



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:15 pm GMT

PDB ID : 3OOJ  
Title : C1A mutant of E. coli GlmS in complex with glucose-6P and glutamate  
Authors : Mouilleron, S.; Golinelli-Pimpaneau, B.  
Deposited on : 2010-08-31  
Resolution : 2.50 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](mailto: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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28986

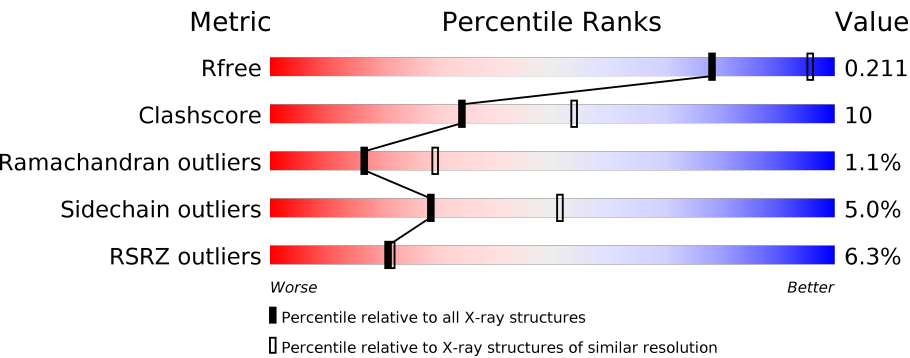
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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  $\geq 3$ , 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	608	<div><div>3%</div><div><div></div><div>84%</div><div>15%</div><div>.</div></div></div>
1	B	608	<div><div>5%</div><div><div></div><div>77%</div><div>20%</div><div>.</div></div></div>
1	C	608	<div><div>4%</div><div><div></div><div>78%</div><div>19%</div><div>..</div></div></div>
1	D	608	<div><div>4%</div><div><div></div><div>76%</div><div>21%</div><div>..</div></div></div>
1	E	608	<div><div>4%</div><div><div></div><div>77%</div><div>19%</div><div>..</div></div></div>
1	F	608	<div><div>16%</div><div><div></div><div>69%</div><div>25%</div><div>..</div></div></div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	G	608	
1	H	608	

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
2	GLU	F	701	-	-	X	-
4	GOL	C	609	-	-	-	X
4	GOL	F	609	-	-	-	X
4	GOL	G	609	-	-	-	X
5	G6Q	A	610	-	-	-	X
5	G6Q	B	610	-	-	-	X
5	G6Q	C	611	-	-	-	X
5	G6Q	D	611	-	-	-	X
5	G6Q	E	610	-	-	-	X
5	G6Q	F	610	-	-	-	X
5	G6Q	G	610	-	-	-	X
5	G6Q	H	610	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 39092 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.

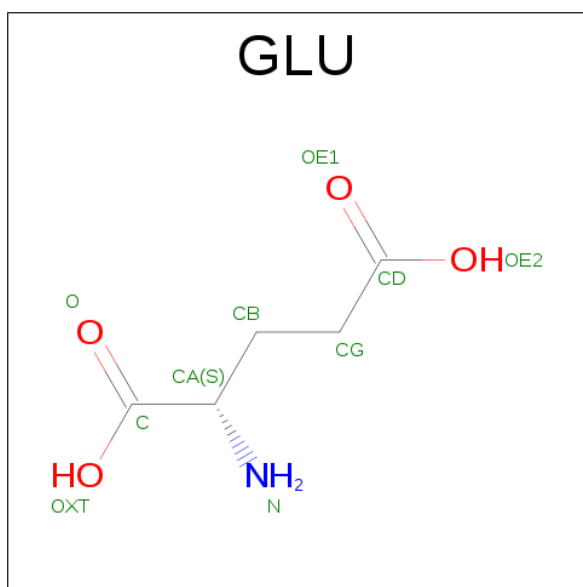
- Molecule 1 is a protein called Glucosamine/fructose-6-phosphate aminotransferase, isomerizing.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	608	Total	C	N	O	S	0	5	0
			4718	2966	838	898	16			
1	B	608	Total	C	N	O	S	0	2	0
			4697	2953	834	894	16			
1	C	601	Total	C	N	O	S	0	2	0
			4631	2915	819	881	16			
1	D	602	Total	C	N	O	S	0	3	0
			4634	2915	821	882	16			
1	E	602	Total	C	N	O	S	0	2	0
			4647	2925	826	880	16			
1	F	594	Total	C	N	O	S	0	0	0
			4583	2887	811	869	16			
1	G	605	Total	C	N	O	S	0	1	0
			4653	2929	823	885	16			
1	H	608	Total	C	N	O	S	0	2	0
			4692	2954	828	894	16			

There are 8 discrepancies between the modelled and reference sequences:

