



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 09:06 am BST

PDB ID : 6R4F  
Title : Crystal structure of human GFAT-1 in complex with Glucose-6-Phosphate  
Authors : Ruegenberg, S.; Horn, M.; Pichlo, C.; Allmeroth, K.; Baumann, U.; Denzel, M.S.  
Deposited on : 2019-03-22  
Resolution : 2.50 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](mailto: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 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 : 2.11  
buster-report : 1.1.7 (2018)  
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) : 2.11

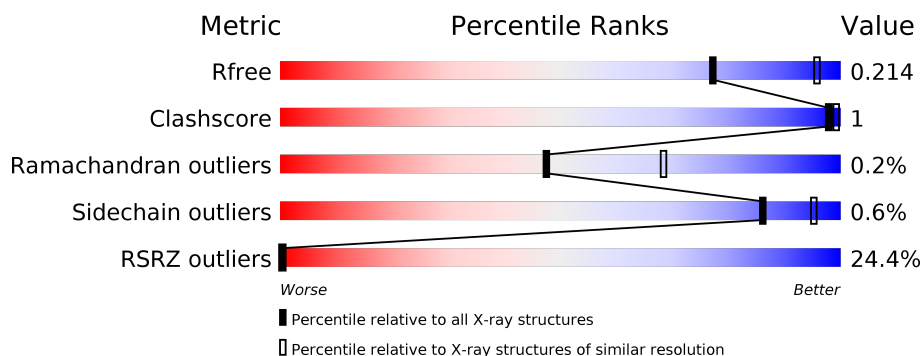
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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	687	<div> <div>11%</div> <div>91%</div> <div>6%</div> </div>
1	B	687	<div> <div>35%</div> <div>92%</div> <div>5%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20577 atoms, of which 10238 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.

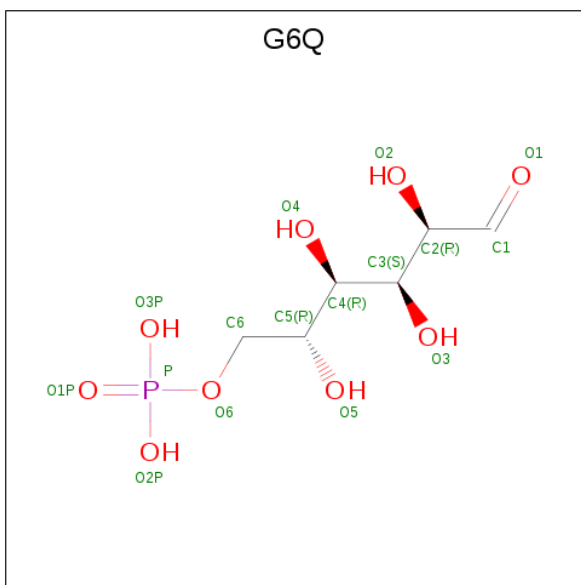
- Molecule 1 is a protein called Glutamine--fructose-6-phosphate aminotransferase [isomerizing] 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	647	Total	C	H	N	O	S	0	0	0
			10171	3222	5070	887	960	32			
1	B	650	Total	C	H	N	O	S	0	0	0
			10277	3242	5142	893	968	32			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	299A	HIS	-	insertion	UNP Q06210
A	299B	HIS	-	insertion	UNP Q06210
A	299C	HIS	-	insertion	UNP Q06210
A	299D	HIS	-	insertion	UNP Q06210
A	299E	HIS	-	insertion	UNP Q06210
A	299F	HIS	-	insertion	UNP Q06210
B	299A	HIS	-	insertion	UNP Q06210
B	299B	HIS	-	insertion	UNP Q06210
B	299C	HIS	-	insertion	UNP Q06210
B	299D	HIS	-	insertion	UNP Q06210
B	299E	HIS	-	insertion	UNP Q06210
B	299F	HIS	-	insertion	UNP Q06210

- Molecule 2 is GLUCOSE-6-PHOSPHATE (three-letter code: G6Q) (formula: C<sub>6</sub>H<sub>13</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			29	6	13	9	1		
2	B	1	Total	C	H	O	P	0	0
			29	6	13	9	1		

