



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 06:55 am BST

PDB ID : 1JXA
Title : GLUCOSAMINE 6-PHOSPHATE SYNTHASE WITH GLUCOSE 6-PHOSPHATE
Authors : Teplyakov, A.; Obmolova, G.; Badet, B.; Badet-Denisot, M.A.
Deposited on : 2001-09-06
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

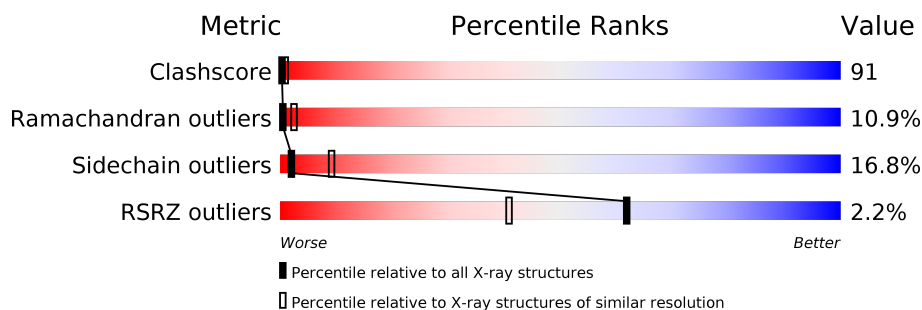
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	608	<div> <div>20%</div> <div>54%</div> <div>23%</div> <div>•</div> </div>
1	B	608	<div> <div>17%</div> <div>60%</div> <div>20%</div> <div>•</div> </div>
1	C	608	<div> <div>5%</div> <div>21%</div> <div>60%</div> <div>17%</div> <div>•</div> </div>

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
2	G6Q	A	700	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14156 atoms, of which 0 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.

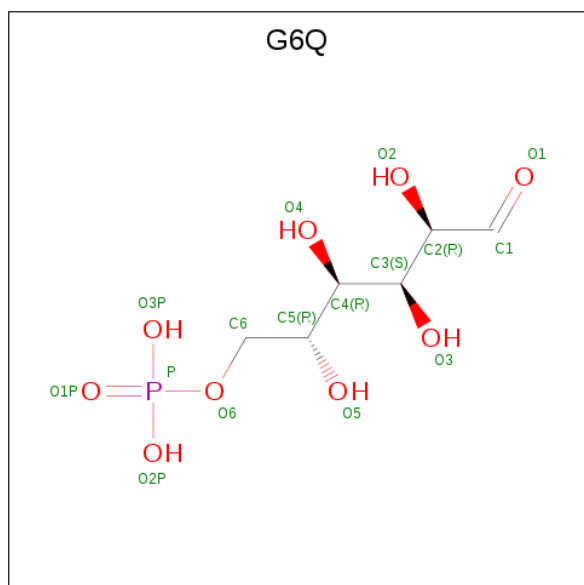
- Molecule 1 is a protein called glucosamine 6-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	608	Total	C	N	O	S	0	0	0
			4695	2953	829	896	17			
1	B	608	Total	C	N	O	S	0	0	0
			4695	2953	829	896	17			
1	C	608	Total	C	N	O	S	0	0	0
			4695	2953	829	896	17			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	421	LYS	ARG	CONFLICT	UNP P17169
B	421	LYS	ARG	CONFLICT	UNP P17169
C	421	LYS	ARG	CONFLICT	UNP P17169

- Molecule 2 is GLUCOSE-6-PHOSPHATE (three-letter code: G6P) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		

