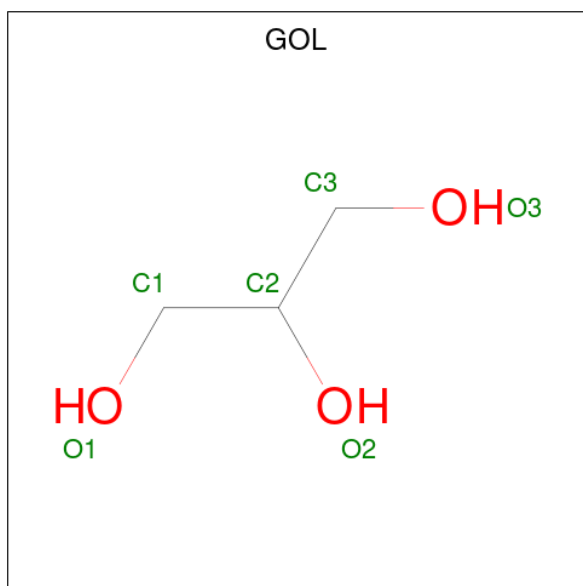
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		

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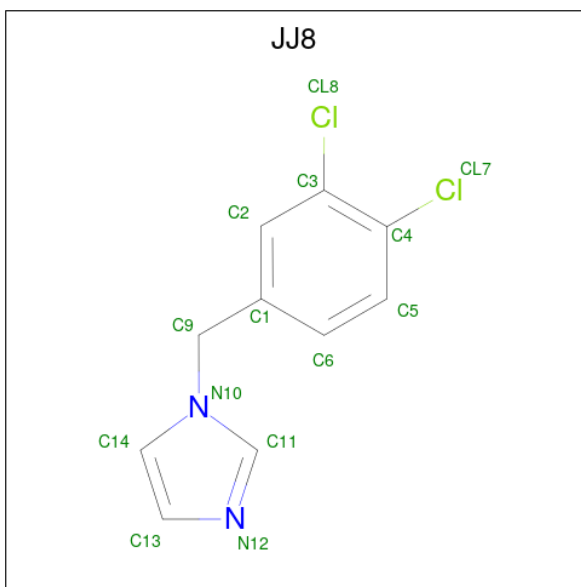
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		
2	G	1	Total	C	O	0	0
			13	6	7		
2	H	1	Total	C	O	0	0
			13	6	7		

- 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		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 1-[(3,4-dichlorophenyl)methyl]imidazole (three-letter code: JJ8) (formula: $C_{10}H_8Cl_2N_2$).

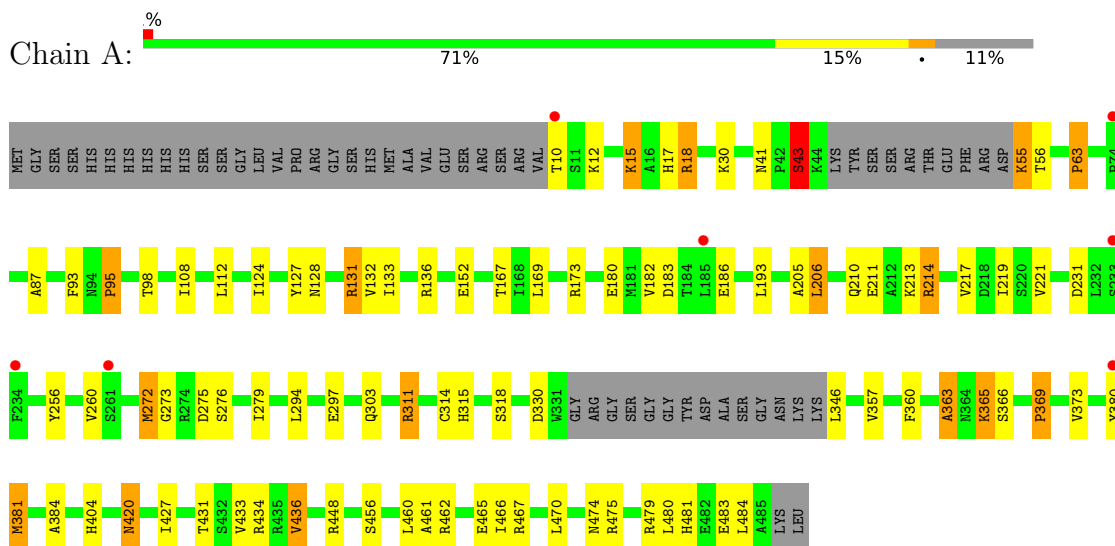


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	0	0
			14	10	2	2		
4	B	1	Total	C	Cl	N	0	0
			14	10	2	2		

