Full wwPDB X-ray Structure Validation Report (i)

Jan 14, 2024 – 12:18 pm GMT

PDB ID	:	6R4J
Title	:	Crystal structure of human GFAT-1 G451E in complex with UDP-GlcNAc
Authors	:	Ruegenberg, S.; Horn, M.; Pichlo, C.; Allmeroth, K.; Baumann, U.; Denzel, M.S.
Deposited on	:	2019-03-22
Resolution	:	2.42 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:

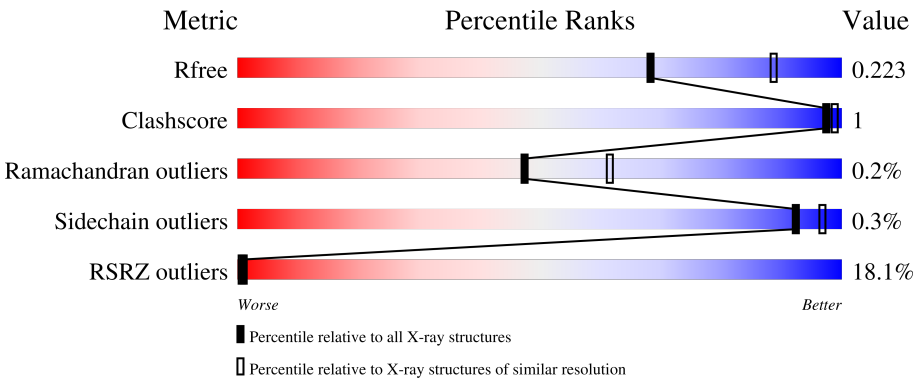
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.42 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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	4% 92% • 6%
1	B	687	31% 93% • 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 21010 atoms, of which 10440 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.

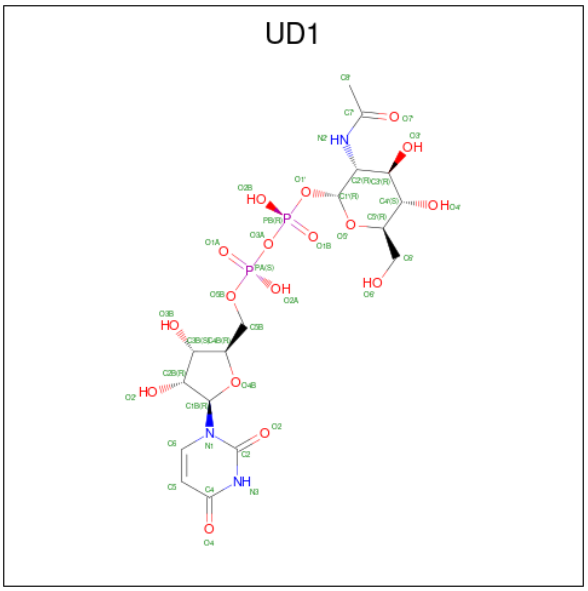
- Molecule 1 is a protein called Glutamine--fructose-6-phosphate aminotransferase [isomerizing] 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	649	10304	3248	5161	895	968	32	0	0	0
1	B	654	10377	3270	5198	899	978	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	451	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	451	GLU	GLY	engineered mutation	UNP Q06210

- Molecule 2 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$).

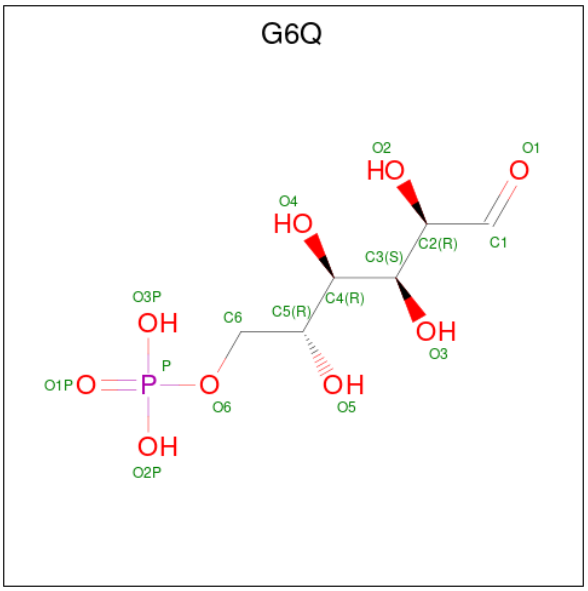


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
2	A	1	64	17	25	3	17	2	0	0
			Total	C	H	N	O	P		
2	B	1	64	17	25	3	17	2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

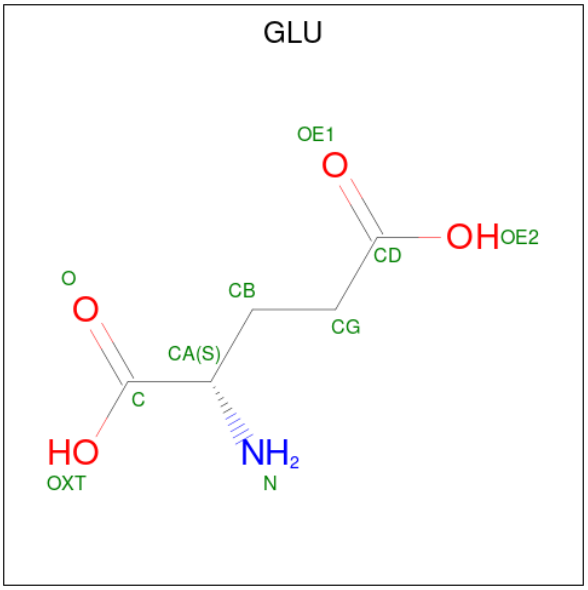
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
			Total	Mg		
3	B	1	1	1	0	0

- Molecule 4 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		
4	A	1	29	6	13	9	1	0	0
			Total	C	H	O	P		
4	B	1	29	6	13	9	1	0	0

- Molecule 5 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



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

- Molecule 6 is water.