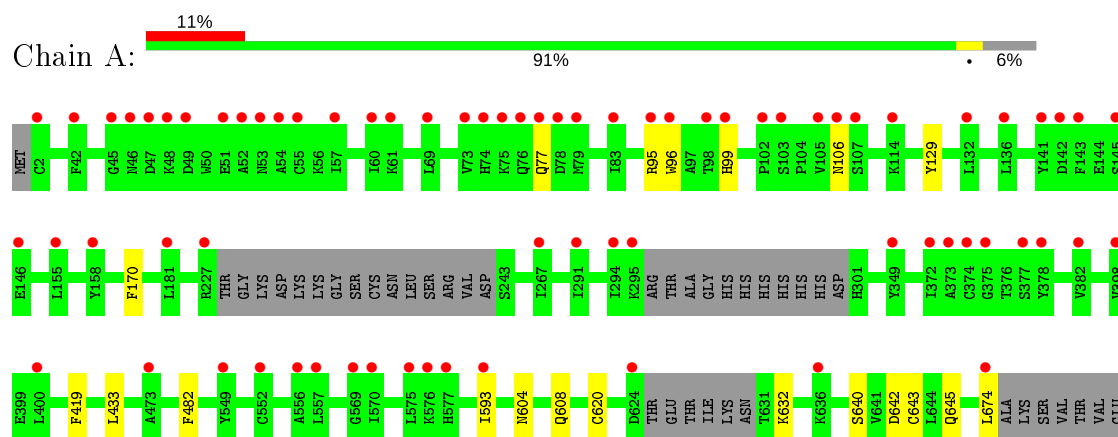
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	24	Total	O	0	0
			24	24		

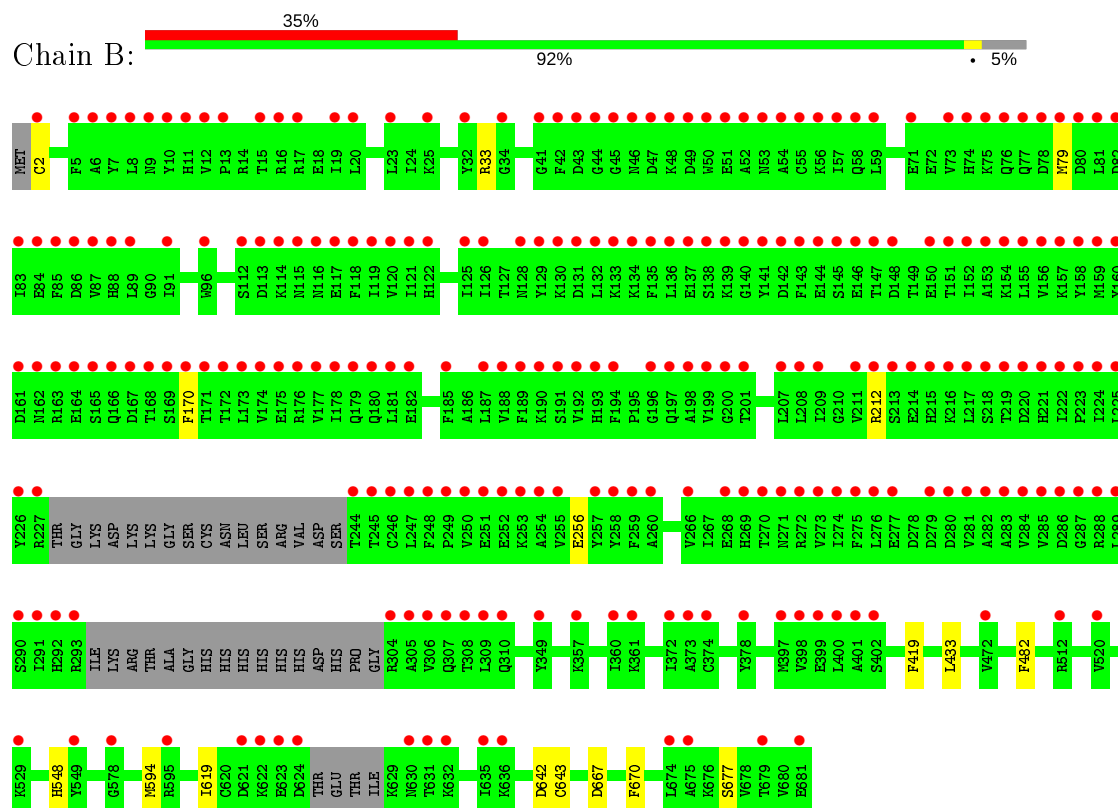
### 3 Residue-property plots

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: Glutamine--fructose-6-phosphate aminotransferase [isomerizing] 1



- Molecule 1: Glutamine--fructose-6-phosphate aminotransferase [isomerizing] 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.02Å 153.02Å 167.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.81 – 2.50 48.81 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.81-2.50) 96.6 (48.81-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 2.51Å)	Xtriage
Refinement program	PHENIX (dev_2499: ???)	Depositor
R, $R_{free}$	0.194 , 0.214 0.194 , 0.214	Depositor DCC
$R_{free}$ test set	1937 reflections (2.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.1	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 63.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	20577	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: 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	0.26	0/5189	0.44	0/7005
1	B	0.25	0/5222	0.43	0/7048
All	All	0.25	0/10411	0.43	0/14053

There are no bond length outliers.