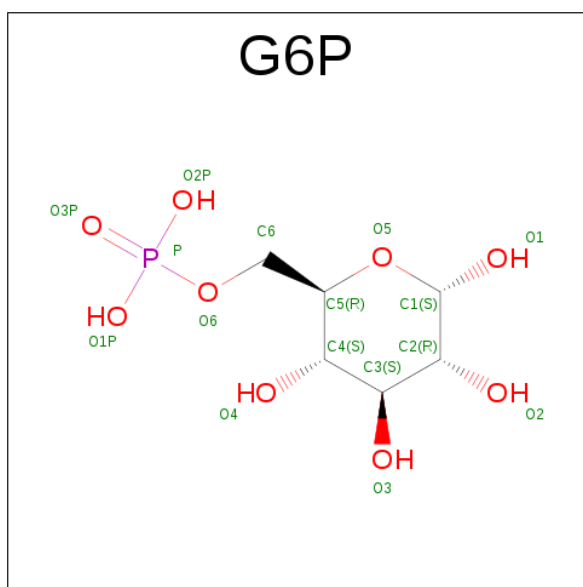
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	CYS	ENGINEERED MUTATION	UNP C9QXA7
B	1	ALA	CYS	ENGINEERED MUTATION	UNP C9QXA7
C	1	ALA	CYS	ENGINEERED MUTATION	UNP C9QXA7
D	1	ALA	CYS	ENGINEERED MUTATION	UNP C9QXA7
E	1	ALA	CYS	ENGINEERED MUTATION	UNP C9QXA7
F	1	ALA	CYS	ENGINEERED MUTATION	UNP C9QXA7
G	1	ALA	CYS	ENGINEERED MUTATION	UNP C9QXA7
H	1	ALA	CYS	ENGINEERED MUTATION	UNP C9QXA7

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	F	1	Total	C	N	O	0	0
			10	5	1	4		
2	G	1	Total	C	N	O	0	0
			10	5	1	4		
2	H	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is SUGAR (ALPHA-D-GLUCOSE-6-PHOSPHATE) (three-letter code: G6P) (formula: C<sub>6</sub>H<sub>13</sub>O<sub>9</sub>P).



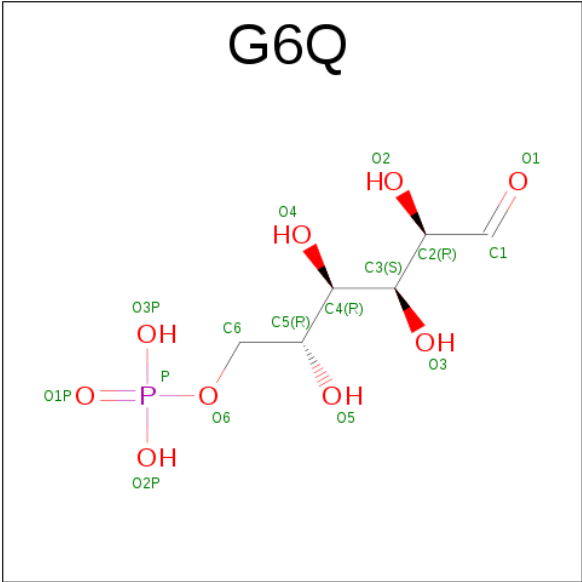
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		
3	C	1	Total	C	O	P	0	0
			16	6	9	1		
3	D	1	Total	C	O	P	0	0
			16	6	9	1		
3	E	1	Total	C	O	P	0	0
			16	6	9	1		
3	F	1	Total	C	O	P	0	0
			16	6	9	1		
3	G	1	Total	C	O	P	0	0
			16	6	9	1		
3	H	1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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SUGAR (GLUCOSE-6-PHOSPHATE) (three-letter code: G6Q) (formula:  $C_6H_{13}O_9P$ ).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	231	Total	O	0	0
			231	231		
6	B	192	Total	O	0	0
			192	192		
6	C	196	Total	O	0	0
			196	196		
6	D	244	Total	O	0	0
			244	244		

Continued on next page...



