



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:16 am BST

PDB ID : 6R4I
Title : Crystal structure of human GFAT-1 G461E
Authors : Ruegenberg, S.; Horn, M.; Pichlo, C.; Allmeroth, K.; Baumann, U.; Denzel, M.S.
Deposited on : 2019-03-22
Resolution : 2.59 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

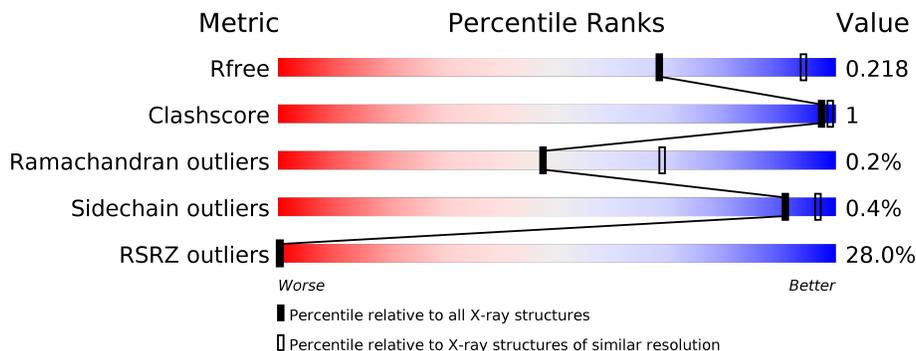
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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 $\leq 5\%$. 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	
1	B	687	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20882 atoms, of which 10419 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.

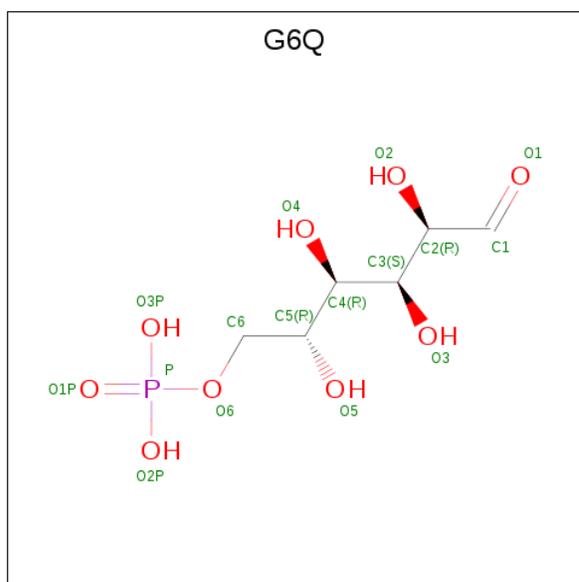
- Molecule 1 is a protein called Glutamine--fructose-6-phosphate aminotransferase [isomerizing] 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	659	10417	3284	5213	906	982	32	0	0	0
1	B	650	10328	3254	5175	894	973	32	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

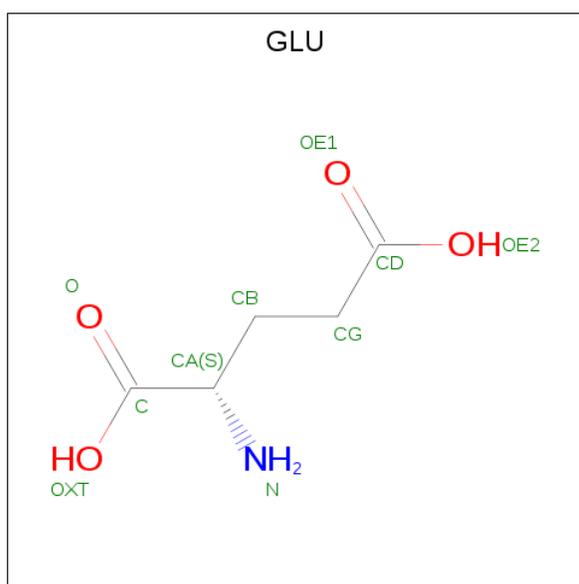
Chain	Residue	Modelled	Actual	Comment	Reference
A	299A	HIS	-	insertion	UNP Q06210
A	299B	HIS	-	insertion	UNP Q06210
A	299C	HIS	-	insertion	UNP Q06210
A	299D	HIS	-	insertion	UNP Q06210
A	299E	HIS	-	insertion	UNP Q06210
A	299F	HIS	-	insertion	UNP Q06210
A	461	GLU	GLY	engineered mutation	UNP Q06210
B	299A	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
B	461	GLU	GLY	engineered mutation	UNP Q06210

