wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:58 PM GMT

PDB ID	:	1MTO
Title	:	Crystal structure of a Phosphofructokinase mutant from Bacillus stearothermophilus bound with fructose-6-phosphate
Authors	:	Riley-Lovingshimer, M.R.; Ronning, D.R.; Sacchettini, J.C.; Reinhart, G.D.
Deposited on	:	2002-09-21
Resolution	:	3.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

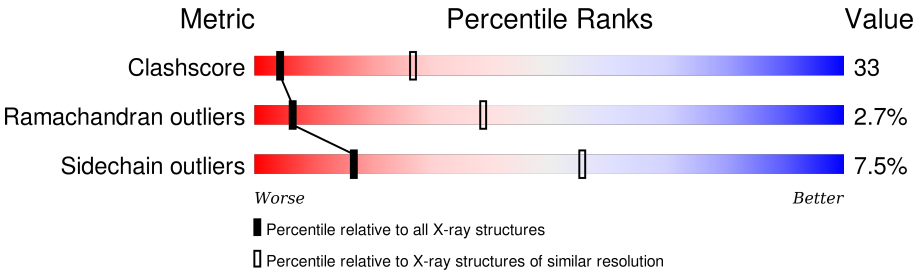
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	319	48% 45% 8%
1	B	319	50% 46% .
1	C	319	46% 50% . .
1	D	319	46% 48% 6%
1	E	319	40% 51% 8%
1	F	319	46% 50% 5%
1	G	319	41% 55% .

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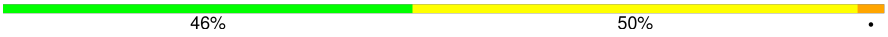
Mol	Chain	Length	Quality of chain
1	H	319	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 19328 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 6-phosphofructokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2400	1499	436	457	8			
1	B	319	Total	C	N	O	S	0	0	0
			2400	1499	436	457	8			
1	C	319	Total	C	N	O	S	0	0	0
			2400	1499	436	457	8			
1	D	319	Total	C	N	O	S	0	0	0
			2400	1499	436	457	8			
1	E	319	Total	C	N	O	S	0	0	0
			2400	1499	436	457	8			
1	F	319	Total	C	N	O	S	0	0	0
			2400	1499	436	457	8			
1	G	319	Total	C	N	O	S	0	0	0
			2400	1499	436	457	8			
1	H	319	Total	C	N	O	S	0	0	0
			2400	1499	436	457	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	TRP	TYR	ENGINEERED	UNP P00512
A	179	TYR	TRP	ENGINEERED	UNP P00512
B	164	TRP	TYR	ENGINEERED	UNP P00512
B	179	TYR	TRP	ENGINEERED	UNP P00512
C	164	TRP	TYR	ENGINEERED	UNP P00512
C	179	TYR	TRP	ENGINEERED	UNP P00512
D	164	TRP	TYR	ENGINEERED	UNP P00512
D	179	TYR	TRP	ENGINEERED	UNP P00512
E	164	TRP	TYR	ENGINEERED	UNP P00512
E	179	TYR	TRP	ENGINEERED	UNP P00512
F	164	TRP	TYR	ENGINEERED	UNP P00512
F	179	TYR	TRP	ENGINEERED	UNP P00512
G	164	TRP	TYR	ENGINEERED	UNP P00512

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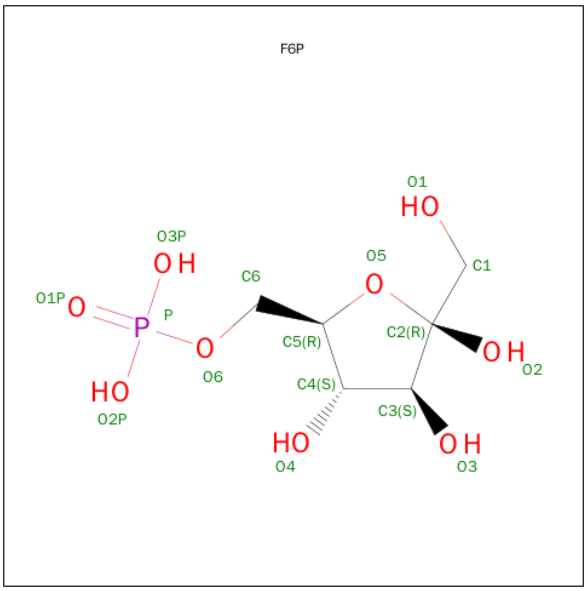
Chain	Residue	Modelled	Actual	Comment	Reference
G	179	TYR	TRP	ENGINEERED	UNP P00512
H	164	TRP	TYR	ENGINEERED	UNP P00512
H	179	TYR	TRP	ENGINEERED	UNP P00512