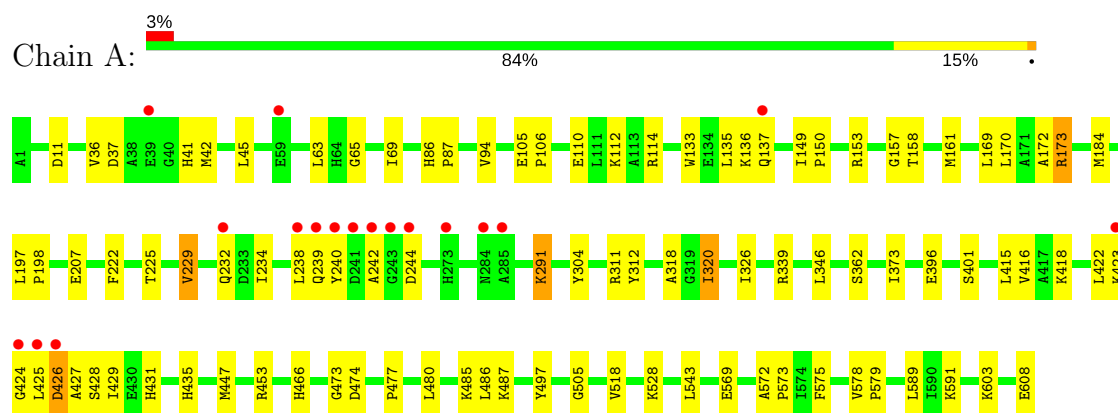
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	123	Total 123	O 123	0	0
6	F	123	Total 123	O 123	0	0
6	G	175	Total 175	O 175	0	0
6	H	169	Total 169	O 169	0	0

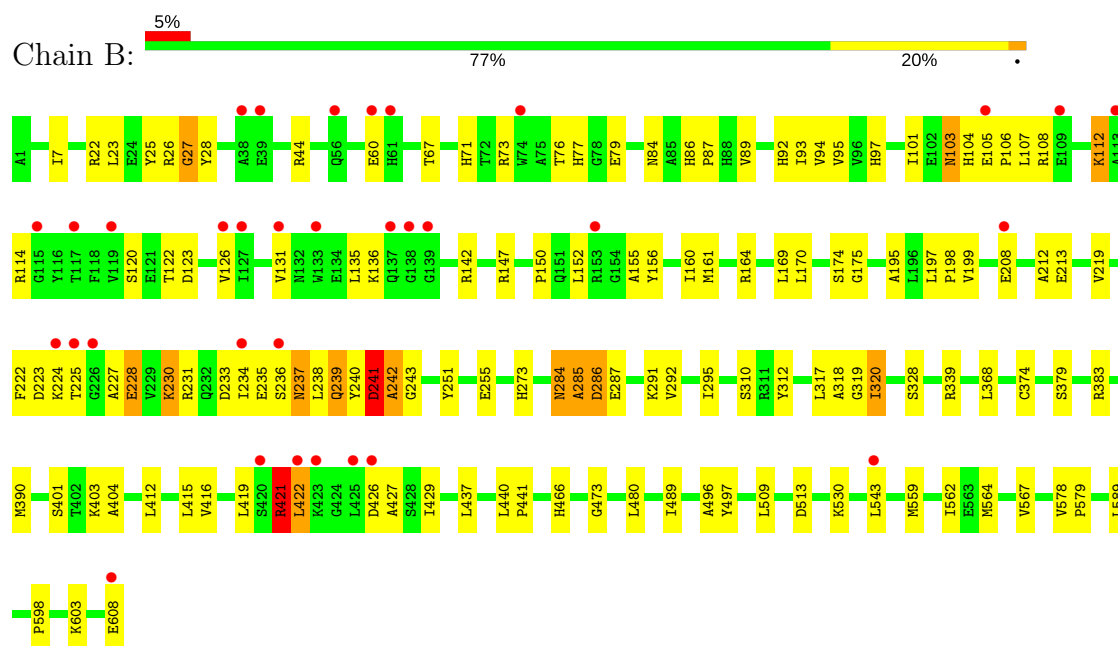
### 3 Residue-property plots

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

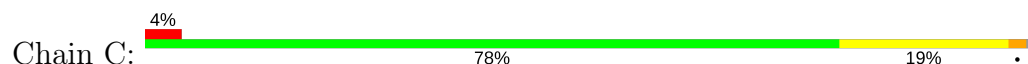
- Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing