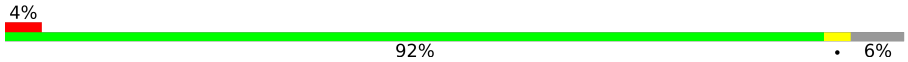
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	79	79	79	0	0
			Total	O		
6	B	47	47	47	0	0

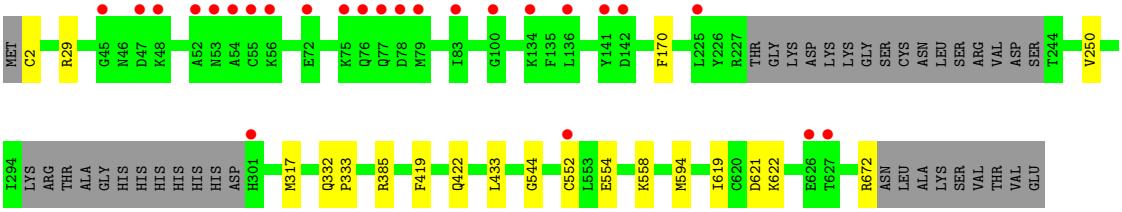
3 Residue-property plots (i)

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

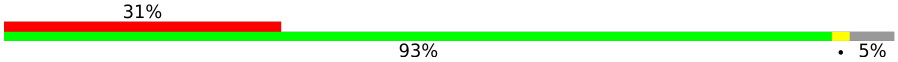
Chain A:

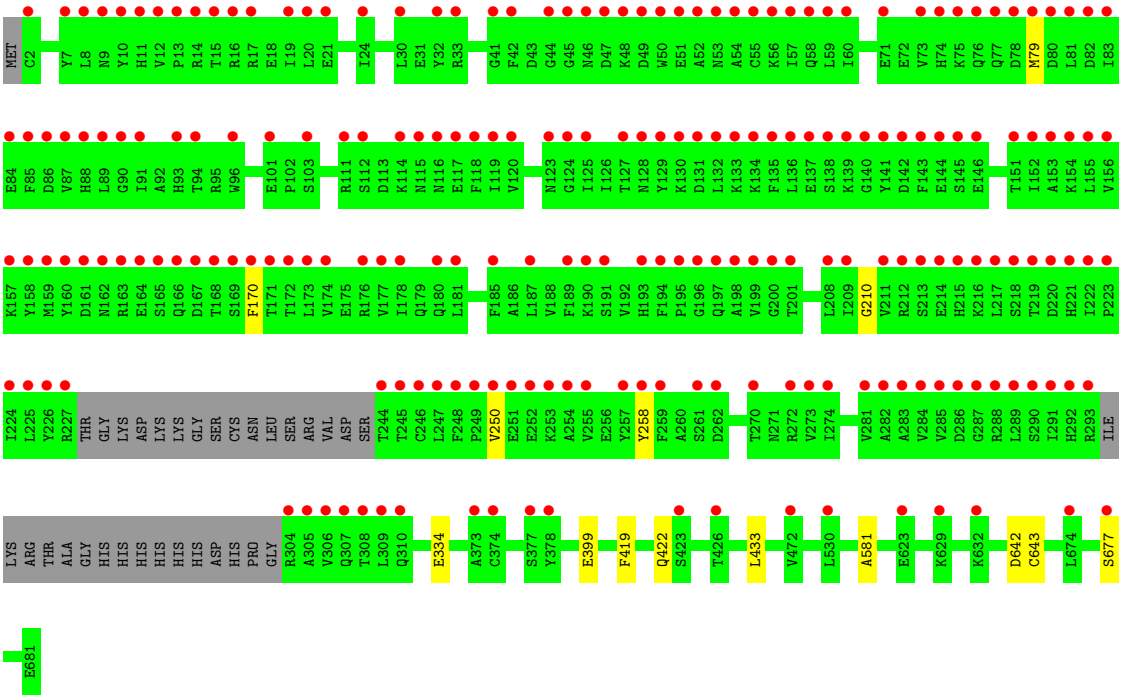




• Molecule 1: Glutamine--fructose-6-phosphate aminotransferase [isomerizing] 1

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	153.23Å 153.23Å 162.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.73 – 2.42 48.73 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.73-2.42) 96.4 (48.73-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.42Å)	Xtriage
Refinement program	PHENIX (dev_2499: ???)	Depositor
R, R_{free}	0.194 , 0.223 0.194 , 0.223	Depositor DCC
R_{free} test set	1991 reflections (2.69%)	wwPDB-VP
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 47.6	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	0.95	EDS
Total number of atoms	21010	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: UD1, MG, 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	0/5232	0.42	0/7061
1	B	0.24	0/5267	0.42	0/7109
All	All	0.24	0/10499	0.42	0/14170

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	5143	5161	5160	12	0
1	B	5179	5198	5197	7	0
2	A	39	25	25	0	0
2	B	39	25	25	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	16	13	11	2	0
4	B	16	13	11	1	0
5	A	10	5	5	1	0
6	A	79	0	0	0	0
6	B	47	0	0	0	0
All	All	10570	10440	10434	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:A:558:LYS:NZ	4:A:703:G6Q:O1	2.15	0.79
1:A:422:GLN:N	4:A:703:G6Q:O2P	2.27	0.68
1:A:621:ASP:OD1	1:A:622:LYS:N	2.34	0.59
1:B:210:GLY:O	1:B:258:TYR:N	2.42	0.51
1:B:334:GLU:OE1	1:B:334:GLU:N	2.47	0.48
1:A:672:ARG:NH1	1:B:581:ALA:O	2.47	0.47
1:A:29:ARG:NH1	1:A:317:MET:SD	2.88	0.47
1:A:544:GLY:N	1:A:552:CYS:SG	2.89	0.46
1:B:422:GLN:N	4:B:703:G6Q:O3P	2.40	0.46
1:A:332:GLN:N	1:A:333:PRO:CD	2.81	0.43
1:B:419:PHE:CZ	1:B:433:LEU:HA	2.53	0.43
1:A:419:PHE:CZ	1:A:433:LEU:HA	2.53	0.42
1:A:594:MET:HE1	1:A:619:ILE:HG22	2.01	0.42
1:A:2:CYS:N	5:A:704:GLU:OE1	2.52	0.42
1:B:642:ASP:OD1	1:B:643:CYS:N	2.52	0.42
1:A:385:ARG:NH2	1:B:399:GLU:OE2	2.42	0.41
1:A:554:GLU:OE2	1:A:558:LYS:HE3	2.21	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	643/687 (94%)	629 (98%)	13 (2%)	1 (0%)	47	61
1	B	648/687 (94%)	628 (97%)	18 (3%)	2 (0%)	41	54
All	All	1291/1374 (94%)	1257 (97%)	31 (2%)	3 (0%)	47	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	250	VAL
1	B	677	SER
1	A	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	567/602 (94%)	566 (100%)	1 (0%)	93 97
1	B	572/602 (95%)	570 (100%)	2 (0%)	92 97
All	All	1139/1204 (95%)	1136 (100%)	3 (0%)	92 97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	PHE
1	B	79	MET
1	B	170	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)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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	UD1	B	701	3	38,41,41	3.11	18 (47%)	57,62,62	1.50	9 (15%)
4	G6Q	B	703	-	14,15,15	0.43	0	20,21,21	0.80	0
4	G6Q	A	703	-	14,15,15	0.43	0	20,21,21	0.85	1 (5%)
2	UD1	A	701	3	38,41,41	3.10	18 (47%)	57,62,62	1.47	7 (12%)
5	GLU	A	704	-	8,9,9	1.07	1 (12%)	10,11,11	1.29	2 (20%)