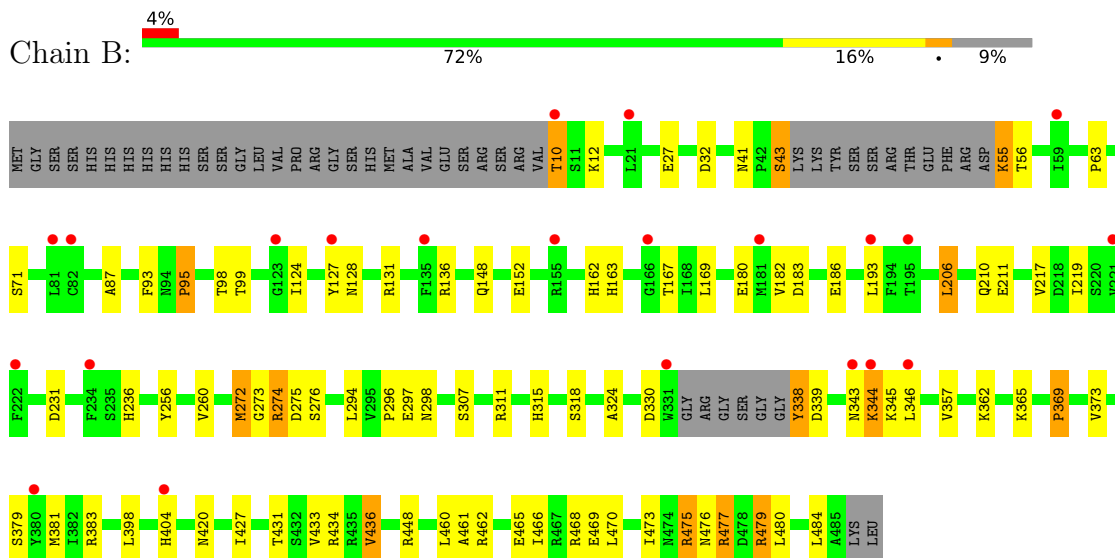
3 Residue-property plots

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: ATP-dependent 6-phosphofructokinase

