



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:43 PM UTC

PDB ID : 1JXA / pdb_00001jxa
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

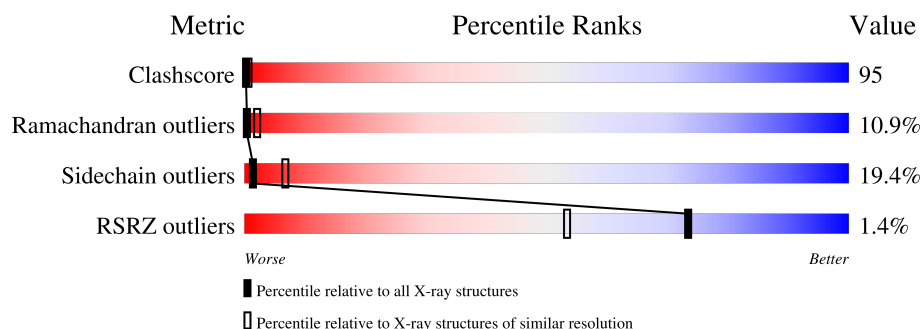
1 Overall quality at a glance

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	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 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 $\leq 5\%$. 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	% 16% 52% 28% .
1	B	608	% 16% 56% 26% .
1	C	608	3% 19% 61% 18% .

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.

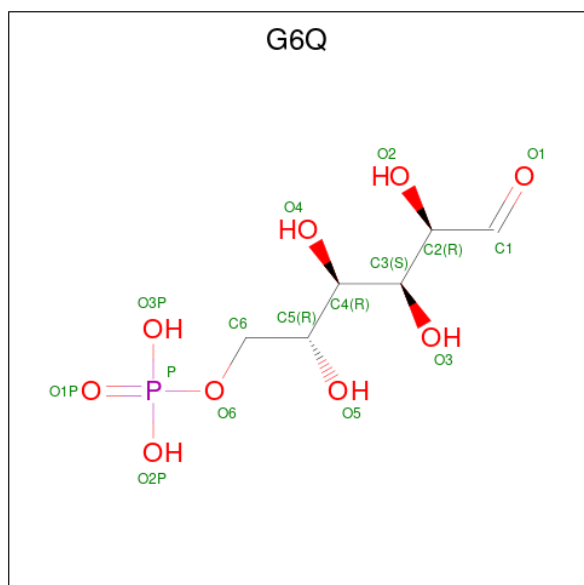
- Molecule 1 is a protein called glucosamine 6-phosphate synthase.

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 (CCD ID: G6Q) (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		

