Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2023 – 06:25 PM EDT

PDB ID	:	4GM6
Title	:	Crystal structure of PfkB family carbohydrate kinase(TARGET EFI-502146 FROM Listeria grayi DSM 20601
Authors	:	Patskovsky, Y.; Toro, R.; Bhosle, R.; Hillerich, B.; Seidel, R.D.; Washington, E.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Zencheck, W.D.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on	:	2012-08-15
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

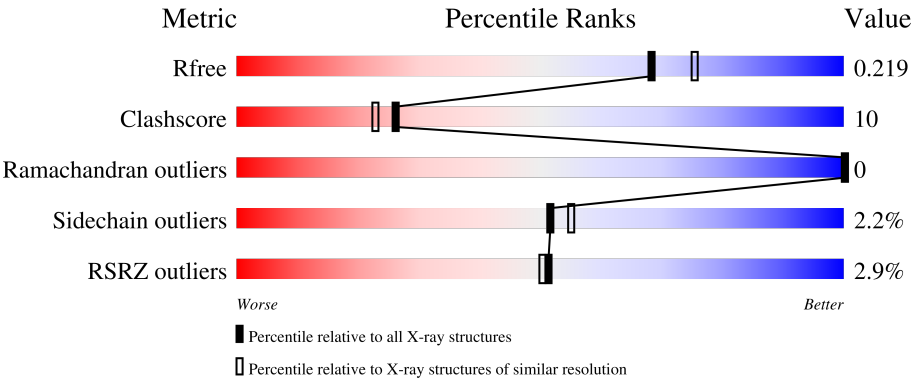
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	351	2% 73% 17% • 9%
1	B	351	3% 74% 17% • 9%
1	C	351	2% 75% 15% • 8%
1	D	351	4% 78% 13% • 8%

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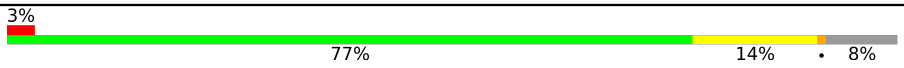
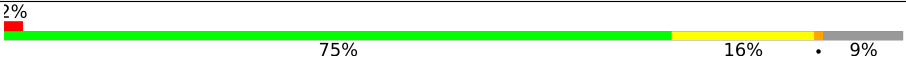
Mol	Chain	Length	Quality of chain
1	E	351	
1	F	351	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16449 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 PfkB family carbohydrate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	10	0
			2572	1648	441	474	9			
1	B	321	Total	C	N	O	S	0	7	0
			2559	1640	434	476	9			
1	C	322	Total	C	N	O	S	0	4	0
			2544	1629	431	475	9			
1	D	322	Total	C	N	O	S	0	5	0
			2563	1642	438	474	9			
1	E	322	Total	C	N	O	S	0	5	0
			2555	1636	435	475	9			
1	F	320	Total	C	N	O	S	0	7	0
			2546	1630	434	473	9			

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP D7UWR6
A	-21	HIS	-	expression tag	UNP D7UWR6
A	-20	HIS	-	expression tag	UNP D7UWR6
A	-19	HIS	-	expression tag	UNP D7UWR6
A	-18	HIS	-	expression tag	UNP D7UWR6
A	-17	HIS	-	expression tag	UNP D7UWR6
A	-16	HIS	-	expression tag	UNP D7UWR6
A	-15	SER	-	expression tag	UNP D7UWR6
A	-14	SER	-	expression tag	UNP D7UWR6
A	-13	GLY	-	expression tag	UNP D7UWR6
A	-12	VAL	-	expression tag	UNP D7UWR6
A	-11	ASP	-	expression tag	UNP D7UWR6
A	-10	LEU	-	expression tag	UNP D7UWR6
A	-9	GLY	-	expression tag	UNP D7UWR6
A	-8	THR	-	expression tag	UNP D7UWR6
A	-7	GLU	-	expression tag	UNP D7UWR6
A	-6	ASN	-	expression tag	UNP D7UWR6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	LEU	-	expression tag	UNP D7UWR6
A	-4	TYR	-	expression tag	UNP D7UWR6
A	-3	PHE	-	expression tag	UNP D7UWR6
A	-2	GLN	-	expression tag	UNP D7UWR6
A	-1	SER	-	expression tag	UNP D7UWR6
A	0	MET	-	expression tag	UNP D7UWR6
B	-22	MET	-	expression tag	UNP D7UWR6
B	-21	HIS	-	expression tag	UNP D7UWR6
B	-20	HIS	-	expression tag	UNP D7UWR6
B	-19	HIS	-	expression tag	UNP D7UWR6
B	-18	HIS	-	expression tag	UNP D7UWR6
B	-17	HIS	-	expression tag	UNP D7UWR6
B	-16	HIS	-	expression tag	UNP D7UWR6
B	-15	SER	-	expression tag	UNP D7UWR6
B	-14	SER	-	expression tag	UNP D7UWR6
B	-13	GLY	-	expression tag	UNP D7UWR6
B	-12	VAL	-	expression tag	UNP D7UWR6
B	-11	ASP	-	expression tag	UNP D7UWR6
B	-10	LEU	-	expression tag	UNP D7UWR6
B	-9	GLY	-	expression tag	UNP D7UWR6
B	-8	THR	-	expression tag	UNP D7UWR6
B	-7	GLU	-	expression tag	UNP D7UWR6
B	-6	ASN	-	expression tag	UNP D7UWR6
B	-5	LEU	-	expression tag	UNP D7UWR6
B	-4	TYR	-	expression tag	UNP D7UWR6
B	-3	PHE	-	expression tag	UNP D7UWR6
B	-2	GLN	-	expression tag	UNP D7UWR6
B	-1	SER	-	expression tag	UNP D7UWR6
B	0	MET	-	expression tag	UNP D7UWR6
C	-22	MET	-	expression tag	UNP D7UWR6
C	-21	HIS	-	expression tag	UNP D7UWR6
C	-20	HIS	-	expression tag	UNP D7UWR6
C	-19	HIS	-	expression tag	UNP D7UWR6
C	-18	HIS	-	expression tag	UNP D7UWR6
C	-17	HIS	-	expression tag	UNP D7UWR6
C	-16	HIS	-	expression tag	UNP D7UWR6
C	-15	SER	-	expression tag	UNP D7UWR6
C	-14	SER	-	expression tag	UNP D7UWR6
C	-13	GLY	-	expression tag	UNP D7UWR6
C	-12	VAL	-	expression tag	UNP D7UWR6
C	-11	ASP	-	expression tag	UNP D7UWR6
C	-10	LEU	-	expression tag	UNP D7UWR6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	GLY	-	expression tag	UNP D7UWR6
C	-8	THR	-	expression tag	UNP D7UWR6
C	-7	GLU	-	expression tag	UNP D7UWR6
C	-6	ASN	-	expression tag	UNP D7UWR6
C	-5	LEU	-	expression tag	UNP D7UWR6
C	-4	TYR	-	expression tag	UNP D7UWR6
C	-3	PHE	-	expression tag	UNP D7UWR6
C	-2	GLN	-	expression tag	UNP D7UWR6
C	-1	SER	-	expression tag	UNP D7UWR6
C	0	MET	-	expression tag	UNP D7UWR6
D	-22	MET	-	expression tag	UNP D7UWR6
D	-21	HIS	-	expression tag	UNP D7UWR6
D	-20	HIS	-	expression tag	UNP D7UWR6
D	-19	HIS	-	expression tag	UNP D7UWR6
D	-18	HIS	-	expression tag	UNP D7UWR6
D	-17	HIS	-	expression tag	UNP D7UWR6
D	-16	HIS	-	expression tag	UNP D7UWR6
D	-15	SER	-	expression tag	UNP D7UWR6
D	-14	SER	-	expression tag	UNP D7UWR6
D	-13	GLY	-	expression tag	UNP D7UWR6
D	-12	VAL	-	expression tag	UNP D7UWR6
D	-11	ASP	-	expression tag	UNP D7UWR6
D	-10	LEU	-	expression tag	UNP D7UWR6
D	-9	GLY	-	expression tag	UNP D7UWR6
D	-8	THR	-	expression tag	UNP D7UWR6
D	-7	GLU	-	expression tag	UNP D7UWR6
D	-6	ASN	-	expression tag	UNP D7UWR6
D	-5	LEU	-	expression tag	UNP D7UWR6
D	-4	TYR	-	expression tag	UNP D7UWR6
D	-3	PHE	-	expression tag	UNP D7UWR6
D	-2	GLN	-	expression tag	UNP D7UWR6
D	-1	SER	-	expression tag	UNP D7UWR6
D	0	MET	-	expression tag	UNP D7UWR6
E	-22	MET	-	expression tag	UNP D7UWR6
E	-21	HIS	-	expression tag	UNP D7UWR6
E	-20	HIS	-	expression tag	UNP D7UWR6
E	-19	HIS	-	expression tag	UNP D7UWR6
E	-18	HIS	-	expression tag	UNP D7UWR6
E	-17	HIS	-	expression tag	UNP D7UWR6
E	-16	HIS	-	expression tag	UNP D7UWR6
E	-15	SER	-	expression tag	UNP D7UWR6
E	-14	SER	-	expression tag	UNP D7UWR6

