Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:04 am BST

PDB ID	:	6R4E
Title	:	Crystal structure of human GFAT-1 in complex with Glucose-6-Phosphate and L-Glu
Authors	:	Ruegenberg, S.; Horn, M.; Pichlo, C.; Allmeroth, K.; Baumann, U.; Denzel, M.S.
Deposited on	:	2019-03-22
Resolution	:	2.35 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 ⓘ symbol.

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

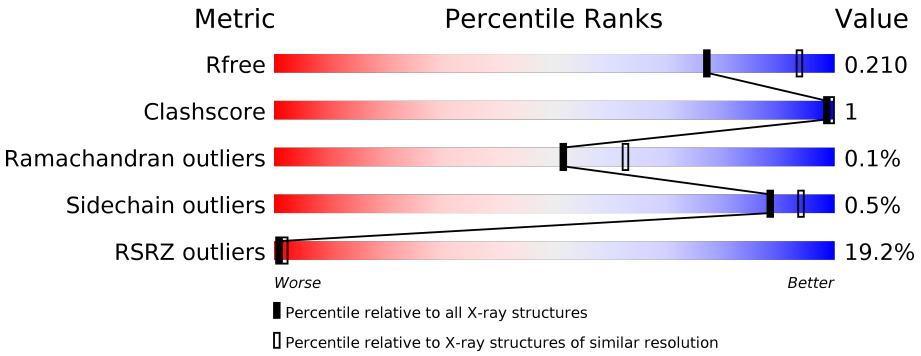
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 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	687	9% 94%
1	B	687	28% 94%

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
1	SEP	B	243	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21023 atoms, of which 10471 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.

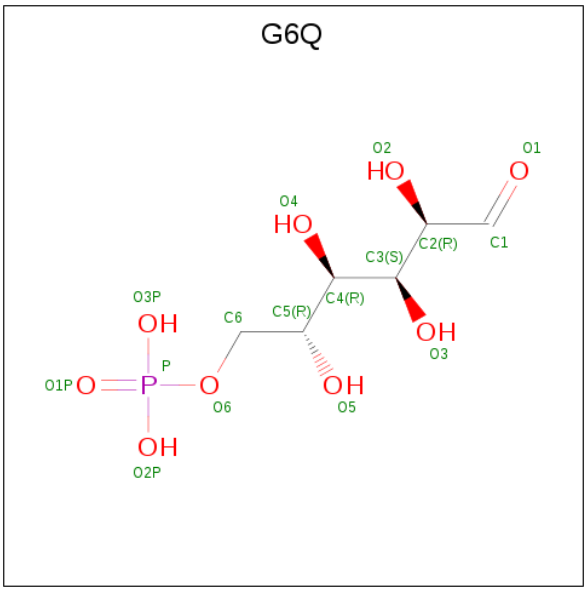
- Molecule 1 is a protein called Glutamine--fructose-6-phosphate aminotransferase [isomerizing] 1.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	663	Total	C	H	N	O	P	S	0	0	0
			10459	3297	5228	910	991	1	32			
1	B	657	Total	C	H	N	O	P	S	0	0	0
			10411	3279	5212	902	985	1	32			

There are 12 discrepancies between the modelled and reference sequences:

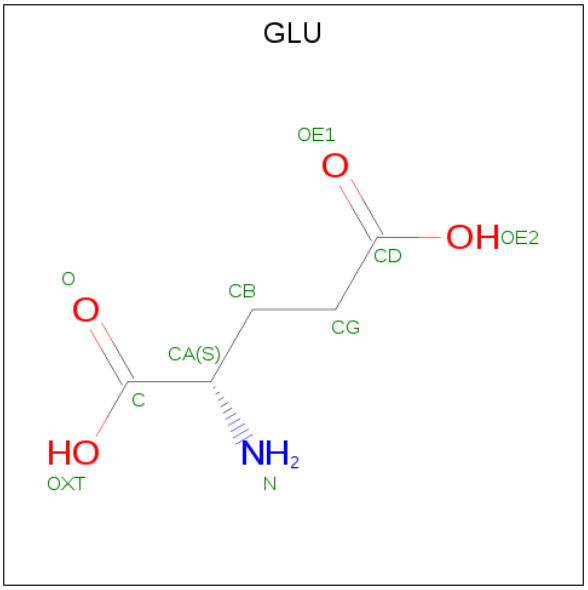
Chain	Residue	Modelled	Actual	Comment	Reference
A	294F	HIS	-	insertion	UNP Q06210
A	294G	HIS	-	insertion	UNP Q06210
A	294H	HIS	-	insertion	UNP Q06210
A	294I	HIS	-	insertion	UNP Q06210
A	294J	HIS	-	insertion	UNP Q06210
A	294K	HIS	-	insertion	UNP Q06210
B	293G	HIS	-	insertion	UNP Q06210
B	293H	HIS	-	insertion	UNP Q06210
B	293I	HIS	-	insertion	UNP Q06210
B	293J	HIS	-	insertion	UNP Q06210
B	293K	HIS	-	insertion	UNP Q06210
B	293L	HIS	-	insertion	UNP Q06210

- Molecule 2 is GLUCOSE-6-PHOSPHATE (three-letter code: G6Q) (formula: $C_6H_{13}O_9P$).