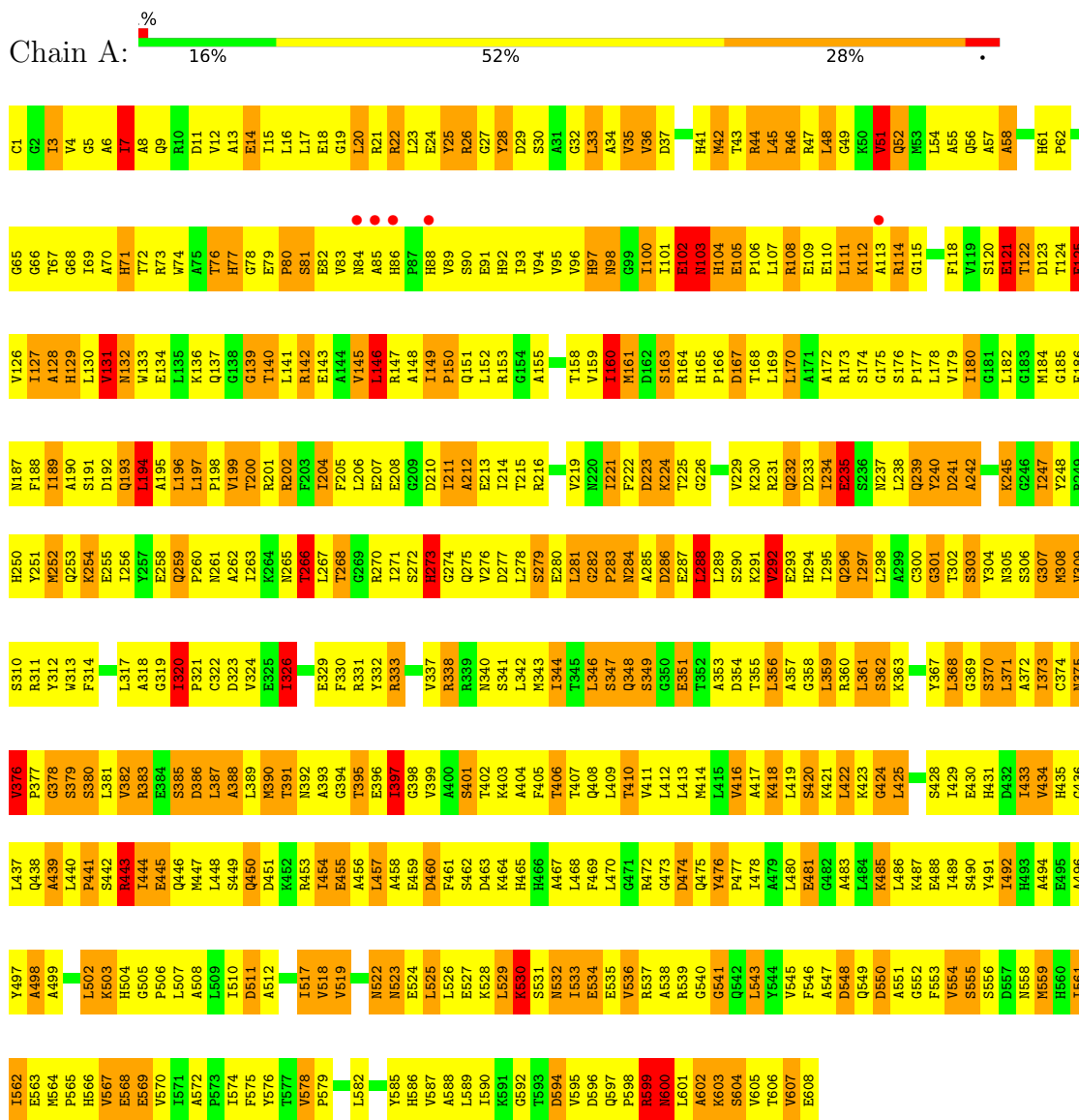
- Molecule 3 is water.

