Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 03:02 PM EDT

PDB ID	:	6SVQ
Title	:	Crystal structure of human GFAT-1 G461E after UDP-GlcNAc soaking
Authors	:	Ruegenberg, S.; Horn, M.; Pichlo, C.; Allmeroth, K.; Baumann, U.; Denzel, M.S.
Deposited on	:	2019-09-18
Resolution	:	2.72 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

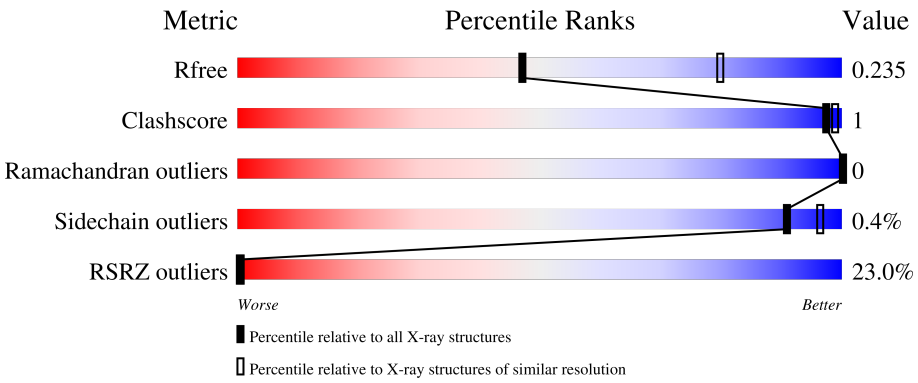
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.72 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 of 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	5%, 93%, • 5%
1	B	687	38%, 90%, • 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20533 atoms, of which 10263 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.

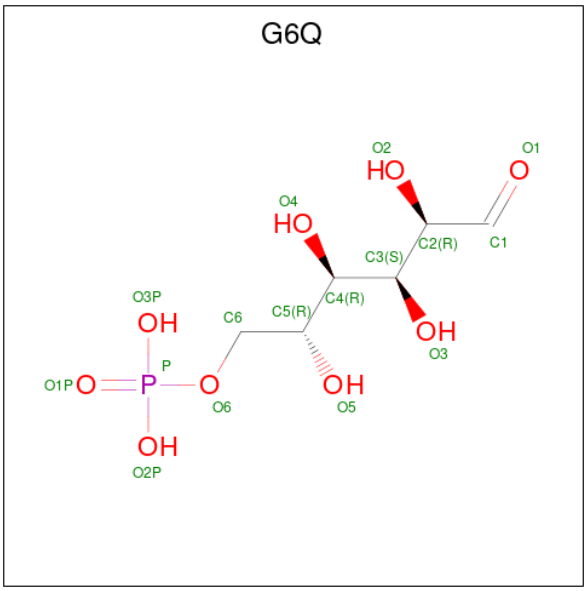
- Molecule 1 is a protein called Glutamine--fructose-6-phosphate-aminotransferase [isomerizing] 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	651	10302	3251	5153	896	970	32	0	0	0
1	B	640	10145	3201	5076	882	955	31	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

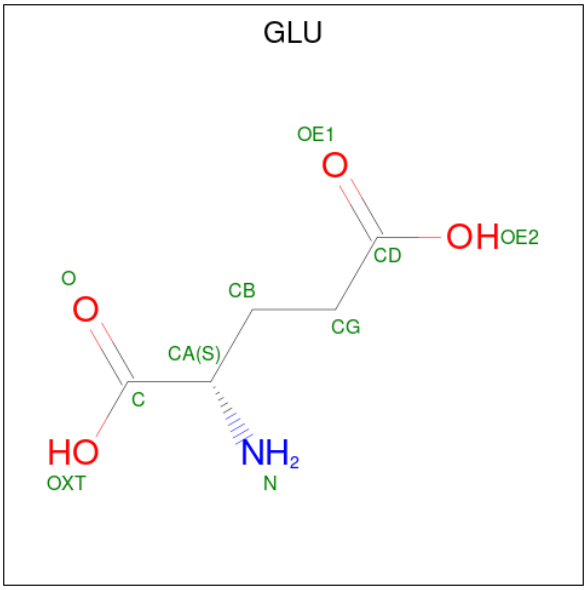
Chain	Residue	Modelled	Actual	Comment	Reference
A	299A	HIS	-	insertion	UNP Q06210
A	299B	HIS	-	insertion	UNP Q06210
A	299C	HIS	-	insertion	UNP Q06210
A	299D	HIS	-	insertion	UNP Q06210
A	299E	HIS	-	insertion	UNP Q06210
A	299F	HIS	-	insertion	UNP Q06210
A	461	GLU	GLY	engineered mutation	UNP Q06210
B	299A	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: $C_6H_{13}O_9P$).