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	UD1	B	701	3	-	6/26/63/63	0/3/3/3
4	G6Q	B	703	-	-	5/18/20/20	-
4	G6Q	A	703	-	-	5/18/20/20	-
2	UD1	A	701	3	-	1/26/63/63	0/3/3/3
5	GLU	A	704	-	-	2/9/9/9	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	UD1	C3B-C2B	-8.20	1.30	1.53
2	A	701	UD1	C3B-C2B	-8.16	1.31	1.53
2	A	701	UD1	C2-N1	7.01	1.49	1.38
2	B	701	UD1	C2-N1	6.97	1.49	1.38
2	B	701	UD1	C2-N3	6.97	1.50	1.38
2	A	701	UD1	C2-N3	6.92	1.50	1.38
2	B	701	UD1	C6-C5	5.69	1.48	1.35
2	A	701	UD1	C6-C5	5.63	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	UD1	O4B-C1B	-4.94	1.30	1.42
2	B	701	UD1	O4B-C1B	-4.90	1.30	1.42
2	B	701	UD1	O4B-C4B	4.40	1.54	1.45
2	A	701	UD1	O4B-C4B	4.38	1.54	1.45
2	B	701	UD1	C4-N3	4.24	1.46	1.38
2	A	701	UD1	C4-N3	4.18	1.46	1.38
2	B	701	UD1	C5B-C4B	-3.50	1.40	1.51
2	A	701	UD1	C5B-C4B	-3.44	1.40	1.51
2	B	701	UD1	O5'-C1'	3.35	1.50	1.41
2	A	701	UD1	O5'-C1'	3.31	1.50	1.41
2	B	701	UD1	C7'-N2'	3.21	1.45	1.34
2	A	701	UD1	C7'-N2'	3.12	1.45	1.34
2	A	701	UD1	O3B-C3B	2.99	1.50	1.43
2	B	701	UD1	O3B-C3B	2.99	1.50	1.43
2	A	701	UD1	C6-N1	2.96	1.45	1.38
2	B	701	UD1	C6-N1	2.92	1.45	1.38
2	A	701	UD1	C2B-C1B	2.82	1.62	1.53
2	B	701	UD1	C2B-C1B	2.80	1.62	1.53
2	B	701	UD1	O4-C4	-2.79	1.19	1.24
2	A	701	UD1	O4-C4	-2.71	1.19	1.24
2	B	701	UD1	C2'-N2'	2.43	1.49	1.45
2	B	701	UD1	C5-C4	2.38	1.48	1.43
2	A	701	UD1	C5-C4	2.35	1.48	1.43
2	A	701	UD1	C3'-C2'	-2.28	1.48	1.53
2	A	701	UD1	C2'-N2'	2.26	1.49	1.45
2	A	701	UD1	O2-C2	-2.25	1.18	1.23
2	B	701	UD1	O2-C2	-2.22	1.19	1.23
2	B	701	UD1	C3'-C2'	-2.20	1.49	1.53
5	A	704	GLU	OXT-C	-2.12	1.23	1.30

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	UD1	C4-N3-C2	-5.14	119.80	126.58
2	A	701	UD1	C4-N3-C2	-5.03	119.94	126.58
2	A	701	UD1	O3A-PB-O1'	3.55	109.65	102.48
2	B	701	UD1	N3-C2-N1	3.55	119.60	114.89
2	A	701	UD1	N3-C2-N1	3.47	119.49	114.89
2	B	701	UD1	C5-C4-N3	3.33	119.82	114.84
2	A	701	UD1	C5-C4-N3	3.31	119.80	114.84
2	B	701	UD1	O3A-PB-O1'	3.31	109.15	102.48
2	A	701	UD1	O4-C4-C5	-2.96	119.96	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	UD1	O4-C4-C5	-2.90	120.07	125.16
2	B	701	UD1	C8'-C7'-N2'	2.78	120.80	116.10
5	A	704	GLU	OXT-C-O	-2.70	117.95	124.09
2	B	701	UD1	PB-O3A-PA	-2.43	124.48	132.83
5	A	704	GLU	OXT-C-CA	2.27	121.10	113.38
2	A	701	UD1	C8'-C7'-N2'	2.18	119.78	116.10
2	A	701	UD1	PB-O3A-PA	-2.17	125.39	132.83
4	A	703	G6Q	O2-C2-C3	2.14	114.54	109.46
2	B	701	UD1	C3B-C2B-C1B	2.08	105.38	101.43
2	B	701	UD1	O2-C2-N1	-2.04	120.08	122.79

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	UD1	PA-O3A-PB-O1'
2	B	701	UD1	C5B-O5B-PA-O1A
4	A	703	G6Q	O2-C2-C3-C4
4	A	703	G6Q	O2-C2-C3-O3
4	A	703	G6Q	C4-C5-C6-O6
4	B	703	G6Q	C1-C2-C3-C4
4	B	703	G6Q	O2-C2-C3-C4
4	B	703	G6Q	O2-C2-C3-O3
4	B	703	G6Q	C4-C5-C6-O6
2	B	701	UD1	C8'-C7'-N2'-C2'
2	B	701	UD1	O7'-C7'-N2'-C2'
4	B	703	G6Q	C1-C2-C3-O3
2	B	701	UD1	C1'-C2'-N2'-C7'
4	A	703	G6Q	C1-C2-C3-O3
2	B	701	UD1	O5'-C5'-C6'-O6'
4	A	703	G6Q	C1-C2-C3-C4
5	A	704	GLU	OE2-CD-CG-CB
5	A	704	GLU	OE1-CD-CG-CB
2	B	701	UD1	C3'-C2'-N2'-C7'

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	703	G6Q	1	0
4	A	703	G6Q	2	0