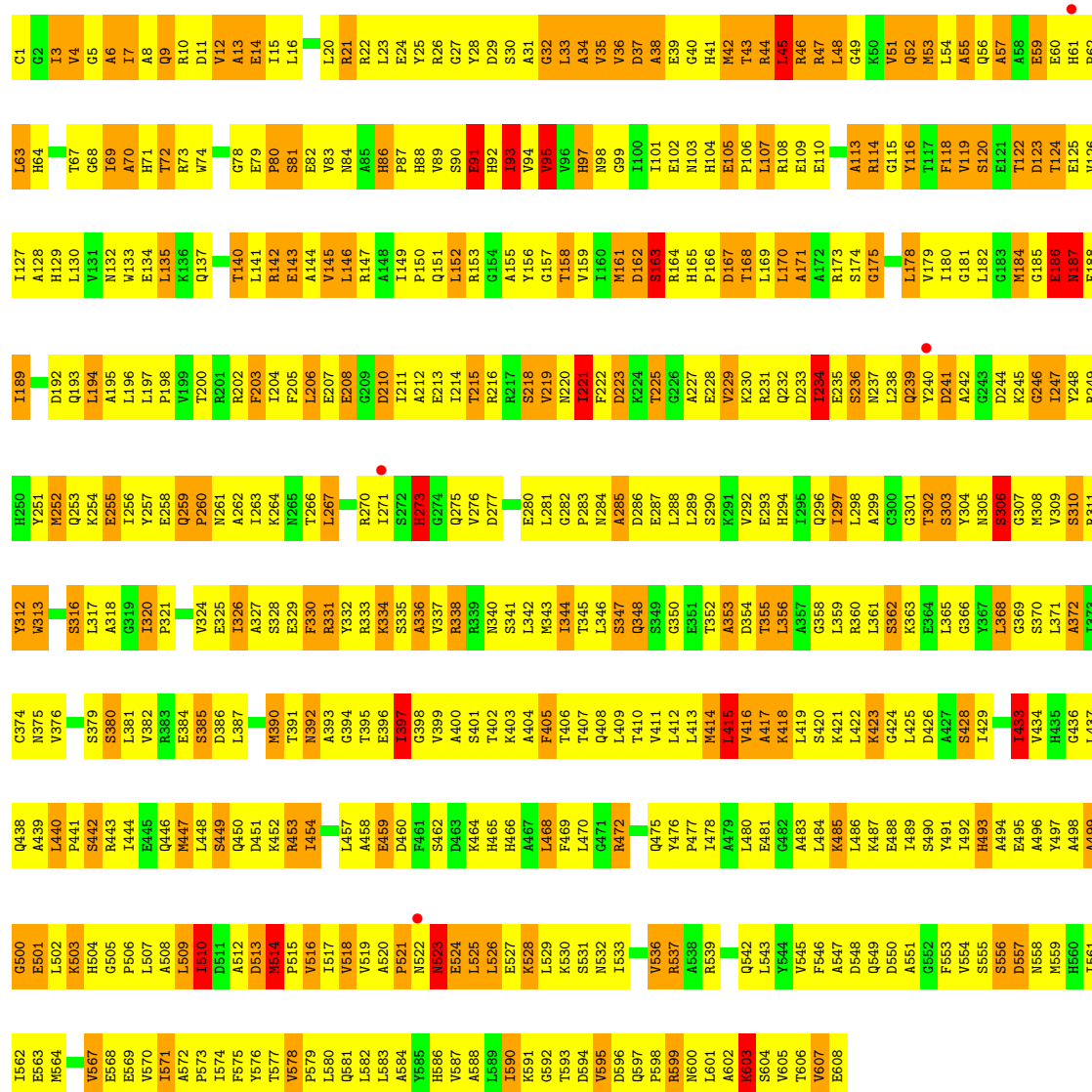
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	26	Total	O	0	0
			26	26		
3	B	10	Total	O	0	0
			10	10		
3	C	3	Total	O	0	0
			3	3		

3 Residue-property plots

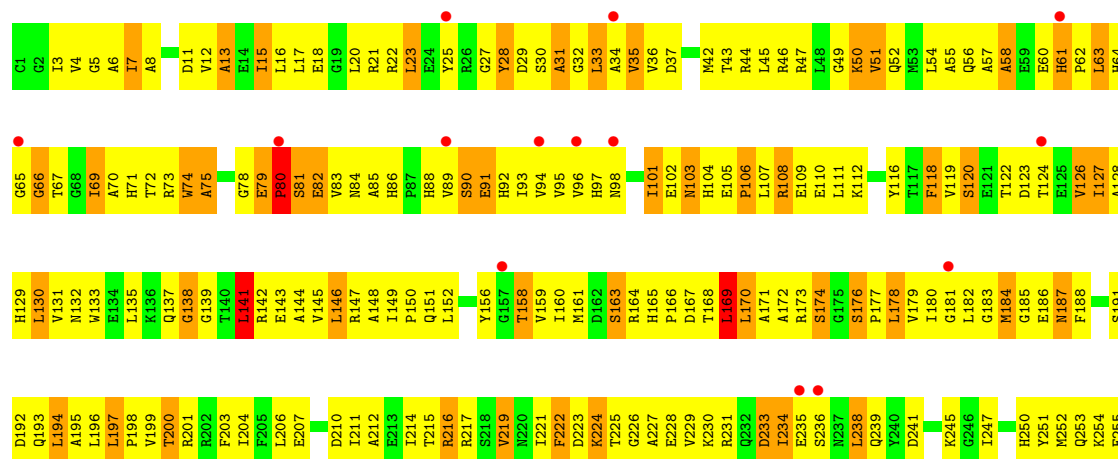
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: glucosamine 6-phosphate synthase