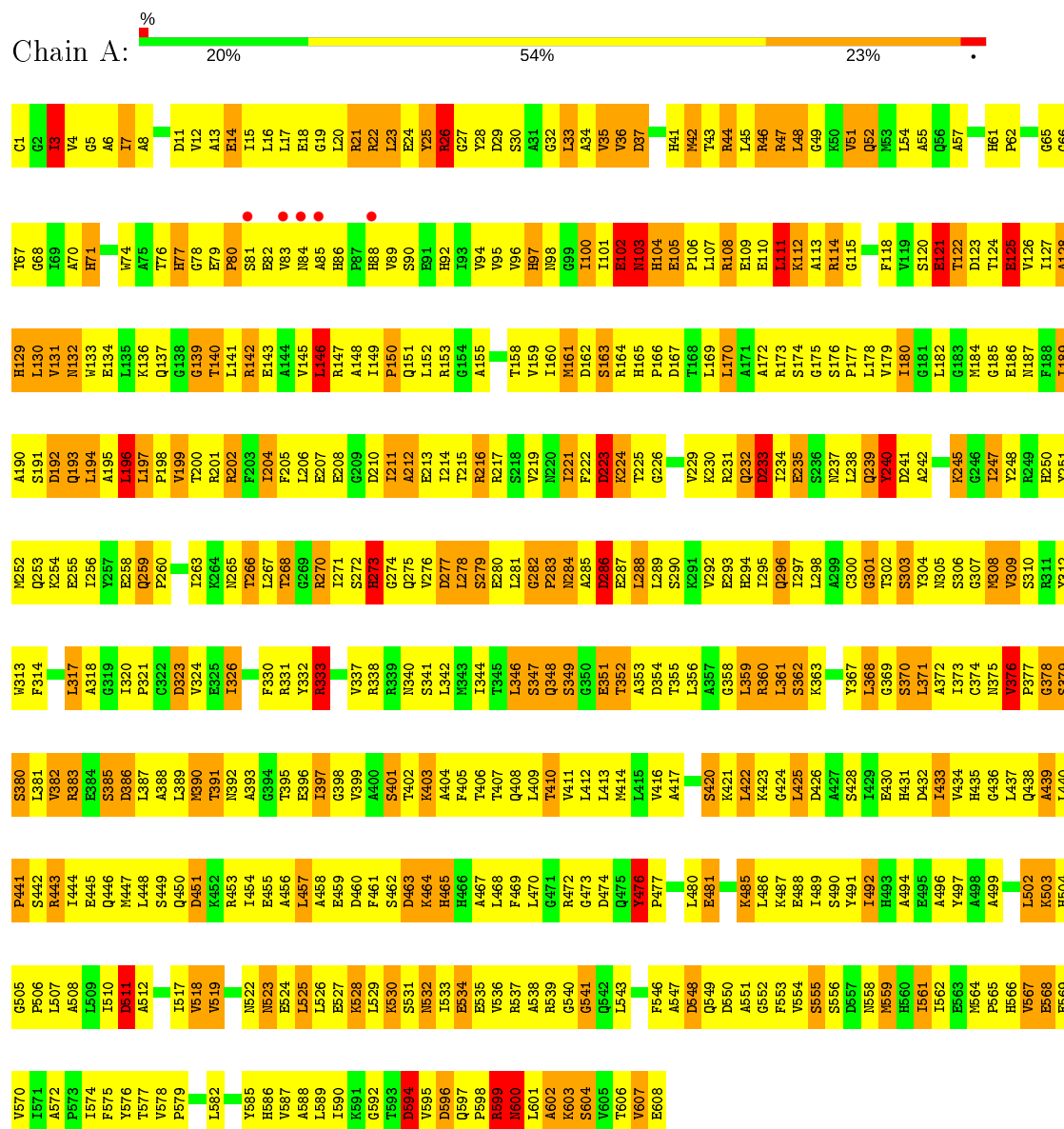
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	26	Total	O	0	0
			26	26		
3	B	10	Total	O	0	0
			10	10		
3	C	3	Total	O	0	0
			3	3		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: glucosamine 6-phosphate synthase