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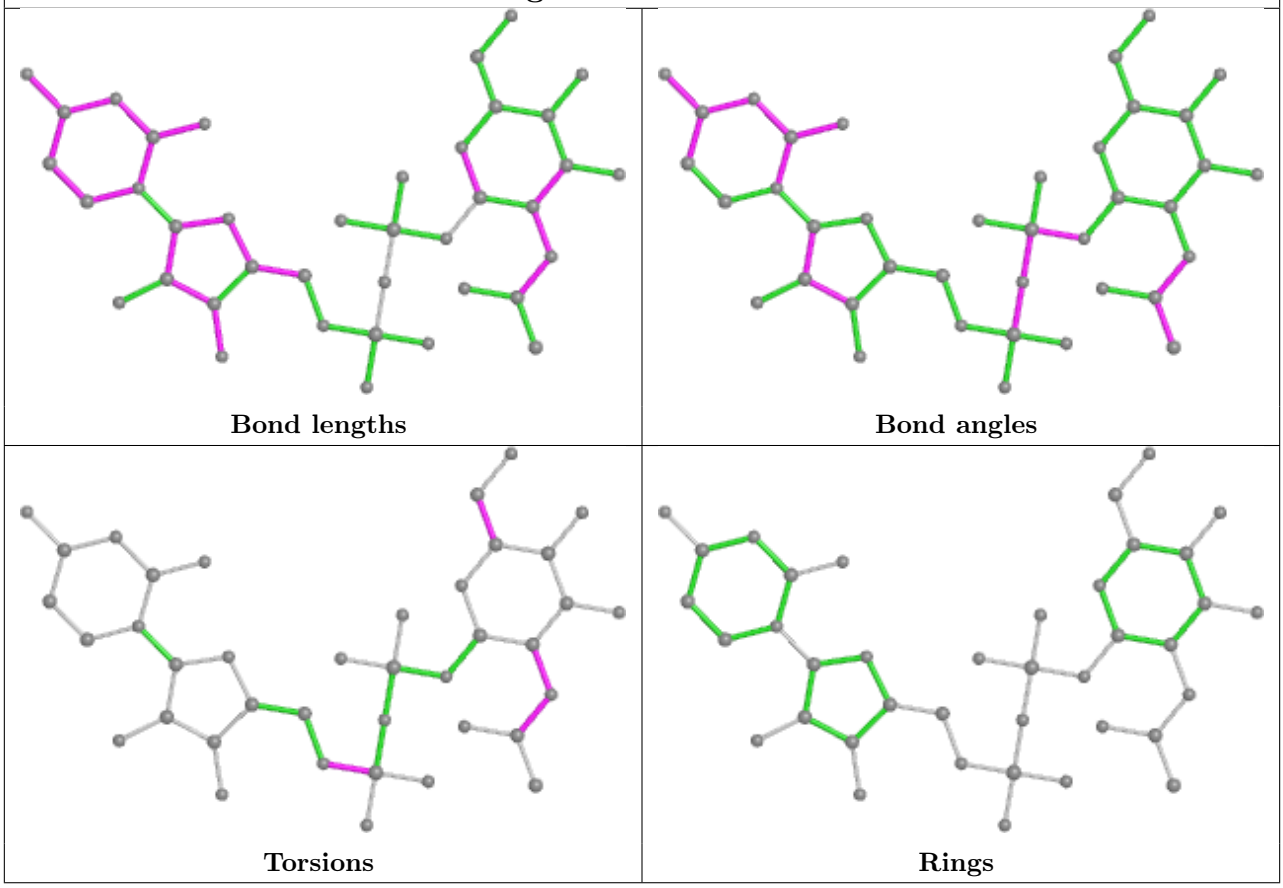
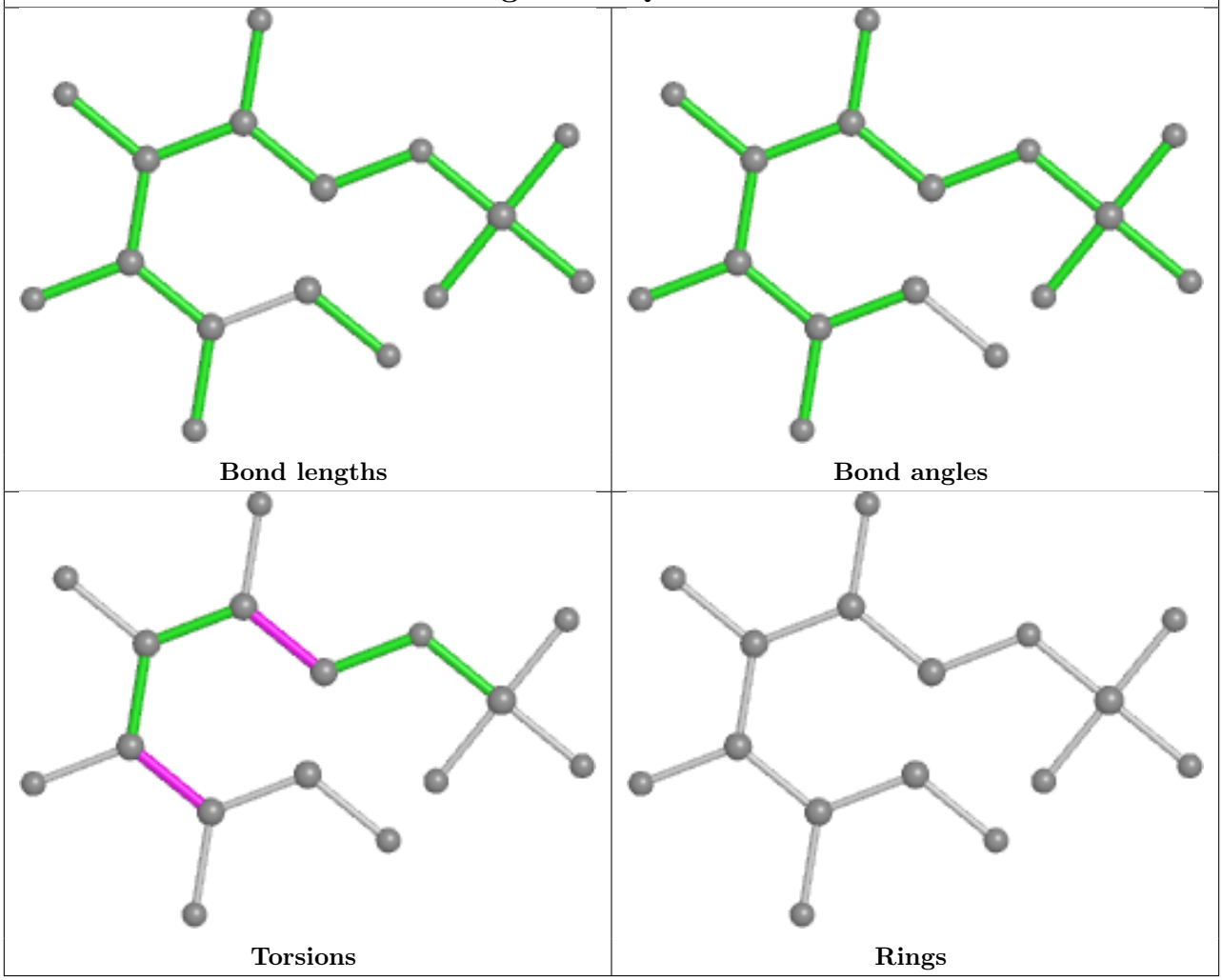
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	704	GLU	1	0

