wwPDB X-ray Structure Validation Summary Report (i)

Jun 11, 2024 – 11:35 PM EDT

PDB ID	:	1DQR
Title	:	CRYSTAL STRUCTURE OF RABBIT PHOSPHOGLUCOSE ISOMERASE, A GLYCOLYTIC ENZYME THAT MOONLIGHTS AS NEUROLEUKIN, AUTOCRINE MOTILITY FACTOR, AND DIFFERENTIATION MEDIATOR
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Deposited on	:	2000-01-05
Resolution	:	2.50 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 (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:

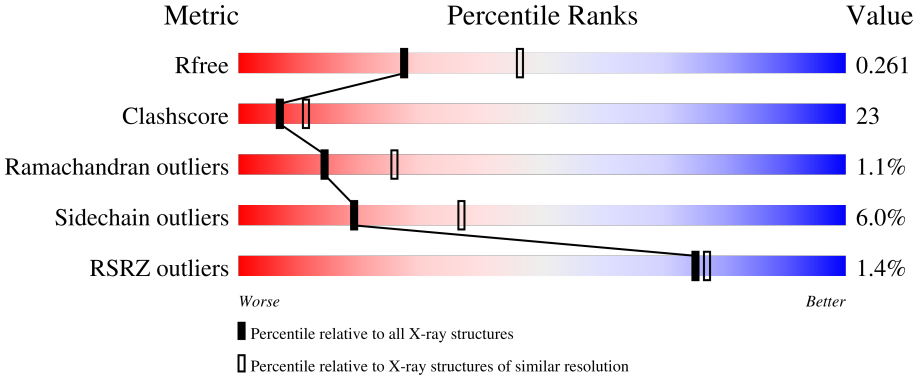
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

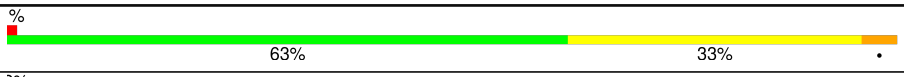
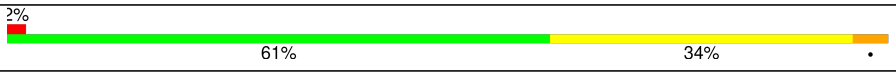
The reported resolution of this entry is 2.50 Å.

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	557	
1	B	557	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9194 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.

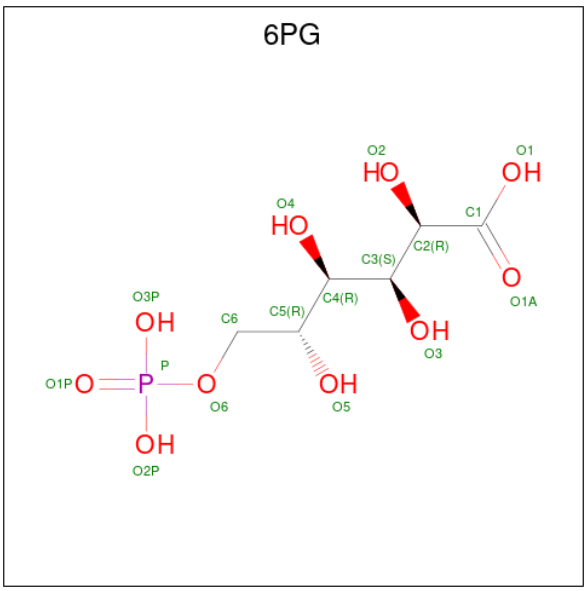
- Molecule 1 is a protein called PHOSPHOGLUCOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	555	4395	2805	765	806	19	0	0	0
1	B	555	4395	2805	765	806	19	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	PRO	LEU	see remark 999	UNP Q9N1E2
A	222	LYS	GLU	see remark 999	UNP Q9N1E2
A	283	ILE	VAL	see remark 999	UNP Q9N1E2
B	109	PRO	LEU	see remark 999	UNP Q9N1E2
B	222	LYS	GLU	see remark 999	UNP Q9N1E2
B	283	ILE	VAL	see remark 999	UNP Q9N1E2

- Molecule 2 is 6-PHOSPHOGLUCONIC ACID (three-letter code: 6PG) (formula: $C_6H_{13}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	17	6	10	1	0	0
			Total	C	O	P		
2	B	1	17	6	10	1	0	0

- Molecule 3 is water.