- Molecule 2 is GLUCOSE-6-PHOSPHATE (three-letter code: G6Q) (formula: C₆H₁₃O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	P		
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
			Total	C	H	N	O		
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	43	Total 43	O 43	0	0
4	B	21	Total 21	O 21	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	152.75Å 152.75Å 165.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.68 – 2.59 48.68 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.68-2.59) 96.5 (48.68-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.58Å)	Xtrriage
Refinement program	PHENIX (dev_2499: ???)	Depositor
R, R_{free}	0.192 , 0.219 0.192 , 0.218	Depositor DCC
R_{free} test set	1967 reflections (3.19%)	wwPDB-VP
Wilson B-factor (Å ²)	60.6	Xtrriage
Anisotropy	0.017	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20882	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.24	0/5293	0.42	0/7146
1	B	0.24	0/5241	0.42	0/7073
All	All	0.24	0/10534	0.42	0/14219

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 [i](#)

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	5204	5213	5212	11	0
1	B	5153	5175	5173	6	0
2	A	16	13	11	1	0
2	B	16	13	11	0	0
3	A	10	5	5	0	0
4	A	43	0	0	0	0
4	B	21	0	0	0	0
All	All	10463	10419	10412	16	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 (16) 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:621:ASP:OD1	1:A:622:LYS:N	2.35	0.60
1:A:604:ASN:ND2	1:A:608:GLN:OE1	2.38	0.56
1:A:640:SER:N	1:A:645:GLN:OE1	2.39	0.54
1:A:544:GLY:N	1:A:552:CYS:SG	2.84	0.51
1:A:533:GLU:OE1	1:A:633:ARG:NE	2.46	0.48
1:B:594:MET:HE1	1:B:619:ILE:HG22	1.98	0.46
1:A:419:PHE:CZ	1:A:433:LEU:HA	2.51	0.46
1:B:393:GLU:OE2	1:B:496:ARG:NH1	2.44	0.45
2:A:701:G6Q:HO5	1:B:577:HIS:HD1	1.66	0.44
1:B:11:HIS:N	1:B:86:ASP:O	2.50	0.43
1:A:225:LEU:HD21	1:A:245:THR:HB	2.02	0.41
1:A:642:ASP:OD2	1:A:643:CYS:N	2.53	0.41
1:A:672:ARG:HE	1:B:612:ARG:NH2	2.19	0.41
1:A:44:GLY:N	1:A:56:LYS:O	2.43	0.41
1:A:226:TYR:HA	1:A:293:ARG:O	2.22	0.40
1:B:642:ASP:OD1	1:B:643:CYS:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	653/687 (95%)	640 (98%)	13 (2%)	0	100	100
1	B	644/687 (94%)	607 (94%)	35 (5%)	2 (0%)	41	62
All	All	1297/1374 (94%)	1247 (96%)	48 (4%)	2 (0%)	47	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	677	SER
1	B	250	VAL

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	573/602 (95%)	571 (100%)	2 (0%)	92	97
1	B	570/602 (95%)	567 (100%)	3 (0%)	88	96
All	All	1143/1204 (95%)	1138 (100%)	5 (0%)	91	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	B	9	ASN

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](#)

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	0.37	0	20,21,21	0.64	0
2	G6Q	A	701	-	14,15,15	0.38	0	20,21,21	0.86	2 (10%)

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	-	-	13/18/20/20	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	G6Q	O2-C2-C3	2.17	114.61	109.46
2	A	701	G6Q	O6-P-O1P	2.07	112.28	106.47

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	G6Q	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

