



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 4, 2023 – 10:08 PM EDT

PDB ID : 6V6Z
Title : Crystal structure of N-[(4-methoxyphenyl)sulfonyl]-N-(4-[[[(4-methoxyphenyl)sulfonyl]amino}naphthalen-1-yl)glycine bound to human Keap1 Kelch domain
Authors : Lazzara, P.R.; David, B.P.; Ankireddy, A.; Richardson, B.G.; Dye, K.; Ratia, K.M.; Reddy, S.P.; Moore, T.W.
Deposited on : 2019-12-06
Resolution : 1.60 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 : **FAILED**
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

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10213 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 Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	285	2200	1370	400	413	17	0	3	0
1	B	286	2208	1377	398	416	17	0	3	0
1	C	285	2192	1363	398	416	15	0	1	0
1	D	285	2207	1375	399	417	16	0	4	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	SER	-	expression tag	UNP Q14145
A	540	ALA	GLU	engineered mutation	UNP Q14145
A	542	ALA	GLU	engineered mutation	UNP Q14145
B	320	SER	-	expression tag	UNP Q14145
B	540	ALA	GLU	engineered mutation	UNP Q14145
B	542	ALA	GLU	engineered mutation	UNP Q14145
C	320	SER	-	expression tag	UNP Q14145
C	540	ALA	GLU	engineered mutation	UNP Q14145
C	542	ALA	GLU	engineered mutation	UNP Q14145
D	320	SER	-	expression tag	UNP Q14145
D	540	ALA	GLU	engineered mutation	UNP Q14145
D	542	ALA	GLU	engineered mutation	UNP Q14145

- Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



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

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

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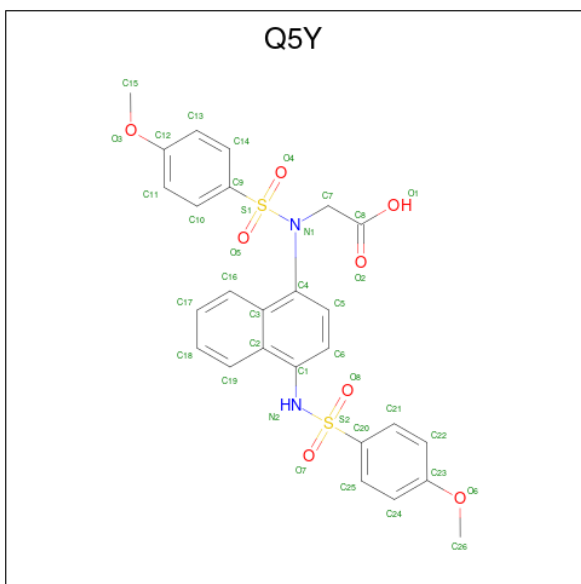
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total 3	C 1	O 2	0	0
2	C	1	Total 3	C 1	O 2	0	0
2	C	1	Total 3	C 1	O 2	0	0
2	C	1	Total 3	C 1	O 2	0	0
2	C	1	Total 3	C 1	O 2	0	0
2	C	1	Total 3	C 1	O 2	0	0
2	C	1	Total 3	C 1	O 2	0	0
2	C	1	Total 3	C 1	O 2	0	0
2	C	1	Total 3	C 1	O 2	0	0
2	C	1	Total 3	C 1	O 2	0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

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

- Molecule 3 is N-[(4-methoxyphenyl)sulfonyl]-N-(4-[(4-methoxyphenyl)sulfonyl]amino)naphthalen-1-yl)glycine (three-letter code: Q5Y) (formula: C₂₆H₂₄N₂O₈S₂) (labeled as "Ligand of Interest" by depositor).