• Molecule 1: glucosamine 6-phosphate synthase



E569	P506	Q446	E384	G322	I256
V570	L507	M447	S385	D323	Y257
I571	A508	L448	D386	V324	E288
A572	L509	S449	L387	E325	Q259
P573	I510	Q450	A388	I326	P260
I511	D511	D451	L389	A327	M261
F575		K452	K390	S328	A262
F576	M514	R453	T391	E329	I263
F577		I454	N392	F330	K264
F578	I517	E455	A393	R331	N265
P579	V518	A456	G394	Y332	T266
L580		L457	T395	R333	
Q581	P521	A458	E396	K334	R270
L582	M522	E459	I397	S335	I271
L583	N523	D460	G398		S272
A584	E524	F461	V399	R338	H273
Y585	L525	S462	A400		L278
H586	L526	D463	S401	S341	S279
V587	E527	K464	T402	I342	E280
A588	K528	H465	K403	M343	L281
L589	L529	H466	A404	I344	G282
I590	K530	A467	F405	T345	P283
K591	S531	L468	T406	L346	N284
G592	N532	F469	T407	S347	A285
T593	I533	L470	Q408	Q348	D286
D594	E534	G471	L409	S349	E287
V595	E535	R472	F410	G350	L288
D596	V536	Q473	V411	E351	L289
Q597	R537	D474	L412	T352	S290
P598	A538	Q475	L413	A353	K291
R599	R539	Y476	M414	D354	V292
N600	G540	P477	L415	T355	E293
L601	G541	I478	V416	L356	H294
A602	Q542	A479	A417	A357	I295
K603	L543	L480	K418	G358	Q296
S604	Y544	E481		L359	I297
V605	V545	G482	K421	R360	L298
T606	F546	A483	L422	L361	A299
V607	A647	L484	K423	S362	C300
E608	D548	K485	G424	K363	G301
	Q549	L486	L425	E364	T302
	D550	K487	D426	L365	S303
	A551	E488	A427	G366	Y304
	G552	I489	S428	Y367	N305
	F553	S490	I429	L368	S306
	V554	Y491	E430	G369	G307
	SS55	I492		S370	M308
	SS56	H493	V433	L371	V309
	D557	A494	V434	A372	S310
	N558	E495	H435	I373	R311
	M559	A496	G436	C374	
	H560	Y497	L437	N375	F314
	I561	A498	L437	N376	E315
	S562	A499	Q438	V376	S316
	E563	G500	A439	P377	L317
	M564	E501	L440	G378	A318
	P565	P441	P441	S379	G319
	H566	L502	S442	S380	I320
	V567	R503	R443	L381	P321
	E568	H504	I444	V382	
		G505	E445	R383	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.40Å 112.40Å 185.10Å 90.00° 96.40° 90.00°	Depositor
Resolution (Å)	12.00 – 3.10 12.00 – 3.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-3.10) 91.0 (12.00-3.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 3.15Å)	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)	0.24 , 70.2	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	0.92	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 ⓘ

5.1 Standard geometry ⓘ

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	1.09	12/4776 (0.3%)	1.64	82/6467 (1.3%)
1	B	0.90	8/4776 (0.2%)	1.36	42/6467 (0.6%)
1	C	0.67	0/4776	1.13	23/6467 (0.4%)
All	All	0.90	20/14328 (0.1%)	1.39	147/19401 (0.8%)

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	578	VAL	CA-CB	-10.04	1.49	1.54
1	A	262	ALA	CA-CB	-6.73	1.42	1.53
1	A	93	ILE	CA-CB	-6.40	1.46	1.54
1	A	100	ILE	CG1-CD1	6.36	1.76	1.51
1	A	388	ALA	CA-CB	-6.24	1.43	1.53

The worst 5 of 147 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	508	ALA	N-CA-C	-9.41	101.03	114.12
1	A	397	ILE	N-CA-C	-9.27	103.69	112.96
1	A	536	VAL	N-CA-C	-9.18	101.61	110.42
1	A	394	GLY	CA-C-O	-8.80	115.57	122.52
1	A	530	LYS	N-CA-C	-8.64	101.77	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4695	0	4715	908	1
1	B	4695	0	4715	957	0
1	C	4695	0	4715	878	0
2	A	16	0	10	4	0
2	B	16	0	11	4	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	2700	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 95.