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	5101	5070	5092	8	0
1	B	5135	5142	5140	7	0
2	A	16	13	11	0	0
2	B	16	13	11	0	0
3	A	47	0	0	0	0
3	B	24	0	0	0	0
All	All	10339	10238	10254	15	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 1.

All (15) 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:640:SER:N	1:A:645:GLN:OE1	2.35	0.58
1:A:96:TRP:CH2	1:A:674:LEU:HD13	2.39	0.58
1:B:2:CYS:N	1:B:33:ARG:O	2.36	0.58
1:A:96:TRP:CZ2	1:A:674:LEU:HD13	2.40	0.57
1:A:95:ARG:NH2	1:A:106:ASN:O	2.36	0.57
1:A:604:ASN:OD1	1:A:608:GLN:NE2	2.43	0.51
1:A:642:ASP:OD2	1:A:643:CYS:N	2.43	0.51
1:B:548:HIS:NE2	1:B:594:MET:HG3	2.26	0.50
1:B:667:ASP:OD2	1:B:670:PHE:N	2.45	0.48
1:A:419:PHE:CZ	1:A:433:LEU:HA	2.53	0.43
1:B:419:PHE:CZ	1:B:433:LEU:HA	2.53	0.43
1:B:212:ARG:NH2	1:B:256:GLU:OE1	2.48	0.42
1:A:593:ILE:O	1:A:620:CYS:HA	2.21	0.41
1:B:594:MET:HE2	1:B:619:ILE:O	2.21	0.41
1:B:642:ASP:OD1	1:B:643:CYS:N	2.54	0.41

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	639/687 (93%)	620 (97%)	17 (3%)	2 (0%)	41 61
1	B	642/687 (93%)	606 (94%)	35 (6%)	1 (0%)	47 68
All	All	1281/1374 (93%)	1226 (96%)	52 (4%)	3 (0%)	47 68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	632	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	677	SER

### 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	559/601 (93%)	555 (99%)	4 (1%)	84	94
1	B	565/601 (94%)	562 (100%)	3 (0%)	88	96
All	All	1124/1202 (94%)	1117 (99%)	7 (1%)	86	95

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	HIS
1	A	129	TYR
1	A	170	PHE
1	A	482	PHE
1	B	79	MET
1	B	170	PHE
1	B	482	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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	G6Q	A	701	-	14,15,15	0.56	0	20,21,21	0.75	1 (5%)
2	G6Q	B	701	-	14,15,15	0.68	1 (7%)	20,21,21	0.76	1 (5%)

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	G6Q	A	701	-	-	6/18/20/20	-
2	G6Q	B	701	-	-	4/18/20/20	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	G6Q	C3-C2	2.45	1.57	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	G6Q	O3-C3-C2	2.12	113.06	109.17
2	A	701	G6Q	O3-C3-C2	2.02	112.86	109.17

There are no chirality outliers.

All (10) torsion outliers are listed below:

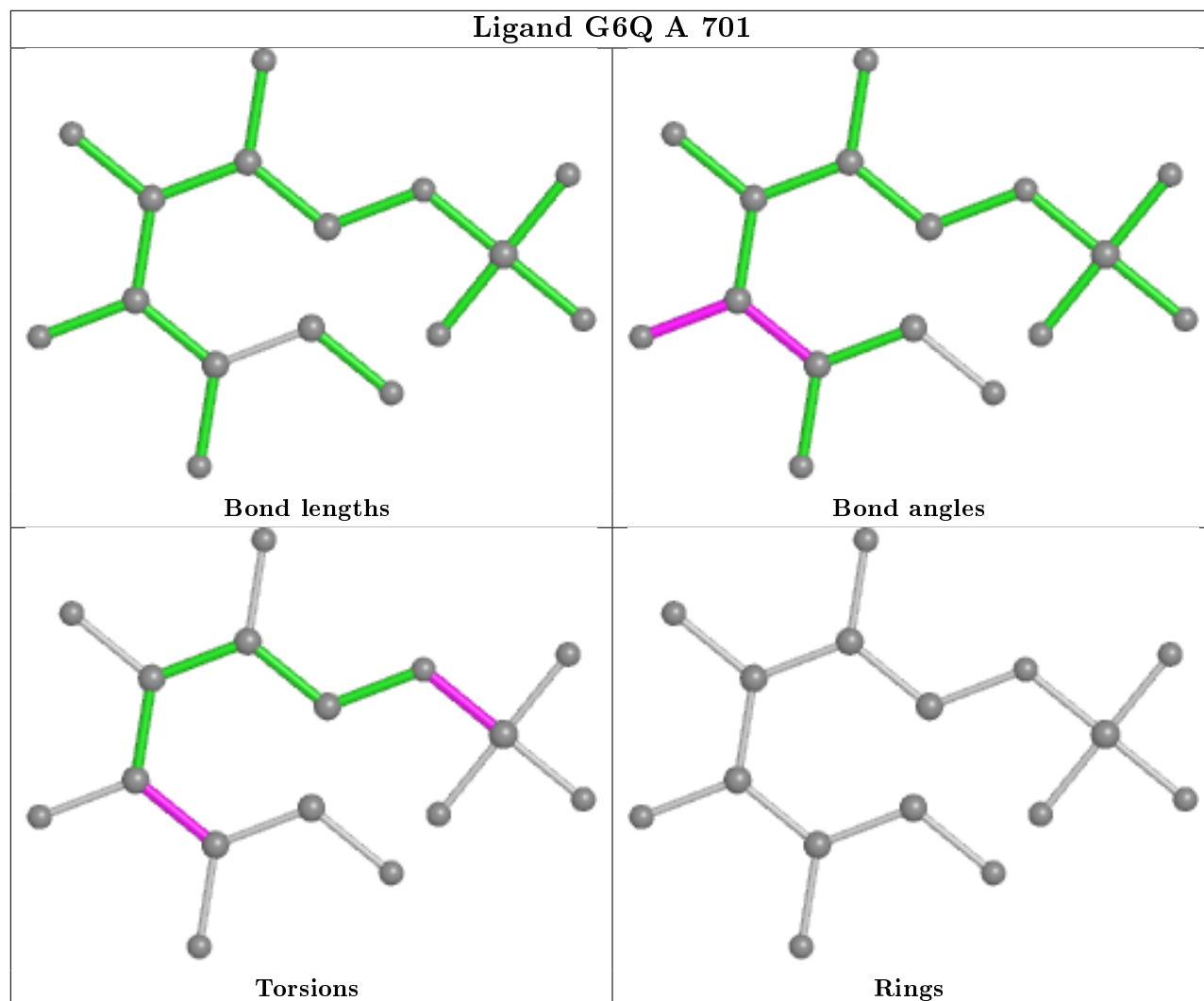
Mol	Chain	Res	Type	Atoms
2	A	701	G6Q	C1-C2-C3-C4
2	A	701	G6Q	C1-C2-C3-O3
2	A	701	G6Q	O2-C2-C3-C4
2	A	701	G6Q	O2-C2-C3-O3
2	B	701	G6Q	C1-C2-C3-C4
2	B	701	G6Q	C1-C2-C3-O3
2	B	701	G6Q	O2-C2-C3-C4
2	B	701	G6Q	O2-C2-C3-O3
2	A	701	G6Q	C6-O6-P-O1P
2	A	701	G6Q	C6-O6-P-O2P