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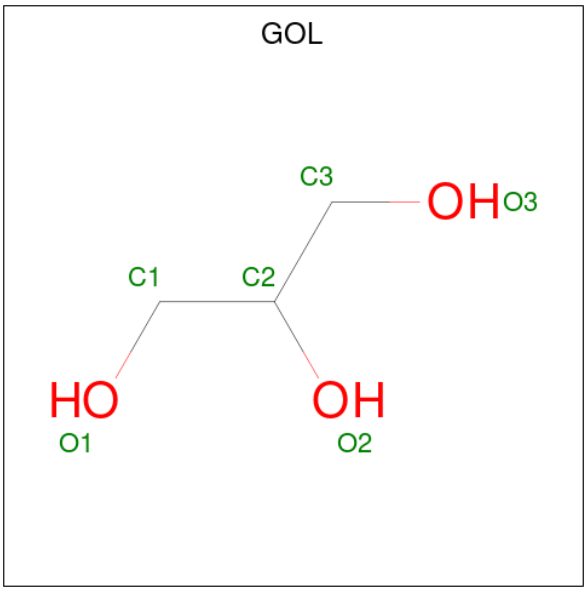
Chain	Residue	Modelled	Actual	Comment	Reference
E	-13	GLY	-	expression tag	UNP D7UWR6
E	-12	VAL	-	expression tag	UNP D7UWR6
E	-11	ASP	-	expression tag	UNP D7UWR6
E	-10	LEU	-	expression tag	UNP D7UWR6
E	-9	GLY	-	expression tag	UNP D7UWR6
E	-8	THR	-	expression tag	UNP D7UWR6
E	-7	GLU	-	expression tag	UNP D7UWR6
E	-6	ASN	-	expression tag	UNP D7UWR6
E	-5	LEU	-	expression tag	UNP D7UWR6
E	-4	TYR	-	expression tag	UNP D7UWR6
E	-3	PHE	-	expression tag	UNP D7UWR6
E	-2	GLN	-	expression tag	UNP D7UWR6
E	-1	SER	-	expression tag	UNP D7UWR6
E	0	MET	-	expression tag	UNP D7UWR6
F	-22	MET	-	expression tag	UNP D7UWR6
F	-21	HIS	-	expression tag	UNP D7UWR6
F	-20	HIS	-	expression tag	UNP D7UWR6
F	-19	HIS	-	expression tag	UNP D7UWR6
F	-18	HIS	-	expression tag	UNP D7UWR6
F	-17	HIS	-	expression tag	UNP D7UWR6
F	-16	HIS	-	expression tag	UNP D7UWR6
F	-15	SER	-	expression tag	UNP D7UWR6
F	-14	SER	-	expression tag	UNP D7UWR6
F	-13	GLY	-	expression tag	UNP D7UWR6
F	-12	VAL	-	expression tag	UNP D7UWR6
F	-11	ASP	-	expression tag	UNP D7UWR6
F	-10	LEU	-	expression tag	UNP D7UWR6
F	-9	GLY	-	expression tag	UNP D7UWR6
F	-8	THR	-	expression tag	UNP D7UWR6
F	-7	GLU	-	expression tag	UNP D7UWR6
F	-6	ASN	-	expression tag	UNP D7UWR6
F	-5	LEU	-	expression tag	UNP D7UWR6
F	-4	TYR	-	expression tag	UNP D7UWR6
F	-3	PHE	-	expression tag	UNP D7UWR6
F	-2	GLN	-	expression tag	UNP D7UWR6
F	-1	SER	-	expression tag	UNP D7UWR6
F	0	MET	-	expression tag	UNP D7UWR6

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	174	Total O 175 175	0	1
4	B	192	Total O 192 192	0	0

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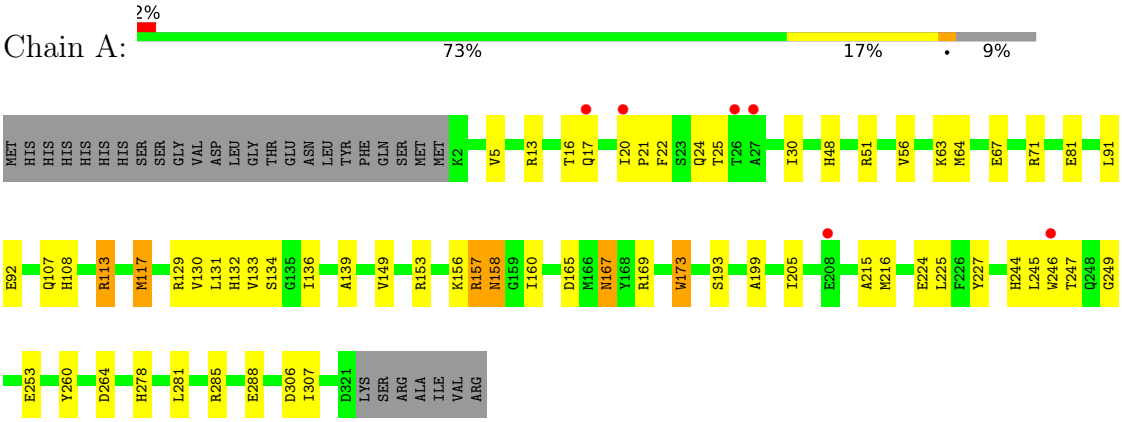
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	171	Total O 171 171	0	0
4	D	188	Total O 188 188	0	0
4	E	173	Total O 173 173	0	0
4	F	179	Total O 179 179	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