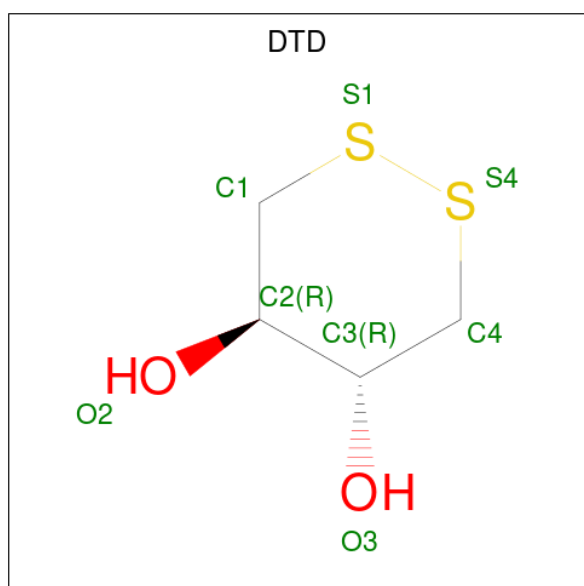


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			38	26	2	8	2		
3	B	1	Total	C	N	O	S	0	0
			38	26	2	8	2		
3	C	1	Total	C	N	O	S	0	0
			38	26	2	8	2		
3	D	1	Total	C	N	O	S	0	0
			38	26	2	8	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

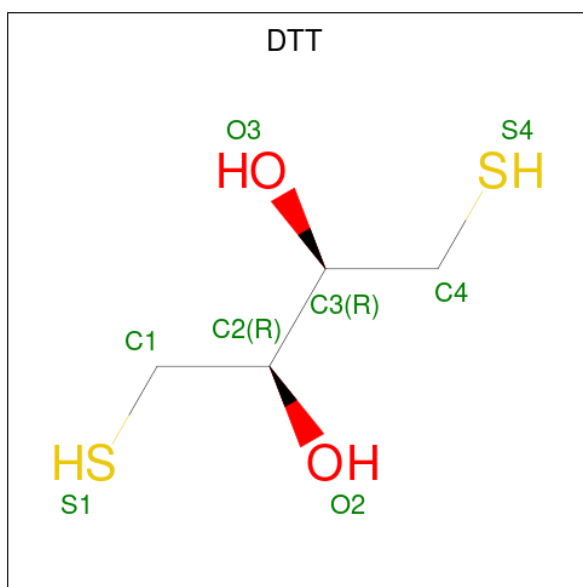
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Na 3 3	0	0
4	B	2	Total Na 2 2	0	0
4	C	1	Total Na 1 1	0	0
4	D	2	Total Na 2 2	0	0

- Molecule 5 is DITHIANE DIOL (three-letter code: DTD) (formula: $C_4H_8O_2S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O S 8 4 2 2	0	0

- Molecule 6 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	308	Total	O	0	0
			308	308		
7	B	274	Total	O	0	0
			274	274		
7	C	242	Total	O	0	0
			242	242		
7	D	223	Total	O	0	0
			223	223		

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

3 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.36Å 75.54Å 97.95Å 74.55° 77.54° 67.48°	Depositor
Resolution (Å)	19.73 – 1.60	Depositor
% Data completeness (in resolution range)	92.0 (19.73-1.60)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 1.60Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.192 , 0.210	Depositor
Wilson B-factor (Å ²)	20.0	Xtrriage
Anisotropy	0.384	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	10213	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 75 ligands modelled in this entry, 8 are monoatomic - leaving 67 for Mogul analysis.

