wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 06:05 PM EDT

PDB ID	:	6P69
Title	:	Crystal structure of FGFR1-Y563C (FGFR4 surrogate) covalently bound to compound 11.
Authors	:	Larsen, N.A.
Deposited on	:	2019-06-03
Resolution	:	2.20 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 (1)) were used in the production of this report:

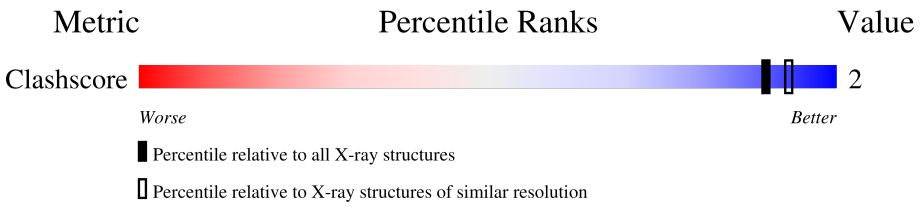
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.20 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	5594 (2.20-2.20)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	309	89% • 7%
1	B	309	88% 5% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4936 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.

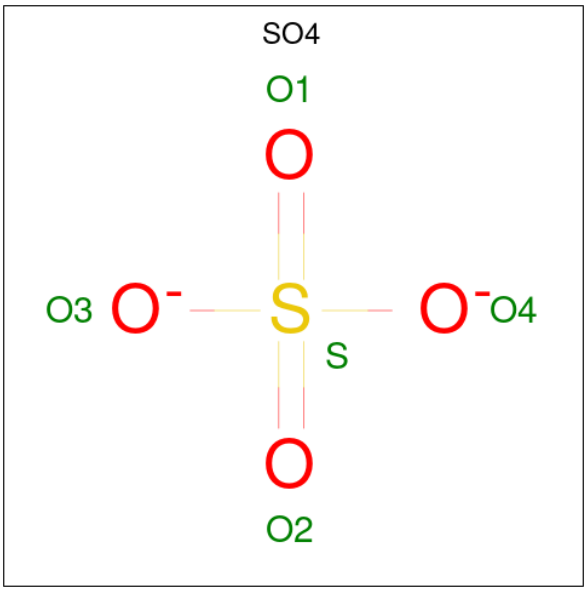
- Molecule 1 is a protein called Fibroblast growth factor receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2301	1463	394	424	20	0	2	0
1	B	286	2272	1446	390	417	19	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

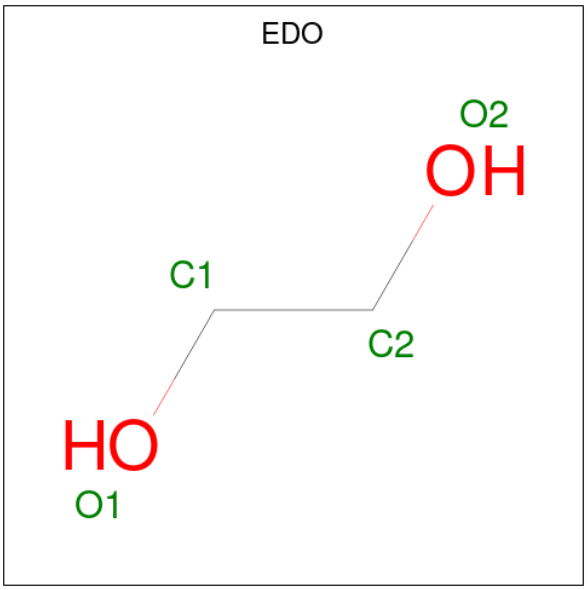
Chain	Residue	Modelled	Actual	Comment	Reference
A	457	GLY	-	expression tag	UNP P11362
A	488	ALA	CYS	engineered mutation	UNP P11362
A	563	CYS	TYR	engineered mutation	UNP P11362
A	584	SER	CYS	conflict	UNP P11362
B	457	GLY	-	expression tag	UNP P11362
B	488	ALA	CYS	engineered mutation	UNP P11362
B	563	CYS	TYR	engineered mutation	UNP P11362
B	584	SER	CYS	conflict	UNP P11362