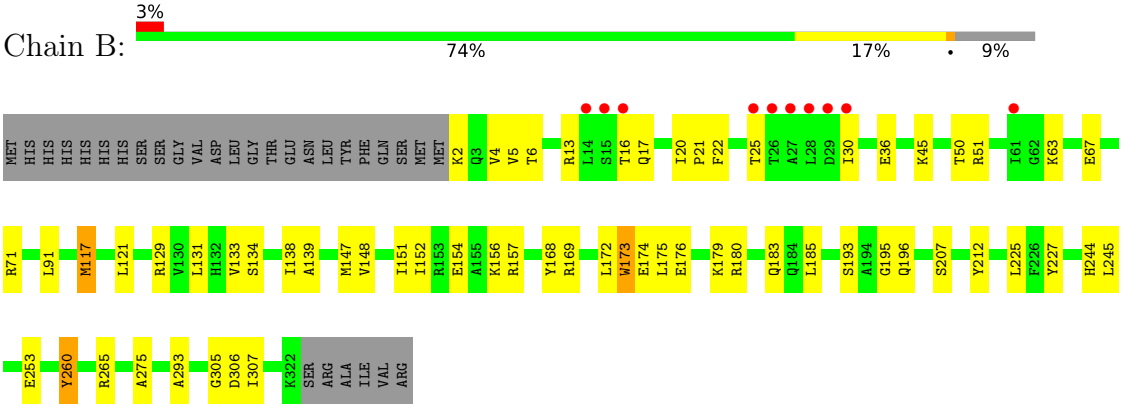
• Molecule 1: PfkB family carbohydrate kinase

Chain A:



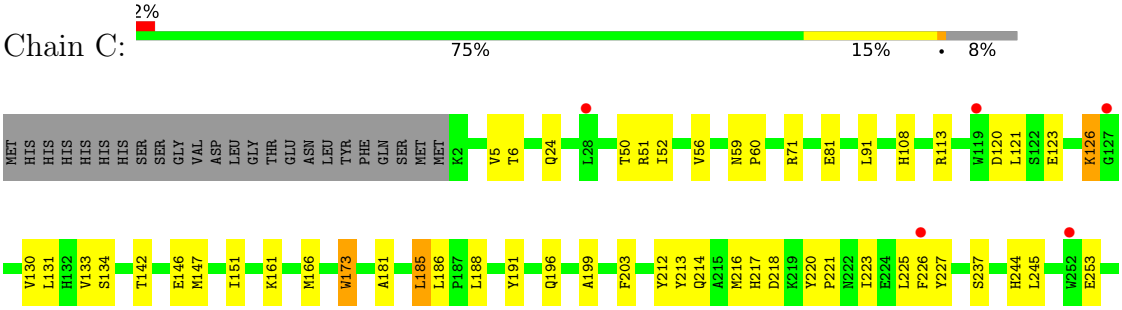
• Molecule 1: PfkB family carbohydrate kinase

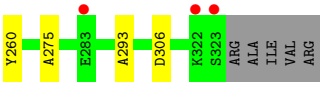
Chain B:



• Molecule 1: PfkB family carbohydrate kinase

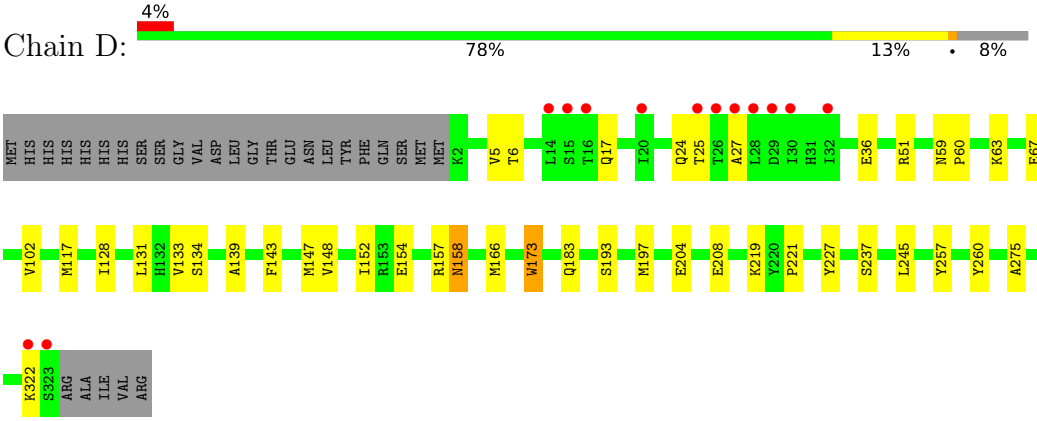
Chain C:





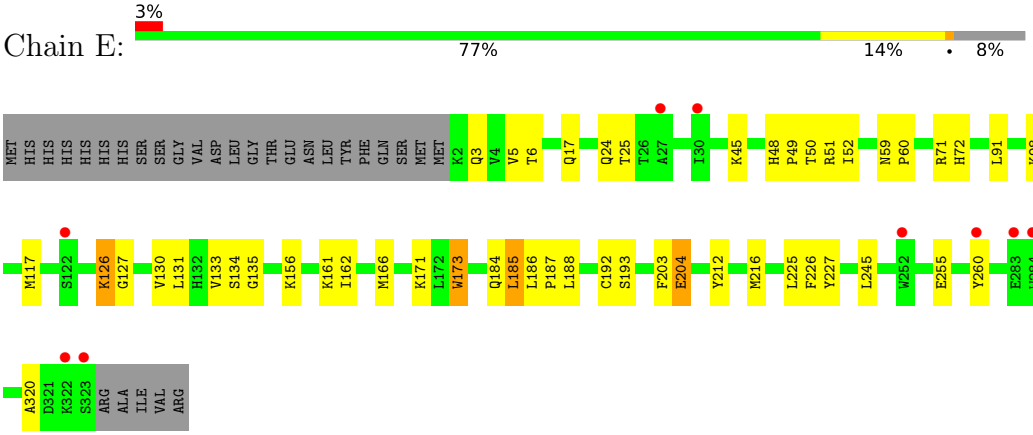
• Molecule 1: PfkB family carbohydrate kinase

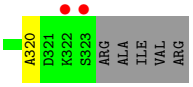
Chain D:



• Molecule 1: PfkB family carbohydrate kinase

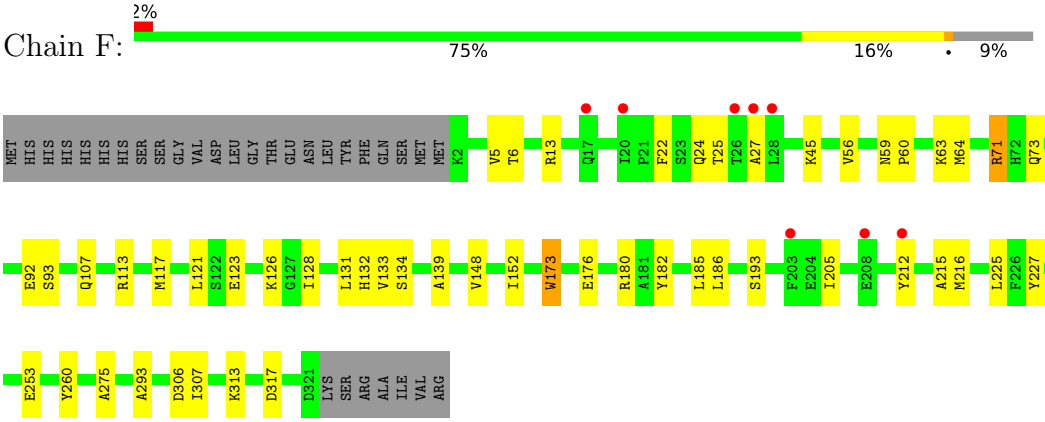
Chain E:





• Molecule 1: PfkB family carbohydrate kinase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.83Å 109.86Å 109.59Å 90.00° 101.92° 90.00°	Depositor
Resolution (Å)	48.23 – 2.00 48.18 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.23-2.00) 99.5 (48.18-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0025	Depositor
R, R_{free}	0.175 , 0.218 0.177 , 0.219	Depositor DCC
R_{free} test set	5084 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	16449	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, 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	0.41	0/2664	0.54	0/3617
1	B	0.41	0/2642	0.54	0/3590
1	C	0.46	1/2618 (0.0%)	0.56	0/3560
1	D	0.39	0/2640	0.55	0/3586
1	E	0.40	0/2632	0.54	0/3576
1	F	0.36	0/2628	0.53	0/3569
All	All	0.41	1/15824 (0.0%)	0.54	0/21498

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	214	GLN	C-N	5.42	1.46	1.34

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	2572	0	2566	70	0
1	B	2559	0	2534	68	0
1	C	2544	0	2504	58	0
1	D	2563	0	2543	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2555	0	2526	50	0
1	F	2546	0	2526	43	0
2	A	6	0	8	1	0
2	B	12	0	16	0	0
2	D	6	0	8	1	0
2	E	6	0	8	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	175	0	0	7	0
4	B	192	0	0	6	0
4	C	171	0	0	2	0
4	D	188	0	0	3	0
4	E	173	0	0	5	0
4	F	179	0	0	6	0
All	All	16449	0	15239	317	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 10.