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.

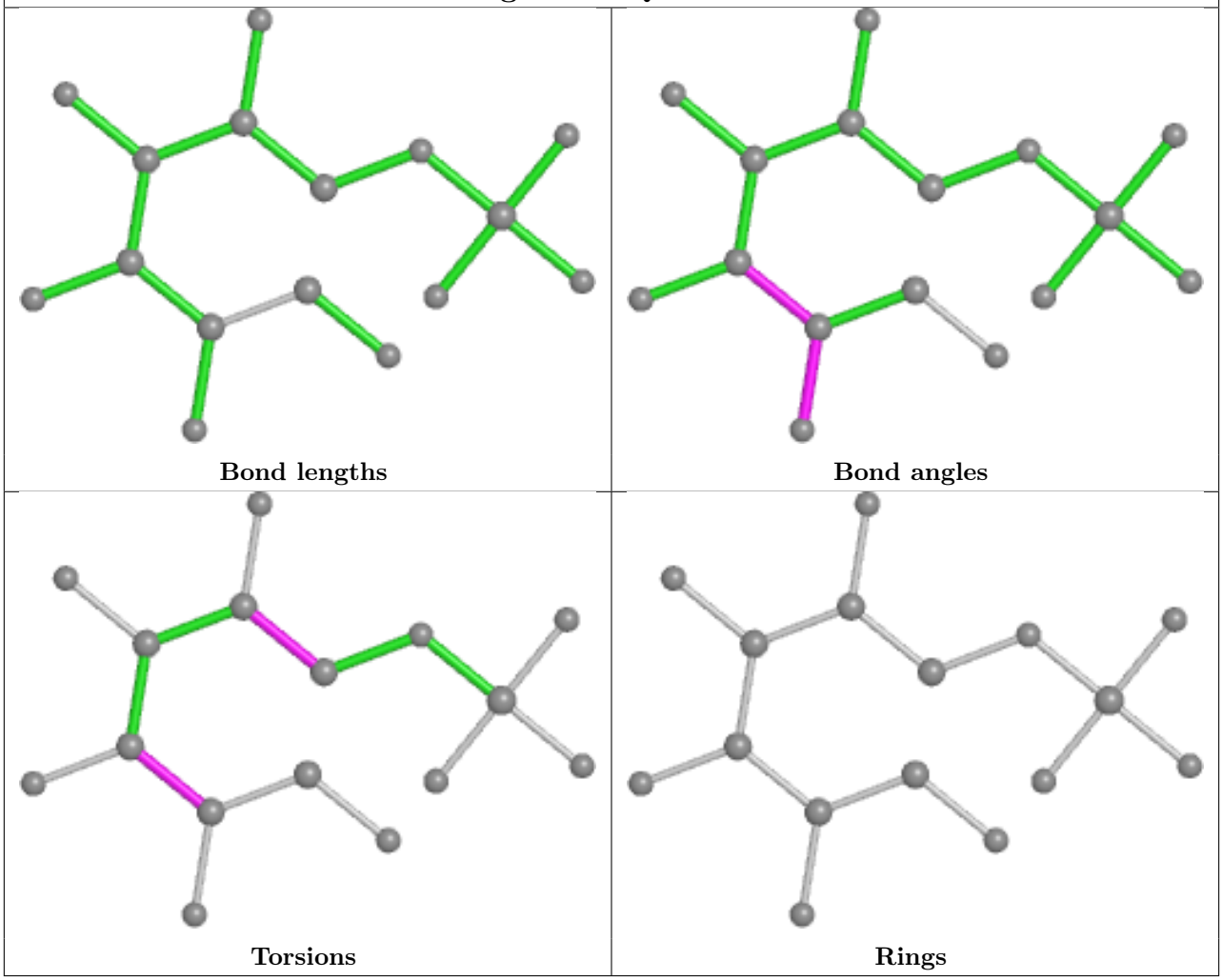
Ligand UD1 B 701



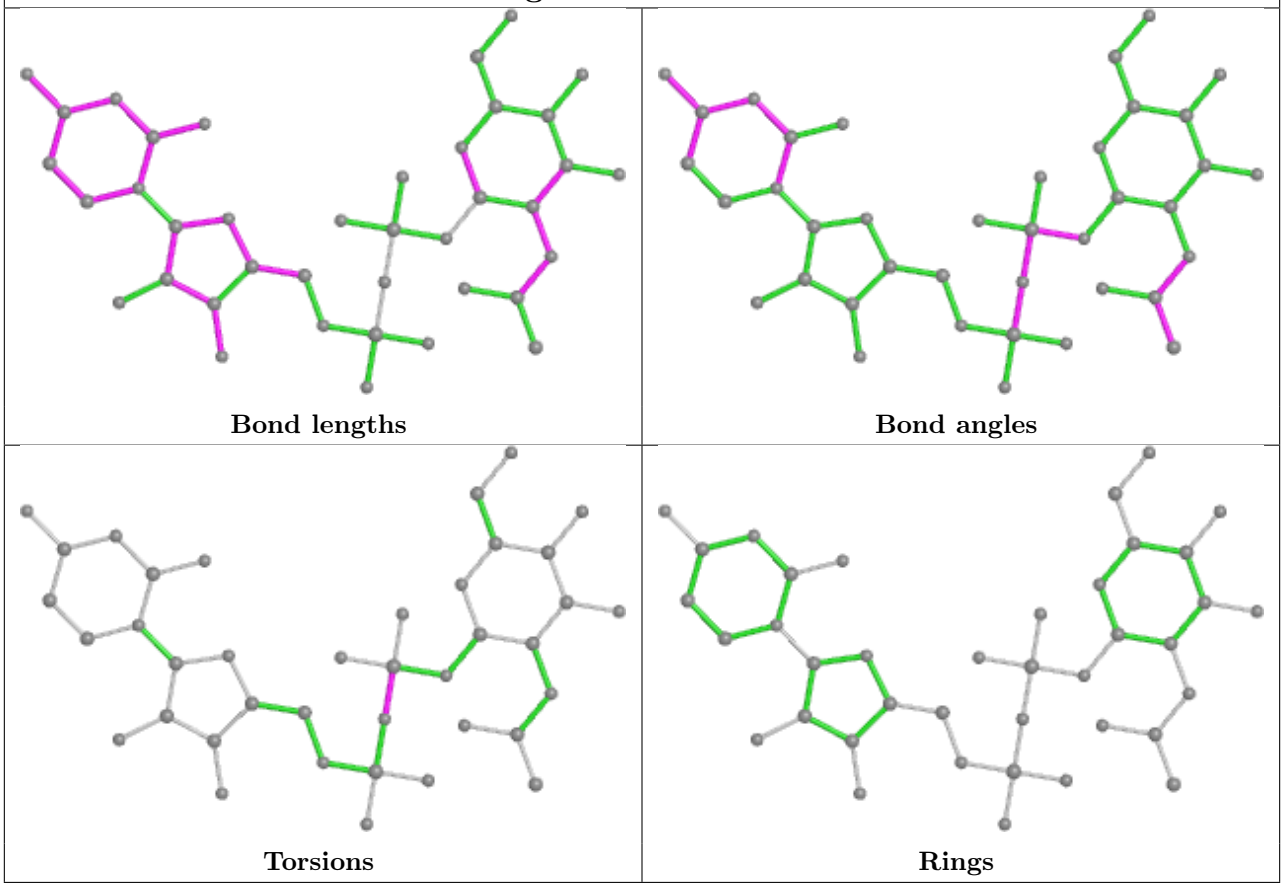
Ligand G6Q B 703



Ligand G6Q A 703



Ligand UD1 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 (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	649/687 (94%)	0.29	25 (3%)	39	37	33, 52, 102, 156	0
1	B	654/687 (95%)	1.98	211 (32%)	0	0	35, 76, 188, 251	0
All	All	1303/1374 (94%)	1.14	236 (18%)	1	1	33, 58, 174, 251	0

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	170	PHE	13.0
1	B	250	VAL	13.0
1	B	255	VAL	12.5
1	B	89	LEU	12.3
1	B	225	LEU	12.3
1	B	54	ALA	11.9
1	B	198	ALA	10.6
1	B	155	LEU	10.4
1	B	159	MET	10.1
1	B	55	CYS	10.1
1	B	247	LEU	9.7
1	B	90	GLY	9.6
1	B	168	THR	9.2
1	B	174	VAL	9.2
1	B	257	TYR	9.0
1	B	249	PRO	9.0
1	B	45	GLY	8.9
1	B	217	LEU	8.8