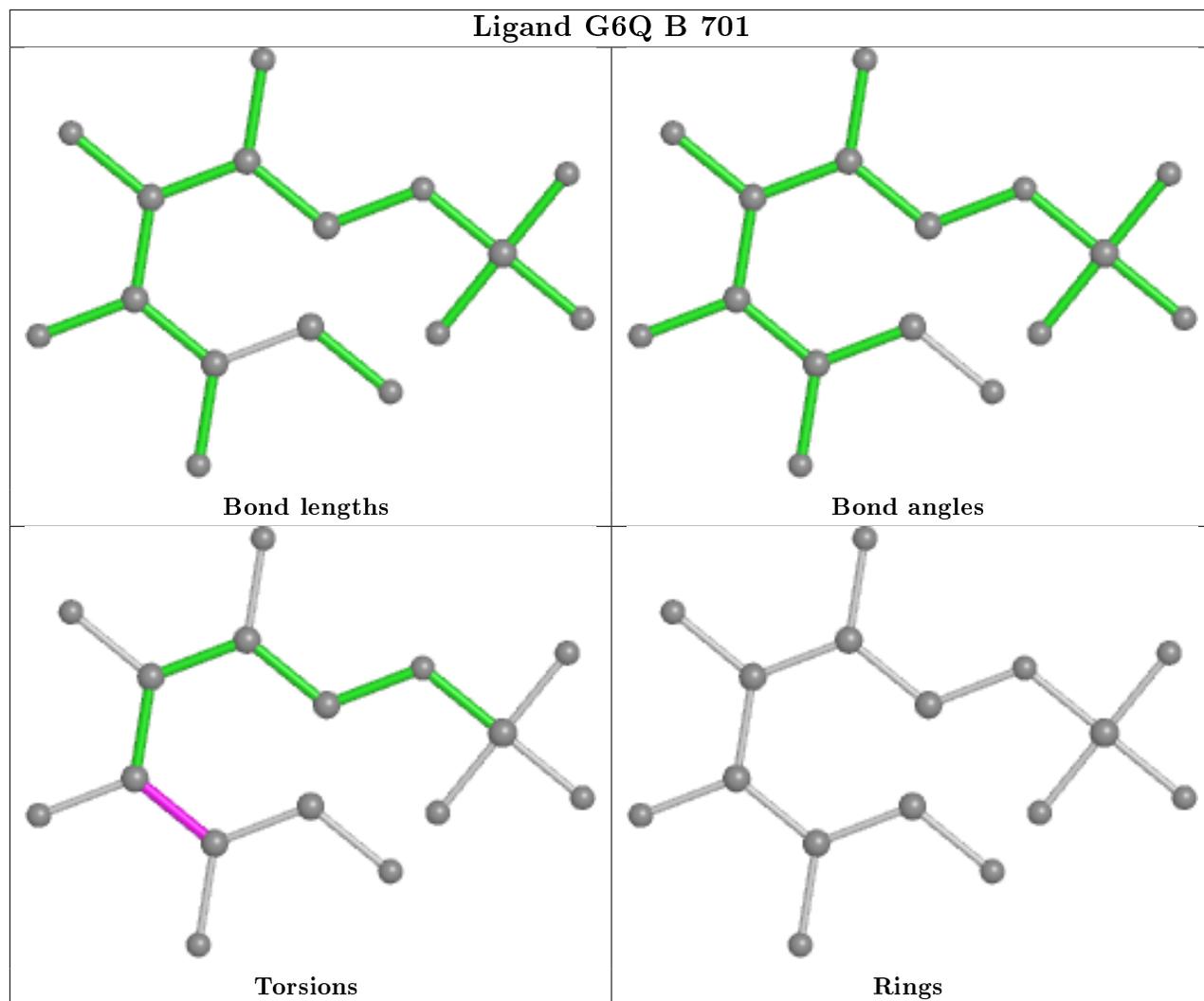
Mol	Chain	Res	Type	Atoms
2	A	701	G6Q	C1-C2-C3-C4
2	A	701	G6Q	O2-C2-C3-C4
2	A	701	G6Q	O2-C2-C3-O3
2	A	701	G6Q	C3-C4-C5-O5
2	A	701	G6Q	O4-C4-C5-O5
2	A	701	G6Q	C4-C5-C6-O6
2	A	701	G6Q	O5-C5-C6-O6
2	A	701	G6Q	O4-C4-C5-C6
2	A	701	G6Q	C3-C4-C5-C6
2	A	701	G6Q	C1-C2-C3-O3
2	B	701	G6Q	C1-C2-C3-O3
2	B	701	G6Q	O2-C2-C3-O3
2	A	701	G6Q	C6-O6-P-O2P
2	A	701	G6Q	C6-O6-P-O3P
2	A	701	G6Q	C2-C3-C4-O4
2	B	701	G6Q	O2-C2-C3-C4