All (317) 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:C:225:LEU:HD12	1:C:245:LEU:HD11	1.29	1.09
1:B:71:ARG:HE	1:C:71:ARG:HH21	1.09	0.98
1:B:169:ARG:HB2	1:B:172:LEU:HD12	1.43	0.97
1:E:126:LYS:HE2	1:E:126:LYS:HA	1.49	0.93
1:A:156[B]:LYS:HE2	1:A:156[B]:LYS:HA	1.55	0.88
1:E:193:SER:HB2	1:E:227:TYR:CE2	2.09	0.86
1:E:225:LEU:HD13	1:E:245:LEU:HD11	1.58	0.86
1:B:138:ILE:HD13	1:B:185:LEU:CD1	2.05	0.85
1:F:244:HIS:CD2	1:F:253:GLU:HG2	2.12	0.85
1:F:131:LEU:C	1:F:131:LEU:HD23	1.97	0.84
1:D:208:GLU:OE1	1:D:208:GLU:HA	1.78	0.82
1:B:16:THR:HG22	1:B:25[A]:THR:HG21	1.62	0.82
1:A:224:GLU:HG2	1:A:225:LEU:HD12	1.62	0.81
1:A:16:THR:HG22	1:A:25[B]:THR:HG21	1.61	0.81
1:F:244:HIS:HD2	1:F:253:GLU:HG2	1.45	0.80
1:B:21:PRO:O	1:B:25[A]:THR:HG23	1.80	0.79
1:E:156:LYS:HE2	1:E:162:ILE:HG12	1.65	0.79
1:A:131:LEU:C	1:A:131:LEU:HD23	2.06	0.77
1:C:121:LEU:HD21	1:C:151:ILE:HD12	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:THR:CG2	1:A:25[B]:THR:HG21	2.14	0.76
1:E:156:LYS:HE3	1:E:188:LEU:O	1.87	0.73
1:A:244:HIS:HD2	1:A:253:GLU:HG2	1.54	0.73
1:A:244:HIS:CD2	1:A:253:GLU:HG2	2.23	0.72
1:C:121:LEU:CD2	1:C:151:ILE:HD12	2.19	0.72
1:B:16:THR:CG2	1:B:25[A]:THR:HG21	2.18	0.72
1:F:73:GLN:HG2	4:F:572:HOH:O	1.89	0.72
1:B:63:LYS:HD3	4:B:645:HOH:O	1.91	0.71
1:B:138:ILE:HD13	1:B:185:LEU:HD12	1.70	0.71
1:B:45:LYS:HE3	4:B:648:HOH:O	1.90	0.71
1:A:21:PRO:O	1:A:25[B]:THR:HG23	1.90	0.70
1:C:121:LEU:HD21	1:C:151:ILE:CD1	2.22	0.69
1:B:2:LYS:HG2	1:B:129:ARG:CB	2.24	0.68
1:C:6:THR:HG23	1:C:52:ILE:HG13	1.74	0.67
1:B:71:ARG:NE	1:C:71:ARG:HH21	1.88	0.67
1:F:13[A]:ARG:HG3	1:F:89:TYR:CZ	2.29	0.67
1:A:67[A]:GLU:OE1	1:F:71:ARG:HD2	1.94	0.67
1:B:131:LEU:HD23	1:B:131:LEU:C	2.15	0.66
1:D:257:TYR:CE1	1:D:322:LYS:HG3	2.31	0.66
1:B:20:ILE:HG22	1:B:25[A]:THR:HG22	1.77	0.65
1:B:196:GLN:HG2	1:B:212:TYR:CE1	2.31	0.65
1:E:126:LYS:HE2	1:E:126:LYS:CA	2.25	0.65
1:D:148:VAL:O	1:D:152:ILE:HG12	1.97	0.65
1:D:158:ASN:N	1:D:158:ASN:HD22	1.92	0.65
1:A:156[B]:LYS:HA	1:A:156[B]:LYS:CE	2.25	0.65
1:A:193:SER:HB2	1:A:227:TYR:CE2	2.31	0.64
1:B:22:PHE:O	1:B:25[B]:THR:HG22	1.97	0.64
1:A:5:VAL:HG23	1:A:51:ARG:HG3	1.80	0.64
1:F:225:LEU:C	1:F:225:LEU:HD12	2.18	0.64
1:B:148:VAL:O	1:B:152:ILE:HG12	1.98	0.64
1:A:133:VAL:HG22	1:A:134:SER:H	1.63	0.63
1:A:169[A]:ARG:HH22	2:A:401:GOL:H31	1.63	0.63
1:A:22:PHE:O	1:A:25[A]:THR:HG22	1.97	0.63
1:B:117:MET:SD	1:B:147:MET:CE	2.87	0.63
1:E:225:LEU:HD13	1:E:245:LEU:CD1	2.29	0.63
1:A:136:ILE:HD12	1:A:167:ASN:HB3	1.81	0.63
1:B:4:VAL:O	1:B:50[A]:THR:HG23	1.99	0.62
1:D:221:PRO:HG3	4:D:661:HOH:O	1.99	0.62
1:C:131:LEU:C	1:C:131:LEU:HD23	2.20	0.62
1:B:138:ILE:HD13	1:B:185:LEU:HD11	1.82	0.62
1:A:20:ILE:HG22	1:A:25[B]:THR:HG22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260[A]:TYR:CE2	1:E:260[A]:TYR:HD2	2.18	0.61
1:D:204:GLU:HG2	1:D:219:LYS:NZ	2.14	0.61
1:F:25[B]:THR:CG2	1:F:27:ALA:O	2.48	0.61
1:A:224:GLU:HG2	1:A:225:LEU:CD1	2.29	0.61
1:A:133:VAL:HG22	1:A:134:SER:N	2.15	0.61
1:B:307:ILE:C	1:B:307:ILE:HD12	2.21	0.61
1:D:24:GLN:NE2	4:D:554:HOH:O	2.33	0.61
1:A:246:TRP:CZ2	1:A:249:GLY:HA2	2.36	0.60
1:B:138:ILE:HG21	1:B:185:LEU:HD11	1.83	0.60
1:E:212:TYR:O	1:E:216:MET:HG3	2.00	0.60
1:B:13[B]:ARG:NH2	1:B:306:ASP:OD1	2.29	0.60
1:A:71[B]:ARG:HD3	4:A:637:HOH:O	1.99	0.60
1:A:24:GLN:NE2	4:A:543:HOH:O	2.34	0.60
1:C:24:GLN:NE2	4:C:471:HOH:O	2.35	0.59
1:D:183:GLN:HG2	4:D:671:HOH:O	2.01	0.59
1:D:208:GLU:OE1	1:D:208:GLU:CA	2.51	0.59
1:C:147:MET:O	1:C:151:ILE:HG12	2.02	0.59
1:E:59:ASN:HB2	1:E:60:PRO:HD2	1.85	0.59
1:F:176:GLU:H	1:F:176:GLU:CD	2.06	0.59
1:A:158:ASN:N	1:A:158:ASN:HD22	2.02	0.58
1:B:176:GLU:CD	1:B:176:GLU:H	2.05	0.58
1:A:117:MET:SD	1:A:117:MET:C	2.82	0.58
1:B:117:MET:SD	1:B:147:MET:HE1	2.44	0.58
1:B:6:THR:OG1	1:B:36:GLU:HB3	2.03	0.57
1:B:63:LYS:O	1:B:67:GLU:HG3	2.04	0.57
1:B:45:LYS:NZ	4:B:692:HOH:O	2.33	0.57
1:C:191:TYR:HD1	1:C:225:LEU:HD23	1.69	0.57
1:E:185:LEU:HD23	1:E:185:LEU:N	2.19	0.57
1:B:179:LYS:O	1:B:183:GLN:HG3	2.03	0.57
1:C:50[B]:THR:HG22	1:C:51:ARG:N	2.20	0.57
1:E:185:LEU:N	1:E:185:LEU:CD2	2.67	0.57
1:A:17:GLN:CD	1:A:17:GLN:H	2.08	0.57
1:D:59:ASN:HB2	1:D:60:PRO:HD2	1.87	0.57
1:C:191:TYR:CD1	1:C:225:LEU:CD2	2.87	0.57
1:C:227:TYR:HB3	1:C:245:LEU:HD13	1.86	0.56
1:C:191:TYR:CD1	1:C:225:LEU:HD21	2.40	0.56
1:D:91[A]:LEU:HD13	1:D:102:VAL:HG22	1.87	0.56
1:B:20:ILE:CG2	1:B:25[A]:THR:HG22	2.36	0.56
1:A:199:ALA:HB1	1:A:205:ILE:HD12	1.87	0.56
1:F:131:LEU:HD23	1:F:132:HIS:N	2.20	0.56
1:F:131:LEU:C	1:F:131:LEU:CD2	2.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ASP:OD1	1:C:123:GLU:HG2	2.05	0.56
1:A:167:ASN:ND2	4:A:644:HOH:O	2.39	0.55
1:B:176:GLU:O	1:B:180:ARG:HG3	2.05	0.55
1:D:154:GLU:HA	1:D:157:ARG:NH1	2.21	0.55
1:E:91:LEU:HD23	1:E:91:LEU:C	2.26	0.55
1:E:71:ARG:NH2	4:E:574:HOH:O	2.37	0.55