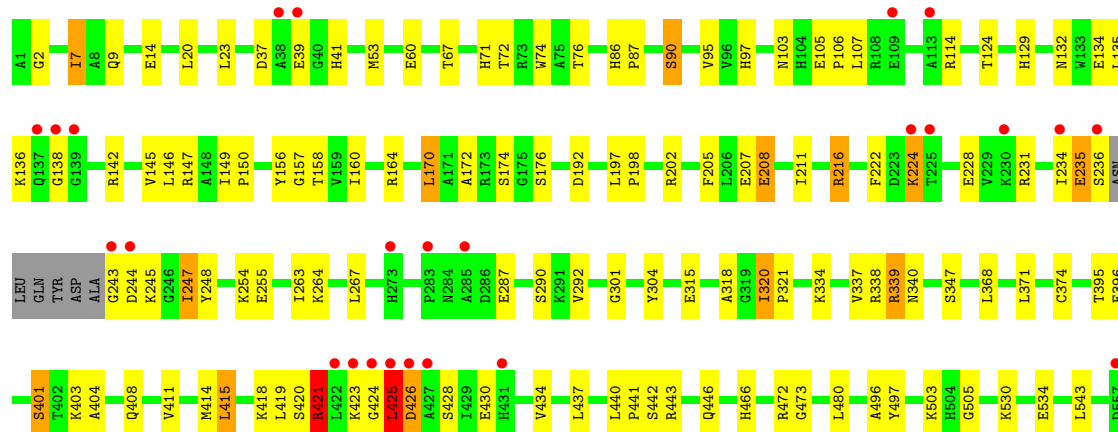


- Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing



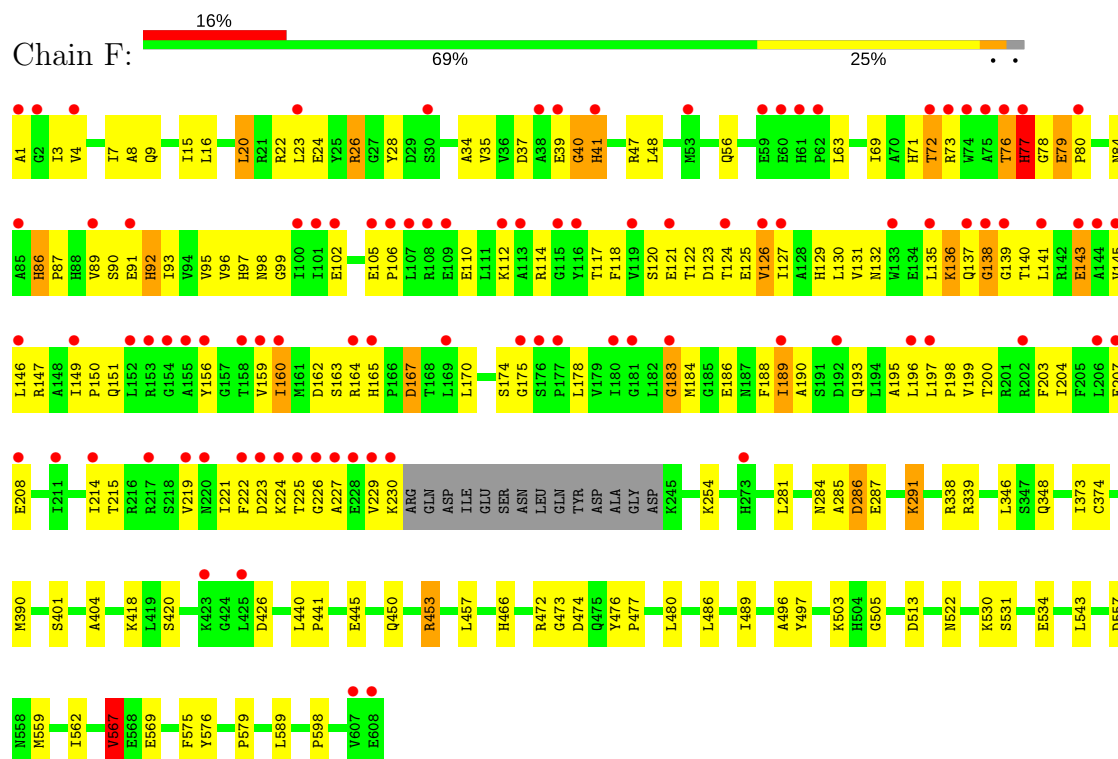
- Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing



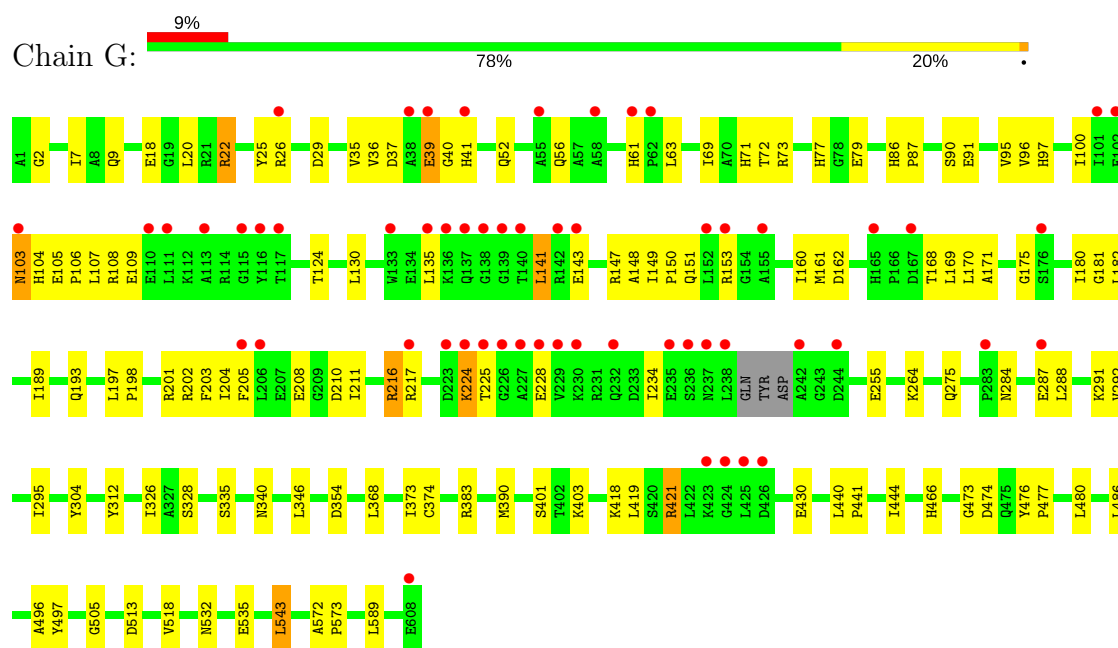




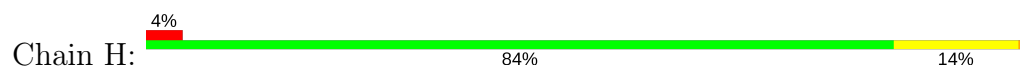
- Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing

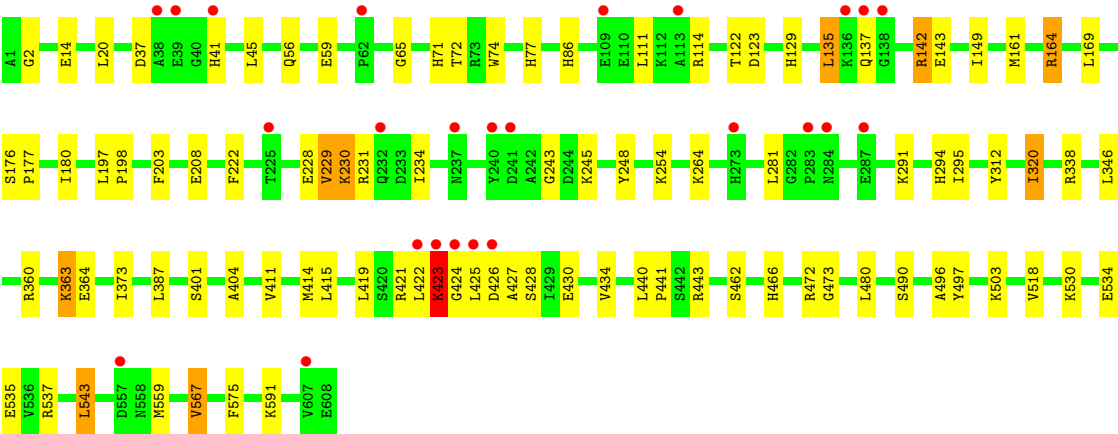


- Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing



- Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	247.60Å 247.60Å 630.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.50 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.99-2.50) 98.5 (19.99-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.178 , 0.220 0.163 , 0.211	Depositor DCC
$R_{free}$ test set	12636 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 58.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.000 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.000 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	39092	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, G6P, G6Q

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	0.44	0/4805	0.61	1/6510 (0.0%)
1	B	0.41	0/4783	0.59	1/6478 (0.0%)
1	C	0.43	0/4714	0.59	0/6384
1	D	0.42	0/4712	0.59	1/6380 (0.0%)
1	E	0.41	0/4734	0.58	2/6409 (0.0%)
1	F	0.40	0/4662	0.57	1/6312 (0.0%)
1	G	0.41	0/4736	0.56	0/6414
1	H	0.42	0/4780	0.57	0/6475
All	All	0.42	0/37926	0.58	6/51362 (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	E	0	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	567	VAL	CB-CA-C	-6.09	99.84	111.40
1	E	157	GLY	N-CA-C	-5.81	98.57	113.10
1	B	421	ARG	N-CA-C	5.72	126.44	111.00
1	D	518	VAL	CB-CA-C	-5.54	100.87	111.40
1	A	320	ILE	CB-CA-C	-5.25	101.09	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	425	LEU	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	4718	0	4704	61	0
1	B	4697	0	4698	106	0
1	C	4631	0	4638	99	0
1	D	4634	0	4640	89	0
1	E	4647	0	4666	81	0
1	F	4583	0	4617	149	0
1	G	4653	0	4669	72	0
1	H	4692	0	4703	68	0
2	A	10	0	5	0	0
2	B	10	0	5	2	0
2	C	10	0	5	2	0
2	D	10	0	5	1	0
2	E	10	0	5	2	0
2	F	10	0	5	4	0
2	G	10	0	5	0	0
2	H	10	0	5	1	0
3	A	16	0	11	0	0
3	B	16	0	11	0	0
3	C	16	0	11	0	0
3	D	16	0	11	0	0
3	E	16	0	11	0	0
3	F	16	0	11	0	0
3	G	16	0	11	0	0
3	H	16	0	11	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
4	E	6	0	8	1	0
4	F	6	0	8	0	0
4	G	6	0	8	0	0
4	H	6	0	8	0	0
5	A	16	0	11	3	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	16	0	11	0	0
5	C	16	0	11	3	0
5	D	16	0	11	1	0
5	E	16	0	11	1	0
5	F	16	0	11	4	0
5	G	16	0	11	2	0
5	H	16	0	11	0	0
6	A	231	0	0	2	0
6	B	192	0	0	3	0
6	C	196	0	0	3	0
6	D	244	0	0	5	0
6	E	123	0	0	1	0
6	F	123	0	0	2	0
6	G	175	0	0	2	0
6	H	169	0	0	2	0
All	All	39092	0	37615	720	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.