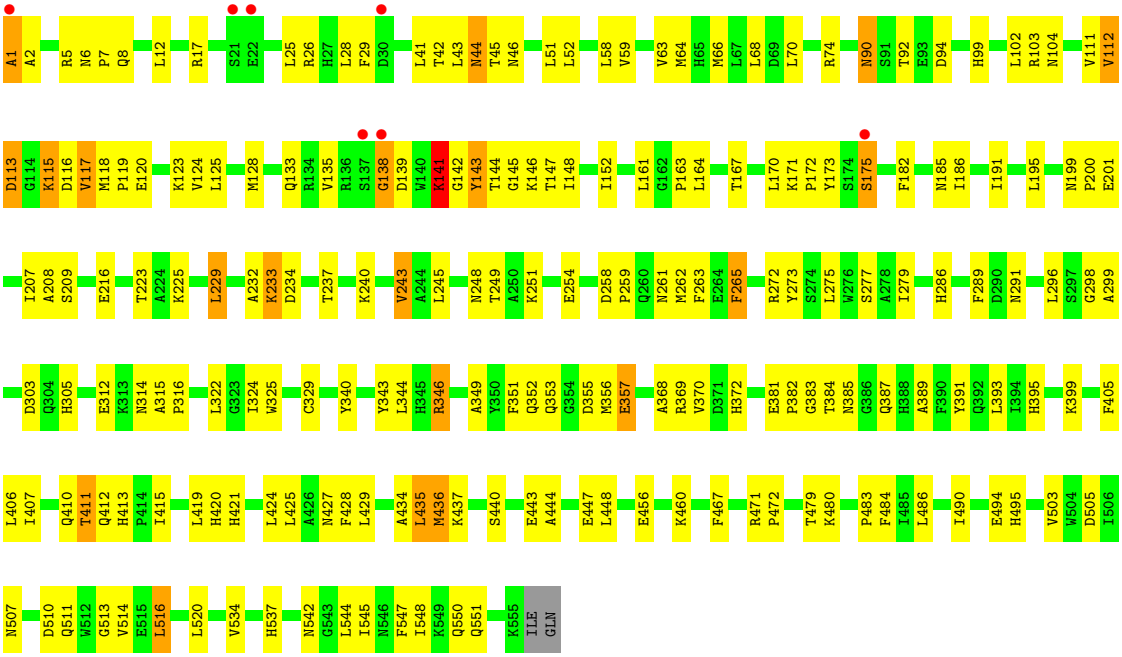
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	176	176	176	0	0
			Total	O		
3	B	194	194	194	0	0

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.

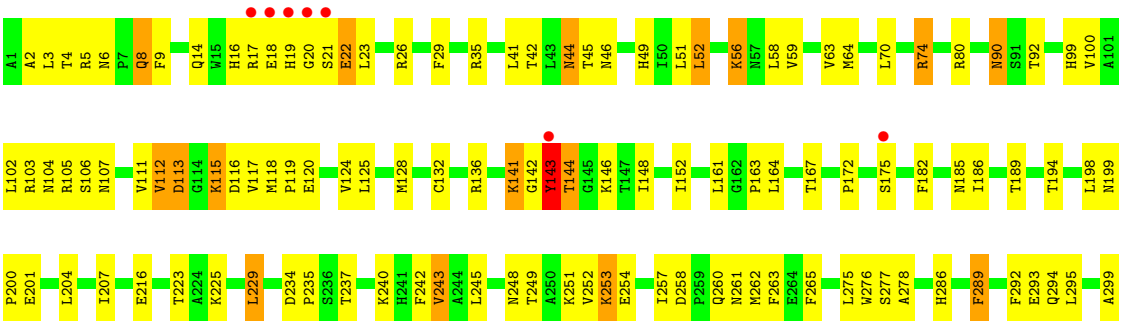
• Molecule 1: PHOSPHOGLUCOSE ISOMERASE

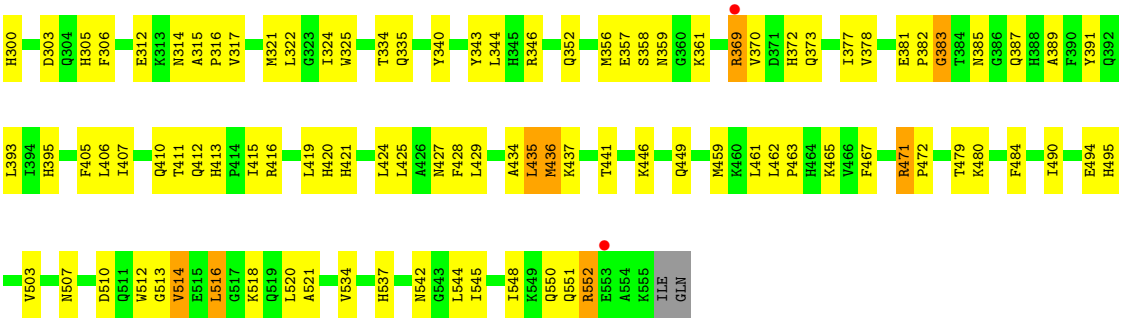
Chain A:



• Molecule 1: PHOSPHOGLUCOSE ISOMERASE

Chain B:




H300 D303 Q304 H305 F306 E312 K313 N314 A315 P316 V317 M321 L322 G323 I324 W325 T334 Q335 Y340 Y343 L344 H345 R346 Q352 M356 E357 S358 N359 G360 K361 R369 V370 D371 H372 Q373 I377 V378 E381 P382 G383 T384 N385 G386 Q387 H388 A389 F390 Y391 Q392
L393 I394 H395 F405 L406 I407 Q410 T411 Q412 H413 P414 I415 R416 L419 H420 H421 L424 L425 A426 N427 F428 L429 A434 L435 M436 K437 T441 K446 Q449 M459 K460 L461 L462 P463 H464 K465 V466 F467 R471 P472 T479 K480 F484 I490 E494 H495
V503 N507 D510 Q511 W512 G513 V514 E515 L516 G517 K518 Q519 L520 A521 V534 H537 N542 G543 L544 I545 I548 K549 Q550 Q551 R552 E553 A554 K555 ILE GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	82.69Å 115.27Å 271.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.50 19.94 – 2.51	Depositor EDS
% Data completeness (in resolution range)	90.9 (35.00-2.50) 92.2 (19.94-2.51)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.48 (at 2.50Å)	Xtriage
Refinement program	CNS, XTALVIEW	Depositor
R, R_{free}	0.212 , 0.265 0.209 , 0.261	Depositor DCC
R_{free} test set	4152 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9194	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: 6PG

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	0.42	3/4504 (0.1%)	0.65	3/6101 (0.0%)
1	B	0.44	3/4504 (0.1%)	0.64	2/6101 (0.0%)
All	All	0.43	6/9008 (0.1%)	0.65	5/12202 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	514	VAL	CB-CG1	-8.29	1.35	1.52
1	B	514	VAL	CB-CG2	-6.59	1.39	1.52
1	A	514	VAL	CB-CG2	-6.17	1.39	1.52
1	A	1	ALA	CA-CB	-5.96	1.40	1.52
1	B	143	TYR	CD2-CE2	-5.91	1.30	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	112	VAL	CB-CA-C	-6.89	98.31	111.40
1	A	112	VAL	CB-CA-C	-6.76	98.56	111.40
1	A	141	LYS	N-CA-C	6.75	129.22	111.00
1	A	175	SER	N-CA-C	6.72	129.16	111.00
1	B	175	SER	N-CA-C	6.38	128.23	111.00

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	4395	0	4352	219	0
1	B	4395	0	4352	216	0
2	A	17	0	10	1	0
2	B	17	0	10	1	0
3	A	176	0	0	12	0
3	B	194	0	0	15	0
All	All	9194	0	8724	408	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 23.

The worst 5 of 408 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:143:TYR:CE2	3:B:787:HOH:O	1.87	1.24
1:A:1:ALA:CB	3:A:774:HOH:O	1.95	1.10
1:A:113:ASP:CG	3:A:724:HOH:O	1.89	1.10
1:B:112:VAL:HG23	1:B:112:VAL:O	1.48	1.10
1:A:112:VAL:HG23	1:A:112:VAL:O	1.38	1.08

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	553/557 (99%)	514 (93%)	34 (6%)	5 (1%)	17 31
1	B	553/557 (99%)	511 (92%)	35 (6%)	7 (1%)	12 21
All	All	1106/1114 (99%)	1025 (93%)	69 (6%)	12 (1%)	14 26

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	TYR
1	A	138	GLY
1	B	113	ASP
1	A	113	ASP
1	A	175	SER

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	475/478 (99%)	446 (94%)	29 (6%)	18	36
1	B	475/478 (99%)	447 (94%)	28 (6%)	19	37
All	All	950/956 (99%)	893 (94%)	57 (6%)	19	37