- Molecule 2 is SUGAR (FRUCTOSE-6-PHOSPHATE) (three-letter code: F6P) (formula: $C_6H_{13}O_9P$).



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

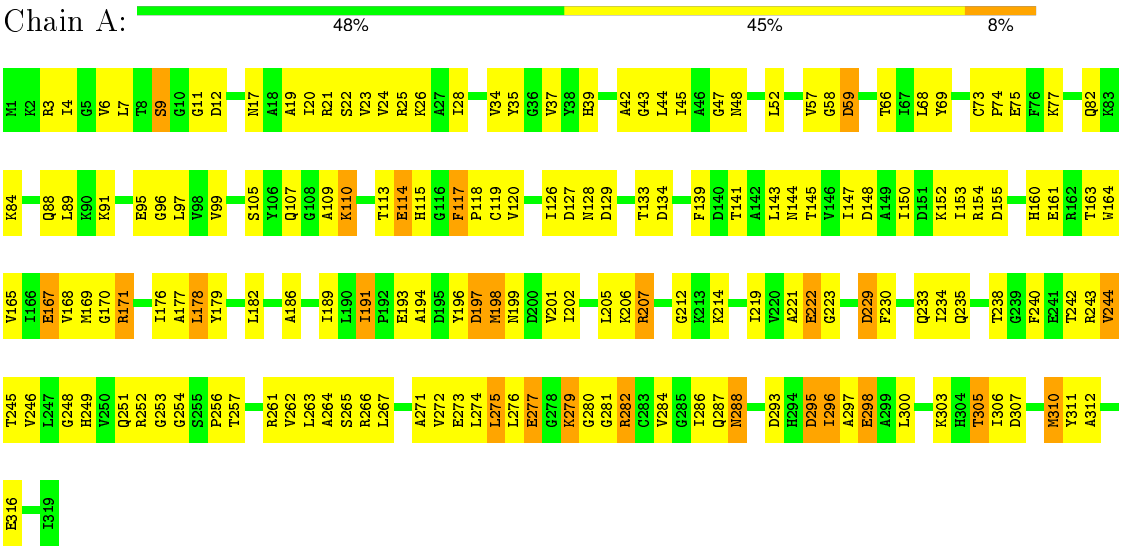
3 Residue-property plots (i)

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

Note EDS was not executed.