• Molecule 1: glucosamine 6-phosphate synthase





I571	A508	I447	R383	I320	Q253
A572	L509	I446	D386	F321	K284
P573	I510	S449	L387	C322	E256
I574	D511	Q450	A388	D323	I256
F575	M514	K451	L389	V324	Y257
F576	M517	K452	K390	E325	E258
F577	I517	K453	T391	I326	Q259
F578	V518	I454	R392	A327	P260
F579	V519	E455	A393	E328	I261
L580	P521	A456	E396	F330	I263
Q581	N522	L457	I397	R331	K264
L582	N523	A458	I397	Y332	I265
L583	E524	E459	G398	R333	T266
A584	E524	D460	V399	R334	
Y585	L525	F461	A400	S335	
H586	L526	S462	S401	R338	R270
V587	E527	D463	T402		I271
A588	K528	K464	K403		S272
L589	L529	H465	K403		
I590	K530	H466	A404		
K591	S531	A467	F405		
G592	N532	L468	T406		L278
T593	I533	F469	T407		S279
D594	E534	L470	Q408		E280
V595	E535	G471	I409		L281
D596	V536	R472	T410		G282
Q597	R537		V411		P283
P598	A538	Q475	L412		I284
R599	R539	Y476	L413		A285
N600	G540	P477	N414		D286
L601	G541	T478	L415		E287
A602	Q542	L479	V416		L288
K603	L543	L480	A417		L289
S604	Y544	E481	K418		S290
V605	Y545	Q482			K291
T606	F546	A483			V292
V607	A547	L484	K421		E293
E608	D548	K485	L422		H294
	Q549	L486	K423		I295
	D550	K487	G424		Q296
	A551	E488	L425		I297
	G552	I489	D426		L298
	F553	S490	A427		A299
	V554	Y491	S428		C300
	S555	L492	L429		G301
	S556	H493	E430		T302
	D557	A494	D432		S303
	N558	E495	I433		Y304
	M559	A496	Y434		N305
	H560	Y497	H435		S306
	I561	A498	G436		G307
	L562	A499	L437		M308
	E563	G500	Q438		V309
	M564	P565	A439		S310
	P565	L502	L440		R311
	H566	K503	P441		F314
	V567	H504	S442		F315
	E568	G505	R443		S316
	E569	P506			S317
	V570	L507	Q446		A318
					G319

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.40 Å 112.40 Å 185.10 Å 90.00° 96.40° 90.00°	Depositor
Resolution (Å)	12.00 – 3.10 19.97 – 3.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-3.10) 92.7 (19.97-3.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 3.15 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.280 0.213 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	67.7	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 83.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14156	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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	0.82	1/4776 (0.0%)	1.34	47/6467 (0.7%)
1	B	0.67	0/4776	1.10	29/6467 (0.4%)
1	C	0.51	0/4776	0.90	18/6467 (0.3%)
All	All	0.68	1/14328 (0.0%)	1.13	94/19401 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	476	TYR	CD1-CE1	-5.16	1.31	1.39

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	ASP	CB-CG-OD2	9.78	127.10	118.30
1	A	22	ARG	NE-CZ-NH1	-8.83	115.88	120.30
1	B	47	ARG	NE-CZ-NH1	-8.83	115.89	120.30
1	B	142	ARG	NE-CZ-NH1	-8.83	115.89	120.30
1	B	114	ARG	NE-CZ-NH1	8.76	124.68	120.30

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	4695	0	4715	862	1
1	B	4695	0	4715	918	0
1	C	4695	0	4715	826	0
2	A	16	0	10	4	0
2	B	16	0	11	2	0
3	A	26	0	0	2	0
3	B	10	0	0	2	0
3	C	3	0	0	0	0
All	All	14156	0	14166	2564	1

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 91.

The worst 5 of 2564 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:100:ILE:CG1	1:A:100:ILE:CD1	1.76	1.63
1:A:304:TYR:CE1	1:A:326:ILE:HD13	1.47	1.48
1:A:304:TYR:CD1	1:A:326:ILE:CD1	2.18	1.26
1:B:484:LEU:O	1:B:485:LYS:HG2	1.27	1.25
1:B:223:ASP:OD2	1:B:225:THR:HG23	1.32	1.25

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:LYS:NZ	1:A:497:TYR:OH[2_555]	2.05	0.15

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	606/608 (100%)	417 (69%)	128 (21%)	61 (10%)	0	3
1	B	606/608 (100%)	423 (70%)	113 (19%)	70 (12%)	0	2
1	C	606/608 (100%)	374 (62%)	164 (27%)	68 (11%)	0	2
All	All	1818/1824 (100%)	1214 (67%)	405 (22%)	199 (11%)	0	2