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

- 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	18	5	8	1	4	0	0

- Molecule 4 is water.

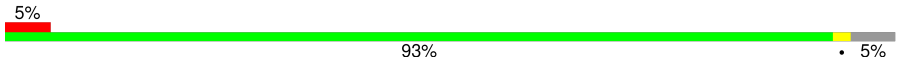
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	9	9	9	0	0
			Total	O		
4	B	1	1	1	0	0

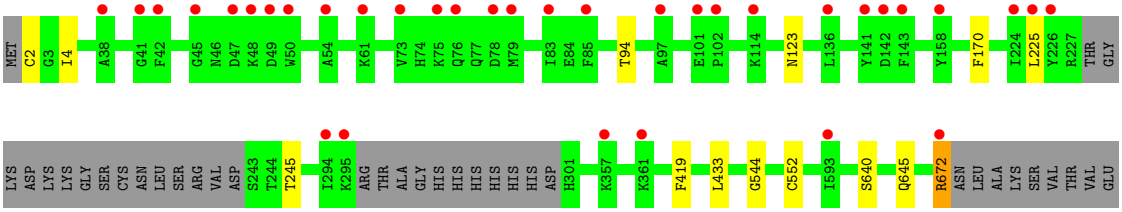
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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

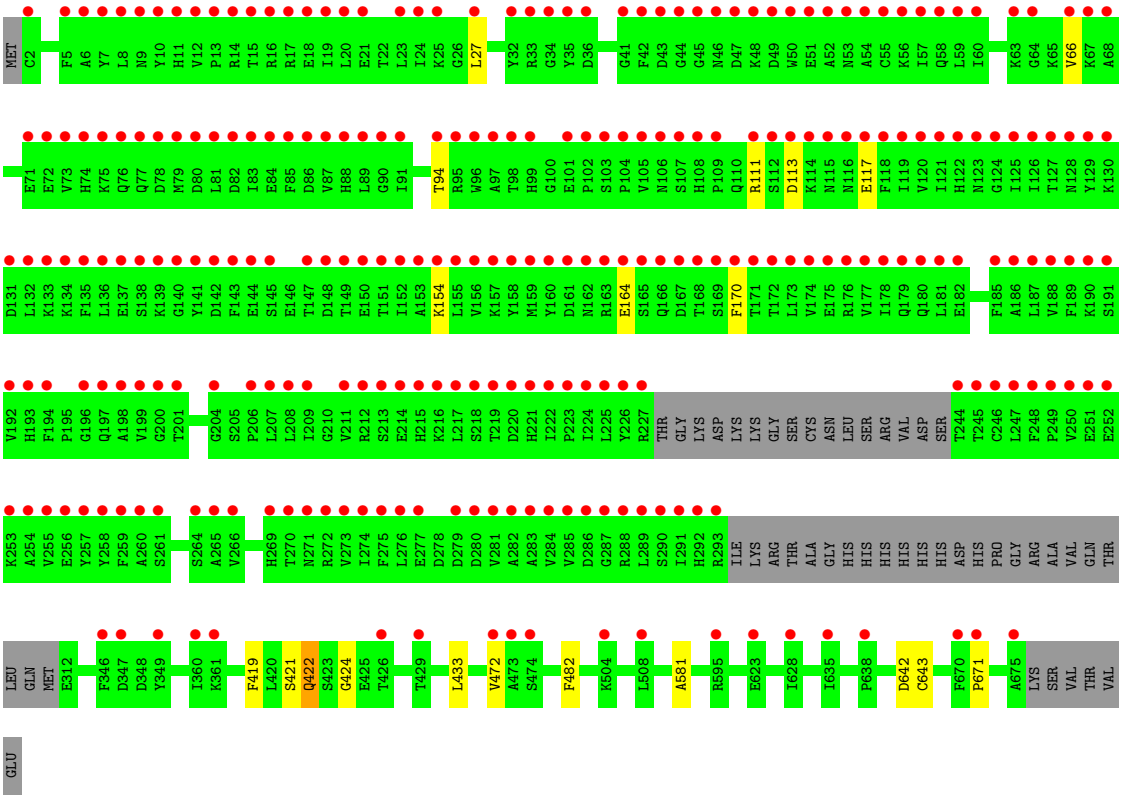
Chain A:





• 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	152.45Å 152.45Å 164.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.97 – 2.72 48.97 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.97-2.72) 96.4 (48.97-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.73Å)	Xtriage
Refinement program	PHENIX dev_2499	Depositor
R, R_{free}	0.205 , 0.234 0.207 , 0.235	Depositor DCC
R_{free} test set	1940 reflections (3.68%)	wwPDB-VP
Wilson B-factor (Å^2)	66.3	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 58.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20533	wwPDB-VP
Average B, all atoms (Å^2)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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 (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	0.25	0/5238	0.42	0/7071
1	B	0.24	0/5157	0.42	0/6960
All	All	0.24	0/10395	0.42	0/14031

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	5149	5153	5153	7	0
1	B	5069	5076	5076	11	0
2	A	16	13	11	0	0
2	B	16	13	11	1	0
3	A	10	8	5	0	0
4	A	9	0	0	0	0
4	B	1	0	0	0	0
All	All	10270	10263	10256	17	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 (17) 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:422:GLN:N	2:B:701:G6Q:O1P	2.28	0.66
1:A:640:SER:N	1:A:645:GLN:OE1	2.44	0.51
1:B:642:ASP:OD1	1:B:643:CYS:N	2.46	0.48
1:A:544:GLY:N	1:A:552:CYS:SG	2.87	0.48
1:B:111:ARG:O	1:B:154:LYS:NZ	2.47	0.47
1:B:27:LEU:HD22	1:B:94:THR:HG23	1.96	0.46
1:B:164:GLU:OE1	1:B:164:GLU:N	2.49	0.45
1:A:2:CYS:N	1:A:94:THR:O	2.49	0.45
1:B:113:ASP:OD2	1:B:117:GLU:HB2	2.17	0.44
1:A:225:LEU:HD21	1:A:245:THR:HB	2.00	0.43
1:B:421:SER:OG	1:B:424:GLY:N	2.51	0.42
1:A:4:ILE:HG12	1:A:123:ASN:ND2	2.35	0.42
1:B:419:PHE:CZ	1:B:433:LEU:HA	2.55	0.41
1:A:419:PHE:CZ	1:A:433:LEU:HA	2.54	0.41
1:B:472:VAL:HG21	1:B:671:PRO:HD2	2.02	0.41
1:B:66:VAL:HG22	1:B:94:THR:HG21	2.03	0.41
1:A:672:ARG:NH1	1:B:581:ALA:O	2.54	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	645/687 (94%)	627 (97%)	18 (3%)	0	100	100
1	B	634/687 (92%)	599 (94%)	35 (6%)	0	100	100
All	All	1279/1374 (93%)	1226 (96%)	53 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	566/602 (94%)	564 (100%)	2 (0%)	91 96
1	B	558/602 (93%)	555 (100%)	3 (0%)	88 95
All	All	1124/1204 (93%)	1119 (100%)	5 (0%)	91 96

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

Mol	Chain	Res	Type
1	A	170	PHE
1	A	672	ARG
1	B	170	PHE
1	B	422	GLN
1	B	482	PHE

Sometimes 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)

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
3	GLU	A	702	-	8,9,9	1.09	1 (12%)	8,11,11	1.18	1 (12%)
2	G6Q	A	701	-	14,15,15	0.34	0	19,21,21	0.68	1 (5%)
2	G6Q	B	701	-	14,15,15	0.40	0	19,21,21	0.82	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
3	GLU	A	702	-	-	3/9/9/9	-
2	G6Q	A	701	-	-	5/19/20/20	-
2	G6Q	B	701	-	-	10/19/20/20	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	GLU	OXT-C	-2.24	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	702	GLU	OXT-C-O	-2.62	118.14	124.08
2	A	701	G6Q	O2-C2-C3	2.05	114.27	109.46

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	G6Q	O1-C1-C2-C3
2	A	701	G6Q	C1-C2-C3-C4
2	A	701	G6Q	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	701	G6Q	O2-C2-C3-C4
2	A	701	G6Q	O2-C2-C3-O3
2	B	701	G6Q	O1-C1-C2-C3
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	B	701	G6Q	C4-C5-C6-O6
2	B	701	G6Q	O5-C5-C6-O6
2	B	701	G6Q	C2-C3-C4-C5
3	A	702	GLU	OE1-CD-CG-CB
2	B	701	G6Q	C2-C3-C4-O4
3	A	702	GLU	OE2-CD-CG-CB
2	B	701	G6Q	C6-O6-P-O3P
3	A	702	GLU	OXT-C-CA-N