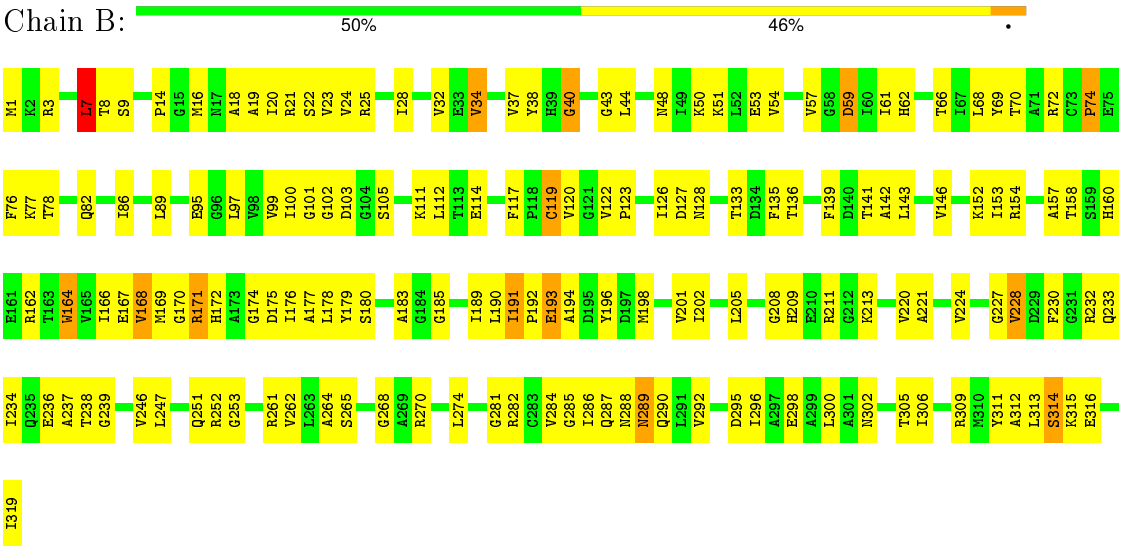
- Molecule 1: 6-phosphofructokinase

Chain A:



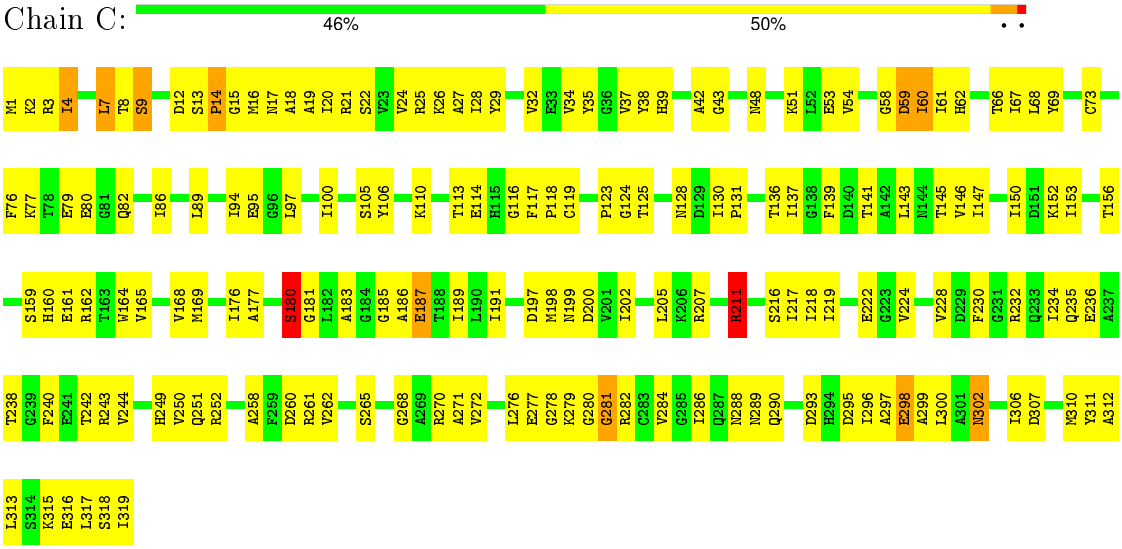
- Molecule 1: 6-phosphofructokinase

Chain B:



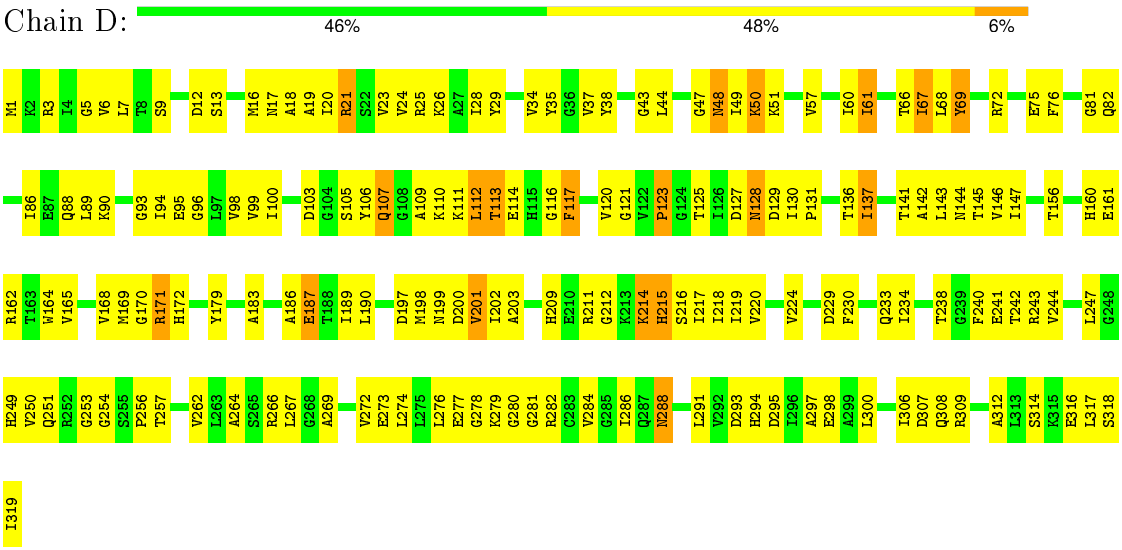
- Molecule 1: 6-phosphofructokinase

Chain C:



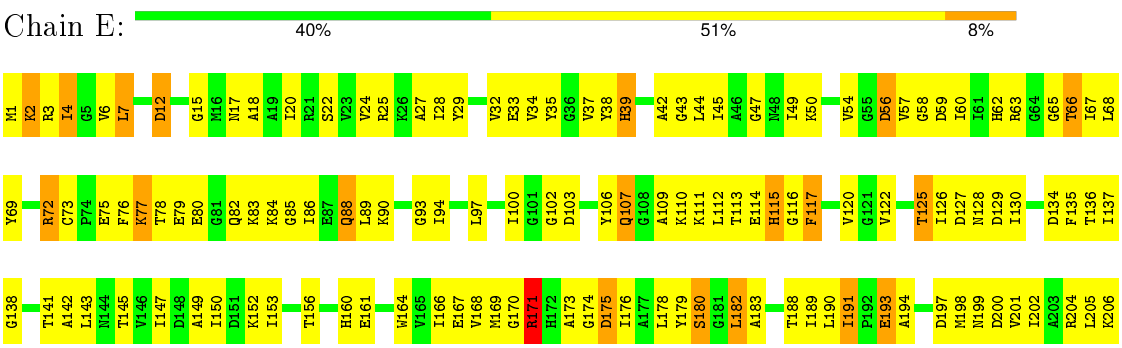
- Molecule 1: 6-phosphofructokinase

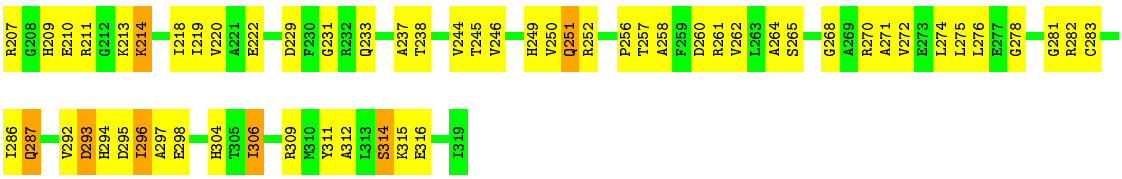
Chain D:



- Molecule 1: 6-phosphofructokinase

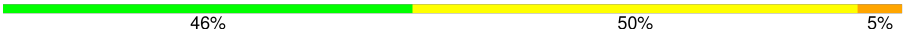
Chain E:

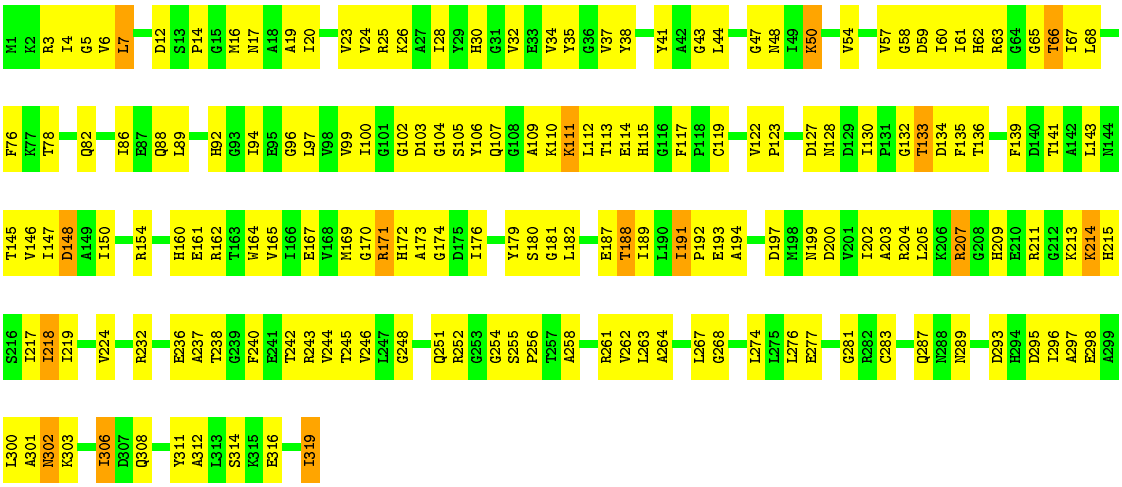




- Molecule 1: 6-phosphofructokinase

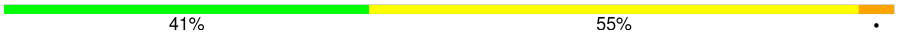
Chain F:

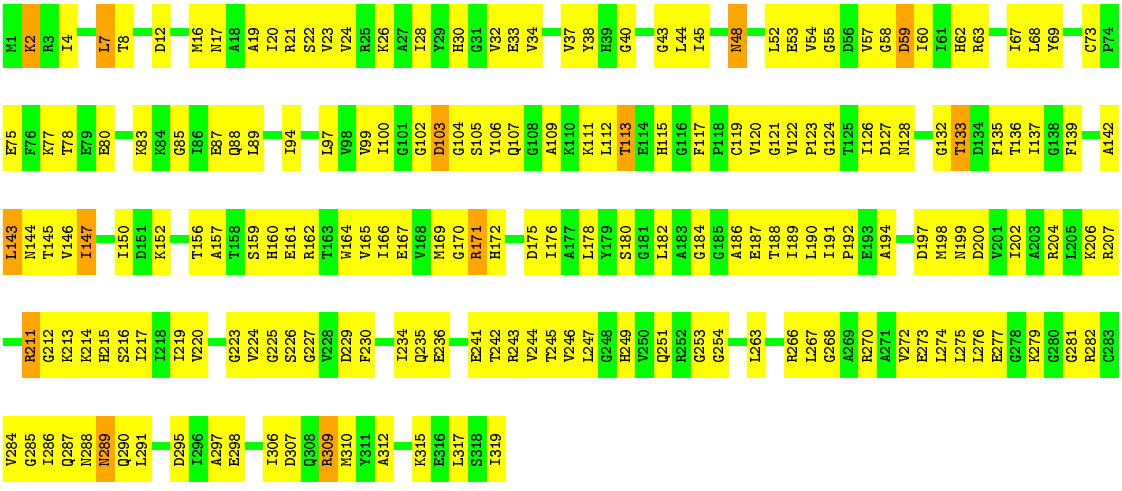




- Molecule 1: 6-phosphofructokinase

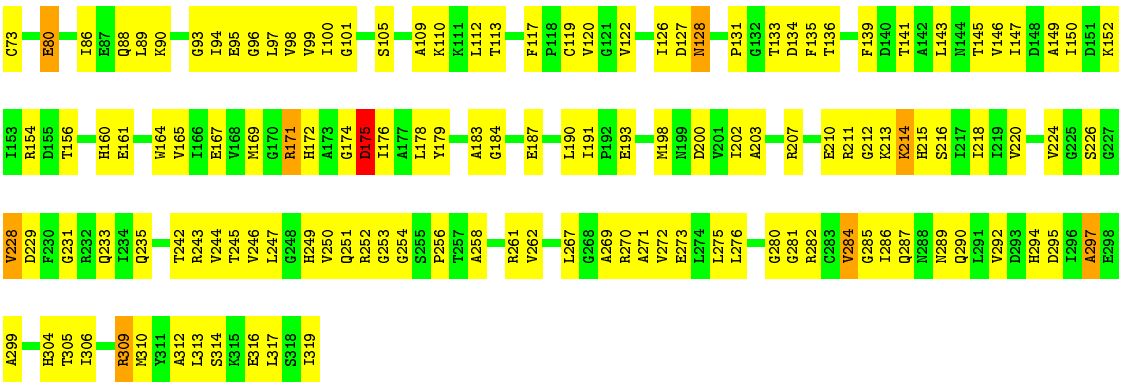
Chain G:





- Molecule 1: 6-phosphofructokinase

Chain H:


C73 E80 I86 E87 Q88 L89 K90 G93 I94 E95 G96 L97 V98 V99 I100 G101 S105 A109 K110 K111 L112 T113 F117 P118 C119 V120 G121 V122 I126 D127 N128 P131 G132 T133 D134 F135 T136 F139 D140 T141 A142 L143 N144 T145 V146 I147 D148 A149 I150 D151 K152
I153 R154 D155 T156 H160 E161 W164 V165 I166 E167 V168 M169 G170 R171 H172 A173 G174 D175 I176 A177 L178 Y179 A183 G184 E187 L190 I191 P192 E193 M198 N199 D200 V201 I202 A203 R207 E210 R211 G212 K213 K214 H215 S216 I217 I218 I219 V220 V224 G225 S226 G227
V228 D229 F230 G231 R232 Q233 I234 Q235 T242 R243 V244 T245 V246 L247 G248 H249 V250 Q251 R252 G253 G254 S255 P256 T257 A258 R261 V262 L267 G268 A269 R270 A271 V272 E273 L274 L275 L276 G280 G281 R282 C283 V284 G285 I286 Q287 N288 N289 Q290 L291 V292 D293 H294 D295 I296 A297 E298
A299 H304 T305 I306 R309 M310 Y311 A312 I313 S314 K315 E316 I317 S318 I319

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	110.68Å 106.87Å 119.59Å 90.00° 113.98° 90.00°	Depositor
Resolution (Å)	29.84 – 3.20	Depositor
% Data completeness (in resolution range)	86.7 (29.84-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.180 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	19328	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F6P

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	0.35	0/2436	0.60	0/3282
1	B	0.38	0/2436	0.63	1/3282 (0.0%)
1	C	0.35	0/2436	0.60	0/3282
1	D	0.38	0/2436	0.62	0/3282
1	E	0.37	0/2436	0.62	0/3282
1	F	0.37	0/2436	0.61	0/3282
1	G	0.39	0/2436	0.62	0/3282
1	H	0.37	0/2436	0.62	0/3282
All	All	0.37	0/19488	0.62	1/26256 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	7	LEU	CA-CB-CG	5.28	127.44	115.30

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	2400	0	2417	172	0
1	B	2400	0	2417	152	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2400	0	2417	151	0
1	D	2400	0	2417	170	0
1	E	2400	0	2417	184	0
1	F	2400	0	2417	180	0
1	G	2400	0	2417	180	0
1	H	2400	0	2417	169	0
2	A	16	0	11	1	0
2	B	16	0	11	0	0
2	C	16	0	11	1	0
2	D	16	0	11	0	0
2	E	16	0	11	0	0
2	F	16	0	11	2	0
2	G	16	0	11	1	0
2	H	16	0	11	3	0
All	All	19328	0	19424	1274	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 33.