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 GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			15	5	5	1	4		

- Molecule 4 is water.

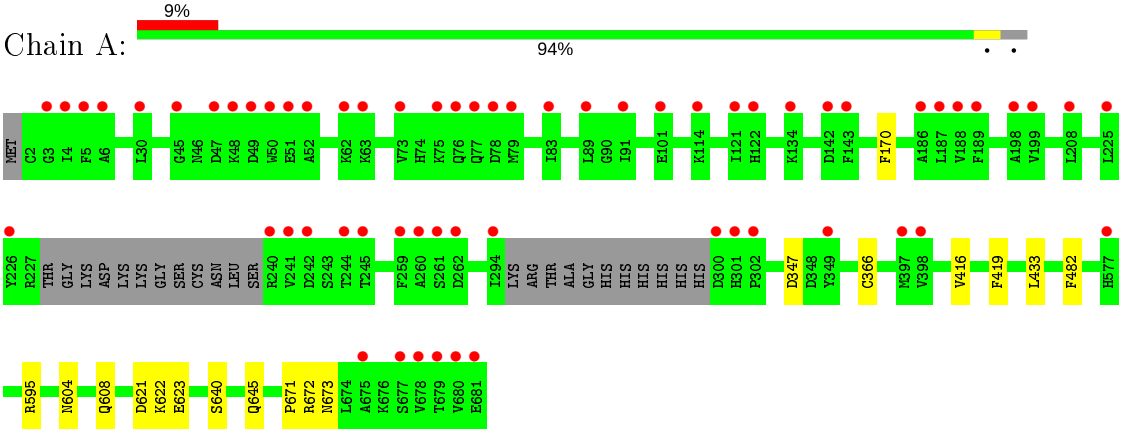
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	52	Total O 52 52	0	0
4	B	28	Total O 28 28	0	0

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 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.

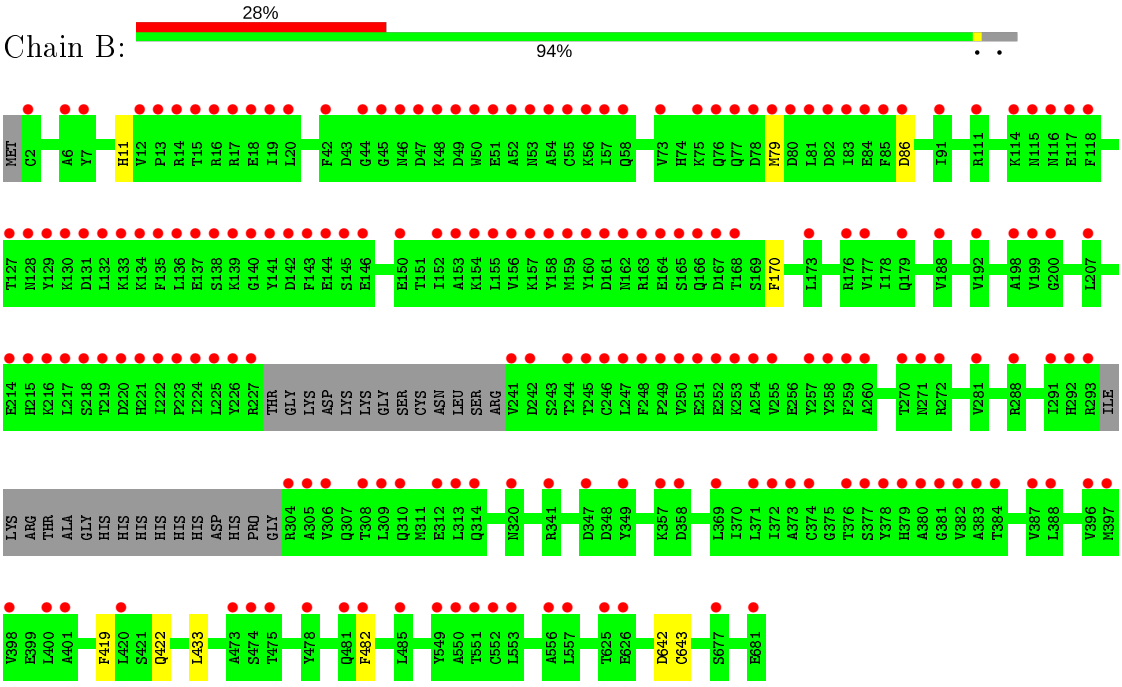
- Molecule 1: Glutamine--fructose-6-phosphate aminotransferase [isomerizing] 1

