



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:11 am BST

PDB ID : 5XGI
Title : Crystal structure of PI3K complex with an inhibitor
Authors : Song, K.; Yang, X.; Zhao, Y.; Jian, Z.
Deposited on : 2017-04-13
Resolution : 2.56 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 ⓘ 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

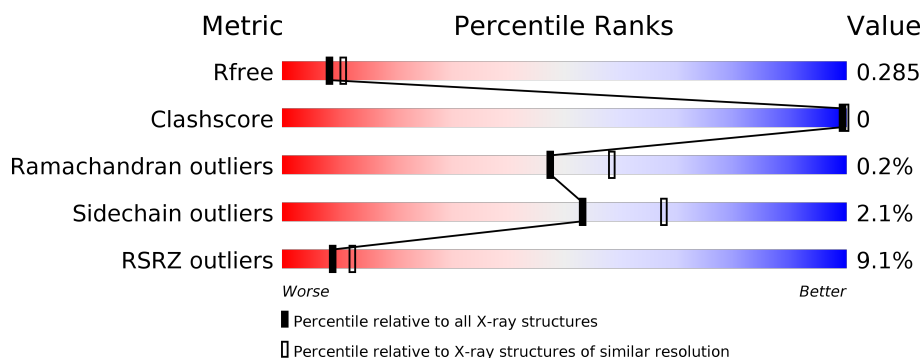
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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	1052	<div> <div>10%</div> <div> <div></div> <div>93%</div> <div></div> </div> <div></div> </div>
2	B	277	<div> <div>6%</div> <div> <div></div> <div>98%</div> <div></div> </div> <div></div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10818 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.

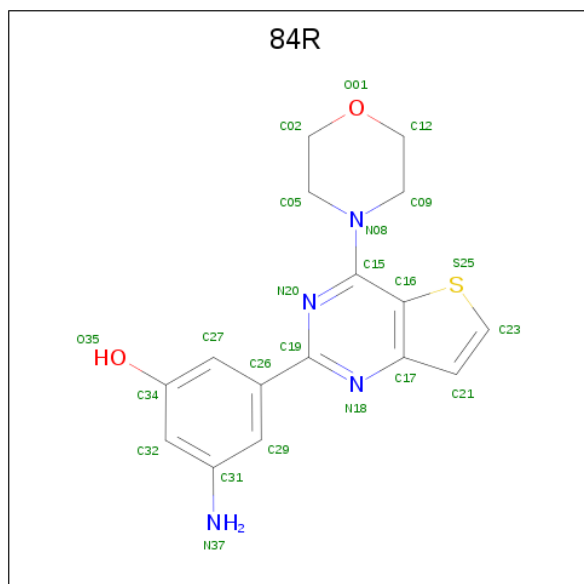
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1013	Total	C	N	O	S	0	0	0
			8293	5307	1414	1504	68			

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

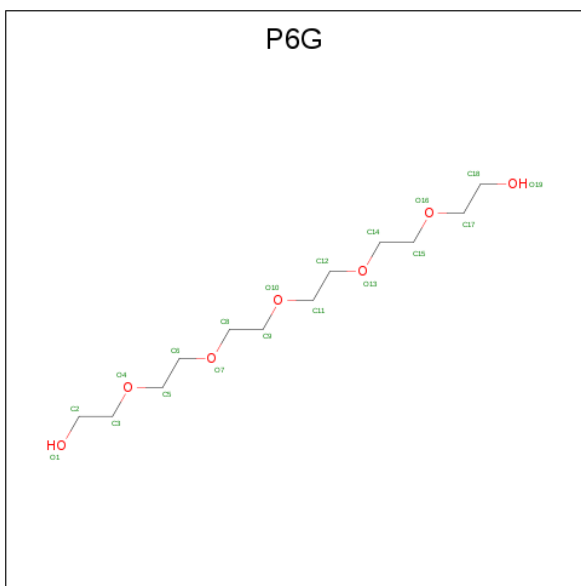
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	277	Total	C	N	O	S	0	0	0
			2354	1474	420	452	8			

- Molecule 3 is 3-azanyl-5-(4-morpholin-4-ylthieno[3,2-d]pyrimidin-2-yl)phenol (three-letter code: 84R) (formula: C₁₆H₁₆N₄O₂S).