The worst 5 of 720 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ALA:HB3	1:B:243:GLY:HA3	1.32	1.10
1:H:230:LYS:HE3	1:H:231:ARG:H	1.11	1.10
1:B:236:SER:HA	1:B:237:ASN:HB2	1.14	1.07
1:B:236:SER:HA	1:B:237:ASN:CB	1.92	0.97
1:F:569:GLU:HG3	5:F:610:G6Q:O2	1.66	0.94

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	611/608 (100%)	586 (96%)	21 (3%)	4 (1%)	25	43
1	B	608/608 (100%)	577 (95%)	21 (4%)	10 (2%)	11	19
1	C	599/608 (98%)	572 (96%)	20 (3%)	7 (1%)	15	27
1	D	601/608 (99%)	576 (96%)	18 (3%)	7 (1%)	15	27
1	E	600/608 (99%)	566 (94%)	28 (5%)	6 (1%)	18	32
1	F	590/608 (97%)	531 (90%)	47 (8%)	12 (2%)	9	14
1	G	602/608 (99%)	576 (96%)	22 (4%)	4 (1%)	25	43
1	H	608/608 (100%)	587 (96%)	19 (3%)	2 (0%)	44	66
All	All	4819/4864 (99%)	4571 (95%)	196 (4%)	52 (1%)	17	29

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	237	ASN
1	B	241	ASP
1	B	242	ALA
1	B	284	ASN
1	B	285	ALA

### 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	498/499 (100%)	472 (95%)	26 (5%)	27	49
1	B	497/499 (100%)	474 (95%)	23 (5%)	31	55
1	C	490/499 (98%)	469 (96%)	21 (4%)	33	58
1	D	488/499 (98%)	464 (95%)	24 (5%)	29	52
1	E	492/499 (99%)	466 (95%)	26 (5%)	26	48
1	F	487/499 (98%)	453 (93%)	34 (7%)	18	33
1	G	493/499 (99%)	471 (96%)	22 (4%)	32	56
1	H	497/499 (100%)	474 (95%)	23 (5%)	31	55

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3942/3992 (99%)	3743 (95%)	199 (5%)	28 51

5 of 199 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	497	TYR
1	E	415	LEU
1	H	164	ARG
1	D	567	VAL
1	E	202	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	446	GLN
1	F	86	HIS
1	G	71	HIS
1	D	52	GLN
1	G	52	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