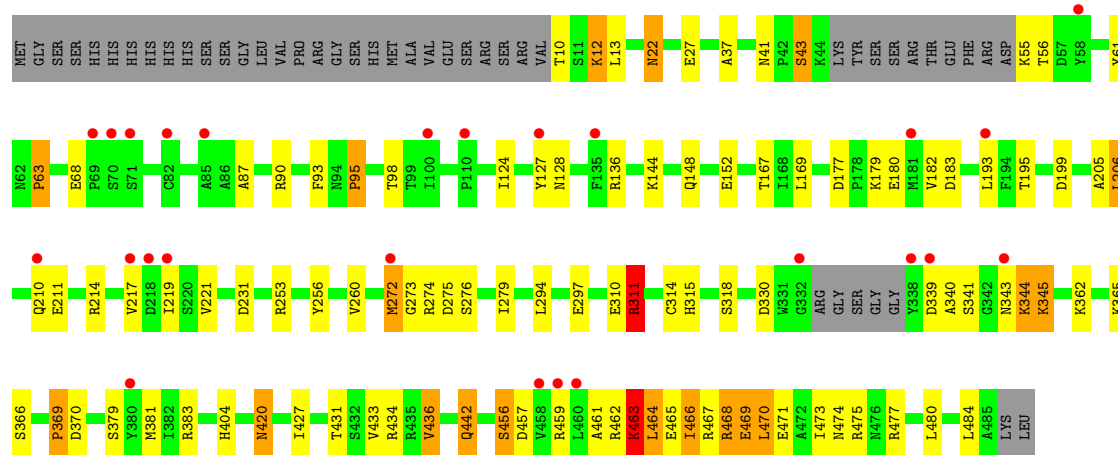


- Molecule 1: ATP-dependent 6-phosphofructokinase

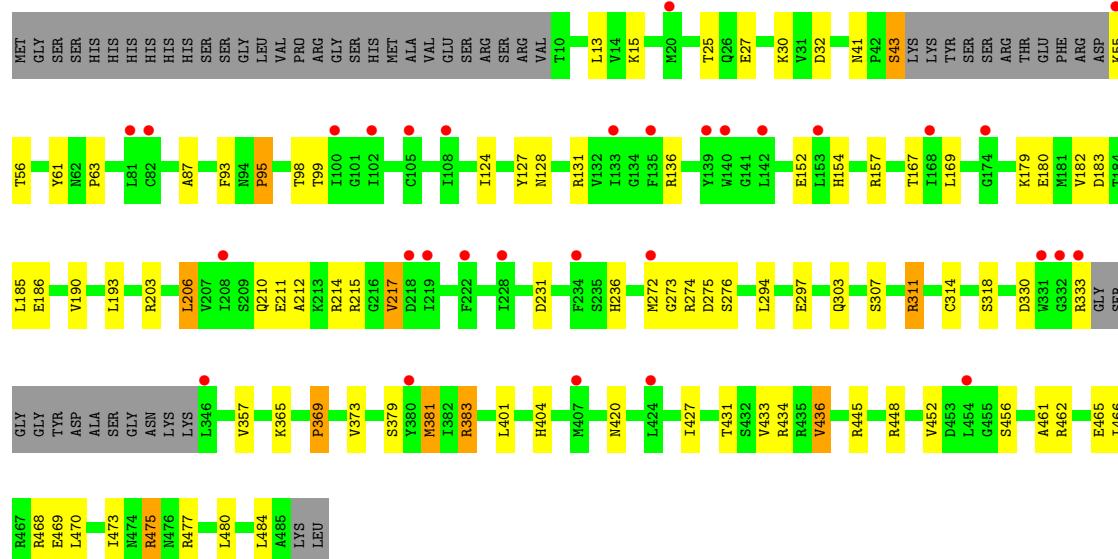


- Molecule 1: ATP-dependent 6-phosphofructokinase

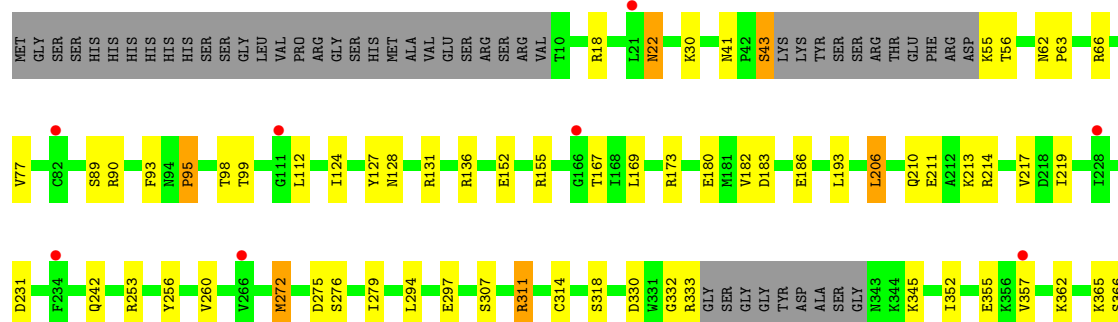