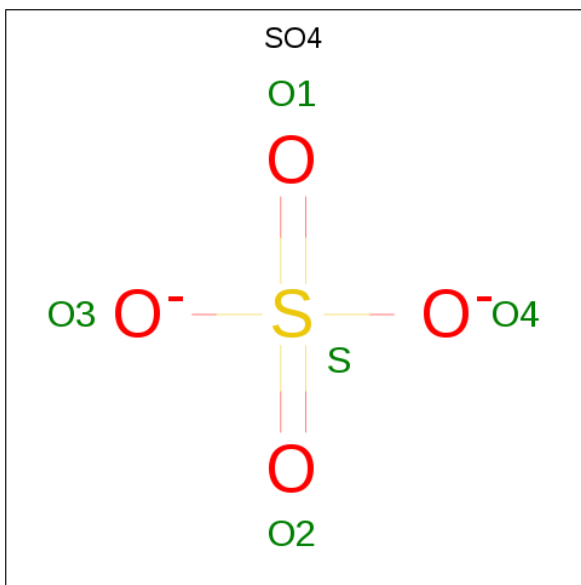
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			23	16	4	2	1		

- Molecule 4 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



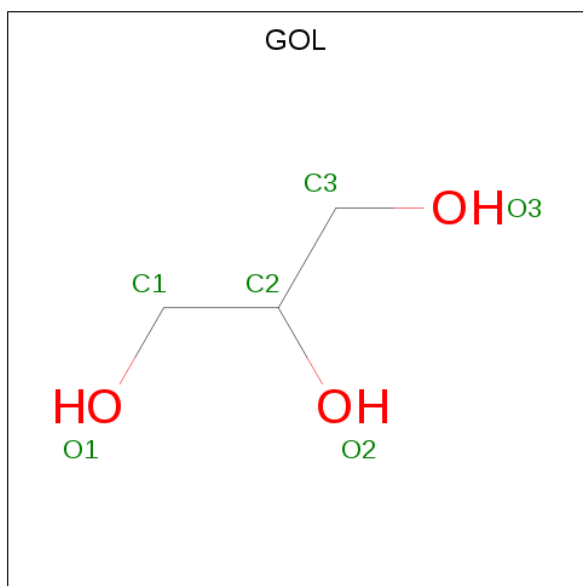
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

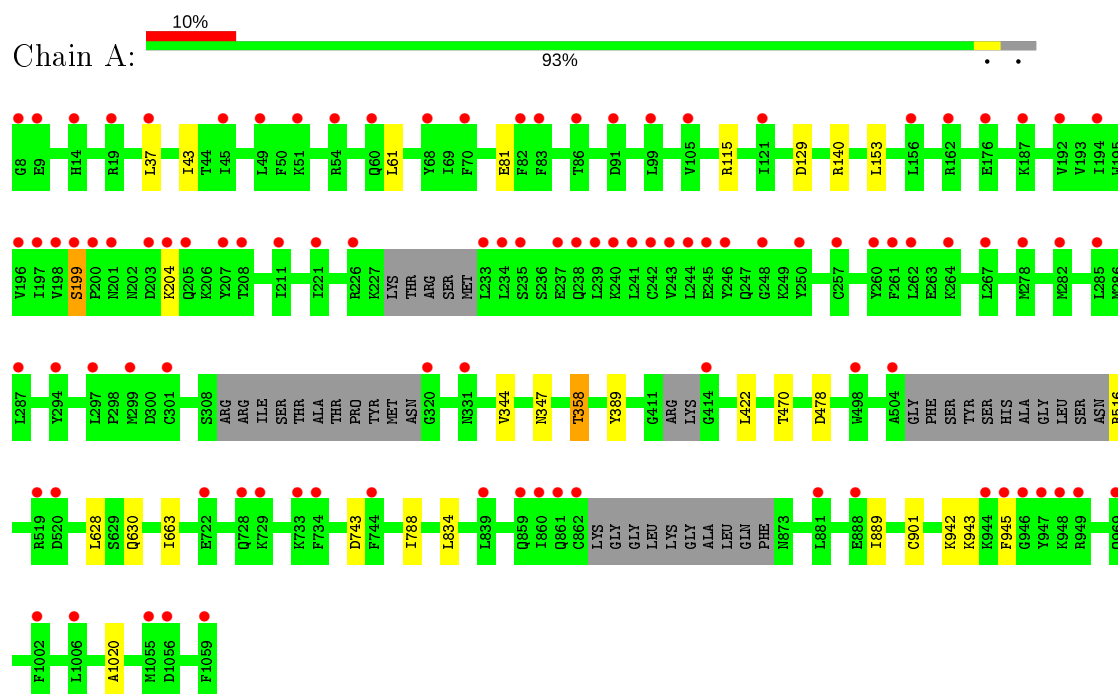
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	84	Total	O	0	0
			84	84		
7	B	18	Total	O	0	0
			18	18		