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0

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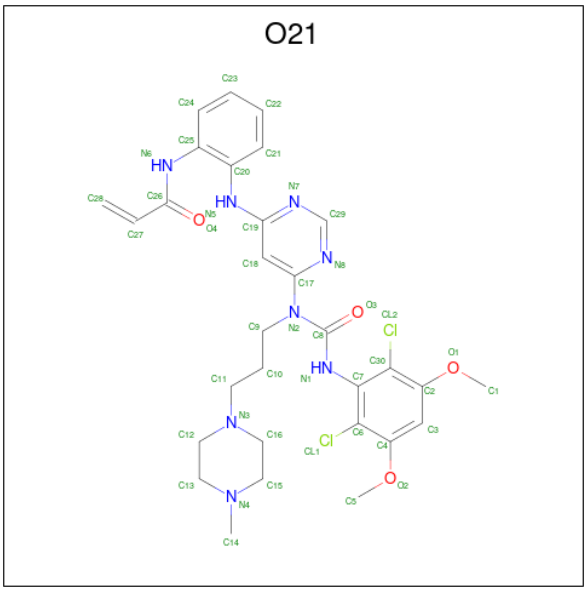
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	2	2	0	0
3	B	1	4	2	2	0	0

- Molecule 4 is N-{2-[(6-{[(2,6-dichloro-3,5-dimethoxyphenyl)carbamoyl][3-(4-methylpiperazin-1-yl)propyl]amino}pyrimidin-4-yl)amino]phenyl}prop-2-enamide (three-letter code: O21) (formula: $C_{30}H_{36}Cl_2N_8O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
4	A	1	44	30	2	8	4	0	0
4	B	1	44	30	2	8	4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	128	128	128	0	0
5	B	120	120	120	0	0

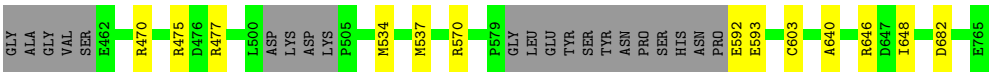
3 Residue-property plots (i)

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. 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. 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.

Note EDS failed to run properly.

• Molecule 1: Fibroblast growth factor receptor 1

Chain A:



• Molecule 1: Fibroblast growth factor receptor 1

Chain B:

4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	205.37Å 58.52Å 66.13Å 90.00° 107.31° 90.00°	Depositor
Resolution (Å)	34.11 – 2.20	Depositor
% Data completeness (in resolution range)	99.6 (34.11-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.14 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.186 , 0.245	Depositor
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.082	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h-2*l,-k,l	Xtriage
Total number of atoms	4936	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.13% 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: O21, SO4, EDO

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	1.23	2/2354 (0.1%)	0.94	8/3179 (0.3%)
1	B	0.90	2/2322 (0.1%)	0.89	1/3137 (0.0%)
All	All	1.08	4/4676 (0.1%)	0.91	9/6316 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	603[A]	CYS	CB-SG	-32.69	1.26	1.82
1	A	603[B]	CYS	CB-SG	-32.69	1.26	1.82
1	B	603[A]	CYS	CB-SG	-12.31	1.61	1.82
1	B	603[B]	CYS	CB-SG	-12.31	1.61	1.82

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	470	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	A	603[A]	CYS	CA-CB-SG	6.20	125.16	114.00
1	A	603[B]	CYS	CA-CB-SG	6.20	125.16	114.00
1	A	534	MET	CG-SD-CE	-6.18	90.32	100.20
1	A	682	ASP	CB-CG-OD2	-6.07	112.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	648	ILE	Peptide

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	2301	0	2313	5	0
1	B	2272	0	2285	10	0
2	A	5	0	0	1	0
2	B	10	0	0	0	0
3	A	8	0	12	0	0
3	B	4	0	6	1	0
4	A	44	0	0	2	0
4	B	44	0	0	2	0
5	A	128	0	0	0	0
5	B	120	0	0	2	0
All	All	4936	0	4616	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 2.

The worst 5 of 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:B:535:MET:CE	1:B:547:LEU:HD13	2.21	0.70
1:B:731:MET:HE2	5:B:941:HOH:O	2.01	0.61
4:A:804:O21:N1	4:A:804:O21:N8	2.51	0.56
1:A:570:ARG:NE	2:A:801:SO4:O1	2.40	0.55
4:B:804:O21:N8	4:B:804:O21:N1	2.52	0.54

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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)

8 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	$\#\|Z\| > 2$
3	EDO	A	803	-	3,3,3	0.43	0	2,2,2	0.30	0
2	SO4	B	802	-	4,4,4	0.51	0	6,6,6	0.12	0
3	EDO	A	802	-	3,3,3	0.35	0	2,2,2	0.53	0
4	O21	A	804	1	47,47,47	1.85	10 (21%)	58,64,64	2.49	18 (31%)
4	O21	B	804	1	47,47,47	1.63	8 (17%)	58,64,64	3.01	15 (25%)
2	SO4	A	801	-	4,4,4	0.61	0	6,6,6	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	801	-	4,4,4	0.23	0	6,6,6	0.79	0
3	EDO	B	803	-	3,3,3	0.29	0	2,2,2	0.87	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
3	EDO	A	803	-	-	1/1/1/1	-
3	EDO	A	802	-	-	0/1/1/1	-
4	O21	A	804	1	-	5/32/42/42	0/4/4/4
4	O21	B	804	1	-	8/32/42/42	0/4/4/4
3	EDO	B	803	-	-	0/1/1/1	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	804	O21	C28-C27	5.39	1.57	1.30
4	B	804	O21	C28-C27	5.16	1.55	1.30
4	A	804	O21	C27-C26	4.84	1.56	1.48
4	A	804	O21	C29-N7	4.54	1.42	1.33
4	B	804	O21	C7-N1	-4.15	1.35	1.43