• Molecule 1: ATP-dependent 6-phosphofructokinase

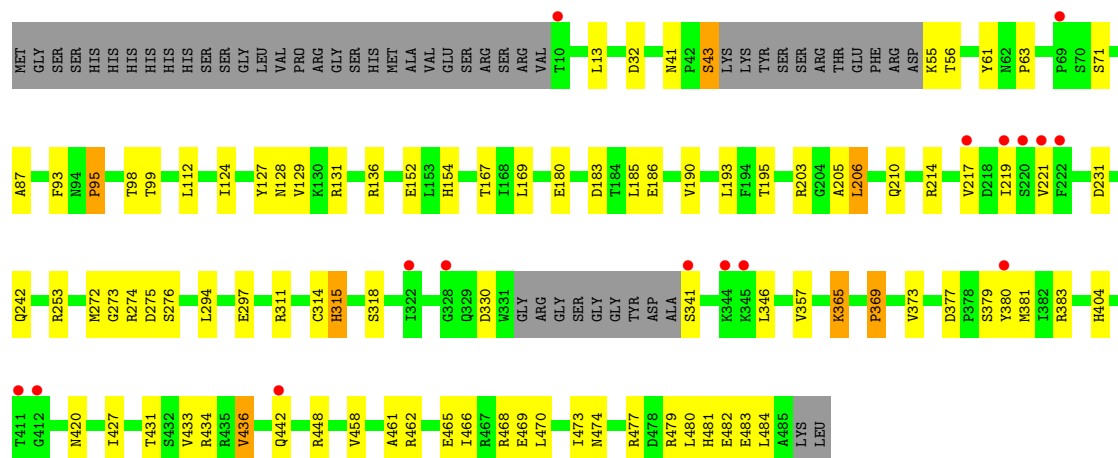


• Molecule 1: ATP-dependent 6-phosphofructokinase

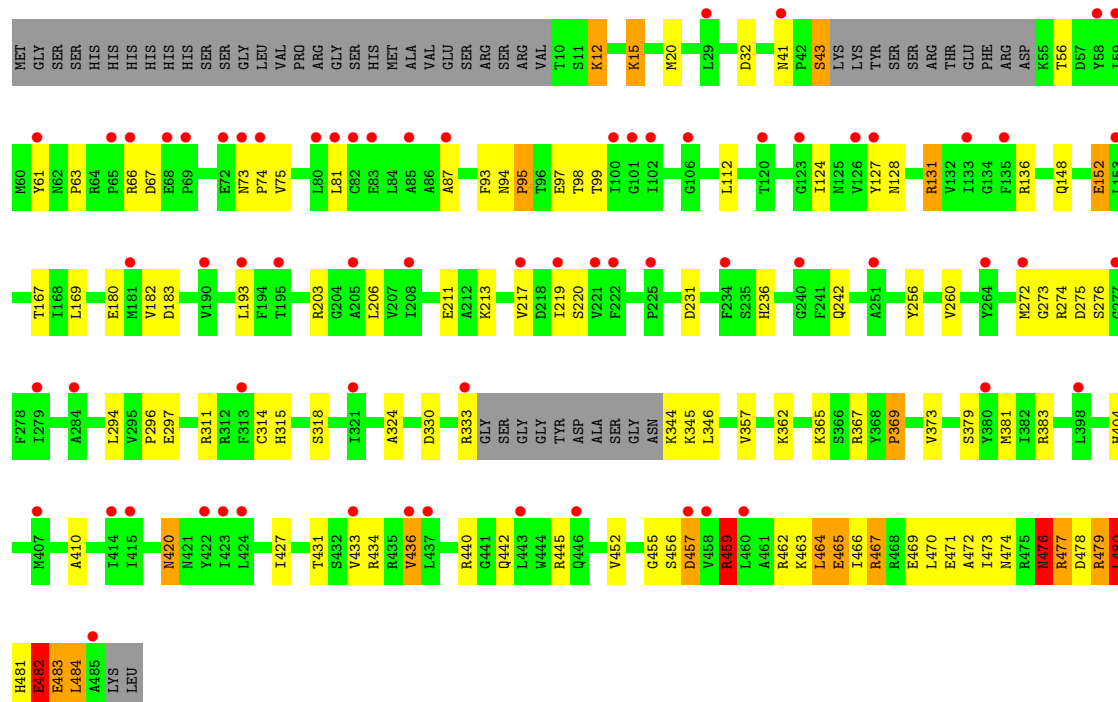




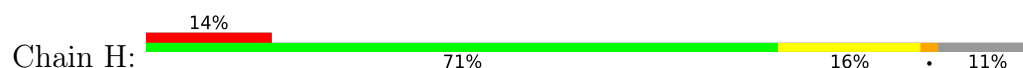
- Molecule 1: ATP-dependent 6-phosphofructokinase