32 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
4	GOL	A	609	-	5,5,5	0.34	0	5,5,5	0.49	0
5	G6Q	A	610	-	15,15,15	1.43	3 (20%)	20,21,21	1.05	1 (5%)
3	G6P	A	611	-	16,16,16	1.41	2 (12%)	24,24,24	0.97	1 (4%)
2	GLU	A	701	-	1,9,9	0.35	0	1,11,11	0.39	0
4	GOL	B	609	-	5,5,5	0.30	0	5,5,5	0.40	0
5	G6Q	B	610	-	15,15,15	1.40	3 (20%)	20,21,21	1.17	2 (10%)
3	G6P	B	612	-	16,16,16	1.41	2 (12%)	24,24,24	0.92	1 (4%)
2	GLU	B	701	-	1,9,9	0.15	0	1,11,11	0.14	0
4	GOL	C	609	-	5,5,5	0.32	0	5,5,5	0.59	0
3	G6P	C	610	-	16,16,16	1.43	2 (12%)	24,24,24	1.06	2 (8%)
5	G6Q	C	611	-	15,15,15	1.35	3 (20%)	20,21,21	1.22	2 (10%)
2	GLU	C	701	-	1,9,9	0.44	0	1,11,11	0.19	0
3	G6P	D	609	-	16,16,16	1.44	3 (18%)	24,24,24	1.12	1 (4%)
4	GOL	D	610	-	5,5,5	0.29	0	5,5,5	0.41	0
5	G6Q	D	611	-	15,15,15	1.56	4 (26%)	20,21,21	1.24	3 (15%)
2	GLU	D	701	-	1,9,9	0.07	0	1,11,11	0.29	0
4	GOL	E	609	-	5,5,5	0.33	0	5,5,5	0.76	0
5	G6Q	E	610	-	15,15,15	1.37	4 (26%)	20,21,21	1.18	1 (5%)
3	G6P	E	616	-	16,16,16	1.49	2 (12%)	24,24,24	1.71	5 (20%)
2	GLU	E	701	-	1,9,9	0.02	0	1,11,11	0.58	0
4	GOL	F	609	-	5,5,5	0.27	0	5,5,5	0.50	0
5	G6Q	F	610	-	15,15,15	1.25	2 (13%)	20,21,21	1.36	4 (20%)
3	G6P	F	615	-	16,16,16	1.44	2 (12%)	24,24,24	0.93	0
2	GLU	F	701	-	1,9,9	0.34	0	1,11,11	0.07	0
4	GOL	G	609	-	5,5,5	0.33	0	5,5,5	0.52	0
5	G6Q	G	610	-	15,15,15	1.39	4 (26%)	20,21,21	1.08	2 (10%)
3	G6P	G	613	-	16,16,16	1.46	2 (12%)	24,24,24	1.27	3 (12%)
2	GLU	G	701	-	1,9,9	0.18	0	1,11,11	0.55	0
4	GOL	H	609	-	5,5,5	0.47	0	5,5,5	0.41	0
5	G6Q	H	610	-	15,15,15	1.36	2 (13%)	20,21,21	1.23	1 (5%)
3	G6P	H	614	-	16,16,16	1.43	2 (12%)	24,24,24	1.14	3 (12%)
2	GLU	H	701	-	1,9,9	0.23	0	1,11,11	0.21	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
4	GOL	A	609	-	-	0/4/4/4	0/0/0/0
5	G6Q	A	610	-	-	0/18/20/20	0/0/0/0
3	G6P	A	611	-	-	0/6/26/26	0/1/1/1
2	GLU	A	701	-	-	0/3/9/9	0/0/0/0
4	GOL	B	609	-	-	0/4/4/4	0/0/0/0
5	G6Q	B	610	-	-	0/18/20/20	0/0/0/0
3	G6P	B	612	-	-	0/6/26/26	0/1/1/1
2	GLU	B	701	-	-	0/3/9/9	0/0/0/0
4	GOL	C	609	-	-	0/4/4/4	0/0/0/0
3	G6P	C	610	-	-	0/6/26/26	0/1/1/1
5	G6Q	C	611	-	-	0/18/20/20	0/0/0/0
2	GLU	C	701	-	-	0/3/9/9	0/0/0/0
3	G6P	D	609	-	-	0/6/26/26	0/1/1/1
4	GOL	D	610	-	-	0/4/4/4	0/0/0/0
5	G6Q	D	611	-	-	0/18/20/20	0/0/0/0
2	GLU	D	701	-	-	0/3/9/9	0/0/0/0
4	GOL	E	609	-	-	0/4/4/4	0/0/0/0
5	G6Q	E	610	-	-	0/18/20/20	0/0/0/0
3	G6P	E	616	-	-	0/6/26/26	0/1/1/1
2	GLU	E	701	-	-	0/3/9/9	0/0/0/0
4	GOL	F	609	-	-	0/4/4/4	0/0/0/0
5	G6Q	F	610	-	-	0/18/20/20	0/0/0/0
3	G6P	F	615	-	-	0/6/26/26	0/1/1/1
2	GLU	F	701	-	-	0/3/9/9	0/0/0/0
4	GOL	G	609	-	-	0/4/4/4	0/0/0/0
5	G6Q	G	610	-	-	0/18/20/20	0/0/0/0
3	G6P	G	613	-	-	0/6/26/26	0/1/1/1
2	GLU	G	701	-	-	0/3/9/9	0/0/0/0
4	GOL	H	609	-	-	0/4/4/4	0/0/0/0
5	G6Q	H	610	-	-	0/18/20/20	0/0/0/0
3	G6P	H	614	-	-	0/6/26/26	0/1/1/1
2	GLU	H	701	-	-	0/3/9/9	0/0/0/0

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	610	G6Q	O2-C2	-2.93	1.37	1.43
5	D	611	G6Q	O2-C2	-2.82	1.37	1.43
5	G	610	G6Q	O2-C2	-2.74	1.38	1.43
5	B	610	G6Q	O2-C2	-2.70	1.38	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	610	G6Q	O2-C2	-2.66	1.38	1.43