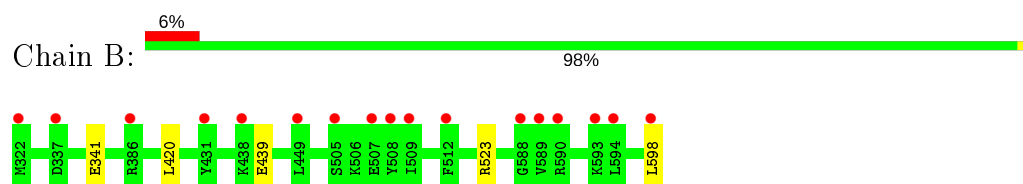
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform



- Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.35Å 135.82Å 150.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.56 49.19 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.56) 99.3 (49.19-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.239 , 0.290 0.238 , 0.285	Depositor DCC
R_{free} test set	2366 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	60.6	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10818	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: GOL, 84R, P6G, SO4

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	0.36	0/8478	0.56	0/11456
2	B	0.37	0/2394	0.57	0/3207
All	All	0.36	0/10872	0.56	0/14663

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

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	8293	0	8293	5	0
2	B	2354	0	2330	1	0
3	A	23	0	0	0	0
4	A	19	0	26	0	0
5	A	5	0	0	0	0
5	B	10	0	0	0	0
6	A	12	0	16	0	0
7	A	84	0	0	0	0
7	B	18	0	0	0	0
All	All	10818	0	10665	5	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 0.

All (5) 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:628:LEU:HD23	1:A:663:ILE:HD13	1.94	0.48
1:A:129:ASP:OD1	1:A:140:ARG:NH1	2.47	0.46
1:A:344:VAL:HG21	1:A:422:LEU:HD13	1.98	0.45
1:A:358:THR:HG21	1:A:389:TYR:OH	2.21	0.40
1:A:1020:ALA:CB	2:B:341:GLU:HG2	2.52	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	1001/1052 (95%)	977 (98%)	22 (2%)	2 (0%)	47	58
2	B	275/277 (99%)	270 (98%)	5 (2%)	0	100	100
All	All	1276/1329 (96%)	1247 (98%)	27 (2%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	SER
1	A	889	ILE

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	928/959 (97%)	907 (98%)	21 (2%)	50	64
2	B	258/258 (100%)	254 (98%)	4 (2%)	62	76
All	All	1186/1217 (98%)	1161 (98%)	25 (2%)	53	67

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	43	ILE
1	A	61	LEU
1	A	81	GLU
1	A	115	ARG
1	A	153	LEU
1	A	199	SER
1	A	204	LYS
1	A	347	ASN
1	A	358	THR
1	A	470	THR
1	A	478	ASP
1	A	516	ARG
1	A	630	GLN
1	A	743	ASP
1	A	788	ILE
1	A	834	LEU
1	A	901	CYS
1	A	942	LYS
1	A	943	LYS
1	A	945	PHE
2	B	420	LEU
2	B	439	GLU
2	B	523	ARG
2	B	598	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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](#)