The worst 5 of 2700 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

5.3.1 Protein backbone

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	1
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%)	383 (77%)	117 (23%)	1	4
1	B	500/500 (100%)	401 (80%)	99 (20%)	1	6
1	C	500/500 (100%)	425 (85%)	75 (15%)	3	13
All	All	1500/1500 (100%)	1209 (81%)	291 (19%)	1	7

5 of 291 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	163	SER
1	C	570	VAL
1	C	194	LEU
1	C	382	VAL
1	A	468	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	265	ASN
1	C	560	HIS
1	B	523	ASN
1	C	558	ASN
1	C	348	GLN

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 oligosaccharides 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	-	14,15,15	1.36	2 (14%)	19,21,21	1.87	5 (26%)
2	G6Q	A	700	-	14,15,15	1.92	5 (35%)	19,21,21	2.84	12 (63%)

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	-	-	8/19/20/20	-
2	G6Q	A	700	-	-	9/19/20/20	-

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	-3.41	1.36	1.43
2	B	701	G6Q	C3-C2	-2.96	1.48	1.53
2	A	700	G6Q	P-O2P	-2.88	1.44	1.54
2	A	700	G6Q	C3-C2	-2.64	1.49	1.53
2	A	700	G6Q	C6-C5	-2.53	1.48	1.51

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	-4.61	103.52	112.22
2	A	700	G6Q	O2-C2-C1	-4.59	100.05	110.48
2	B	701	G6Q	O2-C2-C1	-4.29	100.73	110.48
2	A	700	G6Q	O5-C5-C4	4.15	118.95	109.25