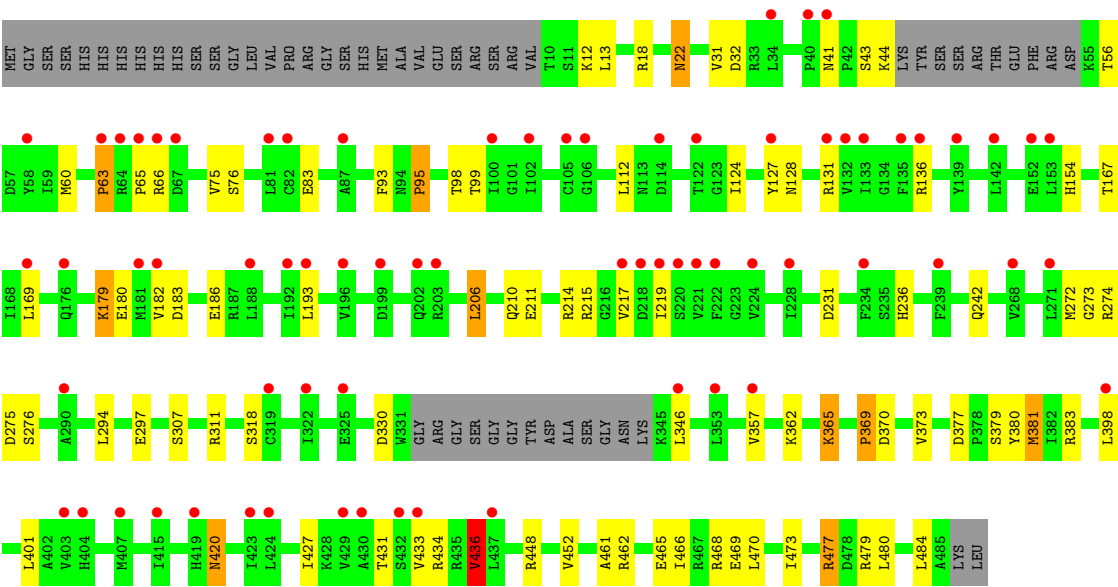


- Molecule 1: ATP-dependent 6-phosphofructokinase



- Molecule 1: ATP-dependent 6-phosphofructokinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.25Å 132.51Å 282.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.67 – 3.40 96.67 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (96.67-3.40) 99.8 (96.67-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.41Å)	Xtriage
Refinement program	REFMAC 5.8.0241	Depositor
R, R_{free}	0.250 , 0.267 0.245 , 0.262	Depositor DCC
R_{free} test set	2969 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	108.7	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28255	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, JJ8, CIT

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	0.72	0/3545	0.85	2/4798 (0.0%)
1	B	0.73	0/3598	0.83	2/4869 (0.0%)
1	C	0.74	0/3611	0.89	4/4885 (0.1%)
1	D	0.72	0/3551	0.81	0/4806
1	E	0.74	0/3577	0.85	0/4839
1	F	0.73	0/3572	0.84	1/4833 (0.0%)
1	G	0.73	0/3569	0.88	3/4828 (0.1%)
1	H	0.71	0/3554	0.81	0/4809
All	All	0.73	0/28577	0.85	12/38667 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
1	G	0	3
All	All	0	7

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	ASP	CB-CA-C	10.89	132.18	110.40
1	G	32	ASP	CB-CA-C	8.20	126.80	110.40
1	A	381	MET	CB-CG-SD	6.38	131.53	112.40
1	B	10	THR	CB-CA-C	6.15	128.21	111.60
1	G	476	ASN	CB-CA-C	5.96	122.32	110.40

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	346	LEU	Peptide
1	A	43	SER	Peptide
1	C	344	LYS	Peptide
1	C	456	SER	Mainchain
1	G	344	LYS	Peptide

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	3487	0	3549	54	0
1	B	3539	0	3594	55	0
1	C	3552	0	3610	76	0
1	D	3493	0	3552	65	0
1	E	3519	0	3584	57	0
1	F	3514	0	3576	59	0
1	G	3511	0	3578	91	0
1	H	3496	0	3560	63	0
2	A	13	0	5	1	0
2	B	13	0	5	1	0
2	C	13	0	5	0	0
2	D	13	0	5	1	0
2	E	13	0	5	0	0
2	F	13	0	5	1	0
2	G	13	0	5	0	0
2	H	13	0	5	0	0
3	A	6	0	8	0	0
3	B	6	0	8	1	0
4	A	14	0	0	1	0
4	B	14	0	0	1	0
All	All	28255	0	28659	463	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 8.