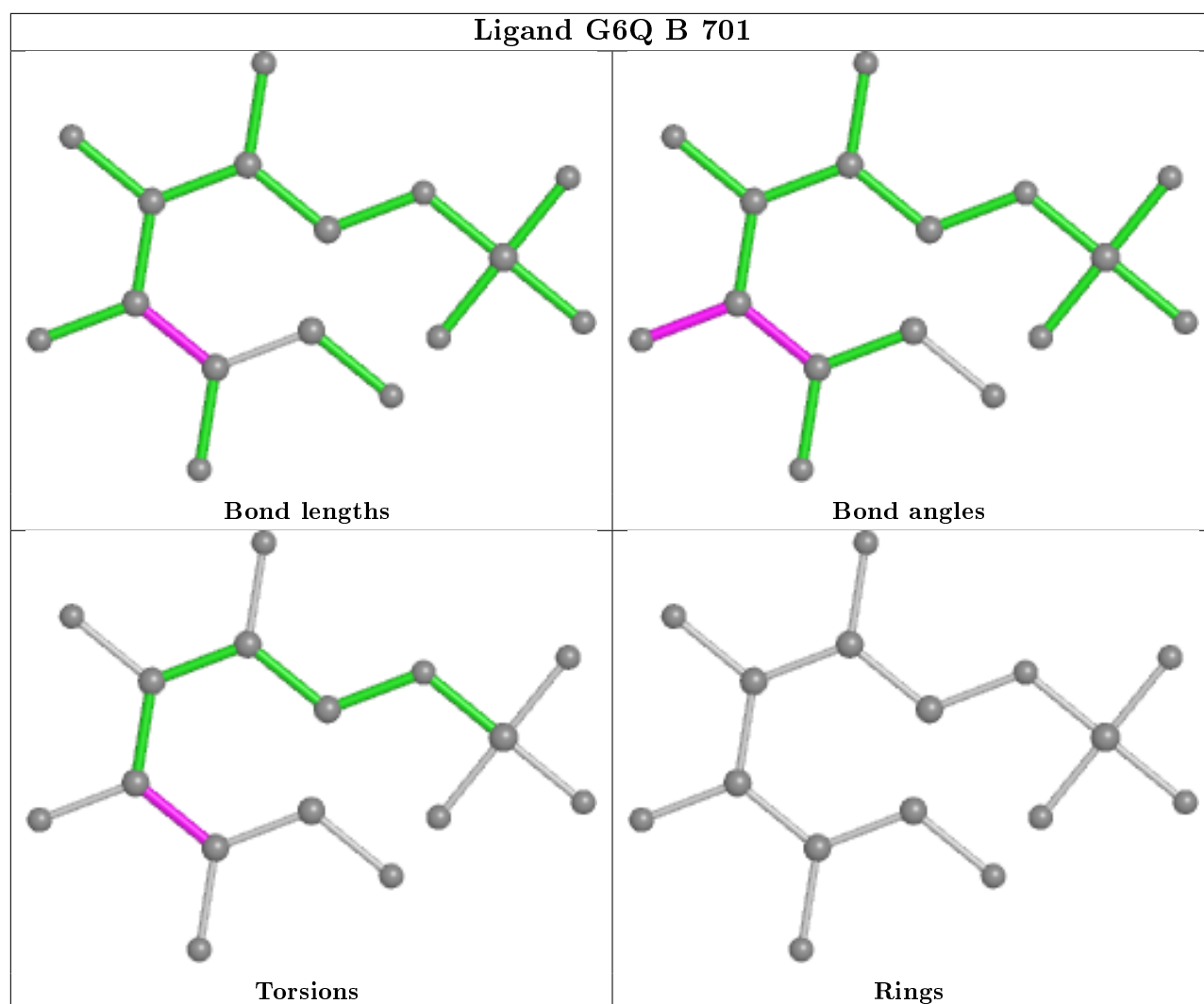
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand G6Q A 701





## 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<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	647/687 (94%)	0.83	73 (11%) 5 4	46, 68, 138, 207	0
1	B	650/687 (94%)	2.57	243 (37%) 0 0	50, 98, 233, 329	0
All	All	1297/1374 (94%)	1.70	316 (24%) 0 0	46, 78, 217, 329	0