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	153.85Å 153.85Å 166.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.13 – 2.35 40.13 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.13-2.35) 97.6 (40.13-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.37Å)	Xtriage
Refinement program	PHENIX (dev_2499: ???)	Depositor
R, R_{free}	0.174 , 0.210 0.176 , 0.210	Depositor DCC
R_{free} test set	1991 reflections (2.41%)	wwPDB-VP
Wilson B-factor (Å^2)	58.8	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 58.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21023	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: G6Q, SEP

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	0.24	0/5309	0.43	0/7167
1	B	0.23	0/5276	0.42	0/7120
All	All	0.24	0/10585	0.42	0/14287

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	5231	5228	5227	7	0
1	B	5199	5212	5211	4	0
2	A	16	13	11	0	0
2	B	16	13	11	1	0
3	A	10	5	5	0	0
4	A	52	0	0	0	0
4	B	28	0	0	0	0
All	All	10552	10471	10465	11	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 (11) 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	2.23	0.71
1:A:604:ASN:OD1	1:A:608:GLN:NE2	2.29	0.66
1:A:621:ASP:OD1	1:A:622:LYS:N	2.46	0.49
1:A:595:ARG:NH2	1:A:623:GLU:O	2.46	0.49
1:A:419:PHE:CZ	1:A:433:LEU:HA	2.52	0.44
1:B:422:GLN:N	2:B:701:G6Q:O1P	2.40	0.43
1:B:642:ASP:OD1	1:B:643:CYS:N	2.52	0.42
1:A:671:PRO:O	1:A:672:ARG:HB3	2.20	0.42
1:B:11:HIS:N	1:B:86:ASP:O	2.53	0.42
1:A:366:CYS:CB	1:A:416:VAL:HG23	2.51	0.41
1:B:419:PHE:CZ	1:B:433:LEU:HA	2.55	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	656/687 (96%)	643 (98%)	12 (2%)	1 (0%)	47 56
1	B	650/687 (95%)	621 (96%)	29 (4%)	0	100 100
All	All	1306/1374 (95%)	1264 (97%)	41 (3%)	1 (0%)	51 63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	673	ASN

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	574/600 (96%)	571 (100%)	3 (0%)	88 94
1	B	573/600 (96%)	570 (100%)	3 (0%)	88 94
All	All	1147/1200 (96%)	1141 (100%)	6 (0%)	88 94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	PHE
1	A	347	ASP
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. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\|>2$
1	SEP	A	243	1	8,9,10	1.56	1 (12%)	8,12,14	1.57	2 (25%)
1	SEP	B	243	1	8,9,10	1.56	1 (12%)	8,12,14	1.50	2 (25%)

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
1	SEP	A	243	1	-	0/5/8/10	-
1	SEP	B	243	1	-	0/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	SEP	P-O1P	3.40	1.61	1.50
1	B	243	SEP	P-O1P	3.39	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	243	SEP	P-OG-CB	-2.85	110.44	118.30
1	A	243	SEP	OG-CB-CA	2.81	110.88	108.14
1	B	243	SEP	P-OG-CB	-2.78	110.62	118.30
1	B	243	SEP	OG-CB-CA	2.59	110.67	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

3 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	B	701	-	14,15,15	0.47	0	20,21,21	0.62	0
2	G6Q	A	701	-	14,15,15	0.50	0	20,21,21	0.70	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	G6Q	B	701	-	-	4/18/20/20	-
2	G6Q	A	701	-	-	4/18/20/20	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	C1-C2-C3-C4
2	A	701	G6Q	O2-C2-C3-C4
2	A	701	G6Q	O2-C2-C3-O3
2	A	701	G6Q	C1-C2-C3-O3

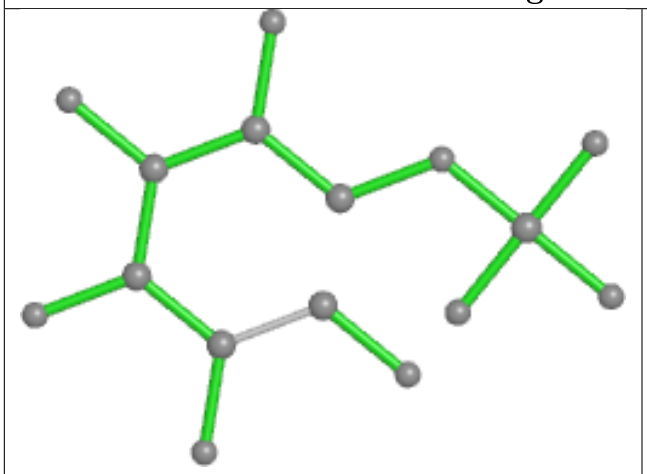
There are no ring outliers.