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	516	LEU
1	B	516	LEU
1	B	90	ASN
1	B	471	ARG
1	B	369	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	104	ASN
1	B	410	GLN
1	B	153	ASN
1	B	385	ASN
1	B	420	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 monosaccharides 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	6PG	B	601	-	16,16,16	1.42	3 (18%)	21,23,23	0.93	1 (4%)
2	6PG	A	600	-	16,16,16	1.36	4 (25%)	21,23,23	0.97	1 (4%)

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	6PG	B	601	-	-	9/22/22/22	-
2	6PG	A	600	-	-	14/22/22/22	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	6PG	O1-C1	-3.37	1.19	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	6PG	O1-C1	-2.90	1.21	1.30
2	B	601	6PG	C3-C2	2.37	1.58	1.53
2	A	600	6PG	P-O6	-2.34	1.52	1.60
2	A	600	6PG	C4-C3	2.15	1.57	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	6PG	O1-C1-C2	2.33	119.80	113.31
2	A	600	6PG	O1-C1-C2	2.24	119.53	113.31

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	6PG	C4-C5-C6-O6
2	A	600	6PG	O5-C5-C6-O6
2	B	601	6PG	C1-C2-C3-C4
2	B	601	6PG	C1-C2-C3-O3
2	B	601	6PG	O2-C2-C3-C4

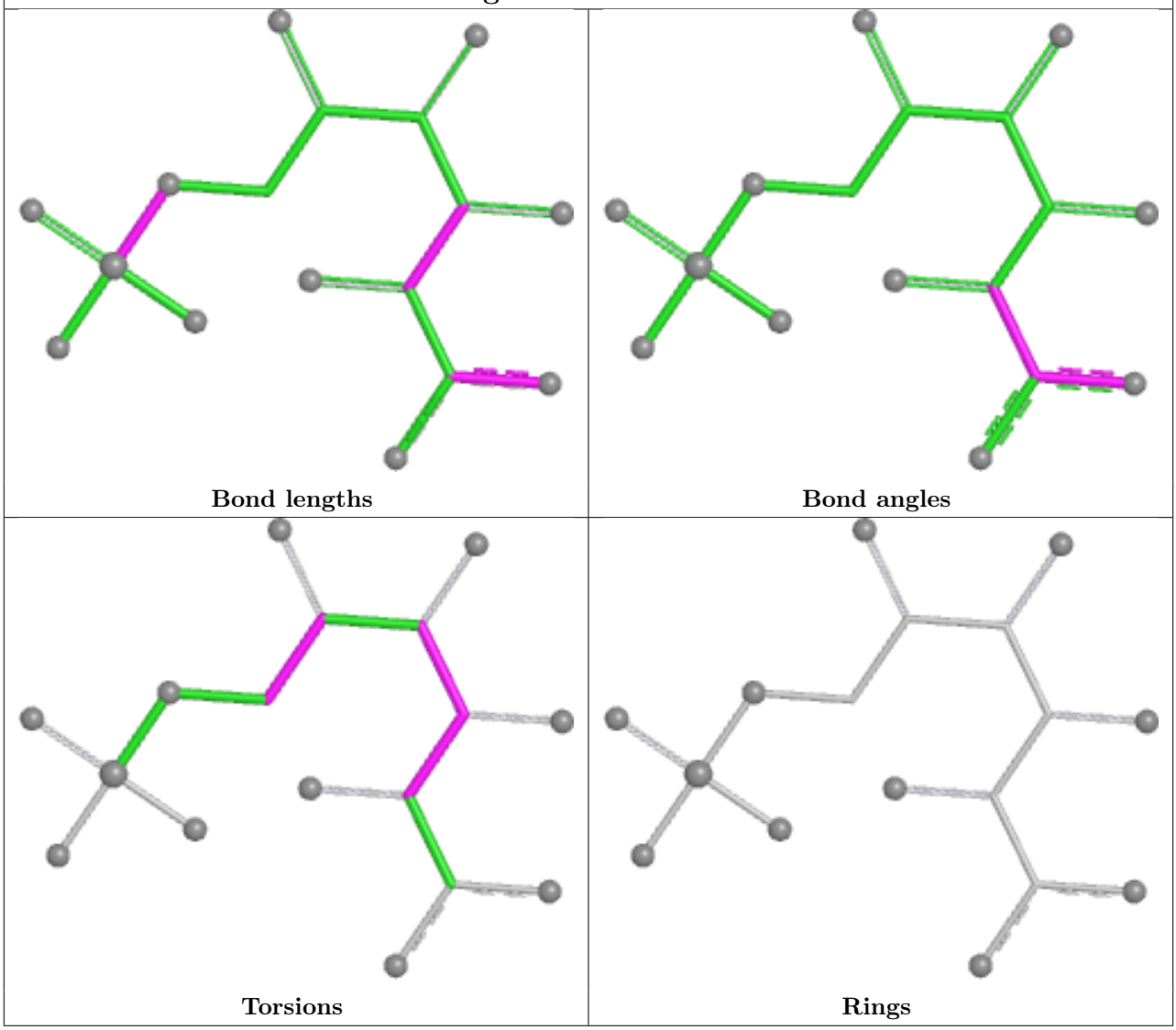
There are no ring outliers.