The worst 5 of 463 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:G:73:ASN:ND2	1:H:76:SER:O	1.64	1.31
1:F:380:TYR:CE2	1:F:381:MET:HG2	1.80	1.17
1:G:464:LEU:O	1:G:467:ARG:HG2	1.47	1.14
1:E:468:ARG:NH2	1:F:129:VAL:O	1.81	1.13
1:A:380:TYR:CE2	1:A:381:MET:HG3	1.91	1.05

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	446/507 (88%)	404 (91%)	38 (8%)	4 (1%)	17	49
1	B	453/507 (89%)	412 (91%)	38 (8%)	3 (1%)	22	55
1	C	455/507 (90%)	402 (88%)	44 (10%)	9 (2%)	7	30
1	D	447/507 (88%)	408 (91%)	35 (8%)	4 (1%)	17	49
1	E	450/507 (89%)	407 (90%)	39 (9%)	4 (1%)	17	49
1	F	450/507 (89%)	411 (91%)	35 (8%)	4 (1%)	17	49
1	G	449/507 (89%)	403 (90%)	35 (8%)	11 (2%)	6	28
1	H	447/507 (88%)	407 (91%)	35 (8%)	5 (1%)	14	44
All	All	3597/4056 (89%)	3254 (90%)	299 (8%)	44 (1%)	13	41

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	369	PRO
1	B	369	PRO
1	C	345	LYS
1	C	369	PRO

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Mol	Chain	Res	Type
1	C	484	LEU

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	377/422 (89%)	345 (92%)	32 (8%)	10	35
1	B	382/422 (90%)	351 (92%)	31 (8%)	11	38
1	C	383/422 (91%)	353 (92%)	30 (8%)	12	39
1	D	377/422 (89%)	349 (93%)	28 (7%)	13	42
1	E	380/422 (90%)	346 (91%)	34 (9%)	9	33
1	F	380/422 (90%)	358 (94%)	22 (6%)	20	50
1	G	379/422 (90%)	351 (93%)	28 (7%)	13	42
1	H	378/422 (90%)	354 (94%)	24 (6%)	18	47
All	All	3036/3376 (90%)	2807 (92%)	229 (8%)	13	41

5 of 229 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	436	VAL
1	H	381	MET
1	E	383	ARG
1	H	365	LYS
1	G	467	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	210	GLN
1	H	420	ASN
1	E	22	ASN
1	G	420	ASN

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Mol	Chain	Res	Type
1	E	17	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	CIT	D	501	-	12,12,12	1.15	1 (8%)	17,17,17	1.18	1 (5%)
2	CIT	B	501	-	12,12,12	1.16	1 (8%)	17,17,17	1.41	2 (11%)
2	CIT	H	501	1	12,12,12	1.24	1 (8%)	17,17,17	1.12	1 (5%)
2	CIT	F	501	-	12,12,12	1.21	1 (8%)	17,17,17	1.45	3 (17%)
2	CIT	C	501	-	12,12,12	1.13	1 (8%)	17,17,17	1.25	2 (11%)
3	GOL	A	502	-	5,5,5	0.09	0	5,5,5	0.27	0
3	GOL	B	502	-	5,5,5	0.11	0	5,5,5	0.31	0
4	JJ8	B	503	-	14,15,15	1.24	4 (28%)	18,20,20	0.96	0
2	CIT	E	501	-	12,12,12	1.23	1 (8%)	17,17,17	1.40	3 (17%)
4	JJ8	A	503	-	14,15,15	1.23	3 (21%)	18,20,20	0.78	0
2	CIT	G	501	-	12,12,12	1.16	1 (8%)	17,17,17	1.45	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CIT	A	501	-	12,12,12	1.11	0	17,17,17	1.33	2 (11%)