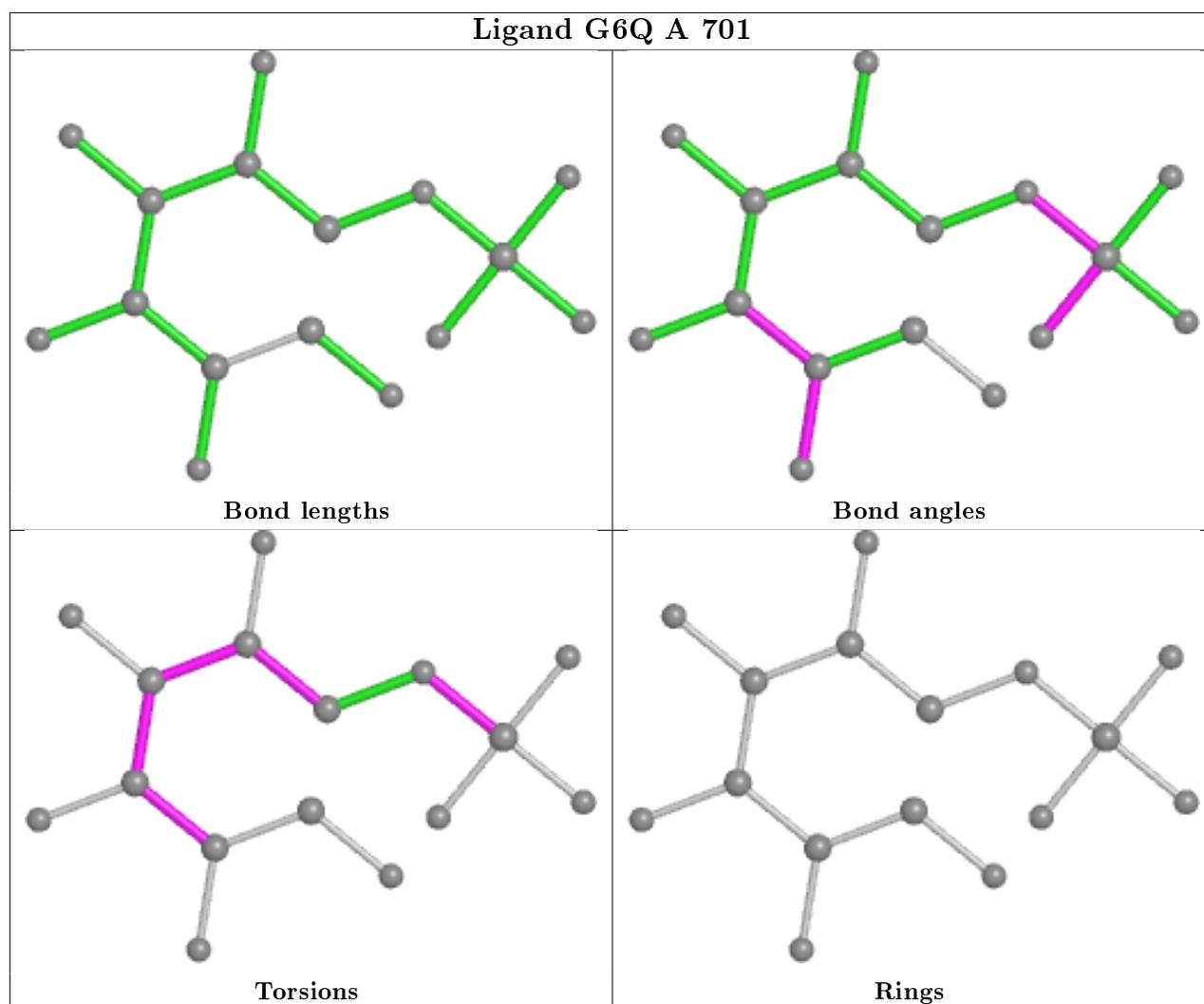
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	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 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.