2 monomers are involved in 2 short contacts:

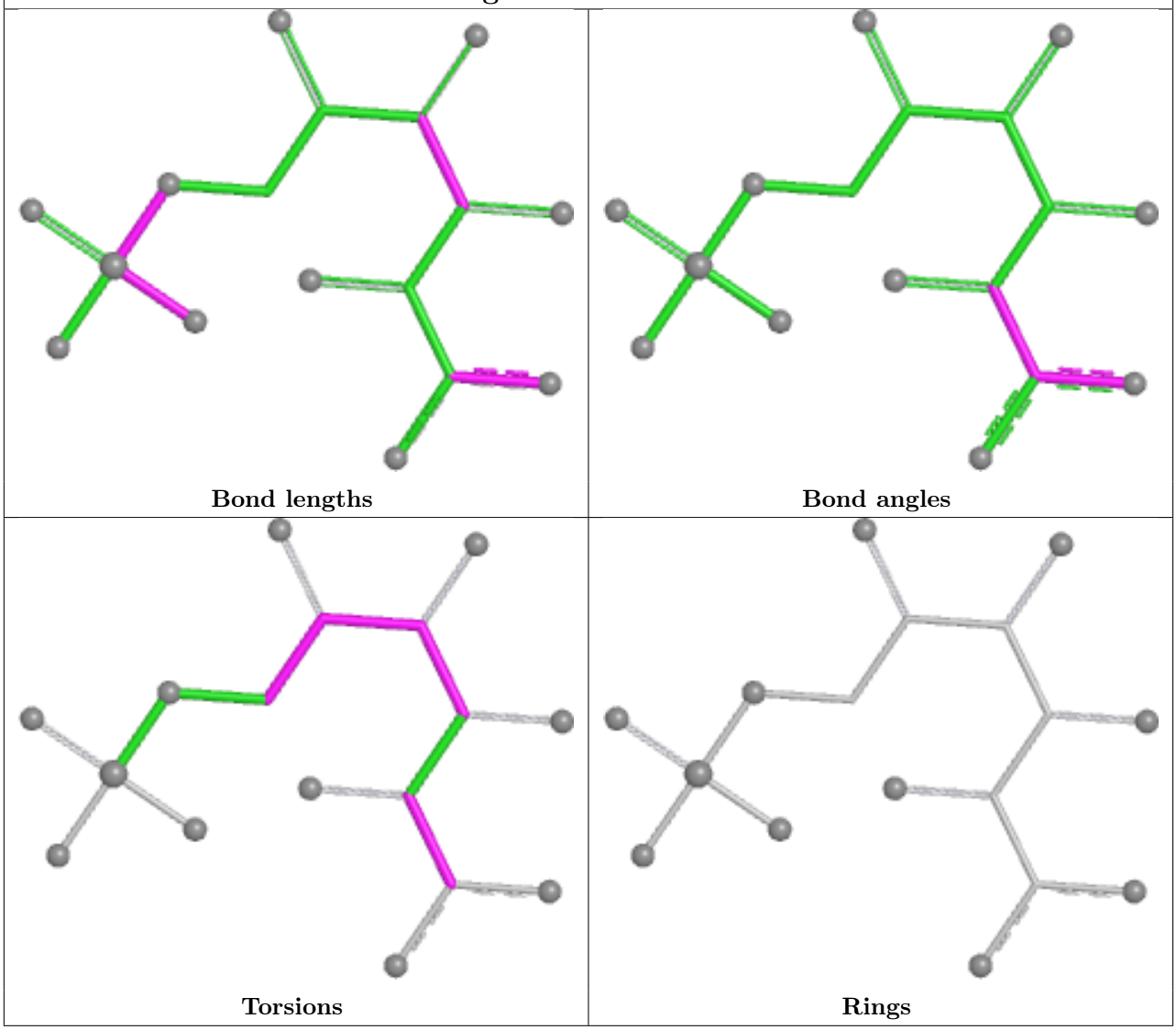
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	6PG	1	0
2	A	600	6PG	1	0