7 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	$\# Z > 2$
6	GOL	A	1104	-	5,5,5	0.33	0	5,5,5	0.28	0
5	SO4	A	1103	-	4,4,4	0.34	0	6,6,6	0.05	0
3	84R	A	1101	-	24,26,26	0.99	1 (4%)	27,37,37	1.85	9 (33%)
6	GOL	A	1105	-	5,5,5	0.31	0	5,5,5	0.20	0
5	SO4	B	601	-	4,4,4	0.30	0	6,6,6	0.06	0
4	P6G	A	1102	-	18,18,18	0.52	0	17,17,17	0.21	0
5	SO4	B	602	-	4,4,4	0.32	0	6,6,6	0.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	1104	-	-	2/4/4/4	-
4	P6G	A	1102	-	-	6/16/16/16	-
3	84R	A	1101	-	-	0/8/16/16	0/4/4/4
6	GOL	A	1105	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	84R	C15-N20	3.72	1.37	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	84R	C16-C15-N08	3.80	129.13	121.57
3	A	1101	84R	C16-C15-N20	-3.65	113.44	122.60
3	A	1101	84R	C21-C17-C16	3.54	113.20	110.62
3	A	1101	84R	C15-N20-C19	3.44	124.24	116.17
3	A	1101	84R	C19-N18-C17	-2.66	114.70	116.50
3	A	1101	84R	N18-C19-N20	-2.39	124.24	126.11
3	A	1101	84R	C26-C27-C34	2.18	121.79	119.78
3	A	1101	84R	C29-C26-C19	2.18	123.26	120.05
3	A	1101	84R	C05-N08-C15	2.13	124.82	118.73

There are no chirality outliers.

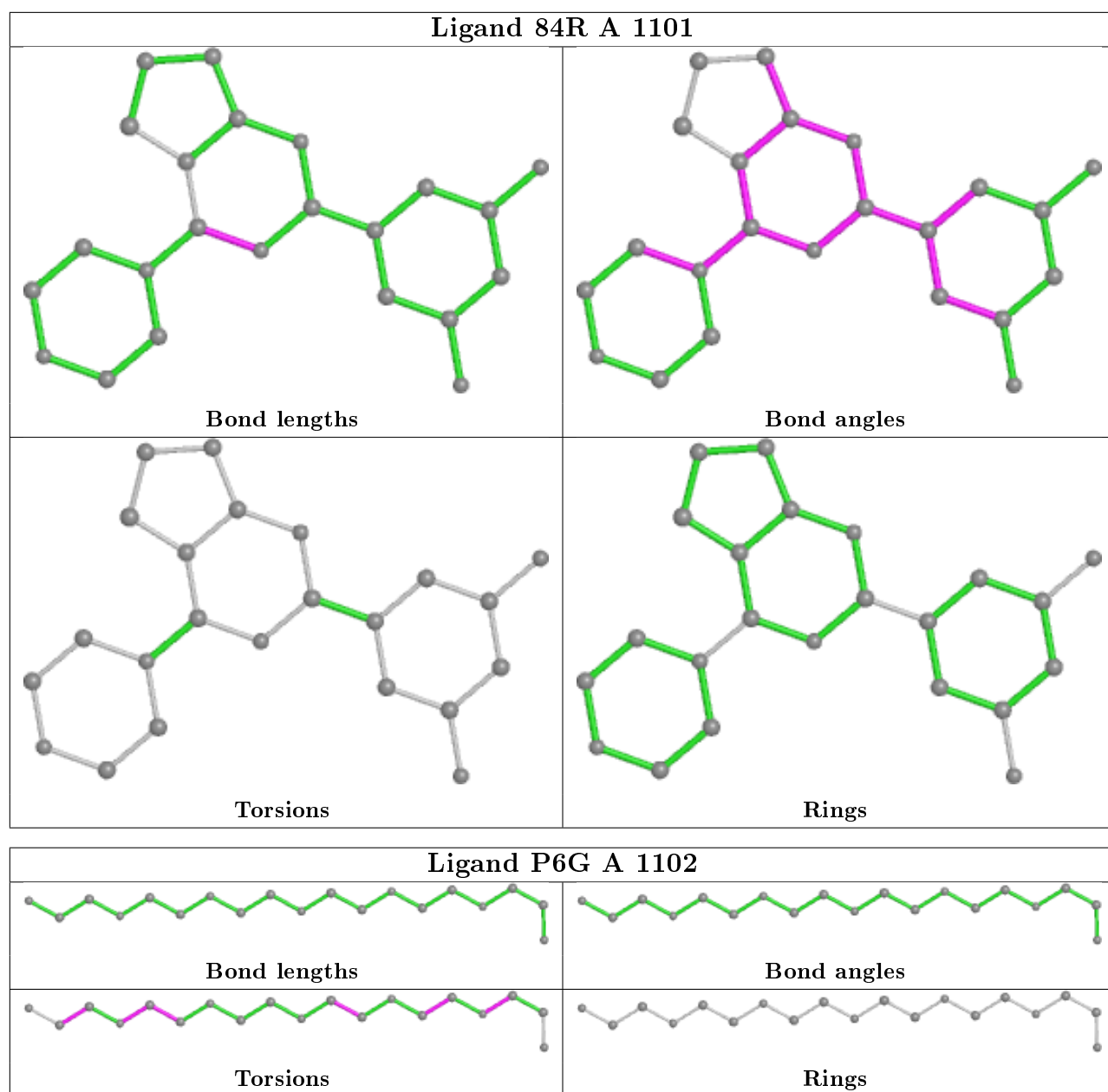
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1104	GOL	C1-C2-C3-O3
4	A	1102	P6G	O13-C14-C15-O16
4	A	1102	P6G	O7-C8-C9-O10
4	A	1102	P6G	O4-C5-C6-O7
6	A	1104	GOL	O2-C2-C3-O3
4	A	1102	P6G	C2-C3-O4-C5
4	A	1102	P6G	C14-C15-O16-C17
4	A	1102	P6G	O16-C17-C18-O19