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, 95th 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	659/687 (95%)	0.83	71 (10%) 5 4	46, 68, 125, 190	0
1	B	650/687 (94%)	3.33	295 (45%) 0 0	48, 97, 284, 404	0
All	All	1309/1374 (95%)	2.07	366 (27%) 0 0	46, 76, 260, 404	0

All (366) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	155	LEU	21.1
1	B	223	PRO	19.8
1	B	247	LEU	18.6
1	B	153	ALA	18.5
1	B	77	GLN	18.2
1	B	53	ASN	16.2
1	B	225	LEU	15.4
1	B	15	THR	14.8
1	B	50	TRP	14.2
1	B	54	ALA	14.1
1	B	255	VAL	14.0
1	B	222	ILE	13.5
1	B	55	CYS	13.3
1	B	52	ALA	13.3
1	B	46	ASN	13.2
1	B	47	ASP	13.2
1	B	213	SER	13.2
1	B	258	TYR	13.1
1	B	224	ILE	12.8
1	B	135	PHE	12.7
1	B	73	VAL	12.5
1	B	79	MET	12.5
1	B	57	ILE	12.4
1	B	218	SER	12.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	89	LEU	12.3
1	B	156	VAL	12.0
1	B	141	TYR	11.6
1	B	245	THR	11.6
1	B	78	ASP	11.6
1	B	201	THR	11.6
1	B	51	GLU	11.5
1	B	158	TYR	11.5
1	B	198	ALA	11.3
1	B	166	GLN	11.3
1	B	115	ASN	11.3
1	B	19	ILE	11.2
1	B	114	LYS	11.1
1	B	48	LYS	10.8
1	B	85	PHE	10.7
1	B	76	GLN	10.7
1	B	246	CYS	10.7
1	B	154	LYS	10.6
1	B	217	LEU	10.6
1	B	170	PHE	10.5
1	B	20	LEU	10.5
1	B	177	VAL	10.3
1	B	189	PHE	10.2
1	B	105	VAL	10.2
1	B	118	PHE	10.2
1	B	272	ARG	10.0
1	B	249	PRO	10.0
1	B	309	LEU	10.0
1	B	219	THR	10.0
1	B	45	GLY	10.0
1	B	81	LEU	9.8
1	B	167	ASP	9.8
1	B	281	VAL	9.8
1	B	160	TYR	9.7
1	B	116	ASN	9.7
1	B	44	GLY	9.6
1	B	165	SER	9.6
1	B	80	ASP	9.6
1	B	7	TYR	9.5
1	B	136	LEU	9.5
1	B	226	TYR	9.5
1	B	209	ILE	9.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	71	GLU	9.4
1	B	41	GLY	9.3
1	B	10	TYR	9.3
1	A	681	GLU	9.1
1	B	49	ASP	9.0
1	B	59	LEU	8.9
1	B	75	LYS	8.9
1	B	274	ILE	8.9
1	B	168	THR	8.9
1	B	308	THR	8.8
1	B	152	ILE	8.8
1	B	8	LEU	8.6
1	B	140	GLY	8.6
1	B	176	ARG	8.6
1	B	216	LYS	8.5
1	B	174	VAL	8.5
1	B	159	MET	8.4
1	B	270	THR	8.3
1	B	220	ASP	8.3
1	B	257	TYR	8.3
1	A	680	VAL	8.2
1	B	292	HIS	8.2
1	B	24	ILE	8.1
1	B	248	PHE	8.1
1	B	157	LYS	8.0
1	B	58	GLN	8.0
1	B	169	SER	8.0
1	B	142	ASP	7.9
1	B	211	VAL	7.9
1	B	129	TYR	7.9
1	B	83	ILE	7.8
1	B	221	HIS	7.8
1	B	215	HIS	7.8
1	B	185	PHE	7.7
1	B	250	VAL	7.7
1	B	18	GLU	7.6
1	B	291	ILE	7.5
1	B	276	LEU	7.4
1	B	137	GLU	7.4
1	B	244	THR	7.4
1	B	254	ALA	7.3
1	B	132	LEU	7.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	87	VAL	7.3
1	B	259	PHE	7.2
1	B	283	ALA	7.2
1	B	111	ARG	7.0
1	B	113	ASP	7.0
1	B	145	SER	7.0
1	B	164	GLU	6.9
1	B	196	GLY	6.9
1	B	86	ASP	6.9
1	B	286	ASP	6.9
1	B	43	ASP	6.8
1	B	200	GLY	6.8
1	B	310	GLN	6.7
1	B	16	ARG	6.7
1	B	227	ARG	6.7
1	B	172	THR	6.6
1	B	128	ASN	6.6
1	B	134	LYS	6.6
1	B	194	PHE	6.5
1	B	289	LEU	6.5
1	B	143	PHE	6.4
1	B	112	SER	6.4
1	B	151	THR	6.4
1	B	42	PHE	6.3
1	B	88	HIS	6.2
1	B	63	LYS	6.2
1	B	138	SER	6.2
1	B	82	ASP	6.2
1	B	187	LEU	6.2
1	A	675	ALA	6.1
1	B	271	ASN	6.1
1	B	117	GLU	6.1
1	B	131	ASP	6.1
1	B	60	ILE	6.1
1	B	12	VAL	6.0
1	B	180	GLN	6.0
1	B	287	GLY	5.9
1	B	284	VAL	5.9
1	B	74	HIS	5.9
1	B	56	LYS	5.9
1	B	148	ASP	5.9
1	A	79	MET	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	199	VAL	5.8
1	B	161	ASP	5.7
1	B	279	ASP	5.7
1	B	171	THR	5.7
1	A	673	ASN	5.7
1	B	197	GLN	5.6
1	B	214	GLU	5.6
1	B	101	GLU	5.5
1	B	251	GLU	5.5
1	B	275	PHE	5.5
1	B	61	LYS	5.5
1	B	162	ASN	5.4
1	B	253	LYS	5.4
1	B	288	ARG	5.3
1	B	120	VAL	5.3
1	B	100	GLY	5.3
1	B	17	ARG	5.3
1	A	677	SER	5.3
1	B	13	PRO	5.2
1	B	178	ILE	5.2
1	B	280	ASP	5.2
1	B	282	ALA	5.2
1	B	173	LEU	5.1