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	CIT	D	501	-	-	11/16/16/16	-
2	CIT	B	501	-	-	6/16/16/16	-
2	CIT	H	501	1	-	10/16/16/16	-
2	CIT	F	501	-	-	10/16/16/16	-
2	CIT	C	501	-	-	5/16/16/16	-
3	GOL	A	502	-	-	0/4/4/4	-
3	GOL	B	502	-	-	2/4/4/4	-
4	JJ8	B	503	-	-	2/4/4/4	0/2/2/2
2	CIT	E	501	-	-	7/16/16/16	-
4	JJ8	A	503	-	-	2/4/4/4	0/2/2/2
2	CIT	G	501	-	-	6/16/16/16	-
2	CIT	A	501	-	-	10/16/16/16	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	JJ8	C3-CL8	2.70	1.80	1.73
2	E	501	CIT	C3-C6	2.65	1.56	1.53
2	F	501	CIT	C3-C6	2.49	1.56	1.53
2	H	501	CIT	C3-C6	2.39	1.55	1.53
4	B	503	JJ8	C9-N10	-2.37	1.44	1.49

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	501	CIT	O5-C6-C3	-3.86	116.79	122.25
2	B	501	CIT	O5-C6-C3	-3.75	116.95	122.25
2	F	501	CIT	O5-C6-C3	-3.65	117.09	122.25
2	E	501	CIT	O5-C6-C3	-3.42	117.41	122.25
2	A	501	CIT	O5-C6-C3	-3.20	117.72	122.25

There are no chirality outliers.

5 of 71 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	CIT	C1-C2-C3-O7
2	A	501	CIT	C2-C3-C4-C5
2	A	501	CIT	C6-C3-C4-C5
2	A	501	CIT	O7-C3-C6-O5
2	A	501	CIT	O7-C3-C6-O6

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	CIT	1	0
2	B	501	CIT	1	0
2	F	501	CIT	1	0
3	B	502	GOL	1	0
4	B	503	JJ8	1	0
4	A	503	JJ8	1	0
2	A	501	CIT	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 [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	452/507 (89%)	0.35	7 (1%) 73 72	71, 100, 144, 171	0
1	B	459/507 (90%)	0.55	22 (4%) 30 31	77, 109, 137, 156	0
1	C	461/507 (90%)	0.56	25 (5%) 25 26	81, 114, 155, 187	0
1	D	453/507 (89%)	0.56	31 (6%) 17 19	82, 120, 156, 179	0
1	E	456/507 (89%)	0.36	12 (2%) 56 54	80, 109, 152, 204	0
1	F	456/507 (89%)	0.55	16 (3%) 44 43	75, 104, 135, 170	0
1	G	455/507 (89%)	0.86	68 (14%) 2 2	99, 137, 177, 229	0
1	H	453/507 (89%)	0.94	71 (15%) 2 2	116, 152, 188, 208	0
All	All	3645/4056 (89%)	0.59	252 (6%) 16 18	71, 117, 168, 229	0

The worst 5 of 252 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	460	LEU	8.0
1	H	219	ILE	7.2
1	G	82	CYS	7.0
1	G	72	GLU	6.3
1	E	485	ALA	5.9

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
2	CIT	G	501	13/13	0.73	0.25	155,155,155,155	0
2	CIT	A	501	13/13	0.76	0.23	155,155,155,155	0
2	CIT	D	501	13/13	0.77	0.24	155,155,155,155	0
2	CIT	H	501	13/13	0.78	0.27	155,155,155,155	0
2	CIT	E	501	13/13	0.79	0.18	155,155,155,155	0
2	CIT	F	501	13/13	0.79	0.36	155,155,155,155	0
4	JJ8	B	503	14/14	0.79	0.52	155,155,155,155	0
3	GOL	A	502	6/6	0.83	0.51	155,155,155,155	0
3	GOL	B	502	6/6	0.84	0.46	155,155,155,155	0
2	CIT	B	501	13/13	0.84	0.31	155,155,155,155	0
4	JJ8	A	503	14/14	0.87	0.55	155,155,155,155	0
2	CIT	C	501	13/13	0.87	0.23	155,155,155,155	0

6.5 Other polymers [i](#)

There are no such residues in this entry.