All (316) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	LEU	21.5
1	B	257	TYR	21.3
1	B	198	ALA	18.4
1	B	170	PHE	13.8
1	B	224	ILE	13.8
1	B	79	MET	13.6
1	B	155	LEU	13.6
1	B	53	ASN	13.5
1	B	199	VAL	13.5
1	B	225	LEU	13.1
1	B	306	VAL	13.0
1	B	50	TRP	12.8
1	B	246	CYS	12.4
1	B	77	GLN	11.8
1	B	222	ILE	10.9
1	B	274	ILE	10.7
1	B	211	VAL	10.7
1	B	76	GLN	10.4
1	B	223	PRO	9.9
1	B	173	LEU	9.9
1	B	249	PRO	9.9
1	B	189	PHE	9.8
1	B	46	ASN	9.8
1	B	73	VAL	9.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	209	ILE	9.4
1	B	158	TYR	9.4
1	B	217	LEU	9.3
1	B	305	ALA	9.2
1	B	255	VAL	9.2
1	B	118	PHE	9.0
1	B	220	ASP	8.9
1	B	81	LEU	8.9
1	B	167	ASP	8.9
1	B	169	SER	8.9
1	B	152	ILE	8.8
1	B	245	THR	8.6
1	B	304	ARG	8.6
1	B	143	PHE	8.5
1	B	215	HIS	8.4
1	B	85	PHE	8.3
1	B	219	THR	8.3
1	B	272	ARG	8.2
1	B	248	PHE	8.2
1	B	15	THR	8.2
1	B	55	CYS	8.2
1	B	282	ALA	8.1
1	B	213	SER	8.1
1	B	221	HIS	8.0
1	B	197	GLN	8.0
1	B	154	LYS	8.0
1	B	54	ALA	8.0
1	B	165	SER	8.0
1	B	292	HIS	7.9
1	B	78	ASP	7.9
1	B	45	GLY	7.9
1	B	250	VAL	7.9
1	B	176	ARG	7.9
1	B	160	TYR	7.8
1	B	58	GLN	7.8
1	B	7	TYR	7.8
1	B	52	ALA	7.7
1	B	80	ASP	7.7
1	B	51	GLU	7.7
1	B	135	PHE	7.5
1	B	218	SER	7.4
1	B	216	LYS	7.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	41	GLY	7.4
1	B	174	VAL	7.4
1	A	99	HIS	7.4
1	B	10	TYR	7.3
1	B	141	TYR	7.3
1	B	75	LYS	7.3
1	B	156	VAL	7.2
1	B	44	GLY	7.1
1	B	168	THR	7.1
1	B	251	GLU	7.1
1	B	281	VAL	6.9
1	B	289	LEU	6.9
1	B	137	GLU	6.9
1	B	166	GLN	6.9
1	B	283	ALA	6.8
1	B	142	ASP	6.8
1	B	117	GLU	6.8
1	B	49	ASP	6.7
1	B	181	LEU	6.7
1	B	259	PHE	6.7
1	B	48	LYS	6.6
1	B	153	ALA	6.4
1	B	16	ARG	6.4
1	B	287	GLY	6.3
1	B	136	LEU	6.3
1	B	308	THR	6.2
1	B	309	LEU	6.2
1	B	258	TYR	6.2
1	B	19	ILE	6.2
1	B	284	VAL	6.1
1	B	307	GLN	6.1
1	B	244	THR	6.0
1	B	192	VAL	6.0
1	B	159	MET	6.0
1	B	177	VAL	5.9
1	A	77	GLN	5.9
1	B	291	ILE	5.9
1	B	273	VAL	5.8
1	B	83	ILE	5.8
1	B	151	THR	5.8
1	B	622	LYS	5.7
1	B	275	PHE	5.7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	74	HIS	5.7
1	B	47	ASP	5.7
1	B	172	THR	5.7
1	B	227	ARG	5.6
1	B	163	ARG	5.6
1	B	290	SER	5.6
1	B	285	VAL	5.5
1	B	162	ASN	5.5
1	B	631	THR	5.5
1	B	200	GLY	5.5
1	B	129	TYR	5.5
1	B	226	TYR	5.5
1	B	132	LEU	5.5
1	B	134	LYS	5.4
1	B	130	LYS	5.4
1	B	116	ASN	5.4
1	B	288	ARG	5.4
1	B	157	LYS	5.3
1	B	8	LEU	5.3
1	A	54	ALA	5.3
1	B	293	ARG	5.3
1	B	190	LYS	5.2
1	B	164	GLU	5.1
1	B	42	PHE	5.1
1	B	20	LEU	5.1
1	B	147	THR	5.1
1	B	254	ALA	5.1
1	A	48	LYS	5.0
1	A	79	MET	4.9
1	B	131	ASP	4.9
1	B	270	THR	4.8
1	B	133	LYS	4.8
1	B	681	GLU	4.8
1	B	214	GLU	4.6
1	B	89	LEU	4.6
1	A	105	VAL	4.6
1	B	23	LEU	4.6
1	B	269	HIS	4.6
1	B	56	LYS	4.6
1	B	57	ILE	4.6
1	B	253	LYS	4.4
1	B	194	PHE	4.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	102	PRO	4.4
1	B	12	VAL	4.4
1	B	201	THR	4.3
1	B	150	GLU	4.3
1	B	43	ASP	4.2
1	B	138	SER	4.2
1	B	180	GLN	4.2
1	A	143	PHE	4.1
1	B	88	HIS	4.1
1	B	185	PHE	4.0
1	A	78	ASP	4.0
1	B	2	CYS	4.0
1	B	196	GLY	4.0
1	A	294	ILE	3.9
1	B	119	ILE	3.9
1	B	86	ASP	3.9
1	A	136	LEU	3.9
1	A	45	GLY	3.9
1	B	191	SER	3.8
1	B	276	LEU	3.8
1	B	252	GLU	3.8
1	A	674	LEU	3.8
1	B	126	ILE	3.8
1	B	193	HIS	3.8
1	B	140	GLY	3.8
1	B	120	VAL	3.8
1	B	187	LEU	3.8
1	B	82	ASP	3.7
1	B	161	ASP	3.7
1	A	295	LYS	3.7
1	B	59	LEU	3.6
1	B	188	VAL	3.6
1	B	398	VAL	3.6
1	A	103	SER	3.5
1	B	623	GLU	3.5
1	B	630	ASN	3.5
1	B	357	LYS	3.5
1	B	266	VAL	3.5
1	A	49	ASP	3.4
1	B	9	ASN	3.4
1	B	632	LYS	3.4
1	B	310	GLN	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	529	LYS	3.3
1	B	208	LEU	3.3
1	B	268	GLU	3.3
1	B	636	LYS	3.3
1	A	60	ILE	3.3
1	A	55	CYS	3.3
1	A	47	ASP	3.3
1	B	145	SER	3.3
1	A	52	ALA	3.2
1	A	75	LYS	3.2
1	B	13	PRO	3.2
1	A	145	SER	3.2
1	B	112	SER	3.1
1	B	91	ILE	3.1
1	B	378	TYR	3.1
1	A	107	SER	3.0
1	B	178	ILE	3.0
1	A	76	GLN	3.0
1	A	142	ASP	3.0
1	B	280	ASP	2.9
1	B	271	ASN	2.9
1	A	73	VAL	2.9
1	B	212	ARG	2.9
1	B	125	ILE	2.9
1	A	181	LEU	2.9
1	B	397	MET	2.9
1	B	146	GLU	2.9
1	B	121	ILE	2.9
1	A	398	VAL	2.8
1	B	635	ILE	2.8
1	B	6	ALA	2.8
1	B	17	ARG	2.8
1	A	106	ASN	2.8
1	A	636	LYS	2.8
1	B	11	HIS	2.8
1	B	624	ASP	2.8
1	B	207	LEU	2.8
1	B	179	GLN	2.7
1	B	374	CYS	2.7
1	B	349	TYR	2.7
1	A	569	GLY	2.7
1	A	83	ILE	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	141	TYR	2.7
1	B	175	GLU	2.7
1	A	61	LYS	2.7
1	A	51	GLU	2.7
1	A	98	THR	2.7
1	B	148	ASP	2.7
1	B	182	GLU	2.7
1	B	260	ALA	2.7
1	B	5	PHE	2.7
1	B	372	ILE	2.7
1	A	227	ARG	2.6
1	A	400	LEU	2.6
1	B	595	ARG	2.6
1	A	96	TRP	2.6
1	B	115	ASN	2.6
1	B	675	ALA	2.6
1	B	25	LYS	2.6
1	B	400	LEU	2.6
1	A	2	CYS	2.5
1	B	128	ASN	2.5
1	B	71	GLU	2.5
1	B	171	THR	2.5
1	A	374	CYS	2.5
1	A	577	HIS	2.5
1	B	373	ALA	2.5
1	A	575	LEU	2.5
1	B	87	VAL	2.5
1	B	113	ASP	2.5
1	A	69	LEU	2.4
1	B	32	TYR	2.4
1	B	114	LYS	2.4
1	B	549	TYR	2.4
1	A	132	LEU	2.4
1	A	378	TYR	2.4
1	B	139	LYS	2.4
1	A	375	GLY	2.4
1	B	122	HIS	2.4
1	B	520	VAL	2.3
1	B	277	GLU	2.3
1	B	286	ASP	2.2
1	A	74	HIS	2.2
1	A	349	TYR	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	373	ALA	2.2
1	A	53	ASN	2.2
1	B	360	ILE	2.2
1	B	399	GLU	2.2
1	B	279	ASP	2.2
1	A	95	ARG	2.2
1	A	556	ALA	2.2
1	A	552	CYS	2.2
1	A	557	LEU	2.2
1	A	57	ILE	2.2
1	A	570	ILE	2.2
1	A	155	LEU	2.2
1	A	46	ASN	2.1
1	A	158	TYR	2.1
1	B	96	TRP	2.1
1	B	578	GLY	2.1
1	A	114	LYS	2.1
1	B	674	LEU	2.1
1	A	377	SER	2.1
1	B	621	ASP	2.1
1	B	401	ALA	2.1
1	A	372	ILE	2.1
1	A	593	ILE	2.1
1	A	42	PHE	2.1
1	A	382	VAL	2.1
1	A	549	TYR	2.1
1	A	267	ILE	2.1
1	A	291	ILE	2.1
1	A	473	ALA	2.1
1	B	144	GLU	2.1
1	B	472	VAL	2.0
1	B	679	THR	2.0
1	A	146	GLU	2.0
1	B	84	GLU	2.0
1	B	34	GLY	2.0
1	A	576	LYS	2.0
1	B	512	ARG	2.0
1	A	624	ASP	2.0
1	B	361	LYS	2.0
1	B	402	SER	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