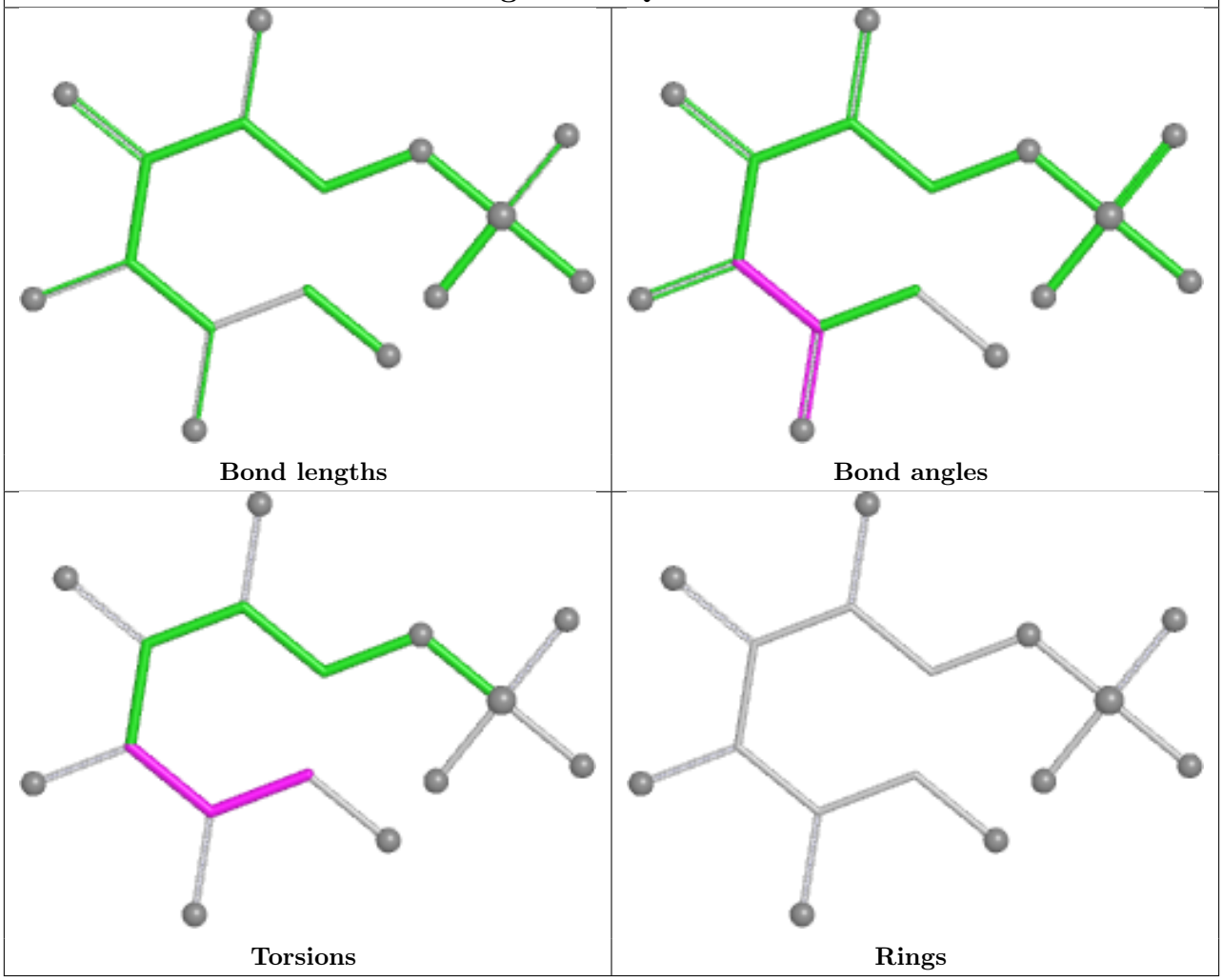
There are no ring outliers.