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	FMT	B	719	-	2,2,2	0.42	0	1,1,1	0.21	0
2	FMT	B	705	-	2,2,2	0.44	0	1,1,1	0.06	0
2	FMT	C	713	-	2,2,2	0.26	0	1,1,1	0.21	0
2	FMT	C	717	-	2,2,2	0.30	0	1,1,1	0.14	0
2	FMT	D	702	-	2,2,2	0.29	0	1,1,1	0.20	0
3	Q5Y	A	703	-	41,41,41	2.01	7 (17%)	56,60,60	2.66	15 (26%)
3	Q5Y	B	707	-	41,41,41	1.90	9 (21%)	56,60,60	2.65	13 (23%)
2	FMT	B	717	-	2,2,2	0.37	0	1,1,1	0.11	0
2	FMT	C	711	4	2,2,2	0.29	0	1,1,1	0.15	0
2	FMT	B	711	-	2,2,2	0.31	0	1,1,1	0.27	0
2	FMT	D	717	-	2,2,2	0.41	0	1,1,1	0.06	0
2	FMT	C	701	-	2,2,2	0.36	0	1,1,1	0.06	0
2	FMT	B	716	-	2,2,2	0.41	0	1,1,1	0.07	0
2	FMT	D	711	-	2,2,2	0.22	0	1,1,1	0.23	0
2	FMT	B	713	-	2,2,2	0.11	0	1,1,1	0.27	0
3	Q5Y	C	706	-	41,41,41	1.86	9 (21%)	56,60,60	2.77	17 (30%)
2	FMT	D	707	-	2,2,2	0.46	0	1,1,1	0.03	0
5	DTD	C	707	-	6,8,8	2.16	1 (16%)	6,10,10	1.64	2 (33%)
2	FMT	C	716	-	2,2,2	0.47	0	1,1,1	0.05	0
2	FMT	D	719	-	2,2,2	0.36	0	1,1,1	0.13	0
2	FMT	A	711	-	2,2,2	0.49	0	1,1,1	0.39	0
2	FMT	B	702	-	2,2,2	0.25	0	1,1,1	0.19	0
2	FMT	B	704	-	2,2,2	0.40	0	1,1,1	0.08	0
2	FMT	A	701	-	2,2,2	0.22	0	1,1,1	0.18	0
2	FMT	B	703	-	2,2,2	0.37	0	1,1,1	0.17	0
2	FMT	A	712	-	2,2,2	0.42	0	1,1,1	0.13	0
2	FMT	B	708	-	2,2,2	0.39	0	1,1,1	0.06	0
2	FMT	A	710	-	2,2,2	0.21	0	1,1,1	0.26	0
2	FMT	D	706	-	2,2,2	0.25	0	1,1,1	0.17	0
2	FMT	C	715	-	2,2,2	0.37	0	1,1,1	0.06	0
2	FMT	A	702	-	2,2,2	0.31	0	1,1,1	0.09	0
2	FMT	B	715	4	2,2,2	0.42	0	1,1,1	0.02	0
2	FMT	C	702	-	2,2,2	0.28	0	1,1,1	0.27	0
2	FMT	C	704	-	2,2,2	0.32	0	1,1,1	0.11	0
2	FMT	B	718	4	2,2,2	0.05	0	1,1,1	0.35	0
2	FMT	D	703	-	2,2,2	0.22	0	1,1,1	0.21	0
2	FMT	D	714	-	2,2,2	0.22	0	1,1,1	0.10	0
2	FMT	D	705	4	2,2,2	0.38	0	1,1,1	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMT	A	707	-	2,2,2	0.39	0	1,1,1	0.06	0
6	DTT	D	709	-	7,7,7	0.29	0	4,8,8	0.88	0
2	FMT	D	715	-	2,2,2	0.33	0	1,1,1	0.15	0
3	Q5Y	D	704	-	41,41,41	2.03	10 (24%)	56,60,60	3.04	15 (26%)
2	FMT	D	701	-	2,2,2	0.27	0	1,1,1	0.20	0
2	FMT	C	710	-	2,2,2	0.38	0	1,1,1	0.10	0
2	FMT	C	712	-	2,2,2	0.26	0	1,1,1	0.24	0
2	FMT	B	712	-	2,2,2	0.24	0	1,1,1	0.25	0
2	FMT	A	715	-	2,2,2	0.16	0	1,1,1	0.21	0
2	FMT	B	710	-	2,2,2	0.56	0	1,1,1	0.00	0
2	FMT	C	708	-	2,2,2	0.28	0	1,1,1	0.17	0
2	FMT	C	709	-	2,2,2	0.31	0	1,1,1	0.17	0
2	FMT	D	713	-	2,2,2	0.20	0	1,1,1	0.28	0
2	FMT	C	719	-	2,2,2	0.34	0	1,1,1	0.13	0
2	FMT	B	709	-	2,2,2	0.37	0	1,1,1	0.13	0
2	FMT	D	716	-	2,2,2	0.31	0	1,1,1	0.11	0
2	FMT	C	718	-	2,2,2	0.27	0	1,1,1	0.11	0
2	FMT	A	706	-	2,2,2	0.25	0	1,1,1	0.25	0
2	FMT	D	712	-	2,2,2	0.28	0	1,1,1	0.23	0
2	FMT	B	714	-	2,2,2	0.50	0	1,1,1	0.08	0
2	FMT	C	720	-	2,2,2	0.36	0	1,1,1	0.10	0
2	FMT	A	714	-	2,2,2	0.47	0	1,1,1	0.27	0
2	FMT	C	703	-	2,2,2	0.34	0	1,1,1	0.21	0
2	FMT	B	706	-	2,2,2	0.97	0	1,1,1	0.16	0
2	FMT	B	701	-	2,2,2	0.18	0	1,1,1	0.18	0
2	FMT	C	714	-	2,2,2	0.41	0	1,1,1	0.05	0
2	FMT	A	713	-	2,2,2	0.29	0	1,1,1	0.18	0
2	FMT	D	718	-	2,2,2	0.26	0	1,1,1	0.07	0
2	FMT	A	704	-	2,2,2	0.25	0	1,1,1	0.26	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
5	DTD	C	707	-	-	-	0/0/1/1
3	Q5Y	A	703	-	-	9/35/35/35	0/4/4/4
3	Q5Y	B	707	-	-	15/35/35/35	0/4/4/4
6	DTT	D	709	-	-	3/8/8/8	-
3	Q5Y	D	704	-	-	3/35/35/35	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	Q5Y	C	706	-	-	4/35/35/35	0/4/4/4