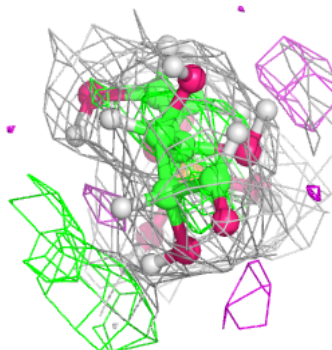
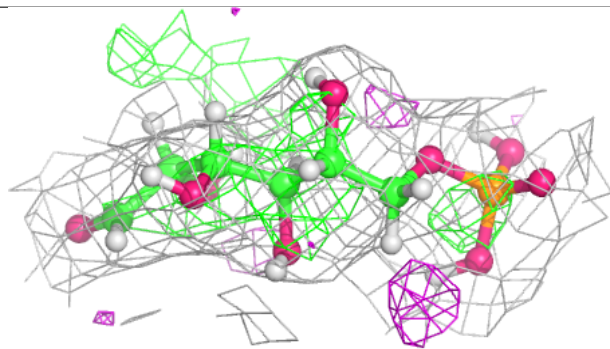
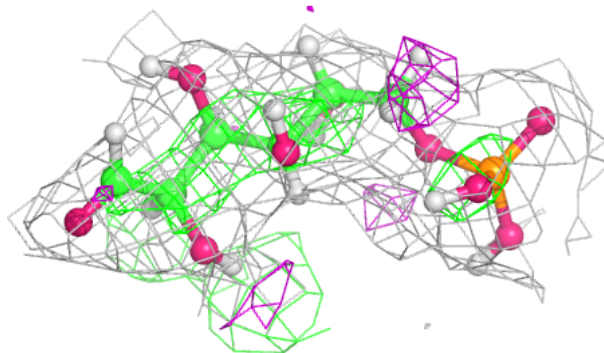
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	G6Q	B	701	16/16	0.96	0.41	71,94,115,117	0
2	G6Q	A	701	16/16	0.97	0.30	51,55,65,67	0