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	1013/1052 (96%)	0.61	100 (9%)	7 10	40, 68, 127, 200	0
2	B	277/277 (100%)	0.36	17 (6%)	21 26	49, 72, 119, 147	0
All	All	1290/1329 (97%)	0.56	117 (9%)	9 12	40, 69, 125, 200	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	LEU	15.7
1	A	238	GLN	12.7
1	A	241	LEU	7.2
1	A	947	TYR	6.6
2	B	322	MET	6.3
1	A	946	GLY	6.2
1	A	201	ASN	6.1
1	A	207	TYR	6.0
1	A	9	GLU	5.9
1	A	37	LEU	5.7
1	A	243	VAL	5.7
1	A	245	GLU	5.4
1	A	203	ASP	5.4
1	A	205	GLN	5.2
1	A	239	LEU	5.0
1	A	504	ALA	5.0
1	A	197	ILE	4.9
1	A	246	TYR	4.6
1	A	234	LEU	4.3
2	B	509	ILE	4.3
1	A	948	LYS	4.3
1	A	233	LEU	4.2
1	A	237	GLU	4.0
1	A	862	CYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	19	ARG	3.9
1	A	54	ARG	3.8
2	B	508	TYR	3.7
1	A	49	LEU	3.6
1	A	1059	PHE	3.6
1	A	176	GLU	3.6
1	A	200	PRO	3.4
1	A	156	LEU	3.4
1	A	287	LEU	3.4
1	A	414	GLY	3.4
1	A	242	CYS	3.4
2	B	438	LYS	3.4
1	A	744	PHE	3.3
1	A	60	GLN	3.3
1	A	199	SER	3.2
1	A	728	GLN	3.2
1	A	105	VAL	3.2
1	A	192	VAL	3.1
1	A	198	VAL	3.1
1	A	240	LYS	3.1
1	A	945	PHE	3.1
1	A	969	GLN	3.1
1	A	235	SER	3.1
1	A	888	GLU	3.0
1	A	1056	ASP	3.0
1	A	250	TYR	3.0
1	A	208	THR	2.9
1	A	520	ASP	2.9
1	A	51	LYS	2.9
1	A	294	TYR	2.9
2	B	386	ARG	2.9
1	A	729	LYS	2.9
1	A	861	GLN	2.8
1	A	285	LEU	2.8
1	A	70	PHE	2.8
1	A	944	LYS	2.8
1	A	519	ARG	2.8
1	A	301	CYS	2.8
1	A	733	LYS	2.8
1	A	498	TRP	2.7
1	A	99	LEU	2.7
2	B	512	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	593	LYS	2.7
1	A	8	GLY	2.6
1	A	211	ILE	2.6
1	A	261	PHE	2.6
1	A	82	PHE	2.6
2	B	431	TYR	2.6
1	A	320	GLY	2.6
1	A	68	TYR	2.6
1	A	260	TYR	2.5
2	B	589	VAL	2.5
2	B	598	LEU	2.5
1	A	162	ARG	2.5
1	A	949	ARG	2.4
1	A	204	LYS	2.4
1	A	226	ARG	2.4
1	A	262	LEU	2.4
1	A	1006	LEU	2.4
1	A	187	LYS	2.4
1	A	299	MET	2.4
2	B	337	ASP	2.4
1	A	297	LEU	2.4
1	A	196	VAL	2.3
1	A	14	HIS	2.3
1	A	86	THR	2.3
1	A	121	ILE	2.3
1	A	282	MET	2.3
1	A	860	ILE	2.3
1	A	194	ILE	2.2
1	A	839	LEU	2.2
1	A	45	ILE	2.2
1	A	221	ILE	2.2
1	A	881	LEU	2.2
2	B	588	GLY	2.2
1	A	1002	PHE	2.2
2	B	449	LEU	2.2
1	A	734	PHE	2.2
1	A	257	CYS	2.2
2	B	505	SER	2.2
1	A	859	GLN	2.2
1	A	1055	MET	2.1
1	A	83	PHE	2.1
1	A	267	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	722	GLU	2.1
2	B	594	LEU	2.1
1	A	331	ASN	2.1
1	A	248	GLY	2.1
1	A	264	LYS	2.0
1	A	278	MET	2.0
2	B	590	ARG	2.0
1	A	91	ASP	2.0
2	B	507	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 carbohydrates in this entry.