1 monomer is involved in 1 short contact:

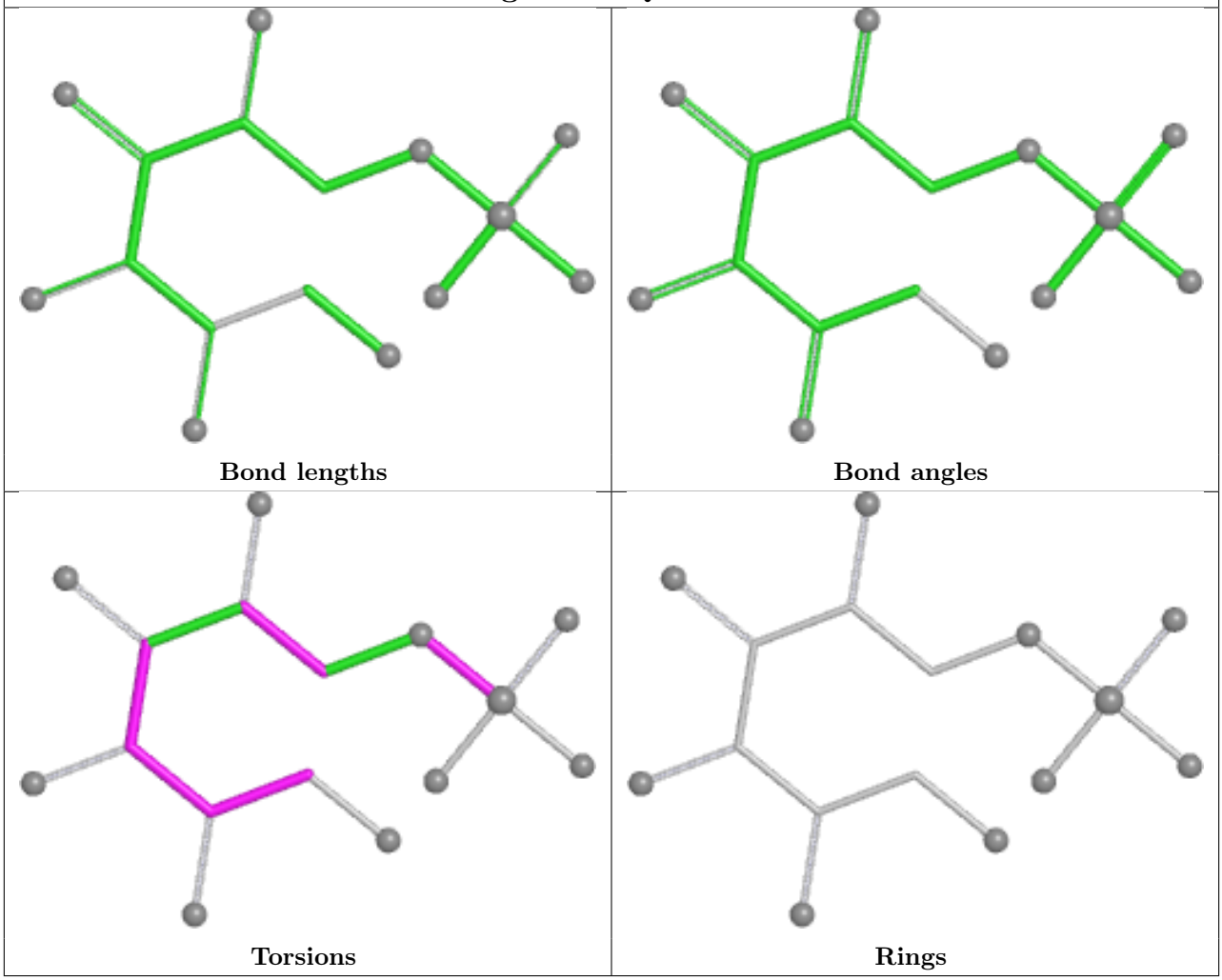
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	G6Q	1	0

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 A 701



Ligand G6Q B 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 (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, 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	651/687 (94%)	0.59	35 (5%)	25	25	47, 70, 125, 193	0
1	B	640/687 (93%)	3.15	262 (40%)	0	0	48, 103, 305, 459	0
All	All	1291/1374 (93%)	1.86	297 (23%)	0	0	47, 79, 281, 459	0

All (297) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	156	VAL	25.2
1	B	153	ALA	24.6
1	B	155	LEU	21.1
1	B	154	LYS	18.7
1	B	57	ILE	17.7
1	B	145	SER	17.6
1	B	20	LEU	17.4
1	B	198	ALA	17.4
1	B	47	ASP	17.4
1	B	19	ILE	17.1
1	B	176	ARG	15.3
1	B	170	PHE	15.0
1	B	24	ILE	14.8
1	B	46	ASN	14.8
1	B	111	ARG	14.5
1	B	281	VAL	14.0
1	B	189	PHE	13.7
1	B	157	LYS	13.5
1	B	200	GLY	13.5
1	B	79	MET	13.4
1	B	245	THR	13.3
1	B	225	LEU	13.3
1	B	258	TYR	13.3
1	B	77	GLN	12.9