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	609	G6P	C6-C5-C4	-2.70	106.25	112.00
5	D	611	G6Q	C5-C4-C3	-2.61	108.25	112.46
5	F	610	G6Q	O2-C2-C1	-2.51	104.34	110.30
3	A	611	G6P	C6-C5-C4	-2.48	106.72	112.00
5	C	611	G6Q	C5-C4-C3	-2.45	108.51	112.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	610	G6Q	3	0
2	B	701	GLU	2	0
5	C	611	G6Q	3	0
2	C	701	GLU	2	0
5	D	611	G6Q	1	0
2	D	701	GLU	1	0
4	E	609	GOL	1	0
5	E	610	G6Q	1	0
2	E	701	GLU	2	0
5	F	610	G6Q	4	0
2	F	701	GLU	4	0
5	G	610	G6Q	2	0
2	H	701	GLU	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	608/608 (100%)	-0.41	18 (2%)	51	53	20, 37, 72, 168	1 (0%)
1	B	608/608 (100%)	-0.15	33 (5%)	26	27	23, 43, 106, 131	1 (0%)
1	C	601/608 (98%)	-0.27	22 (3%)	42	44	18, 39, 96, 137	1 (0%)
1	D	602/608 (99%)	-0.16	27 (4%)	34	36	17, 37, 115, 142	0
1	E	602/608 (99%)	-0.23	25 (4%)	37	39	23, 47, 90, 152	2 (0%)
1	F	594/608 (97%)	0.36	95 (15%)	2	2	24, 47, 129, 158	0
1	G	605/608 (99%)	0.06	57 (9%)	9	9	20, 42, 131, 170	1 (0%)
1	H	608/608 (100%)	-0.34	25 (4%)	38	40	24, 44, 80, 135	2 (0%)
All	All	4828/4864 (99%)	-0.14	302 (6%)	21	21	17, 43, 109, 170	8 (0%)

The worst 5 of 302 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	LEU	10.2
1	G	138	GLY	9.6
1	B	138	GLY	9.1
1	G	238	LEU	8.5
1	A	239	GLN	8.5

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	G6Q	B	610	16/16	0.87	0.31	7.89	60,86,96,100	0
5	G6Q	C	611	16/16	0.88	0.26	6.23	57,77,89,94	0
5	G6Q	F	610	16/16	0.76	0.37	6.05	63,91,104,108	0
5	G6Q	A	610	16/16	0.91	0.24	5.18	56,70,83,88	0
5	G6Q	G	610	16/16	0.86	0.26	4.71	59,90,102,107	0
5	G6Q	H	610	16/16	0.89	0.28	4.02	76,91,103,105	0
5	G6Q	E	610	16/16	0.86	0.30	3.98	95,104,115,118	0
4	GOL	C	609	6/6	0.87	0.27	3.62	56,60,64,66	0
4	GOL	F	609	6/6	0.89	0.21	3.07	55,56,57,59	0
5	G6Q	D	611	16/16	0.92	0.20	3.06	63,71,78,82	0
4	GOL	G	609	6/6	0.90	0.19	2.27	56,58,59,64	0
4	GOL	B	609	6/6	0.90	0.18	1.81	51,54,54,56	0
4	GOL	D	610	6/6	0.95	0.15	1.29	56,56,57,57	0
4	GOL	A	609	6/6	0.90	0.22	1.14	59,62,65,68	0
4	GOL	E	609	6/6	0.94	0.15	1.11	47,51,53,57	0
2	GLU	E	701	10/10	0.95	0.13	1.07	34,42,44,44	0
3	G6P	E	616	16/16	0.98	0.13	0.72	31,37,43,44	0
4	GOL	H	609	6/6	0.96	0.17	0.67	47,53,55,58	0
2	GLU	B	701	10/10	0.91	0.20	0.63	74,83,85,88	0
2	GLU	A	701	10/10	0.98	0.12	0.61	30,35,36,38	0
3	G6P	D	609	16/16	0.99	0.12	0.28	23,27,29,29	0
2	GLU	C	701	10/10	0.95	0.13	0.27	36,46,61,62	0
3	G6P	H	614	16/16	0.99	0.12	0.10	22,29,34,36	0
3	G6P	B	612	16/16	0.99	0.11	-0.02	24,28,34,39	0
2	GLU	D	701	10/10	0.93	0.17	-0.13	64,66,67,67	0
3	G6P	A	611	16/16	0.99	0.11	-0.13	22,26,31,32	0
2	GLU	H	701	10/10	0.97	0.10	-0.23	39,43,48,49	0
3	G6P	F	615	16/16	0.99	0.11	-0.27	29,32,38,39	0
3	G6P	C	610	16/16	0.98	0.11	-0.29	20,25,27,31	0
2	GLU	G	701	10/10	0.91	0.15	-0.36	68,78,81,82	0
3	G6P	G	613	16/16	0.99	0.10	-0.55	24,28,34,34	0
2	GLU	F	701	10/10	0.86	0.20	-0.78	73,75,80,82	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.