1	B	20	LEU	8.8
1	B	46	ASN	8.7
1	B	226	TYR	8.7
1	B	81	LEU	8.7
1	B	222	ILE	8.5
1	B	47	ASP	8.4

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Mol	Chain	Res	Type	RSRZ
1	B	129	TYR	8.4
1	B	79	MET	8.1
1	B	17	ARG	8.0
1	B	246	CYS	8.0
1	B	248	PHE	8.0
1	B	215	HIS	7.9
1	B	132	LEU	7.9
1	B	169	SER	7.7
1	B	214	GLU	7.7
1	B	11	HIS	7.7
1	B	48	LYS	7.7
1	B	75	LYS	7.7
1	B	306	VAL	7.6
1	B	223	PRO	7.6
1	B	143	PHE	7.6
1	B	19	ILE	7.5
1	B	274	ILE	7.5
1	B	50	TRP	7.5
1	B	53	ASN	7.5
1	B	160	TYR	7.4
1	B	153	ALA	7.3
1	B	158	TYR	7.3
1	B	77	GLN	7.3
1	B	51	GLU	7.2
1	B	281	VAL	7.2
1	B	118	PHE	7.0
1	B	259	PHE	6.8
1	B	173	LEU	6.7
1	B	216	LYS	6.7
1	B	114	LYS	6.7
1	B	305	ALA	6.6
1	B	199	VAL	6.5
1	B	85	PHE	6.5
1	B	56	LYS	6.4
1	B	57	ILE	6.4
1	B	52	ALA	6.4
1	B	245	THR	6.4
1	B	253	LYS	6.4
1	A	75	LYS	6.3
1	B	219	THR	6.2
1	B	284	VAL	6.2
1	B	130	LYS	6.2