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Mol	Chain	Res	Type	RSRZ
1	B	159	MET	12.7
1	B	223	PRO	12.6
1	B	15	THR	12.6
1	B	140	GLY	12.5
1	B	158	TYR	12.4
1	B	274	ILE	12.0
1	B	52	ALA	11.9
1	B	45	GLY	11.6
1	B	78	ASP	11.5
1	B	152	ILE	11.4
1	B	255	VAL	11.4
1	B	169	SER	11.3
1	B	177	VAL	11.2
1	B	141	TYR	10.7
1	B	224	ILE	10.5
1	B	247	LEU	10.5
1	B	48	LYS	10.4
1	B	259	PHE	10.3
1	B	71	GLU	10.2
1	B	73	VAL	10.1
1	B	201	THR	10.1
1	B	174	VAL	10.1
1	B	44	GLY	9.9
1	B	105	VAL	9.6
1	B	116	ASN	9.6
1	B	143	PHE	9.5
1	B	173	LEU	9.5
1	B	291	ILE	9.4
1	B	221	HIS	9.4
1	B	50	TRP	9.3
1	B	135	PHE	9.3
1	B	54	ALA	9.2
1	B	272	ARG	9.1
1	B	199	VAL	9.1
1	B	142	ASP	9.1
1	B	137	GLU	9.0
1	B	161	ASP	9.0
1	B	160	TYR	8.8
1	B	222	ILE	8.7
1	B	254	ALA	8.7
1	B	53	ASN	8.7
1	B	129	TYR	8.6

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Mol	Chain	Res	Type	RSRZ
1	B	139	LYS	8.4
1	B	250	VAL	8.4
1	B	115	ASN	8.4
1	B	43	ASP	8.3
1	B	266	VAL	8.3
1	B	59	LEU	8.3
1	B	89	LEU	8.3
1	B	249	PRO	8.2
1	B	246	CYS	8.2
1	B	76	GLN	8.2
1	B	675	ALA	8.1
1	B	107	SER	8.0
1	B	215	HIS	8.0
1	B	60	ILE	8.0
1	B	49	ASP	8.0
1	B	16	ARG	8.0
1	B	219	THR	7.9
1	B	248	PHE	7.9
1	B	168	THR	7.8
1	B	132	LEU	7.8
1	B	56	LYS	7.8
1	B	257	TYR	7.8
1	B	217	LEU	7.8
1	B	214	GLU	7.7
1	B	269	HIS	7.7
1	B	118	PHE	7.7
1	B	80	ASP	7.6
1	B	292	HIS	7.5
1	B	213	SER	7.4
1	B	283	ALA	7.4
1	B	112	SER	7.4
1	B	63	LYS	7.4
1	B	209	ILE	7.3
1	B	85	PHE	7.2
1	B	136	LEU	7.2
1	B	51	GLU	7.2
1	B	74	HIS	7.2
1	B	81	LEU	7.2
1	B	279	ASP	7.2
1	B	55	CYS	7.1
1	B	286	ASP	7.0
1	B	187	LEU	6.9