1	B	130	LYS	5.1
1	B	6	ALA	5.1
1	B	106	ASN	5.1
1	B	264	SER	5.0
1	B	192	VAL	5.0
1	B	139	LYS	5.0
1	B	144	GLU	5.0
1	B	266	VAL	5.0
1	B	133	LYS	4.9
1	A	78	ASP	4.9
1	B	285	VAL	4.9
1	B	179	GLN	4.8
1	B	35	TYR	4.8
1	B	261	SER	4.8
1	B	147	THR	4.8
1	A	77	GLN	4.7
1	B	163	ARG	4.7
1	B	36	ASP	4.7
1	B	273	VAL	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	122	HIS	4.6
1	B	212	ARG	4.6
1	B	25	LYS	4.5
1	B	252	GLU	4.5
1	B	84	GLU	4.5
1	A	143	PHE	4.4
1	B	9	ASN	4.4
1	B	150	GLU	4.4
1	A	54	ALA	4.3
1	B	2	CYS	4.3
1	B	5	PHE	4.3
1	B	123	ASN	4.3
1	B	269	HIS	4.3
1	B	64	GLY	4.3
1	B	182	GLU	4.2
1	A	75	LYS	4.2
1	B	119	ILE	4.2
1	A	552	CYS	4.2
1	B	293	ARG	4.1
1	B	181	LEU	4.1
1	B	311	MET	4.1
1	A	73	VAL	4.1
1	B	290	SER	4.0
1	B	210	GLY	4.0
1	B	91	ILE	4.0
1	B	126	ILE	4.0
1	B	107	SER	4.0
1	A	45	GLY	4.0
1	B	125	ILE	3.9
1	B	397	MET	3.9
1	A	49	ASP	3.9
1	B	195	PRO	3.9
1	B	674	LEU	3.8
1	B	127	THR	3.8
1	B	628	ILE	3.8
1	B	316	ILE	3.7
1	B	98	THR	3.7
1	A	47	ASP	3.7
1	B	11	HIS	3.7
1	B	121	ILE	3.6
1	A	52	ALA	3.6
1	B	361	LYS	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	48	LYS	3.6
1	B	67	LYS	3.5
1	B	146	GLU	3.5
1	B	109	PRO	3.5
1	B	268	GLU	3.4
1	B	99	HIS	3.4
1	A	679	THR	3.4
1	A	678	VAL	3.4
1	B	40	VAL	3.4
1	B	670	PHE	3.3
1	B	149	THR	3.3
1	B	349	TYR	3.3
1	B	676	LYS	3.3
1	B	104	PRO	3.2
1	A	398	VAL	3.2
1	A	50	TRP	3.2
1	A	76	GLN	3.2
1	B	90	GLY	3.2
1	B	378	TYR	3.2
1	B	191	SER	3.2
1	A	105	VAL	3.2
1	B	193	HIS	3.1
1	B	265	ALA	3.1
1	B	260	ALA	3.1
1	B	677	SER	3.1
1	A	549	TYR	3.0
1	A	569	GLY	3.0
1	B	398	VAL	3.0
1	A	676	LYS	3.0
1	A	55	CYS	3.0
1	B	103	SER	3.0
1	B	27	LEU	3.0
1	B	72	GLU	2.9
1	B	32	TYR	2.9
1	B	400	LEU	2.8
1	B	595	ARG	2.8
1	B	204	GLY	2.8
1	B	206	PRO	2.8
1	B	33	ARG	2.8
1	B	313	LEU	2.7
1	A	401	ALA	2.7
1	B	360	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	14	ARG	2.7
1	B	277	GLU	2.7
1	B	70	ASP	2.7
1	B	552	CYS	2.7
1	A	53	ASN	2.7
1	B	62	LYS	2.6
1	A	400	LEU	2.6
1	B	312	GLU	2.6
1	A	571	LEU	2.6
1	A	374	CYS	2.6
1	B	186	ALA	2.5
1	B	401	ALA	2.5
1	A	136	LEU	2.5
1	B	207	LEU	2.5
1	B	256	GLU	2.5
1	B	175	GLU	2.5
1	A	378	TYR	2.5
1	B	108	HIS	2.5
1	B	102	PRO	2.5
1	B	96	TRP	2.5
1	B	188	VAL	2.5
1	B	208	LEU	2.5
1	B	582	LEU	2.5
1	B	372	ILE	2.5
1	A	134	LYS	2.5
1	B	357	LYS	2.5
1	B	671	PRO	2.5
1	B	578	GLY	2.5
1	A	142	ASP	2.4
1	B	579	PRO	2.4
1	A	375	GLY	2.4
1	A	373	ALA	2.4
1	B	504	LYS	2.4
1	A	83	ILE	2.4
1	B	629	LYS	2.4
1	B	402	SER	2.4
1	A	557	LEU	2.3
1	A	575	LEU	2.3
1	A	595	ARG	2.3
1	A	593	ILE	2.3
1	A	576	LYS	2.3
1	A	555	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	556	ALA	2.3
1	A	629	LYS	2.3
1	B	315	GLN	2.3
1	B	97	ALA	2.3
1	B	373	ALA	2.3
1	B	472	VAL	2.3
1	A	46	ASN	2.3
1	A	573	GLY	2.3
1	B	474	SER	2.3
1	A	399	GLU	2.3
1	A	158	TYR	2.2
1	B	374	CYS	2.2
1	A	81	LEU	2.2
1	B	346	PHE	2.2
1	B	575	LEU	2.2
1	B	429	THR	2.2
1	A	156	VAL	2.2
1	A	577	HIS	2.2
1	B	263	ALA	2.2
1	A	627	THR	2.2
1	A	376	THR	2.2
1	B	553	LEU	2.2
1	B	549	TYR	2.1
1	B	625	THR	2.1
1	A	85	PHE	2.1
1	A	379	HIS	2.1
1	A	599	TYR	2.1
1	B	381	GLY	2.1
1	A	559	ILE	2.1
1	A	553	LEU	2.1
1	B	203	ARG	2.1
1	B	31	GLU	2.1
1	A	396	VAL	2.1
1	B	681	GLU	2.1
1	A	567	SER	2.1
1	A	544	GLY	2.1
1	A	141	TYR	2.1
1	A	397	MET	2.1
1	A	574	GLU	2.1
1	A	56	LYS	2.1
1	A	550	ALA	2.1
1	B	28	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	124	GLY	2.1
1	B	513	LEU	2.0
1	B	622	LYS	2.0
1	B	379	HIS	2.0
1	A	473	ALA	2.0
1	B	21	GLU	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](#)