6.4 Ligands [i](#)

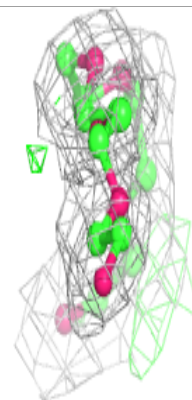
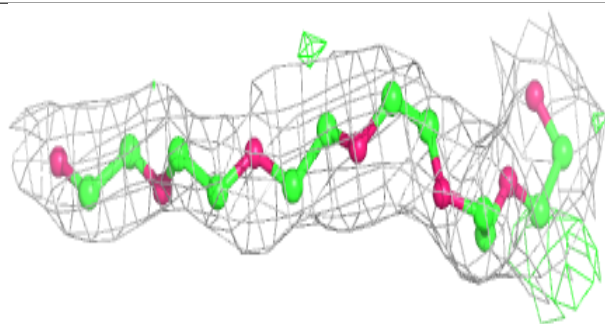
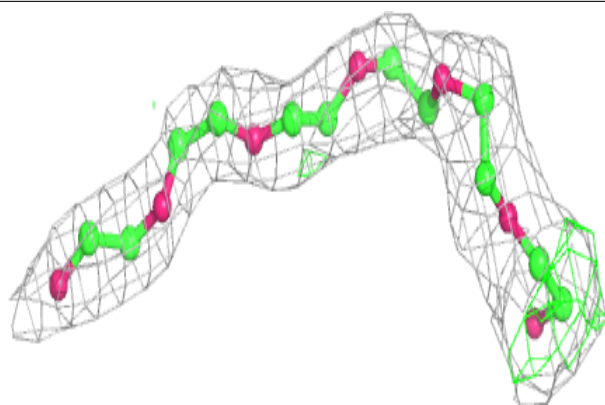
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