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Mol	Chain	Res	Type	RSRZ
1	B	291	ILE	6.2
1	B	244	THR	6.2
1	B	134	LYS	6.2
1	B	272	ARG	6.1
1	B	258	TYR	6.1
1	B	309	LEU	6.1
1	B	292	HIS	6.1
1	B	286	ASP	6.0
1	B	44	GLY	5.9
1	B	213	SER	5.8
1	B	196	GLY	5.8
1	B	251	GLU	5.8
1	B	197	GLN	5.7
1	B	282	ALA	5.7
1	B	287	GLY	5.7
1	B	12	VAL	5.6
1	B	78	ASP	5.5
1	B	137	GLU	5.4
1	B	166	GLN	5.4
1	B	167	ASP	5.4
1	B	135	PHE	5.3
1	B	58	GLN	5.3
1	B	7	TYR	5.3
1	B	13	PRO	5.3
1	B	120	VAL	5.2
1	B	156	VAL	5.2
1	B	164	GLU	5.2
1	B	83	ILE	5.2
1	B	116	ASN	5.1
1	B	142	ASP	5.1
1	B	133	LYS	5.1
1	B	87	VAL	5.1
1	B	152	ILE	5.1
1	B	127	THR	5.1
1	B	131	ASP	5.1
1	B	220	ASP	5.0
1	B	308	THR	5.0
1	B	221	HIS	5.0
1	B	2	CYS	4.9
1	B	211	VAL	4.9
1	B	136	LEU	4.9
1	B	94	THR	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	176	ARG	4.9
1	A	45	GLY	4.9
1	B	111	ARG	4.9
1	B	154	LYS	4.9
1	B	177	VAL	4.9
1	B	76	GLN	4.9
1	B	224	ILE	4.8
1	B	283	ALA	4.8
1	B	289	LEU	4.8
1	B	15	THR	4.7
1	B	146	GLU	4.7
1	B	115	ASN	4.6
1	B	285	VAL	4.6
1	B	172	THR	4.5
1	B	161	ASP	4.5
1	B	162	ASN	4.5
1	B	252	GLU	4.5
1	B	86	ASP	4.5
1	B	59	LEU	4.4
1	B	73	VAL	4.4
1	B	304	ARG	4.4
1	B	84	GLU	4.4
1	B	273	VAL	4.3
1	B	194	PHE	4.3
1	B	42	PHE	4.3
1	B	119	ILE	4.3
1	B	49	ASP	4.2
1	B	16	ARG	4.2
1	B	10	TYR	4.2
1	B	193	HIS	4.2
1	B	310	GLN	4.2
1	B	138	SER	4.2
1	A	48	LYS	4.2
1	B	24	ILE	4.2
1	B	124	GLY	4.1
1	B	139	LYS	4.1
1	B	189	PHE	4.1
1	B	80	ASP	4.1
1	A	76	GLN	4.1
1	B	128	ASN	4.0
1	A	78	ASP	4.0
1	B	112	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	181	LEU	3.8
1	B	32	TYR	3.7
1	B	180	GLN	3.7
1	B	140	GLY	3.6
1	A	77	GLN	3.6
1	B	307	GLN	3.6
1	B	14	ARG	3.6
1	B	187	LEU	3.5
1	B	157	LYS	3.5
1	B	218	SER	3.5
1	B	103	SER	3.5
1	B	74	HIS	3.5
1	B	33	ARG	3.4
1	B	163	ARG	3.4
1	A	79	MET	3.4
1	B	9	ASN	3.3
1	B	165	SER	3.2
1	B	290	SER	3.2
1	B	195	PRO	3.2
1	B	178	ILE	3.1
1	B	227	ARG	3.1
1	B	82	ASP	3.1
1	B	200	GLY	3.1
1	B	254	ALA	3.1
1	B	191	SER	3.0
1	B	293	ARG	3.0
1	B	141	TYR	2.9
1	B	117	GLU	2.9
1	B	91	ILE	2.9
1	B	674	LEU	2.9
1	B	185	PHE	2.8
1	B	190	LYS	2.8
1	B	171	THR	2.8
1	B	201	THR	2.7
1	B	71	GLU	2.7
1	B	151	THR	2.7
1	B	145	SER	2.7
1	B	288	ARG	2.6
1	B	632	LYS	2.6
1	B	261	SER	2.6
1	A	225	LEU	2.6
1	A	72	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	677	SER	2.6
1	A	54	ALA	2.6
1	B	426	THR	2.6
1	B	472	VAL	2.6
1	A	627	THR	2.6
1	B	88	HIS	2.6
1	A	142	ASP	2.6
1	A	136	LEU	2.5
1	B	60	ILE	2.5
1	A	301	HIS	2.5
1	B	209	ILE	2.5
1	B	629	LYS	2.5
1	B	212	ARG	2.5
1	B	30	LEU	2.5
1	A	53	ASN	2.5
1	A	100	GLY	2.5
1	A	47	ASP	2.4
1	A	626	GLU	2.4
1	B	41	GLY	2.4
1	B	270	THR	2.4
1	A	141	TYR	2.4
1	B	8	LEU	2.4
1	A	134	LYS	2.4
1	B	93	HIS	2.4
1	A	52	ALA	2.4
1	B	530	LEU	2.4
1	B	423	SER	2.3
1	B	125	ILE	2.3
1	B	208	LEU	2.3
1	B	373	ALA	2.3
1	A	56	LYS	2.2
1	B	123	ASN	2.2
1	B	262	ASP	2.2
1	B	378	TYR	2.2
1	A	83	ILE	2.2
1	B	374	CYS	2.2
1	A	552	CYS	2.1
1	B	96	TRP	2.1
1	B	144	GLU	2.1
1	B	101	GLU	2.1
1	B	377	SER	2.1
1	A	55	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	21	GLU	2.0
1	B	623	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 monosaccharides in this entry.

6.4 Ligands (i)

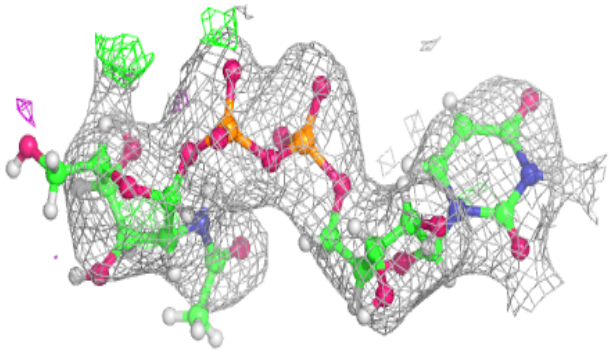
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

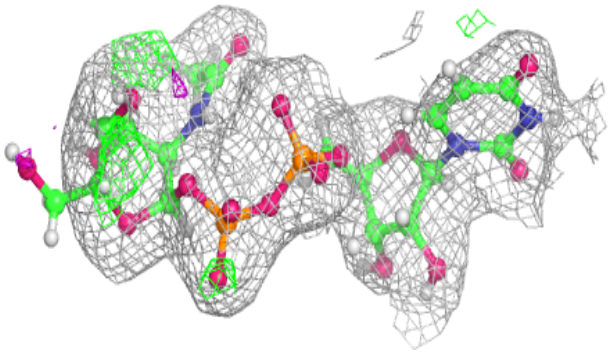
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GLU	A	704	10/10	0.90	0.17	76,80,96,96	0
3	MG	B	702	1/1	0.94	0.18	40,40,40,40	0
2	UD1	B	701	39/39	0.94	0.16	48,72,108,125	0
4	G6Q	B	703	16/16	0.96	0.27	40,49,57,63	0
2	UD1	A	701	39/39	0.97	0.14	41,55,72,79	0
4	G6Q	A	703	16/16	0.97	0.24	34,42,51,56	0
3	MG	A	702	1/1	0.98	0.21	31,31,31,31	0

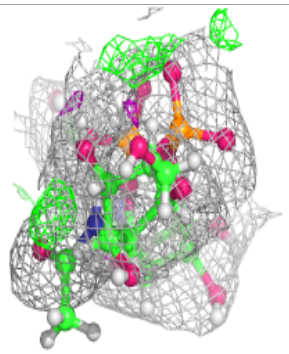
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UD1 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)