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	804	O21	C29-N8-C17	13.05	126.34	114.94
4	A	804	O21	C14-N4-C15	-8.18	98.43	110.66
4	B	804	O21	C27-C26-N6	7.05	118.48	113.84
4	A	804	O21	C27-C26-N6	6.97	118.43	113.84
4	B	804	O21	C16-C15-N4	6.05	117.64	110.80

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	804	O21	N6-C26-C27-C28
4	A	804	O21	O4-C26-C27-C28
4	B	804	O21	N6-C26-C27-C28
4	B	804	O21	O4-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
4	B	804	O21	N8-C17-N2-C9

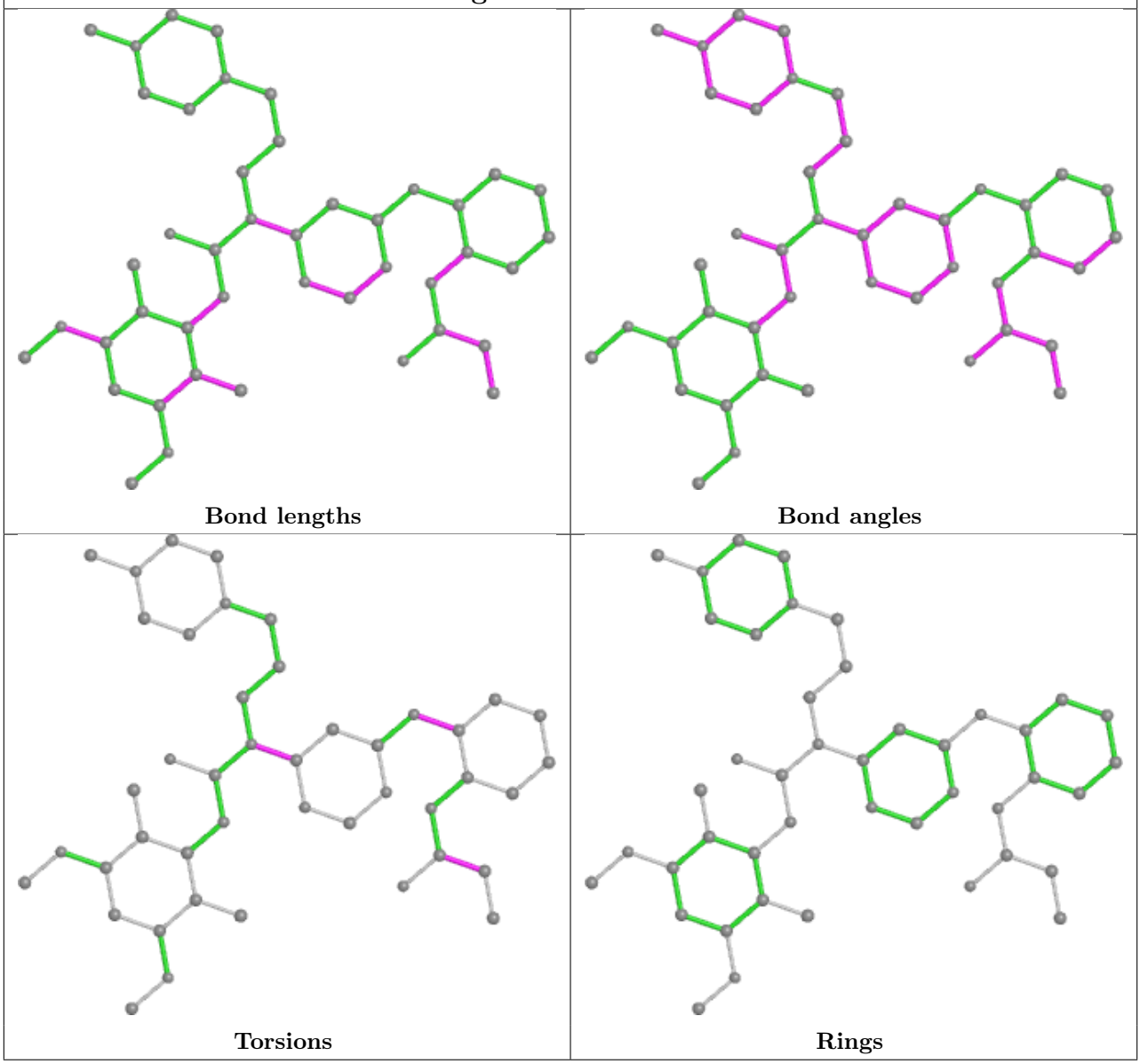
There are no ring outliers.