1:C:225:LEU:HD12	1:C:245:LEU:CD1	2.21	0.55
1:C:225:LEU:CD1	1:C:245:LEU:HD11	2.21	0.55
1:A:225:LEU:HD23	1:A:245:LEU:HD11	1.89	0.55
1:C:212:TYR:O	1:C:216:MET:HG3	2.06	0.55
1:F:148:VAL:O	1:F:152:ILE:HG12	2.07	0.55
1:F:193:SER:HB2	1:F:227:TYR:CE2	2.42	0.54
1:E:193:SER:HB2	1:E:227:TYR:CZ	2.40	0.54
1:D:158:ASN:N	1:D:158:ASN:ND2	2.55	0.54
1:A:113:ARG:NH1	1:A:113:ARG:HB3	2.21	0.54
1:D:5:VAL:HG13	1:D:131:LEU:HD13	1.89	0.54
1:F:313:LYS:HE3	1:F:317:ASP:OD2	2.06	0.54
1:A:156[B]:LYS:HE3	1:A:160:ILE:O	2.07	0.54
1:E:186:LEU:N	1:E:187:PRO:CD	2.71	0.54
1:E:24:GLN:NE2	4:E:523:HOH:O	2.39	0.54
1:C:173:TRP:CD1	1:C:173:TRP:N	2.75	0.54
1:D:5:VAL:HG12	1:D:128:ILE:HG21	1.90	0.54
1:D:71:ARG:HH21	1:E:71:ARG:HD2	1.73	0.54
1:D:204:GLU:CG	1:D:219:LYS:NZ	2.71	0.53
1:A:64:MET:HE3	4:A:584:HOH:O	2.07	0.53
1:B:225:LEU:HD11	1:B:245:LEU:HD21	1.89	0.53
1:B:173:TRP:CD1	1:B:173:TRP:N	2.76	0.53
1:C:126:LYS:HE2	1:C:126:LYS:O	2.08	0.53
1:D:307:ILE:HD12	1:D:307:ILE:C	2.28	0.53
1:B:117:MET:SD	1:B:147:MET:HE2	2.48	0.53
1:B:91:LEU:HD23	1:B:91:LEU:C	2.29	0.53
1:E:126:LYS:HA	1:E:126:LYS:CE	2.30	0.53
1:A:30:ILE:HD12	1:E:25[A]:THR:HG23	1.90	0.52
1:F:63:LYS:NZ	4:F:551:HOH:O	2.31	0.52
1:B:138:ILE:CD1	1:B:185:LEU:HD12	2.39	0.52
1:C:185:LEU:N	1:C:185:LEU:CD2	2.72	0.52
1:C:108:HIS:HA	1:C:113:ARG:HD2	1.92	0.52
1:F:24:GLN:NE2	4:F:493:HOH:O	2.43	0.52
1:C:213:TYR:CE2	1:C:226:PHE:HB3	2.45	0.52
1:C:126:LYS:HE2	1:C:126:LYS:C	2.30	0.51
1:C:181:ALA:O	1:C:185:LEU:HD23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:GLN:HG2	1:E:49:PRO:HB2	1.92	0.51
1:A:130:VAL:CG2	1:A:281:LEU:HD21	2.40	0.51
1:B:244:HIS:CD2	1:B:253[B]:GLU:HG2	2.45	0.51
1:C:275:ALA:CB	1:C:293:ALA:HA	2.40	0.51
1:A:17:GLN:CD	1:A:17:GLN:N	2.62	0.51
1:A:307:ILE:C	1:A:307:ILE:HD12	2.31	0.51
1:F:13[A]:ARG:HG3	1:F:89:TYR:CE1	2.45	0.51
1:C:213:TYR:CE2	1:C:226:PHE:CB	2.94	0.51
1:C:237:SER:O	1:C:260[A]:TYR:HD2	1.93	0.51
1:B:139:ALA:HB2	1:B:173:TRP:CE2	2.46	0.51
1:C:226:PHE:O	1:C:245:LEU:HD12	2.10	0.51
1:D:204:GLU:HG2	1:D:219:LYS:HZ2	1.73	0.51
1:E:156:LYS:HE2	1:E:162:ILE:CG1	2.39	0.51
1:A:165:ASP:OD2	1:A:167:ASN:ND2	2.44	0.51
1:F:5:VAL:HG12	1:F:128:ILE:HG21	1.93	0.51
1:B:169:ARG:CB	1:B:172:LEU:HD12	2.29	0.51
1:A:13:ARG:NH1	1:A:306:ASP:OD1	2.44	0.50
1:B:71:ARG:HE	1:C:71:ARG:NH2	1.93	0.50
1:B:260[A]:TYR:CE2	1:E:260[A]:TYR:CD2	2.98	0.50
1:B:174:GLU:OE1	1:B:174:GLU:HA	2.11	0.50
1:E:126:LYS:HE2	1:E:127:GLY:H	1.76	0.50
1:C:133:VAL:HG22	1:C:134:SER:N	2.26	0.50
1:E:255:GLU:HG2	4:E:516:HOH:O	2.12	0.50
1:D:17:GLN:CD	1:D:17:GLN:H	2.15	0.50
1:D:17:GLN:CD	1:D:17:GLN:N	2.64	0.50
1:A:130:VAL:HG23	1:A:281:LEU:HD21	1.94	0.49
1:C:191:TYR:CD1	1:C:225:LEU:HD23	2.47	0.49
1:D:25[B]:THR:CG2	1:D:27:ALA:O	2.60	0.49
1:A:13:ARG:NH2	1:A:264:ASP:OD2	2.35	0.49
1:B:13[B]:ARG:HG2	4:B:513:HOH:O	2.12	0.49
1:F:225:LEU:HD12	1:F:225:LEU:O	2.13	0.49
1:C:130:VAL:HG22	1:C:161:LYS:HB2	1.95	0.49
1:D:139:ALA:HB2	1:D:173:TRP:CE2	2.48	0.49
1:A:108:HIS:HA	1:A:113:ARG:HD3	1.95	0.49
1:A:139:ALA:HB2	1:A:173:TRP:CE2	2.48	0.49
1:B:30:ILE:HD12	1:D:25[A]:THR:HG23	1.95	0.49
4:A:654:HOH:O	1:F:45[A]:LYS:HE3	2.12	0.48
1:A:131:LEU:HD23	1:A:132:HIS:N	2.27	0.48
1:D:91[A]:LEU:HD13	1:D:102:VAL:CG2	2.43	0.48
1:A:108:HIS:CE1	1:E:113:ARG:HH11	2.31	0.48
1:C:142:THR:O	1:C:146:GLU:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:307:ILE:HD12	1:F:307:ILE:C	2.34	0.48
1:D:6:THR:OG1	1:D:36:GLU:HB3	2.14	0.48
1:C:59:ASN:HB2	1:C:60:PRO:HD2	1.95	0.48
1:C:133:VAL:HG22	1:C:134:SER:H	1.78	0.48
1:F:133:VAL:HG22	1:F:134:SER:N	2.28	0.48
1:C:213:TYR:HE2	1:C:226:PHE:HB3	1.79	0.47
1:F:212:TYR:O	1:F:216:MET:HG3	2.14	0.47
1:F:225:LEU:HB2	1:F:246:TRP:O	2.13	0.47
1:A:260:TYR:HD2	1:C:260[A]:TYR:CZ	2.32	0.47
1:B:156:LYS:HZ2	1:B:156:LYS:HB3	1.79	0.47
1:D:197:MET:HB3	2:D:401:GOL:H2	1.96	0.47
1:E:133:VAL:HG22	1:E:134:SER:N	2.29	0.47
1:B:148:VAL:O	1:B:152:ILE:CG1	2.61	0.47
1:B:5:VAL:HG23	1:B:51:ARG:HG3	1.97	0.47
1:F:123:GLU:OE2	1:F:126:LYS:HE3	2.13	0.47
1:B:133:VAL:HG22	1:B:134:SER:N	2.29	0.47
1:B:139:ALA:HB2	1:B:173:TRP:CZ2	2.50	0.47
1:E:260[B]:TYR:CE2	1:F:260:TYR:HD2	2.33	0.47
1:B:17:GLN:N	1:B:17:GLN:CD	2.69	0.47
1:C:275:ALA:HB1	1:C:293:ALA:HA	1.95	0.46
1:A:56:VAL:O	1:A:81:GLU:HA	2.16	0.46
1:B:147:MET:O	1:B:151:ILE:HG12	2.15	0.46
1:A:173:TRP:CD1	1:A:173:TRP:N	2.84	0.46
1:D:63:LYS:NZ	1:D:67:GLU:OE2	2.32	0.46
1:A:156[B]:LYS:CE	1:A:160:ILE:O	2.63	0.46
1:D:204:GLU:CG	1:D:219:LYS:HZ2	2.28	0.46
1:F:225:LEU:HD13	1:F:245:LEU:HD11	1.96	0.46
1:C:218:ASP:O	1:C:221:PRO:HD3	2.15	0.46
1:B:154:GLU:HA	1:B:154:GLU:OE1	2.15	0.46
1:E:135:GLY:HA3	1:E:166:MET:O	2.15	0.46
1:B:193:SER:HA	1:B:227:TYR:O	2.16	0.46
1:D:143:PHE:CZ	1:D:147:MET:HE2	2.51	0.46
1:E:130:VAL:HG22	1:E:161:LYS:HB2	1.96	0.46
1:F:275:ALA:CB	1:F:293:ALA:HA	2.45	0.46
1:A:136:ILE:CD1	1:A:167:ASN:HB3	2.45	0.46
1:B:50[A]:THR:HG22	1:B:51:ARG:N	2.30	0.46