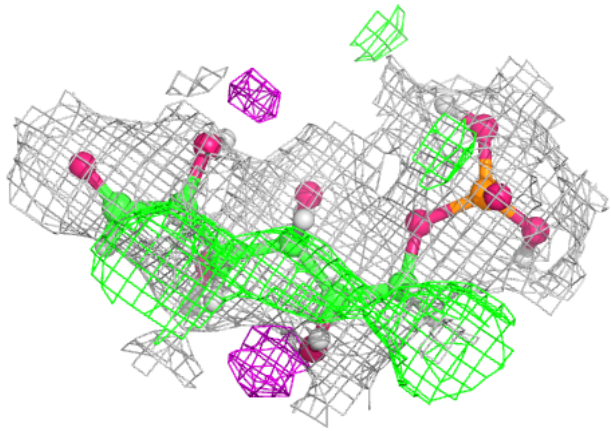


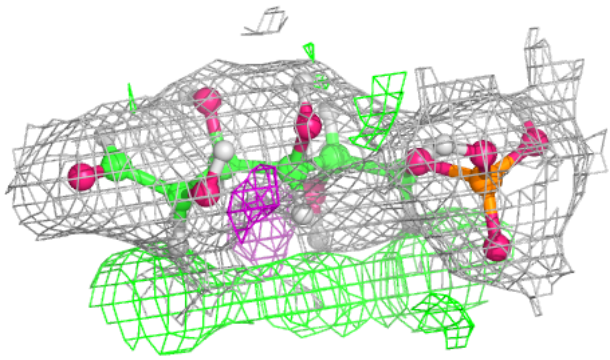


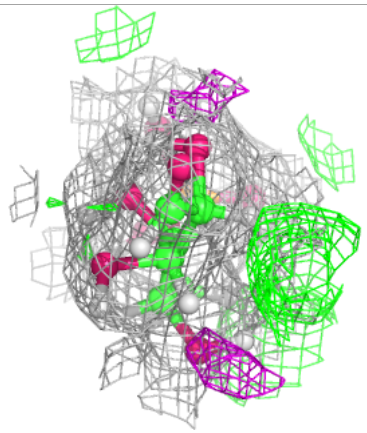


Electron density around G6Q B 703:

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

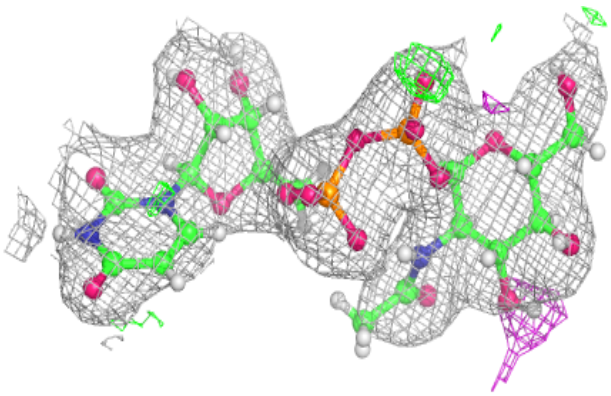


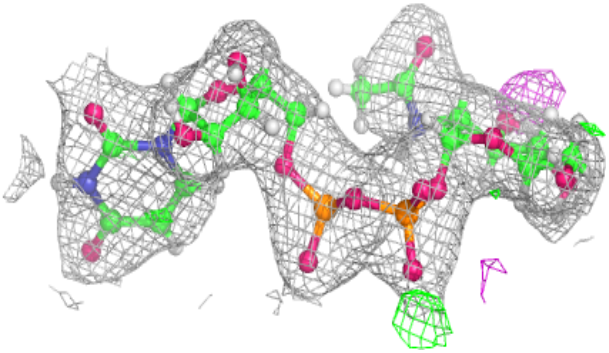


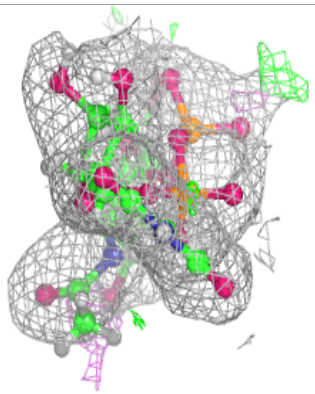


Electron density around UD1 A 701:

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

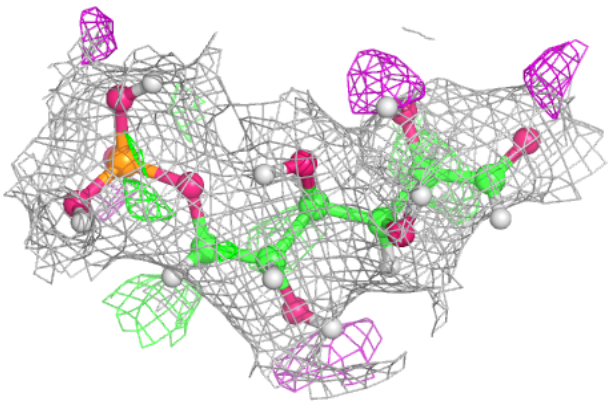


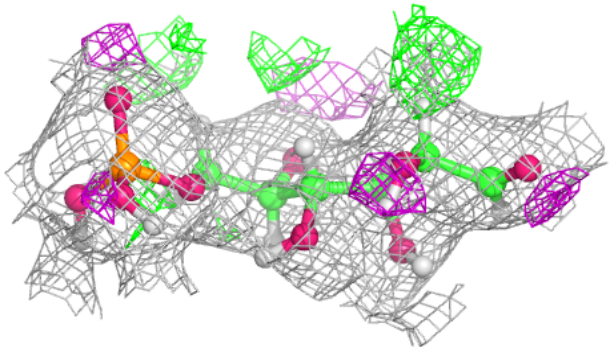


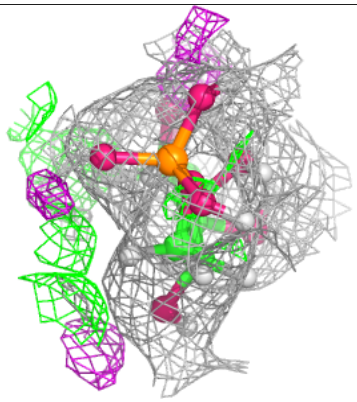


Electron density around G6Q A 703:

$2mF_o$-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.