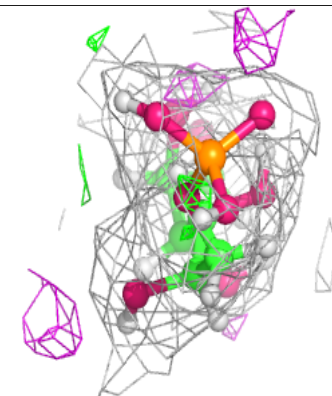
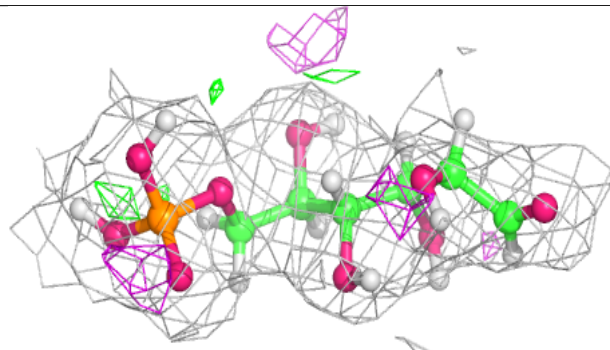
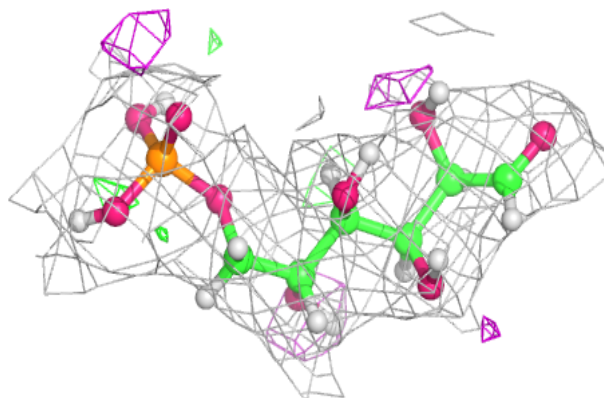
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around G6Q B 701:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around G6Q A 701:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers

There are no such residues in this entry.