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

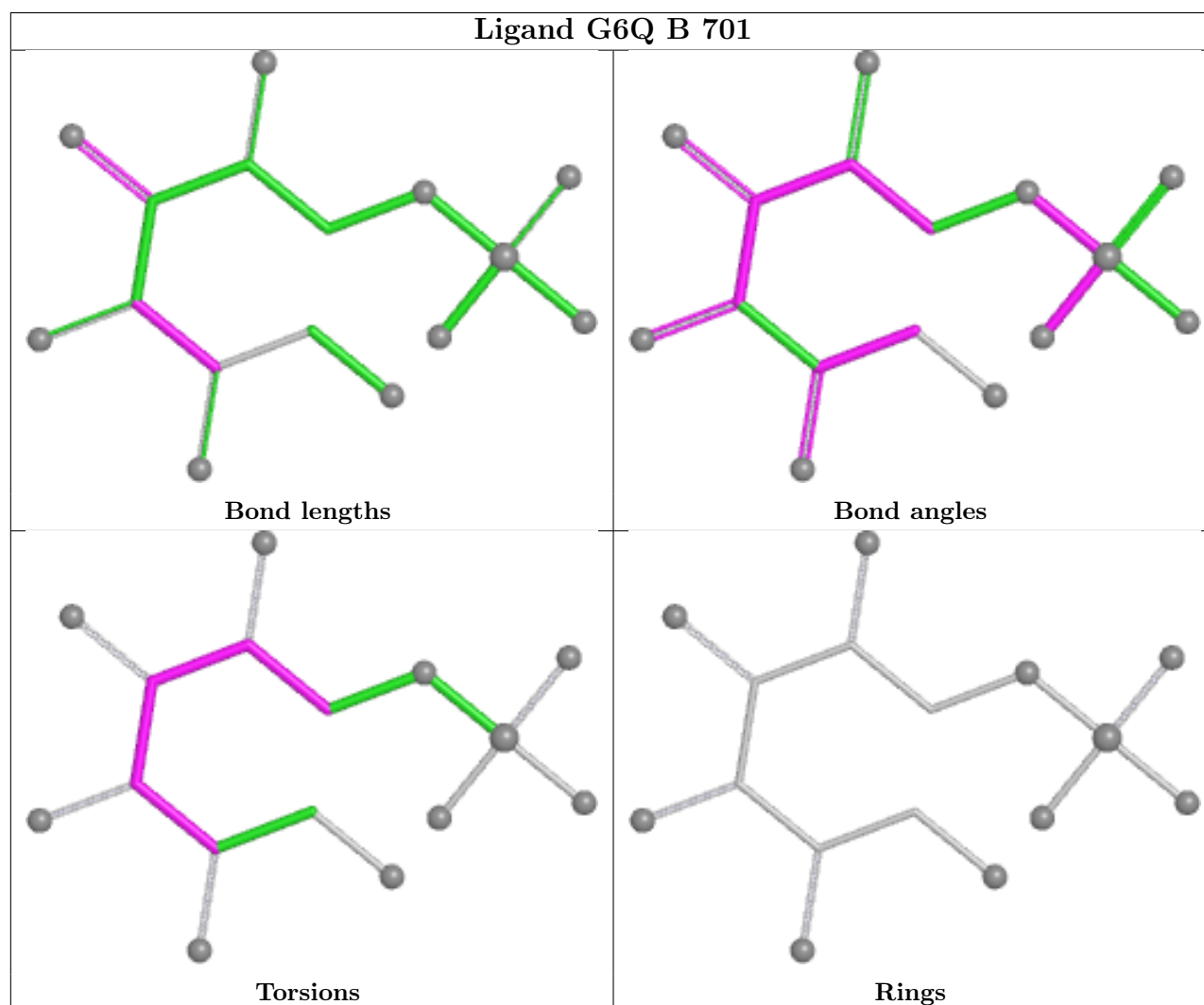
Mol	Chain	Res	Type	Atoms
2	A	700	G6Q	C4-C5-C6-O6
2	A	700	G6Q	O5-C5-C6-O6
2	A	700	G6Q	C6-O6-P-O1P
2	A	700	G6Q	C6-O6-P-O2P
2	A	700	G6Q	C6-O6-P-O3P