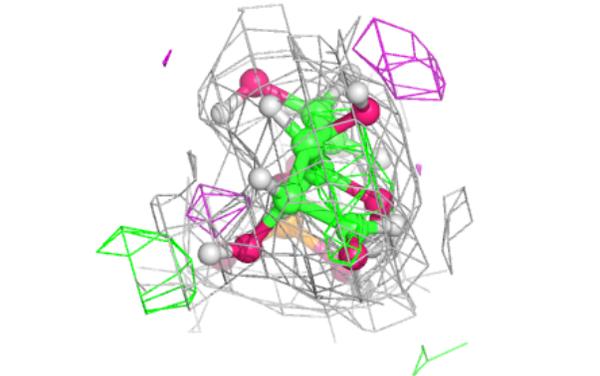
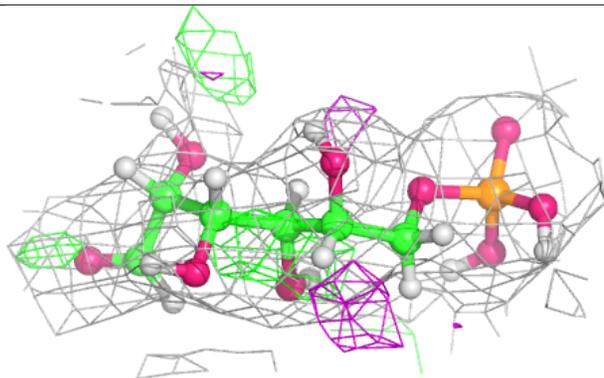
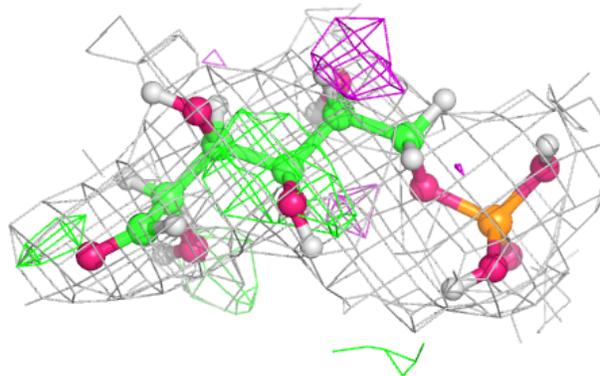
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.90	0.16	83,87,104,104	0
2	G6Q	B	701	16/16	0.94	0.39	73,100,122,126	0
2	G6Q	A	701	16/16	0.95	0.32	56,69,85,89	0