The worst 5 of 1274 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:A:282:ARG:HH12	1:A:293:ASP:HB3	1.04	1.11
1:H:171:ARG:HG3	1:H:172:HIS:H	1.19	1.06
1:F:14:PRO:HG2	1:F:141:THR:HG21	1.38	1.03
1:A:24:VAL:HG21	1:A:57:VAL:HG11	1.45	0.98
1:D:123:PRO:HB2	1:D:136:THR:HG22	1.45	0.96

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	317/319 (99%)	275 (87%)	34 (11%)	8 (2%)	7 41
1	B	317/319 (99%)	263 (83%)	47 (15%)	7 (2%)	8 45
1	C	317/319 (99%)	254 (80%)	52 (16%)	11 (4%)	4 31
1	D	317/319 (99%)	268 (84%)	37 (12%)	12 (4%)	4 28
1	E	317/319 (99%)	270 (85%)	35 (11%)	12 (4%)	4 28
1	F	317/319 (99%)	281 (89%)	34 (11%)	2 (1%)	30 75
1	G	317/319 (99%)	263 (83%)	46 (14%)	8 (2%)	7 41
1	H	317/319 (99%)	261 (82%)	48 (15%)	8 (2%)	7 41
All	All	2536/2552 (99%)	2135 (84%)	333 (13%)	68 (3%)	6 39

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	193	GLU
1	C	279	LYS
1	G	211	ARG
1	H	171	ARG
1	H	213	LYS

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	247/247 (100%)	221 (90%)	26 (10%)	8 35
1	B	247/247 (100%)	231 (94%)	16 (6%)	21 61
1	C	247/247 (100%)	227 (92%)	20 (8%)	15 51
1	D	247/247 (100%)	229 (93%)	18 (7%)	17 57
1	E	247/247 (100%)	225 (91%)	22 (9%)	12 44
1	F	247/247 (100%)	230 (93%)	17 (7%)	19 59
1	G	247/247 (100%)	237 (96%)	10 (4%)	38 77
1	H	247/247 (100%)	228 (92%)	19 (8%)	16 54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1976/1976 (100%)	1828 (92%)	148 (8%)	17 55

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	67	ILE
1	E	4	ILE
1	H	110	LYS
1	D	113	THR
1	D	215	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	288	ASN
1	E	107	GLN
1	H	62	HIS
1	D	294	HIS
1	E	39	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

8 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	F6P	A	1002	-	15,16,16	1.04	0	16,25,25	0.83	0
2	F6P	B	1001	-	15,16,16	1.06	0	16,25,25	0.89	0
2	F6P	C	1004	-	15,16,16	1.01	0	16,25,25	0.90	0
2	F6P	D	1003	-	15,16,16	1.07	1 (6%)	16,25,25	0.81	0
2	F6P	E	1006	-	15,16,16	1.10	1 (6%)	16,25,25	0.89	0
2	F6P	F	1005	-	15,16,16	1.07	1 (6%)	16,25,25	0.97	0
2	F6P	G	1008	-	15,16,16	1.02	1 (6%)	16,25,25	0.89	0
2	F6P	H	1007	-	15,16,16	0.95	0	16,25,25	0.94	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	F6P	A	1002	-	-	0/9/28/28	0/1/1/1
2	F6P	B	1001	-	-	0/9/28/28	0/1/1/1
2	F6P	C	1004	-	-	0/9/28/28	0/1/1/1
2	F6P	D	1003	-	-	0/9/28/28	0/1/1/1
2	F6P	E	1006	-	-	0/9/28/28	0/1/1/1
2	F6P	F	1005	-	-	0/9/28/28	0/1/1/1
2	F6P	G	1008	-	-	0/9/28/28	0/1/1/1
2	F6P	H	1007	-	-	0/9/28/28	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1003	F6P	O5-C2	-2.63	1.39	1.43
2	G	1008	F6P	O5-C2	-2.44	1.39	1.43
2	F	1005	F6P	O5-C2	-2.36	1.39	1.43
2	E	1006	F6P	C1-C2	2.30	1.56	1.52

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 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	F6P	1	0
2	C	1004	F6P	1	0
2	F	1005	F6P	2	0
2	G	1008	F6P	1	0
2	H	1007	F6P	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.