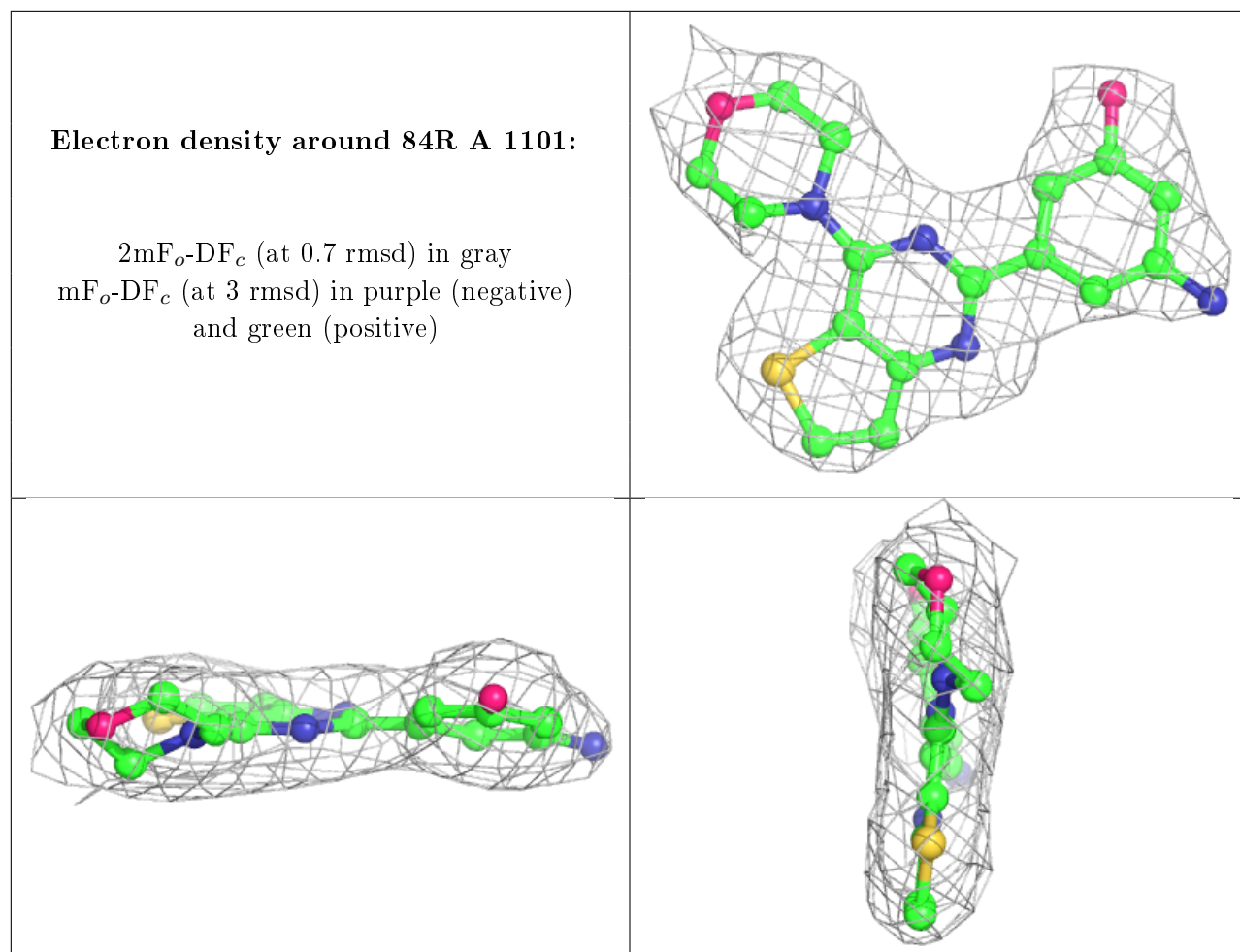
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	A	1104	6/6	0.64	0.26	104,107,107,107	0
6	GOL	A	1105	6/6	0.66	0.21	90,91,92,92	0
5	SO4	A	1103	5/5	0.77	0.21	113,114,116,117	0
4	P6G	A	1102	19/19	0.78	0.24	88,93,97,97	0
5	SO4	B	602	5/5	0.82	0.26	110,112,113,115	0
3	84R	A	1101	23/23	0.93	0.17	46,48,51,52	0
5	SO4	B	601	5/5	0.98	0.14	82,84,86,87	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 P6G A 1102:

$2mF_o - DF_c$ (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.