5 of 199 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	71	HIS
1	A	77	HIS
1	A	103	ASN
1	A	111	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	500/500 (100%)	393 (79%)	107 (21%)	1	4
1	B	500/500 (100%)	422 (84%)	78 (16%)	2	11
1	C	500/500 (100%)	433 (87%)	67 (13%)	4	16
All	All	1500/1500 (100%)	1248 (83%)	252 (17%)	2	9

5 of 252 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	53	MET
1	B	232	GLN
1	C	461	PHE
1	B	86	HIS
1	B	170	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	165	HIS
1	B	375	ASN
1	C	438	GLN
1	B	187	ASN
1	B	250	HIS

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	G6Q	B	701	1	14,15,15	1.34	2 (14%)	20,21,21	1.76	5 (25%)
2	G6Q	A	700	-	14,15,15	1.89	5 (35%)	20,21,21	2.72	12 (60%)

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	1	-	6/18/20/20	-
2	G6Q	A	700	-	-	9/18/20/20	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	G6Q	O5-C5	-3.38	1.36	1.43
2	B	701	G6Q	C3-C2	-2.82	1.48	1.53
2	A	700	G6Q	P-O2P	-2.79	1.44	1.54
2	A	700	G6Q	C3-C2	-2.52	1.49	1.53
2	B	701	G6Q	O4-C4	-2.48	1.37	1.43

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	G6Q	O6-C6-C5	4.67	121.82	109.36
2	A	700	G6Q	C6-C5-C4	-4.50	103.52	112.20
2	A	700	G6Q	O2-C2-C1	-4.25	100.05	110.08
2	A	700	G6Q	O5-C5-C4	4.05	118.95	109.10
2	B	701	G6Q	O2-C2-C1	-3.96	100.73	110.08

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	G6Q	O2-C2-C3-O3
2	B	701	G6Q	O5-C5-C6-O6
2	A	700	G6Q	C4-C5-C6-O6
2	A	700	G6Q	O5-C5-C6-O6
2	A	700	G6Q	C6-O6-P-O1P