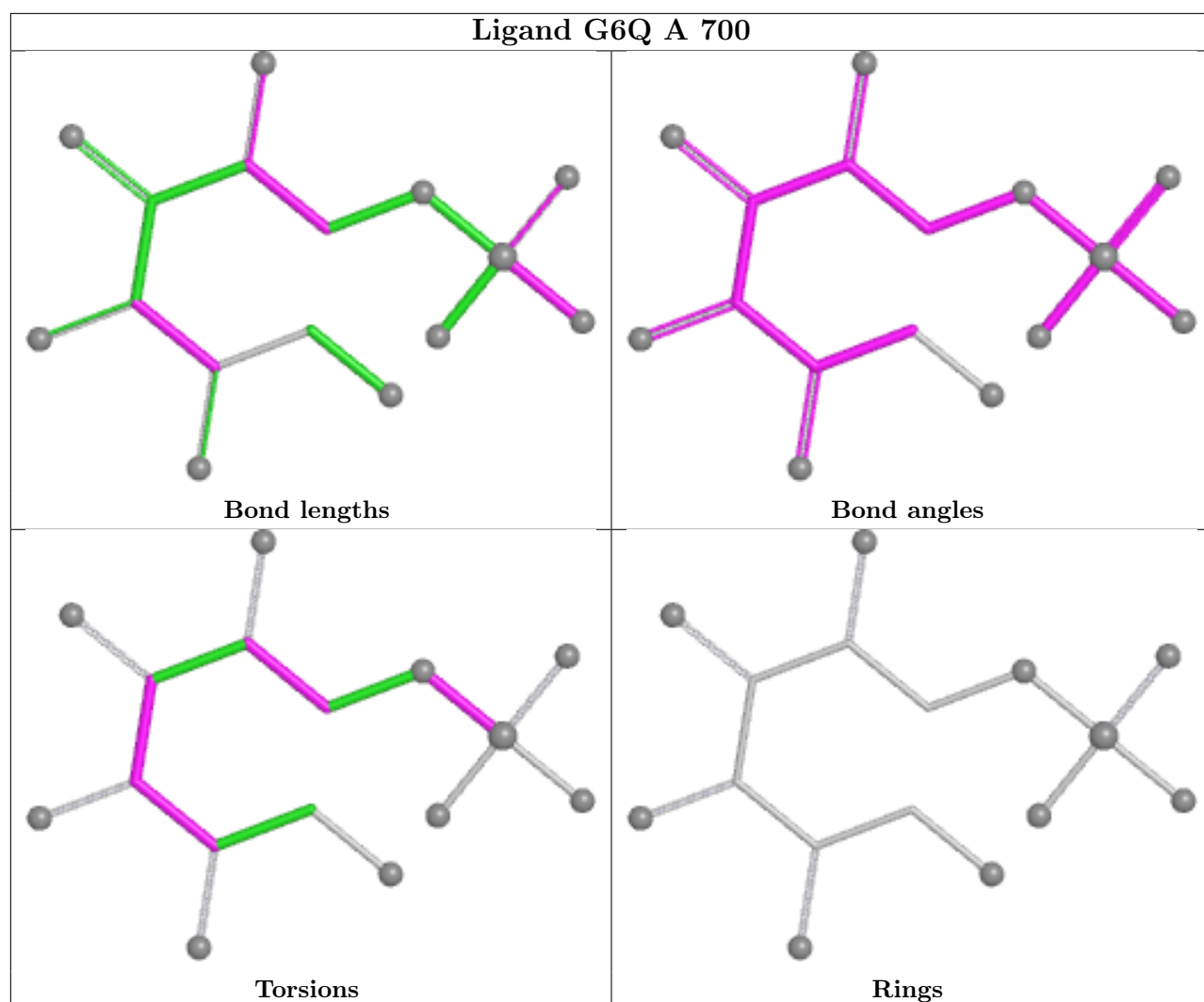
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	G6Q	4	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%)	-0.65	5 (0%) 82 65	9, 38, 101, 133	0
1	B	608/608 (100%)	-0.35	4 (0%) 84 68	19, 78, 125, 138	0
1	C	608/608 (100%)	0.16	17 (2%) 55 34	44, 113, 137, 151	0
All	All	1824/1824 (100%)	-0.28	26 (1%) 73 53	9, 79, 131, 151	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	ASN	4.1
1	C	124	THR	3.2
1	C	435	HIS	3.0
1	C	522	ASN	2.8
1	A	88	HIS	2.8

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

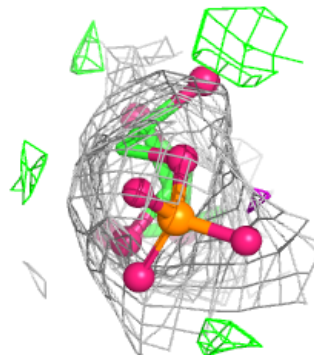
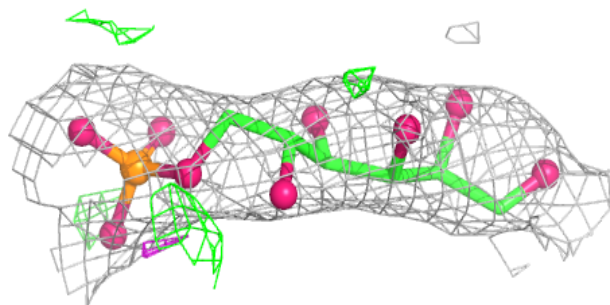
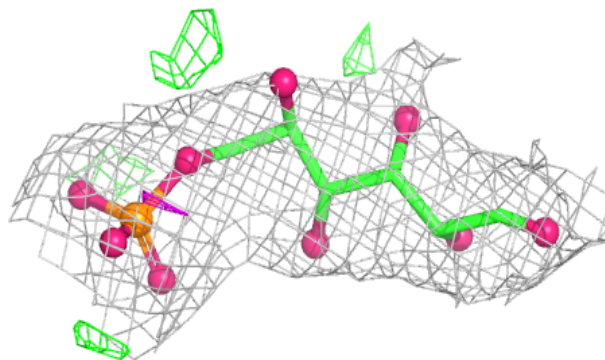
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