1:B:121:LEU:HD21	1:B:151:ILE:CD1	2.46	0.46
1:B:275:ALA:CB	1:B:293:ALA:HA	2.45	0.46
1:E:6:THR:HG23	1:E:52:ILE:HG13	1.98	0.46
1:A:205:ILE:CD1	1:A:216:MET:HG3	2.46	0.45
1:C:220:TYR:HB2	1:C:223:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:ARG:C	1:D:158:ASN:HD22	2.19	0.45
1:D:193:SER:HB2	1:D:227:TYR:CE2	2.51	0.45
1:A:285:ARG:HD3	1:A:288:GLU:OE1	2.16	0.45
1:F:225:LEU:HD13	1:F:245:LEU:CD1	2.47	0.45
1:A:153:ARG:O	1:A:157:ARG:HG2	2.17	0.45
1:C:199:ALA:HB2	1:C:216:MET:SD	2.57	0.45
1:C:217:HIS:O	1:C:221:PRO:HD3	2.17	0.45
1:D:5:VAL:HG13	1:D:131:LEU:CD1	2.45	0.45
1:F:182:TYR:O	1:F:186:LEU:HG	2.16	0.45
1:F:205:ILE:HD12	1:F:215:ALA:HB1	1.97	0.45
1:A:131:LEU:C	1:A:131:LEU:CD2	2.78	0.45
1:D:245:LEU:C	1:D:245:LEU:HD23	2.37	0.45
1:D:59:ASN:HB2	1:D:60:PRO:CD	2.46	0.45
1:F:22:PHE:CE2	1:F:92:GLU:HB2	2.52	0.45
1:F:59:ASN:HB2	1:F:60:PRO:CD	2.47	0.45
1:A:63:LYS:NZ	4:A:650:HOH:O	2.42	0.45
1:C:166:MET:HE2	1:C:203:PHE:HE2	1.80	0.45
1:D:133:VAL:HG22	1:D:134:SER:N	2.32	0.45
1:D:237:SER:O	1:D:260[B]:TYR:HD1	1.98	0.45
1:A:48:HIS:NE2	1:A:278:HIS:ND1	2.45	0.44
1:E:17:GLN:CD	1:E:17:GLN:H	2.20	0.44
1:E:59:ASN:HB2	1:E:60:PRO:CD	2.47	0.44
1:E:192:CYS:O	1:E:226:PHE:HA	2.17	0.44
1:B:196:GLN:HG2	1:B:212:TYR:CD1	2.51	0.44
1:F:107:GLN:HG3	4:F:418:HOH:O	2.18	0.44
1:B:121:LEU:CD2	1:B:151:ILE:CD1	2.96	0.44
1:F:6:THR:HG22	1:F:132:HIS:HB3	2.00	0.44
1:C:91:LEU:C	1:C:91:LEU:HD23	2.39	0.44
1:C:185:LEU:O	1:C:188:LEU:HB2	2.17	0.44
1:B:193:SER:HB2	1:B:227:TYR:CE2	2.53	0.44
1:E:5:VAL:HG23	1:E:51:ARG:HG3	2.00	0.43
1:F:173:TRP:N	1:F:173:TRP:CD1	2.86	0.43
1:C:185:LEU:N	1:C:185:LEU:HD22	2.34	0.43
1:E:17:GLN:CD	1:E:17:GLN:N	2.72	0.43
1:A:165:ASP:CG	1:A:167:ASN:ND2	2.72	0.43
1:B:13[B]:ARG:HH22	1:B:305:GLY:C	2.22	0.43
1:C:186:LEU:HD13	1:C:203:PHE:CE1	2.53	0.43
1:A:20:ILE:CG2	1:A:25[B]:THR:HG22	2.47	0.43
1:B:195:GLY:C	4:B:666:HOH:O	2.57	0.43
1:E:45:LYS:NZ	1:E:72:HIS:ND1	2.59	0.43
1:F:45[B]:LYS:HD2	4:F:543:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:VAL:O	1:A:153:ARG:HG2	2.18	0.42
1:C:50[B]:THR:CG2	1:C:51:ARG:N	2.82	0.42
1:D:71:ARG:HH21	1:E:71:ARG:CD	2.32	0.42
1:D:275:ALA:CB	1:D:293:ALA:HA	2.49	0.42
1:A:107:GLN:NE2	4:A:605:HOH:O	2.51	0.42
1:E:203:PHE:O	1:E:204:GLU:CB	2.65	0.42
1:C:121:LEU:HD22	1:C:151:ILE:HD12	1.97	0.42
1:C:220:TYR:N	1:C:221:PRO:CD	2.82	0.42
1:D:5:VAL:HG23	1:D:51:ARG:HG3	2.02	0.42
1:E:193:SER:HA	1:E:227:TYR:O	2.20	0.42
1:A:157:ARG:HG2	1:A:157:ARG:H	1.64	0.42
1:A:225:LEU:HG	1:A:247:THR:HB	2.02	0.42
1:B:17:GLN:CD	1:B:17:GLN:H	2.22	0.42
1:A:91:LEU:C	1:A:91:LEU:HD23	2.41	0.42
1:B:168:TYR:CZ	1:B:175:LEU:HD23	2.55	0.42
1:C:56:VAL:O	1:C:81:GLU:HA	2.20	0.42
1:E:166:MET:HG2	1:E:193:SER:O	2.20	0.42
1:F:139:ALA:HB2	1:F:173:TRP:CE2	2.55	0.42
1:A:133:VAL:CG2	1:A:134:SER:N	2.83	0.42
1:B:20:ILE:HG22	1:B:25[A]:THR:CG2	2.46	0.42
1:A:205:ILE:HD13	1:A:215:ALA:HB3	2.01	0.41
1:D:193:SER:HA	1:D:227:TYR:O	2.20	0.41
1:C:5:VAL:HG23	1:C:51:ARG:HG3	2.01	0.41
1:E:126:LYS:HE2	1:E:127:GLY:N	2.34	0.41
1:A:67[A]:GLU:OE1	1:F:71:ARG:CD	2.64	0.41
1:A:193:SER:HA	1:A:227:TYR:O	2.21	0.41
1:E:184:GLN:NE2	4:E:559:HOH:O	2.54	0.41
1:C:244:HIS:CD2	1:C:253:GLU:HG2	2.55	0.41
1:F:56:VAL:O	1:F:81:GLU:HA	2.20	0.41
1:B:154:GLU:CD	1:B:157:ARG:HE	2.24	0.41
1:B:275:ALA:HB1	1:B:293:ALA:HA	2.02	0.41
1:C:52:ILE:O	1:C:52:ILE:HG23	2.20	0.41
4:C:519:HOH:O	1:F:64:MET:HE3	2.20	0.41
1:E:186:LEU:HD23	1:E:186:LEU:HA	1.83	0.41
1:E:5:VAL:HG13	1:E:131:LEU:CD1	2.51	0.41
1:A:108:HIS:CE1	1:E:113:ARG:NH1	2.88	0.41
1:C:196:GLN:HG3	1:C:212:TYR:CD1	2.56	0.41
1:C:223:ILE:HG21	1:C:226:PHE:CZ	2.56	0.41
1:D:166:MET:HG2	1:D:193:SER:O	2.21	0.41
1:E:48:HIS:O	1:E:50:THR:HG23	2.21	0.41
1:E:173:TRP:N	1:E:173:TRP:CD1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:VAL:CG2	1:A:134:SER:H	2.32	0.41
1:B:265:ARG:HG2	4:B:515:HOH:O	2.21	0.41
1:A:205:ILE:HD11	1:A:216:MET:HG3	2.02	0.40
1:F:93[A]:SER:HB2	4:F:541:HOH:O	2.21	0.40
1:A:113:ARG:HB3	1:A:113:ARG:CZ	2.52	0.40
1:A:22:PHE:CZ	1:A:92:GLU:HB2	2.56	0.40
1:E:320:ALA:HB2	4:E:609:HOH:O	2.22	0.40
1:F:121:LEU:HA	1:F:121:LEU:HD23	1.82	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	328/351 (93%)	323 (98%)	5 (2%)	0	100	100
1	B	326/351 (93%)	320 (98%)	6 (2%)	0	100	100
1	C	324/351 (92%)	317 (98%)	7 (2%)	0	100	100
1	D	325/351 (93%)	320 (98%)	5 (2%)	0	100	100
1	E	325/351 (93%)	318 (98%)	7 (2%)	0	100	100
1	F	325/351 (93%)	321 (99%)	4 (1%)	0	100	100
All	All	1953/2106 (93%)	1919 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/292 (94%)	267 (97%)	7 (3%)	46	48
1	B	271/292 (93%)	266 (98%)	5 (2%)	59	63
1	C	268/292 (92%)	264 (98%)	4 (2%)	65	69
1	D	271/292 (93%)	267 (98%)	4 (2%)	65	69
1	E	270/292 (92%)	261 (97%)	9 (3%)	38	37
1	F	270/292 (92%)	263 (97%)	7 (3%)	46	48
All	All	1624/1752 (93%)	1588 (98%)	36 (2%)	52	55