1 monomer is involved in 1 short contact:

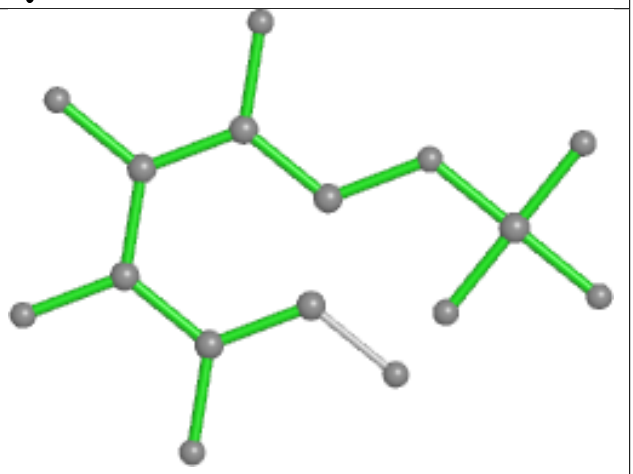
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	G6Q	1	0

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 then 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.

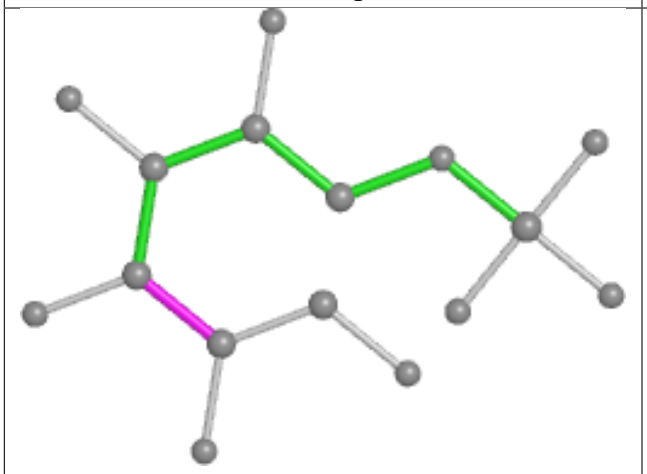
Ligand G6Q B 701



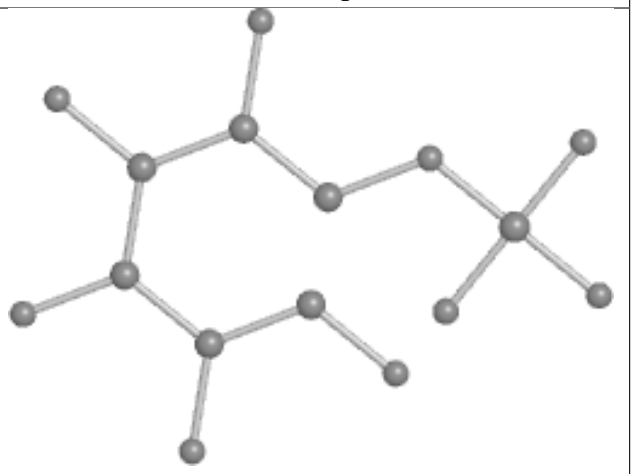
Bond lengths



Bond angles

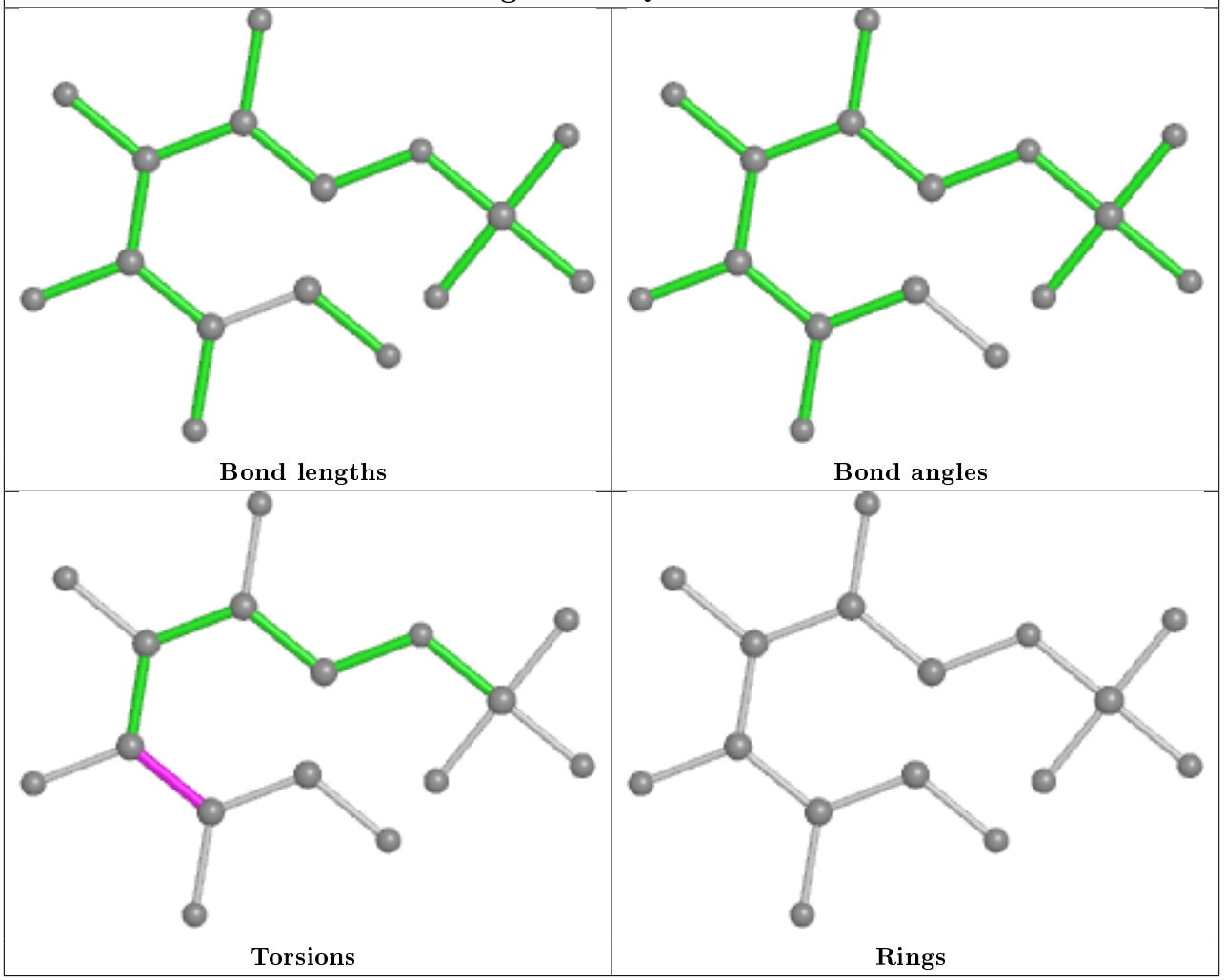


Torsions



Rings

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^{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	662/687 (96%)	0.61	62 (9%) 8 13	44, 68, 122, 159	0
1	B	656/687 (95%)	1.53	191 (29%) 0 0	50, 90, 168, 235	0
All	All	1318/1374 (95%)	1.07	253 (19%) 1 2	44, 76, 158, 235	0

All (253) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	241	VAL	14.4
1	B	77	GLN	9.8
1	B	155	LEU	9.0
1	B	75	LYS	8.6
1	B	217	LEU	8.6
1	B	55	CYS	8.5
1	B	79	MET	8.2
1	B	53	ASN	8.2
1	A	680	VAL	8.2
1	B	226	TYR	8.1
1	B	52	ALA	8.1
1	B	50	TRP	7.9
1	B	250	VAL	7.4
1	B	255	VAL	7.2
1	B	78	ASP	7.1
1	B	160	TYR	7.0
1	B	49	ASP	6.9
1	B	129	TYR	6.8
1	B	143	PHE	6.8
1	B	158	TYR	6.8
1	B	159	MET	6.8
1	B	141	TYR	6.6
1	B	245	THR	6.6
1	B	47	ASP	6.6