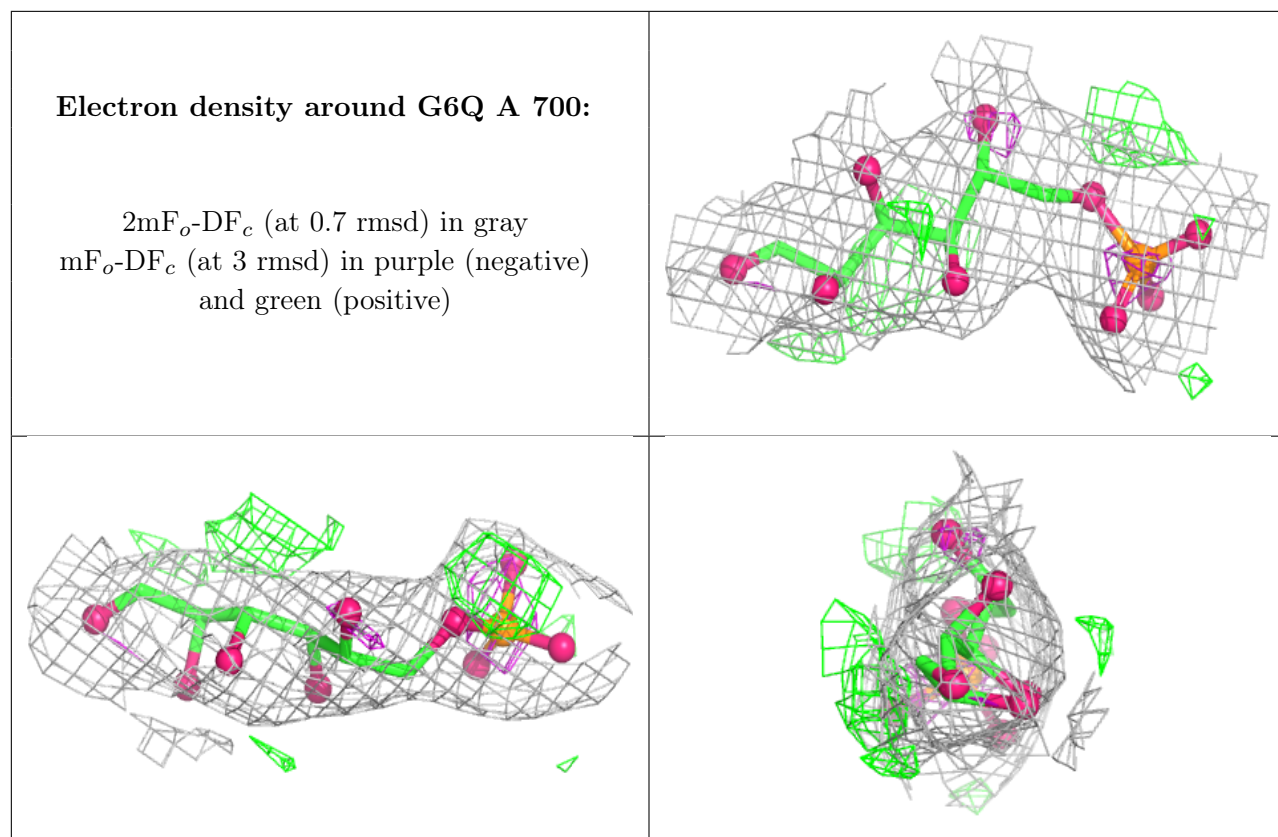
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	G6Q	B	701	16/16	0.90	0.10	62,73,81,84	0
2	G6Q	A	700	16/16	0.94	0.11	25,31,35,36	0

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.