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	ARG
1	A	117	MET
1	A	129	ARG
1	A	157	ARG
1	A	158	ASN
1	A	167	ASN
1	A	173	TRP
1	B	117	MET
1	B	173	TRP
1	B	207	SER
1	B	260[A]	TYR
1	B	260[B]	TYR
1	C	126	LYS
1	C	173	TRP
1	C	185	LEU
1	C	306	ASP
1	D	117	MET
1	D	158	ASN
1	D	173	TRP
1	D	306	ASP
1	E	98	LYS
1	E	101	SER
1	E	117	MET
1	E	126	LYS
1	E	171	LYS
1	E	173	TRP
1	E	185	LEU

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Mol	Chain	Res	Type
1	E	204	GLU
1	E	306	ASP
1	F	71	ARG
1	F	113	ARG
1	F	117	MET
1	F	173	TRP
1	F	180	ARG
1	F	185	LEU
1	F	306	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	24	GLN
1	A	107	GLN
1	A	108	HIS
1	A	158	ASN
1	A	196	GLN
1	A	244	HIS
1	B	31	HIS
1	B	158	ASN
1	B	244	HIS
1	C	24	GLN
1	C	31	HIS
1	C	196	GLN
1	C	244	HIS
1	D	24	GLN
1	D	158	ASN
1	D	183	GLN
1	D	196	GLN
1	D	244	HIS
1	E	24	GLN
1	E	158	ASN
1	E	183	GLN
1	F	24	GLN
1	F	183	GLN
1	F	244	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	GOL	A	401	-	5,5,5	0.37	0	5,5,5	0.28	0
2	GOL	E	401	-	5,5,5	0.36	0	5,5,5	0.51	0
2	GOL	D	401	-	5,5,5	0.28	0	5,5,5	0.46	0
2	GOL	B	401	-	5,5,5	0.32	0	5,5,5	0.40	0
2	GOL	B	402	-	5,5,5	0.30	0	5,5,5	0.29	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	GOL	A	401	-	-	2/4/4/4	-
2	GOL	E	401	-	-	4/4/4/4	-
2	GOL	D	401	-	-	3/4/4/4	-
2	GOL	B	401	-	-	0/4/4/4	-
2	GOL	B	402	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GOL	O1-C1-C2-C3
2	D	401	GOL	O1-C1-C2-C3
2	E	401	GOL	O1-C1-C2-O2
2	E	401	GOL	O1-C1-C2-C3
2	D	401	GOL	O1-C1-C2-O2
2	A	401	GOL	O1-C1-C2-O2
2	E	401	GOL	O2-C2-C3-O3
2	D	401	GOL	C1-C2-C3-O3
2	E	401	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	GOL	1	0
2	D	401	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, 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	320/351 (91%)	-0.16	6 (1%)	66	65	24, 47, 85, 133	0
1	B	321/351 (91%)	0.03	10 (3%)	49	48	27, 49, 85, 121	0
1	C	322/351 (91%)	0.02	8 (2%)	57	56	23, 52, 97, 139	0
1	D	322/351 (91%)	-0.06	13 (4%)	38	37	23, 43, 74, 108	0
1	E	322/351 (91%)	0.02	10 (3%)	49	48	27, 51, 87, 128	0
1	F	320/351 (91%)	-0.29	8 (2%)	57	56	25, 42, 78, 132	0
All	All	1927/2106 (91%)	-0.07	55 (2%)	51	50	23, 47, 87, 139	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	323	SER	5.2
1	E	323	SER	5.1
1	A	208	GLU	4.5
1	D	27	ALA	4.2
1	B	28	LEU	4.1
1	B	25[A]	THR	4.0
1	D	323	SER	4.0
1	B	27	ALA	4.0
1	B	30	ILE	3.7
1	D	14	LEU	3.6
1	D	28	LEU	3.5
1	D	30	ILE	3.5
1	F	17[A]	GLN	3.5
1	B	14	LEU	3.3
1	F	208	GLU	3.3
1	B	26	THR	3.1
1	D	26	THR	3.0
1	C	127	GLY	2.9
1	D	15	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	252	TRP	2.9
1	D	25[A]	THR	2.9
1	F	27	ALA	2.8
1	D	20	ILE	2.7
1	D	16	THR	2.7
1	C	119	TRP	2.7
1	E	322	LYS	2.6
1	A	27	ALA	2.6
1	A	20	ILE	2.6
1	D	32	ILE	2.5
1	F	20	ILE	2.5
1	B	15	SER	2.4
1	E	284	TRP	2.4
1	E	27	ALA	2.4
1	E	122	SER	2.4
1	B	16	THR	2.4
1	F	212	TYR	2.4
1	E	252	TRP	2.3
1	E	283	GLU	2.3
1	A	26	THR	2.3
1	C	28	LEU	2.3
1	F	26	THR	2.3
1	C	226	PHE	2.2
1	E	287	ASP	2.2
1	C	283	GLU	2.2
1	F	203	PHE	2.1
1	E	260[A]	TYR	2.1
1	D	29	ASP	2.1
1	E	30	ILE	2.1
1	D	322	LYS	2.1
1	B	29	ASP	2.1
1	C	322	LYS	2.0
1	A	246	TRP	2.0
1	B	61	ILE	2.0
1	F	28	LEU	2.0
1	A	17	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
2	GOL	D	401	6/6	0.83	0.21	39,57,65,68	0
2	GOL	E	401	6/6	0.89	0.15	55,58,66,67	0
2	GOL	A	401	6/6	0.91	0.09	41,49,54,69	0
2	GOL	B	402	6/6	0.91	0.29	50,64,68,69	0
2	GOL	B	401	6/6	0.93	0.10	46,59,69,77	0
3	CL	B	403	1/1	0.98	0.07	42,42,42,42	0
3	CL	A	402	1/1	1.00	0.09	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.