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Mol	Chain	Res	Type	RSRZ
1	B	45	GLY	6.6
1	B	225	LEU	6.5
1	B	164	GLU	6.5
1	B	51	GLU	6.3
1	B	81	LEU	6.2
1	B	135	PHE	6.2
1	B	251	GLU	6.0
1	B	54	ALA	6.0
1	B	46	ASN	5.9
1	B	48	LYS	5.8
1	B	136	LEU	5.7
1	B	44	GLY	5.7
1	B	137	GLU	5.6
1	B	223	PRO	5.6
1	A	79	MET	5.5
1	B	224	ILE	5.5
1	B	15	THR	5.5
1	B	247	LEU	5.5
1	B	80	ASP	5.5
1	B	118	PHE	5.4
1	A	241	VAL	5.3
1	B	166	GLN	5.3
1	B	306	VAL	5.2
1	A	300	ASP	5.2
1	A	45	GLY	5.2
1	B	254	ALA	5.1
1	A	77	GLN	5.0
1	B	244	THR	5.0
1	B	246	CYS	5.0
1	B	73	VAL	4.9
1	A	48	LYS	4.8
1	B	167	ASP	4.8
1	B	397	MET	4.8
1	A	677	SER	4.7
1	B	57	ILE	4.7
1	B	176	ARG	4.7
1	A	681	GLU	4.6
1	B	249	PRO	4.6
1	B	76	GLN	4.5
1	B	157	LYS	4.5
1	B	216	LYS	4.4
1	B	140	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	85	PHE	4.4
1	B	380	ALA	4.3
1	B	165	SER	4.3
1	B	168	THR	4.3
1	B	378	TYR	4.3
1	B	222	ILE	4.2
1	A	6	ALA	4.2
1	B	134	LYS	4.1
1	B	398	VAL	4.1
1	B	215	HIS	4.1
1	B	308	THR	4.1
1	B	20	LEU	4.1
1	A	49	ASP	4.1
1	B	145	SER	4.1
1	B	142	ASP	4.0
1	B	248	PHE	4.0
1	A	397	MET	4.0
1	B	199	VAL	4.0
1	B	56	LYS	3.9
1	B	138	SER	3.9
1	A	675	ALA	3.9
1	B	258	TYR	3.9
1	B	218	SER	3.9
1	B	163	ARG	3.9
1	B	83	ILE	3.9
1	B	382	VAL	3.8
1	B	86	ASP	3.8
1	B	153	ALA	3.8
1	A	259	PHE	3.7
1	B	114	LYS	3.7
1	A	226	TYR	3.7
1	B	221	HIS	3.7
1	A	260	ALA	3.6
1	B	259	PHE	3.6
1	B	242	ASP	3.6
1	B	379	HIS	3.6
1	B	383	ALA	3.6
1	A	302	PRO	3.6
1	A	75	LYS	3.6
1	A	73	VAL	3.6
1	A	678	VAL	3.6
1	B	309	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	154	LYS	3.5
1	B	146	GLU	3.5
1	B	162	ASN	3.5
1	B	2	CYS	3.5
1	B	257	TYR	3.5
1	A	50	TRP	3.4
1	B	349	TYR	3.4
1	B	310	GLN	3.4
1	B	474	SER	3.4
1	B	260	ALA	3.4
1	B	384	THR	3.3
1	B	357	LYS	3.3
1	B	156	VAL	3.3
1	A	188	VAL	3.3
1	B	252	GLU	3.3
1	B	132	LEU	3.3
1	A	5	PHE	3.2
1	B	381	GLY	3.2
1	A	78	ASP	3.2
1	B	131	ASP	3.2
1	B	6	ALA	3.2
1	B	478	TYR	3.2
1	B	130	LYS	3.2
1	B	358	ASP	3.2
1	A	301	HIS	3.2
1	B	82	ASP	3.2
1	B	227	ARG	3.2
1	A	189	PHE	3.1
1	B	177	VAL	3.1
1	B	139	LYS	3.1
1	B	272	ARG	3.1
1	B	553	LEU	3.1
1	A	83	ILE	3.1
1	B	219	THR	3.1
1	B	19	ILE	3.1
1	B	220	ASP	3.0
1	B	192	VAL	3.0
1	B	161	ASP	3.0
1	A	47	ASP	3.0
1	A	225	LEU	3.0
1	B	116	ASN	3.0
1	B	320	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	18	GLU	3.0
1	B	115	ASN	3.0
1	A	142	ASP	3.0
1	B	253	LYS	3.0
1	A	187	LEU	2.9
1	B	549	TYR	2.9
1	B	127	THR	2.9
1	B	188	VAL	2.9
1	B	133	LYS	2.9
1	B	552	CYS	2.9
1	B	313	LEU	2.9
1	A	52	ALA	2.9
1	B	200	GLY	2.8
1	B	111	ARG	2.8
1	B	117	GLU	2.8
1	A	262	ASP	2.8
1	B	347	ASP	2.8
1	B	550	ALA	2.8
1	B	482	PHE	2.7
1	A	4	ILE	2.7
1	B	388	LEU	2.7
1	B	293	ARG	2.7
1	B	305	ALA	2.7
1	B	144	GLU	2.7
1	A	76	GLN	2.7
1	B	291	ILE	2.6
1	A	134	LYS	2.6
1	B	374	CYS	2.6
1	B	84	GLU	2.6
1	A	398	VAL	2.6
1	B	91	ILE	2.6
1	B	271	ASN	2.6
1	A	577	HIS	2.6
1	B	42	PHE	2.6
1	A	240	ARG	2.6
1	B	207	LEU	2.6
1	A	261	SER	2.5
1	B	377	SER	2.5
1	B	387	VAL	2.5
1	B	372	ILE	2.5
1	B	400	LEU	2.5
1	B	625	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	349	TYR	2.5
1	B	7	TYR	2.5
1	A	294	ILE	2.5
1	B	12	VAL	2.5
1	B	304	ARG	2.5
1	A	245	THR	2.5
1	B	13	PRO	2.5
1	B	681	GLU	2.5
1	B	198	ALA	2.4
1	B	281	VAL	2.4
1	B	14	ARG	2.4
1	B	312	GLU	2.4
1	A	121	ILE	2.4
1	B	270	THR	2.4
1	B	420	LEU	2.4
1	B	376	THR	2.4
1	A	199	VAL	2.4
1	B	475	THR	2.3
1	A	63	LYS	2.3
1	A	143	PHE	2.3
1	A	208	LEU	2.3
1	B	314	GLN	2.3
1	B	626	GLU	2.3
1	B	401	ALA	2.3
1	B	473	ALA	2.3
1	A	186	ALA	2.3
1	B	214	GLU	2.2
1	B	373	ALA	2.2
1	A	51	GLU	2.2
1	A	242	ASP	2.2
1	B	288	ARG	2.2
1	A	244	THR	2.2
1	B	179	GLN	2.2
1	B	557	LEU	2.2
1	A	679	THR	2.2
1	B	16	ARG	2.2
1	A	101	GLU	2.2
1	A	89	LEU	2.2
1	B	396	VAL	2.1
1	A	198	ALA	2.1
1	B	17	ARG	2.1
1	A	62	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	152	ILE	2.1
1	B	58	GLN	2.1
1	A	91	ILE	2.1
1	B	173	LEU	2.1
1	B	369	LEU	2.1
1	B	556	ALA	2.1
1	B	371	LEU	2.1
1	B	292	HIS	2.1
1	B	551	THR	2.1
1	A	122	HIS	2.1
1	B	677	SER	2.1
1	B	481	GLN	2.0
1	A	30	LEU	2.0
1	B	341	ARG	2.0
1	B	485	LEU	2.0
1	B	128	ASN	2.0
1	B	150	GLU	2.0
1	A	114	LYS	2.0
1	A	3	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	SEP	B	243	10/11	0.64	0.44	145,185,219,219	0
1	SEP	A	243	10/11	0.87	0.26	108,151,178,178	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