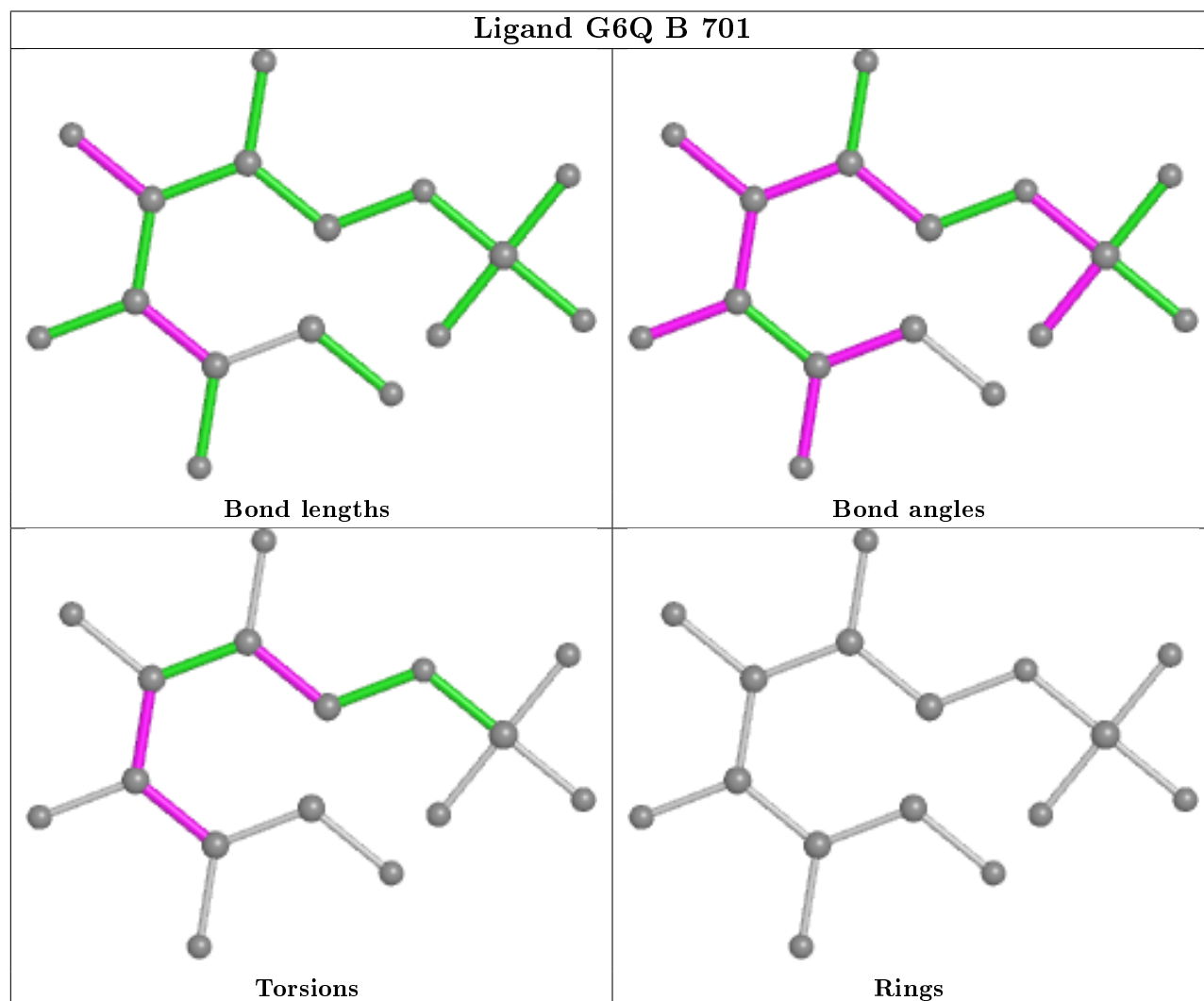
There are no ring outliers.