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Mol	Chain	Res	Type	RSRZ
1	B	82	ASP	6.9
1	B	18	GLU	6.8
1	B	114	LYS	6.8
1	B	270	THR	6.8
1	B	147	THR	6.7
1	B	109	PRO	6.7
1	B	218	SER	6.7
1	B	211	VAL	6.7
1	B	87	VAL	6.7
1	B	282	ALA	6.6
1	B	151	THR	6.6
1	B	90	GLY	6.6
1	B	276	LEU	6.4
1	B	138	SER	6.3
1	B	167	ASP	6.3
1	B	284	VAL	6.3
1	B	148	ASP	6.2
1	B	75	LYS	6.2
1	B	226	TYR	6.1
1	B	130	LYS	6.1
1	B	33	ARG	6.1
1	B	180	GLN	6.1
1	B	83	ILE	6.0
1	B	126	ILE	6.0
1	B	144	GLU	6.0
1	B	150	GLU	6.0
1	B	124	GLY	6.0
1	B	165	SER	5.9
1	B	113	ASP	5.8
1	B	5	PHE	5.8
1	B	131	ASP	5.8
1	B	244	THR	5.8
1	B	179	GLN	5.7
1	B	25	LYS	5.7
1	B	172	THR	5.7
1	B	178	ILE	5.7
1	B	166	GLN	5.6
1	B	285	VAL	5.6
1	B	216	LYS	5.5
1	B	164	GLU	5.5
1	B	171	THR	5.5
1	B	190	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	7	TYR	5.5
1	B	10	TYR	5.5
1	B	134	LYS	5.5
1	B	220	ASP	5.5
1	B	9	ASN	5.4
1	B	212	ARG	5.3
1	B	91	ILE	5.3
1	B	2	CYS	5.2
1	B	86	ASP	5.2
1	B	182	GLU	5.2
1	B	117	GLU	5.2
1	B	67	LYS	5.1
1	B	106	ASN	5.0
1	B	185	PHE	5.0
1	A	79	MET	4.9
1	B	251	GLU	4.9
1	B	34	GLY	4.9
1	B	181	LEU	4.9
1	B	58	GLN	4.9
1	B	289	LEU	4.8
1	B	120	VAL	4.8
1	B	288	ARG	4.7
1	B	133	LYS	4.6
1	B	163	ARG	4.6
1	A	226	TYR	4.6
1	B	35	TYR	4.6
1	B	6	ALA	4.6
1	B	273	VAL	4.6
1	B	191	SER	4.5
1	B	275	PHE	4.5
1	B	36	ASP	4.4
1	B	13	PRO	4.3
1	B	227	ARG	4.3
1	B	41	GLY	4.3
1	B	102	PRO	4.2
1	B	68	ALA	4.2
1	B	197	GLN	4.2
1	B	119	ILE	4.1
1	B	252	GLU	4.1
1	B	194	PHE	4.1
1	B	162	ASN	4.1
1	B	208	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	360	ILE	4.0
1	B	42	PHE	4.0
1	B	121	ILE	4.0
1	B	94	THR	3.9
1	B	196	GLY	3.9
1	B	280	ASP	3.9
1	B	66	VAL	3.9
1	B	287	GLY	3.8
1	B	17	ARG	3.8
1	B	88	HIS	3.8
1	B	290	SER	3.7
1	B	123	ASN	3.7
1	B	12	VAL	3.7
1	B	128	ASN	3.7
1	B	96	TRP	3.6
1	B	149	THR	3.6
1	B	207	LEU	3.6
1	B	11	HIS	3.5
1	B	122	HIS	3.5
1	A	78	ASP	3.4
1	A	49	ASP	3.4
1	B	186	ALA	3.4
1	B	64	GLY	3.4
1	B	99	HIS	3.3
1	B	204	GLY	3.3
1	B	193	HIS	3.2
1	B	14	ARG	3.2
1	B	84	GLU	3.1
1	B	8	LEU	3.1
1	A	50	TRP	3.0
1	B	108	HIS	3.0
1	B	260	ALA	3.0
1	A	45	GLY	3.0
1	B	27	LEU	3.0
1	A	294	ILE	3.0
1	A	295	LYS	3.0
1	A	143	PHE	3.0
1	A	114	LYS	2.9
1	B	670	PHE	2.9
1	A	75	LYS	2.9
1	A	158	TYR	2.9
1	B	98	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	97	ALA	2.9
1	B	192	VAL	2.8
1	B	32	TYR	2.8
1	A	48	LYS	2.8
1	A	54	ALA	2.8
1	B	346	PHE	2.8
1	A	142	ASP	2.8
1	B	508	LEU	2.8
1	B	347	ASP	2.8
1	A	47	ASP	2.7
1	A	357	LYS	2.7
1	B	175	GLU	2.7
1	B	628	ILE	2.7
1	B	474	SER	2.7
1	A	225	LEU	2.7
1	B	253	LYS	2.6
1	B	72	GLU	2.6
1	B	277	GLU	2.6
1	B	293	ARG	2.6
1	A	361	LYS	2.6
1	B	271	ASN	2.6
1	B	103	SER	2.6
1	B	21	GLU	2.5
1	B	261	SER	2.5
1	B	361	LYS	2.5
1	A	38	ALA	2.5
1	B	125	ILE	2.5
1	A	672	ARG	2.5
1	B	671	PRO	2.4
1	B	206	PRO	2.4
1	A	83	ILE	2.4
1	B	101	GLU	2.4
1	B	504	LYS	2.4
1	B	23	LEU	2.4
1	A	76	GLN	2.3
1	B	349	TYR	2.3
1	B	473	ALA	2.3
1	A	61	LYS	2.3
1	B	472	VAL	2.3
1	A	141	TYR	2.3
1	B	256	GLU	2.3
1	B	95	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	593	ILE	2.2
1	B	265	ALA	2.2
1	A	73	VAL	2.2
1	A	102	PRO	2.2
1	B	104	PRO	2.1
1	A	85	PHE	2.1
1	B	264	SER	2.1
1	B	127	THR	2.1
1	B	635	ILE	2.1
1	A	101	GLU	2.1
1	A	42	PHE	2.1
1	B	623	GLU	2.1
1	B	638	PRO	2.1
1	A	97	ALA	2.1
1	B	188	VAL	2.1
1	A	224	ILE	2.0
1	B	595	ARG	2.0
1	A	41	GLY	2.0
1	B	426	THR	2.0
1	B	429	THR	2.0
1	A	136	LEU	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 monosaccharides 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	0.93	0.17	90,93,110,110	0
2	G6Q	B	701	16/16	0.95	0.33	61,67,81,89	0