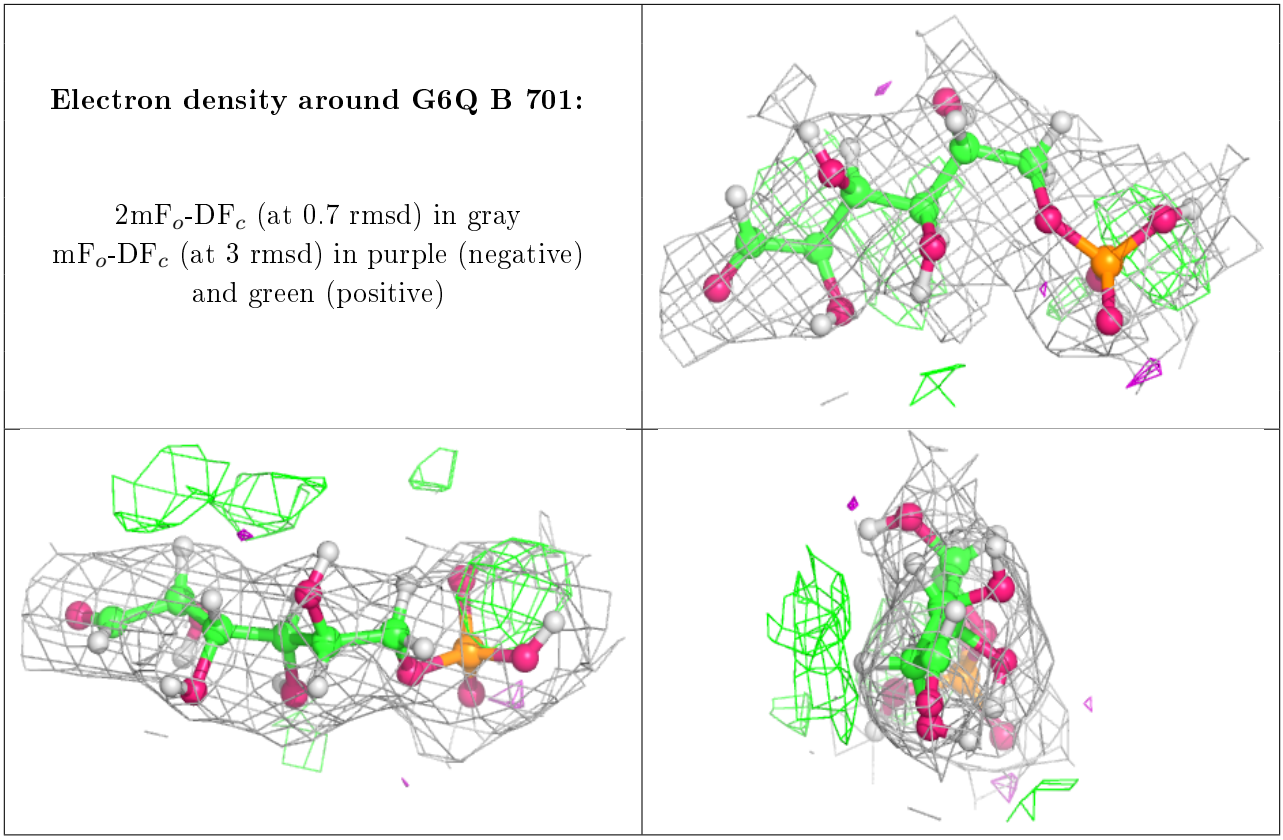
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	GLU	A	702	10/10	0.93	0.15	78,94,121,121	0
2	G6Q	B	701	16/16	0.97	0.31	51,68,96,118	0
2	G6Q	A	701	16/16	0.98	0.19	47,60,68,73	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.