4 monomers are involved in 6 short contacts:

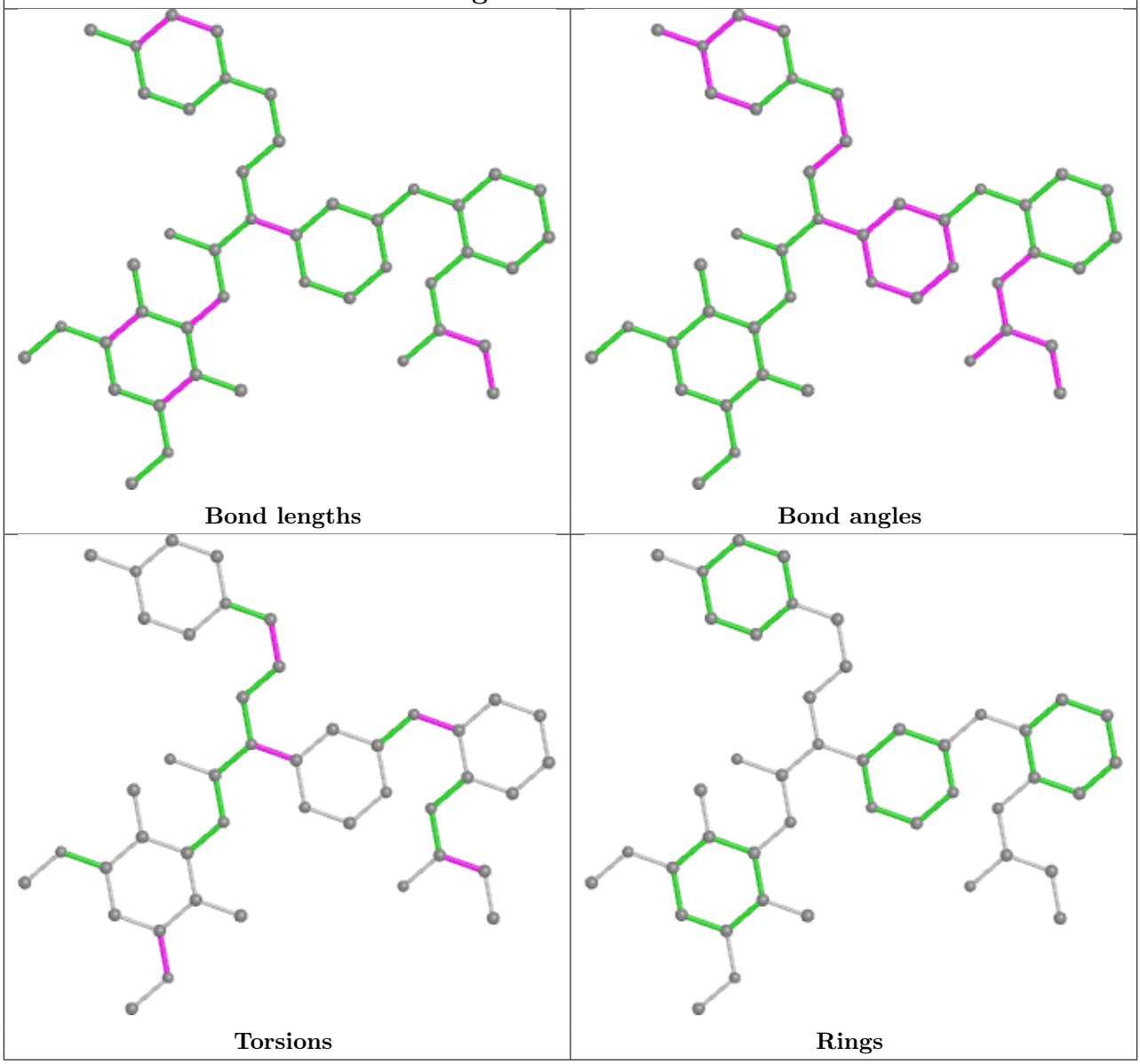
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	804	O21	2	0
4	B	804	O21	2	0
2	A	801	SO4	1	0
3	B	803	EDO	1	0

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 O21 A 804



Ligand O21 B 804



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)

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.