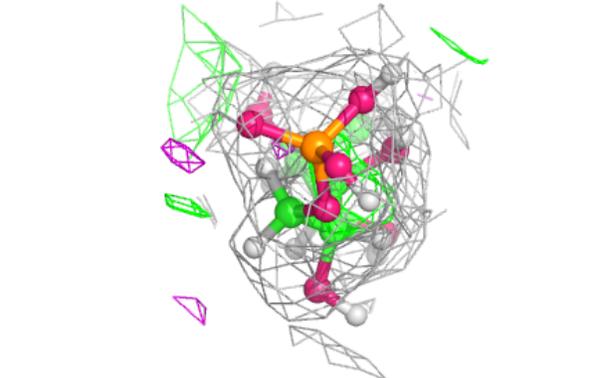
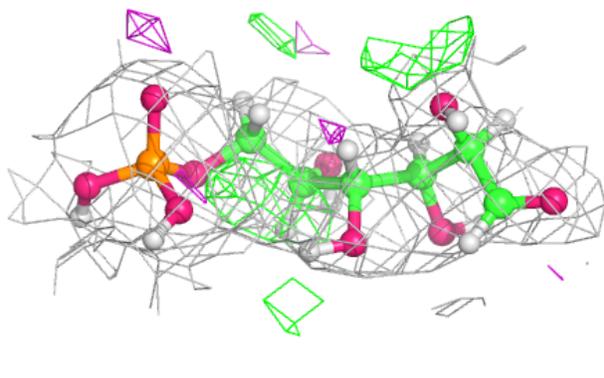
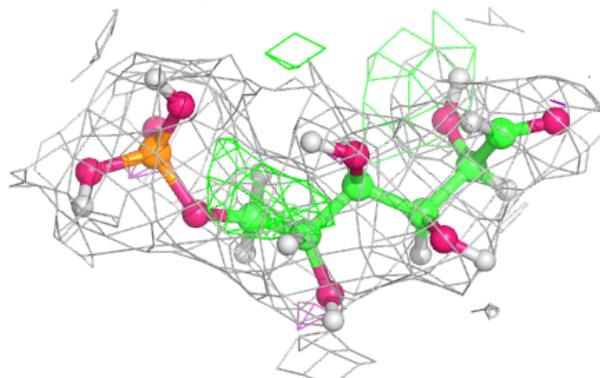
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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