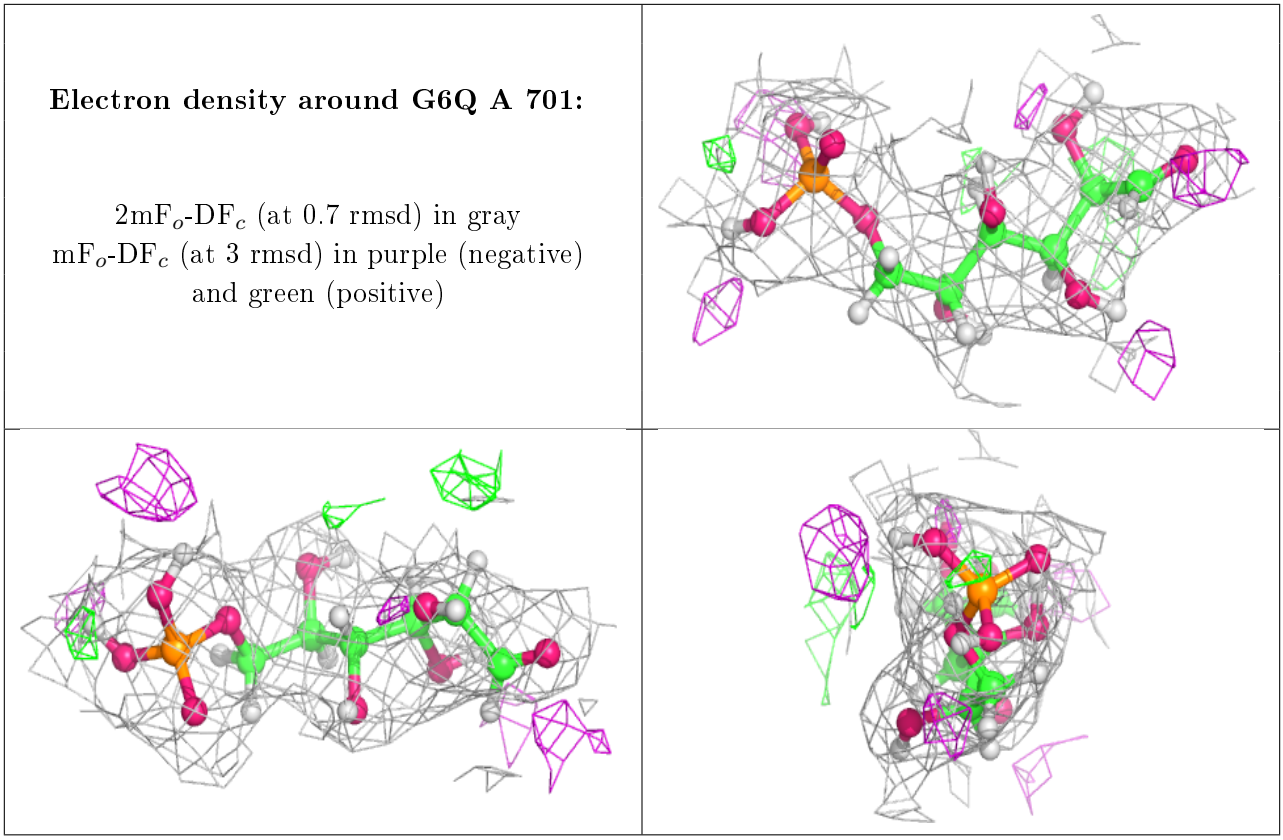
Electron density around G6Q B 701:

$2mF_o$-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 (i)

There are no such residues in this entry.