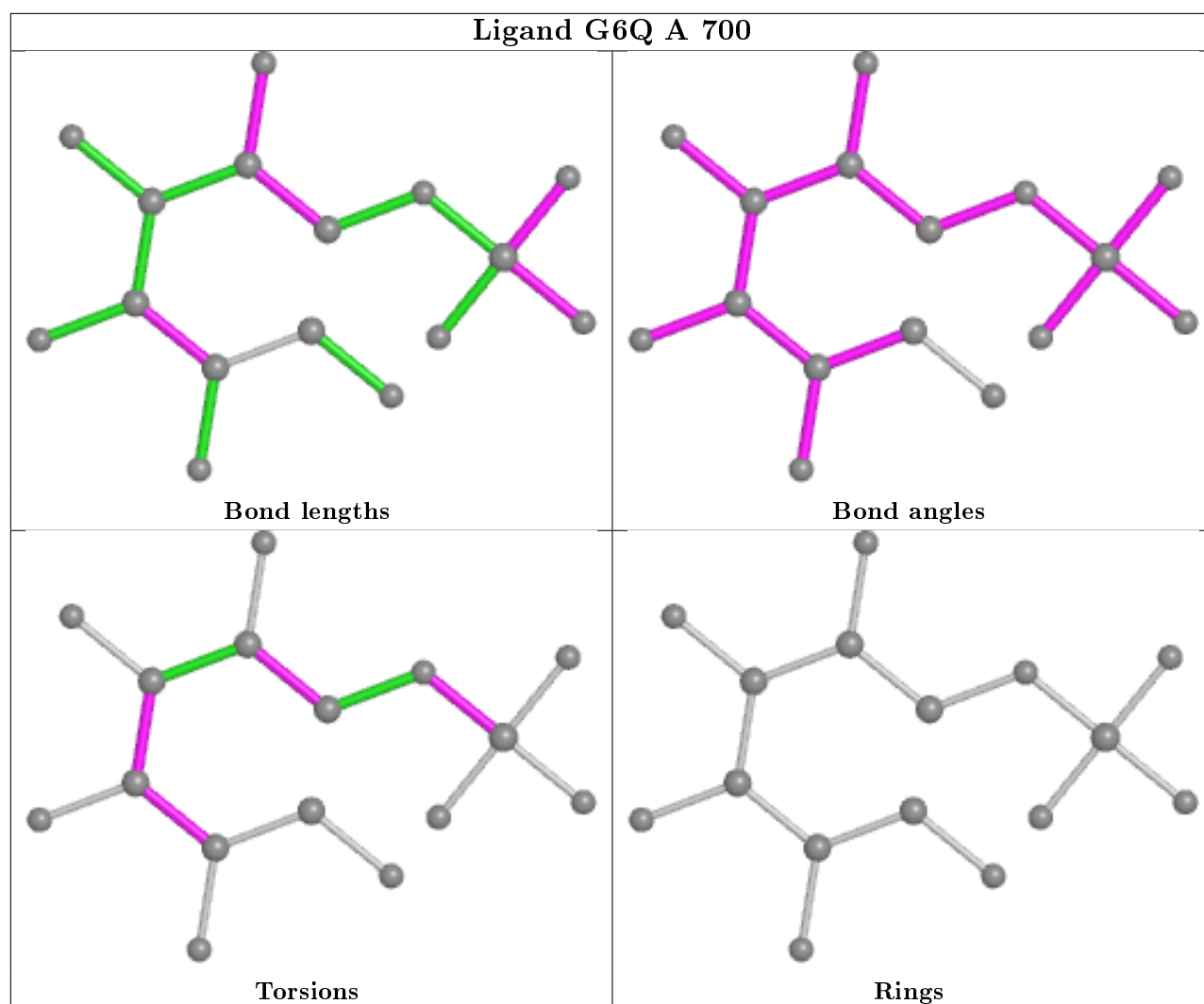
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	G6Q	2	0
2	A	700	G6Q	4	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 [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	608/608 (100%)	-0.73	5 (0%) 86 72	9, 38, 101, 133	0
1	B	608/608 (100%)	-0.52	6 (0%) 82 67	19, 78, 125, 138	0
1	C	608/608 (100%)	0.06	29 (4%) 30 14	44, 113, 137, 151	0
All	All	1824/1824 (100%)	-0.40	40 (2%) 62 41	9, 79, 131, 151	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	ASN	8.6
1	C	89	VAL	5.6
1	C	81	SER	5.6
1	B	240	TYR	4.7
1	A	85	ALA	4.6

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](#)

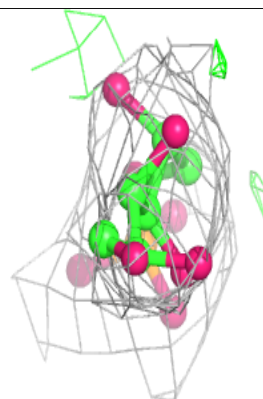
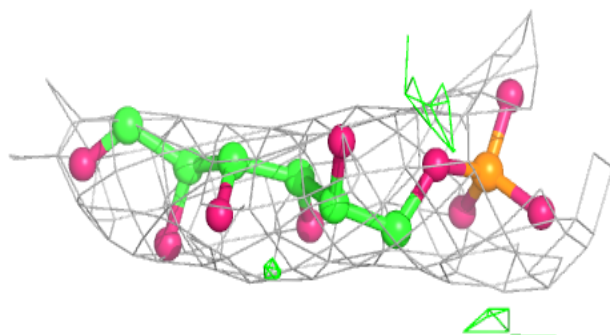
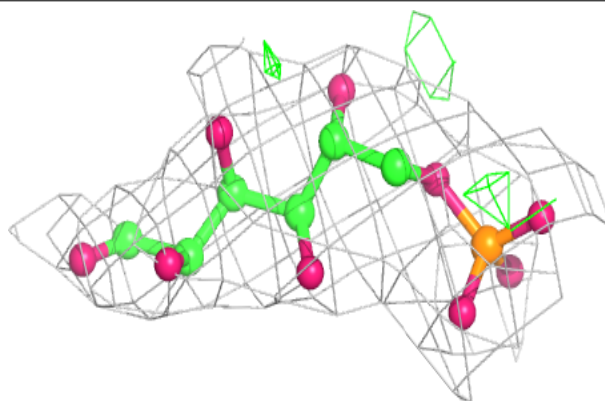
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