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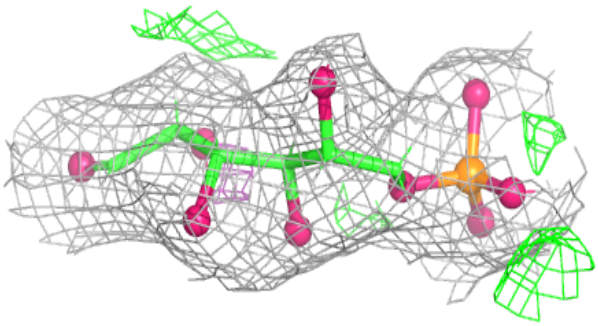
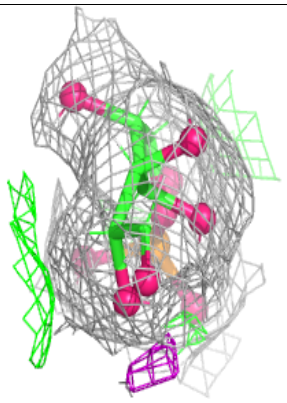
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	G6Q	A	701	16/16	0.95	0.34	54,60,71,81	0

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:

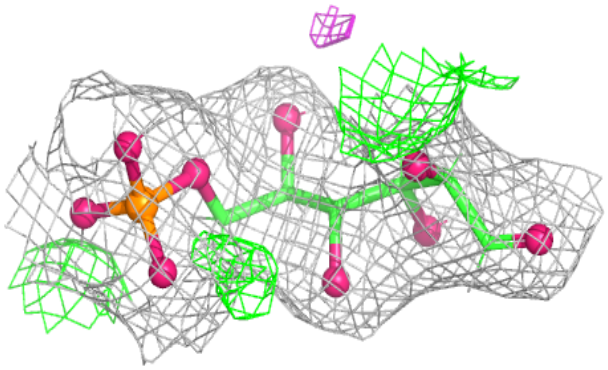
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

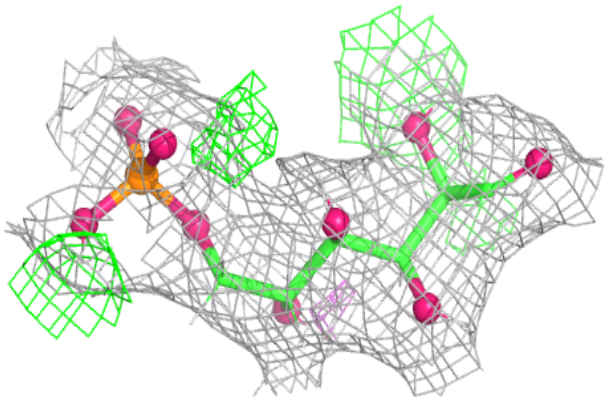


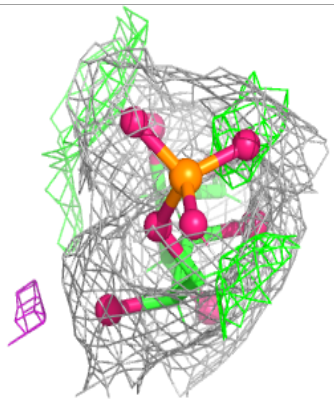


Electron density around G6Q A 701:

$2mF_o$-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.