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 6PG B 601



Ligand 6PG A 600



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	555/557 (99%)	-0.25	7 (1%)	77	79	10, 27, 61, 87	0
1	B	555/557 (99%)	-0.34	9 (1%)	72	74	9, 25, 52, 86	0
All	All	1110/1114 (99%)	-0.29	16 (1%)	75	77	9, 26, 57, 87	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	20	GLY	5.3
1	B	21	SER	5.1
1	B	18	GLU	4.9
1	A	1	ALA	4.1
1	B	175	SER	3.9

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)

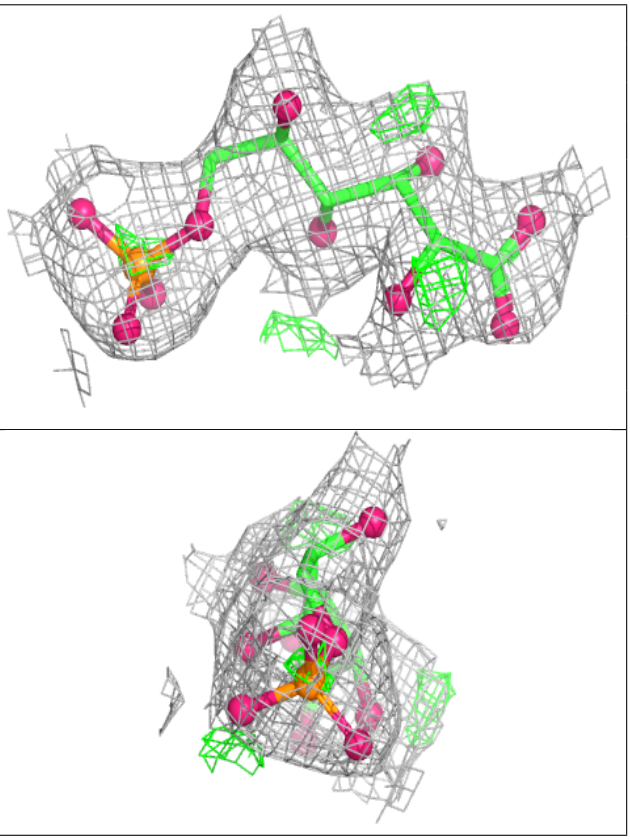
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	6PG	B	601	17/17	0.93	0.17	31,41,49,54	0
2	6PG	A	600	17/17	0.94	0.21	42,57,73,74	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.

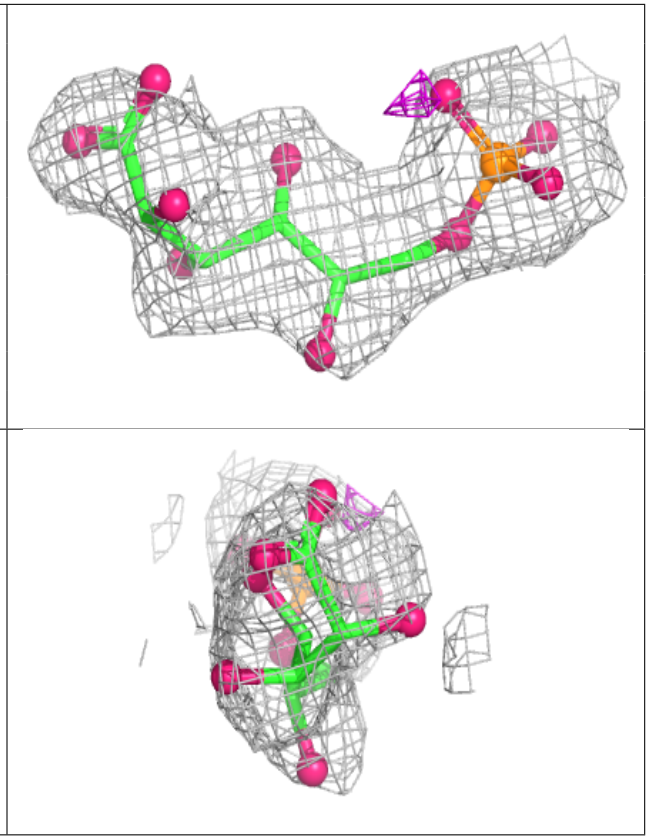
Electron density around 6PG B 601:

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 6PG A 600:

$2mF_o$-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.