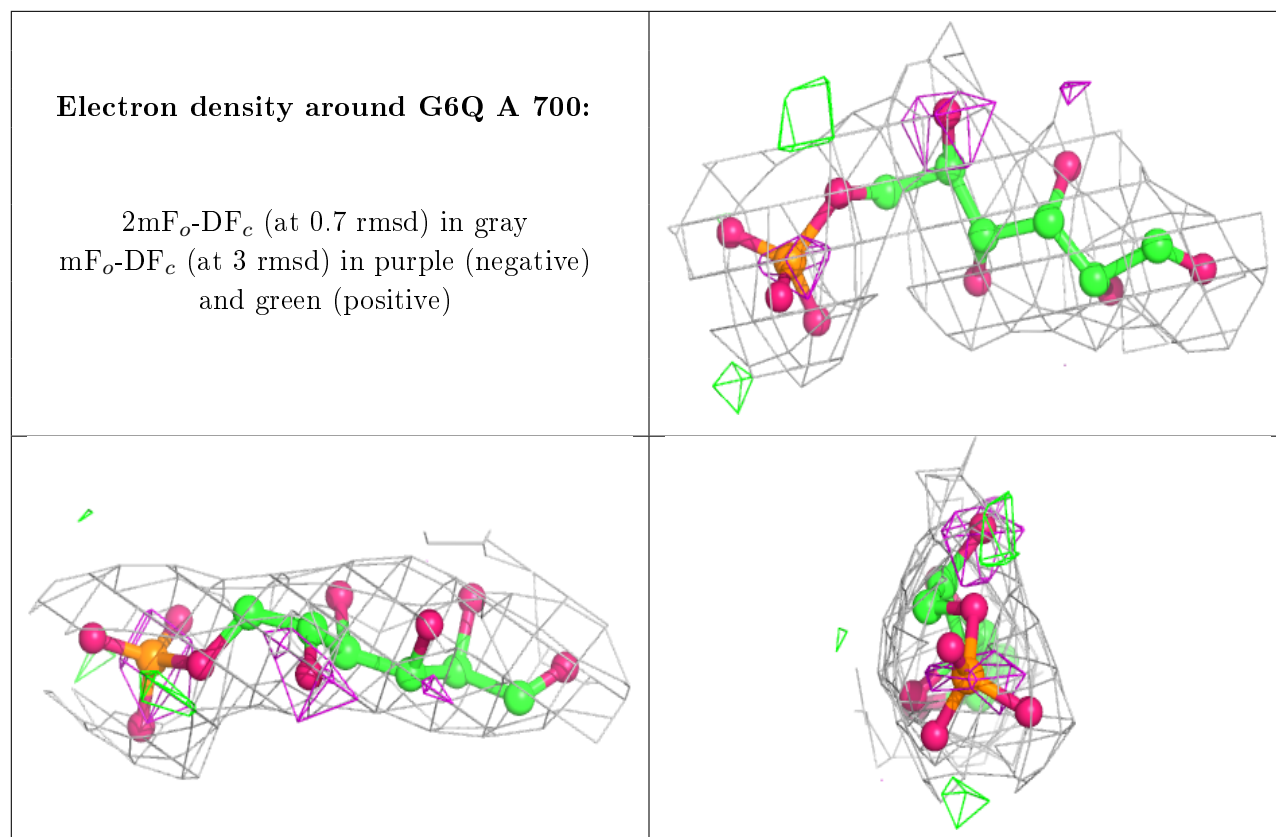
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	G6Q	B	701	16/16	0.94	0.17	62,73,81,84	0
2	G6Q	A	700	16/16	0.96	0.13	25,31,35,36	0

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)





6.5 Other polymers [i](#)

There are no such residues in this entry.