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	Q5Y	S1-N1	9.64	1.78	1.65
3	C	706	Q5Y	S1-N1	6.92	1.74	1.65
3	D	704	Q5Y	S1-N1	6.68	1.74	1.65
3	B	707	Q5Y	S1-N1	5.88	1.73	1.65
5	C	707	DTD	S4-S1	5.03	2.51	2.01

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	704	Q5Y	O5-S1-N1	11.99	120.90	106.71
3	A	703	Q5Y	O5-S1-N1	10.90	119.60	106.71
3	B	707	Q5Y	O5-S1-O4	-10.23	102.95	119.52
3	B	707	Q5Y	O4-S1-C9	10.00	120.69	108.05
3	C	706	Q5Y	O5-S1-N1	9.87	118.39	106.71

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

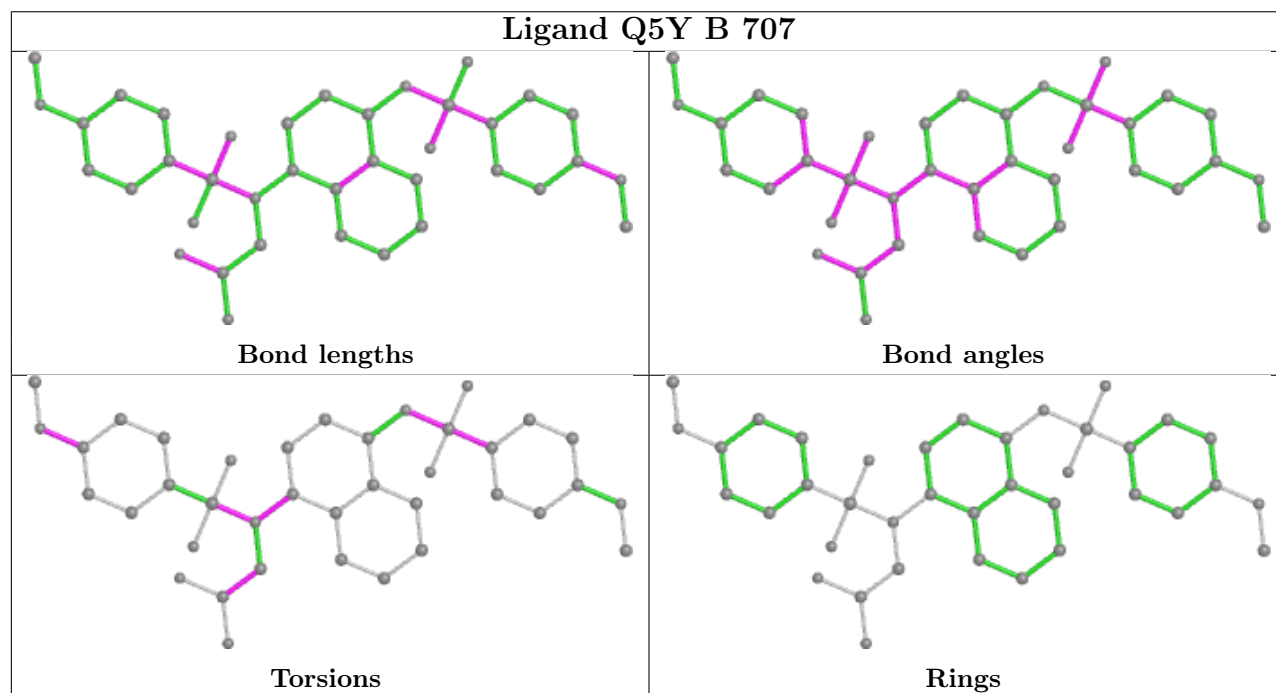
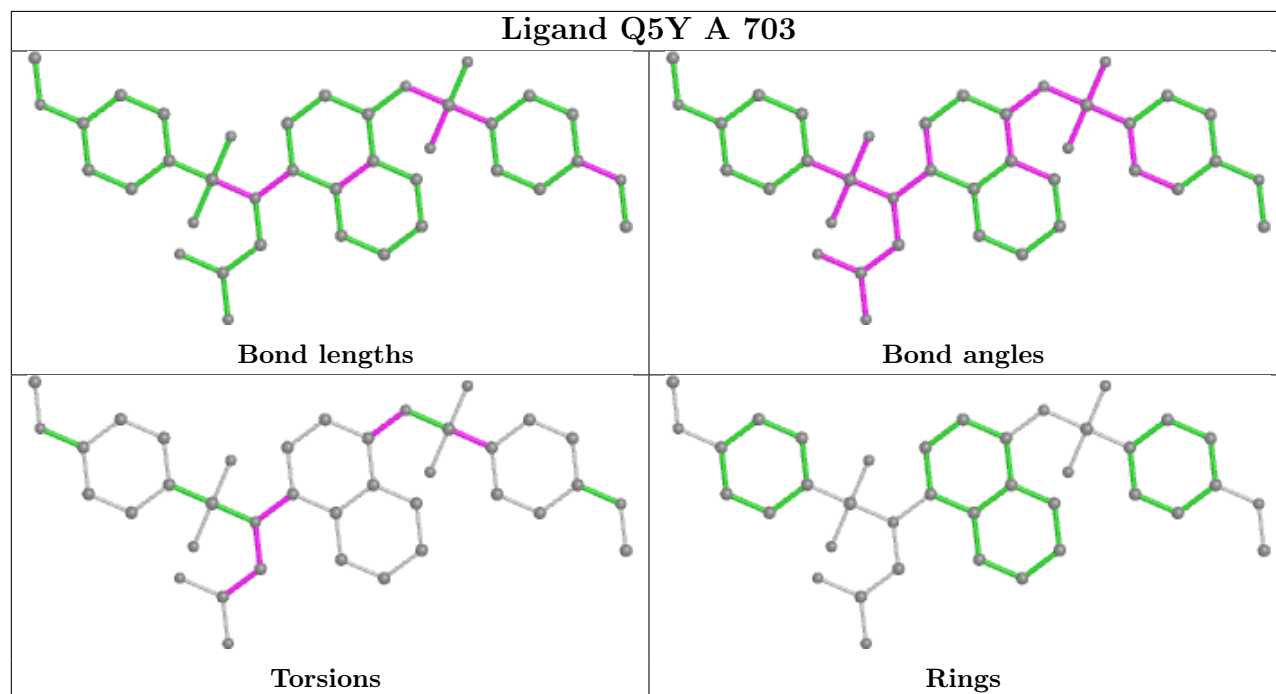
Mol	Chain	Res	Type	Atoms
3	A	703	Q5Y	C8-C7-N1-C4
3	D	704	Q5Y	C24-C23-O6-C26
3	D	704	Q5Y	C22-C23-O6-C26
3	B	707	Q5Y	C11-C12-O3-C15
3	B	707	Q5Y	C13-C12-O3-C15

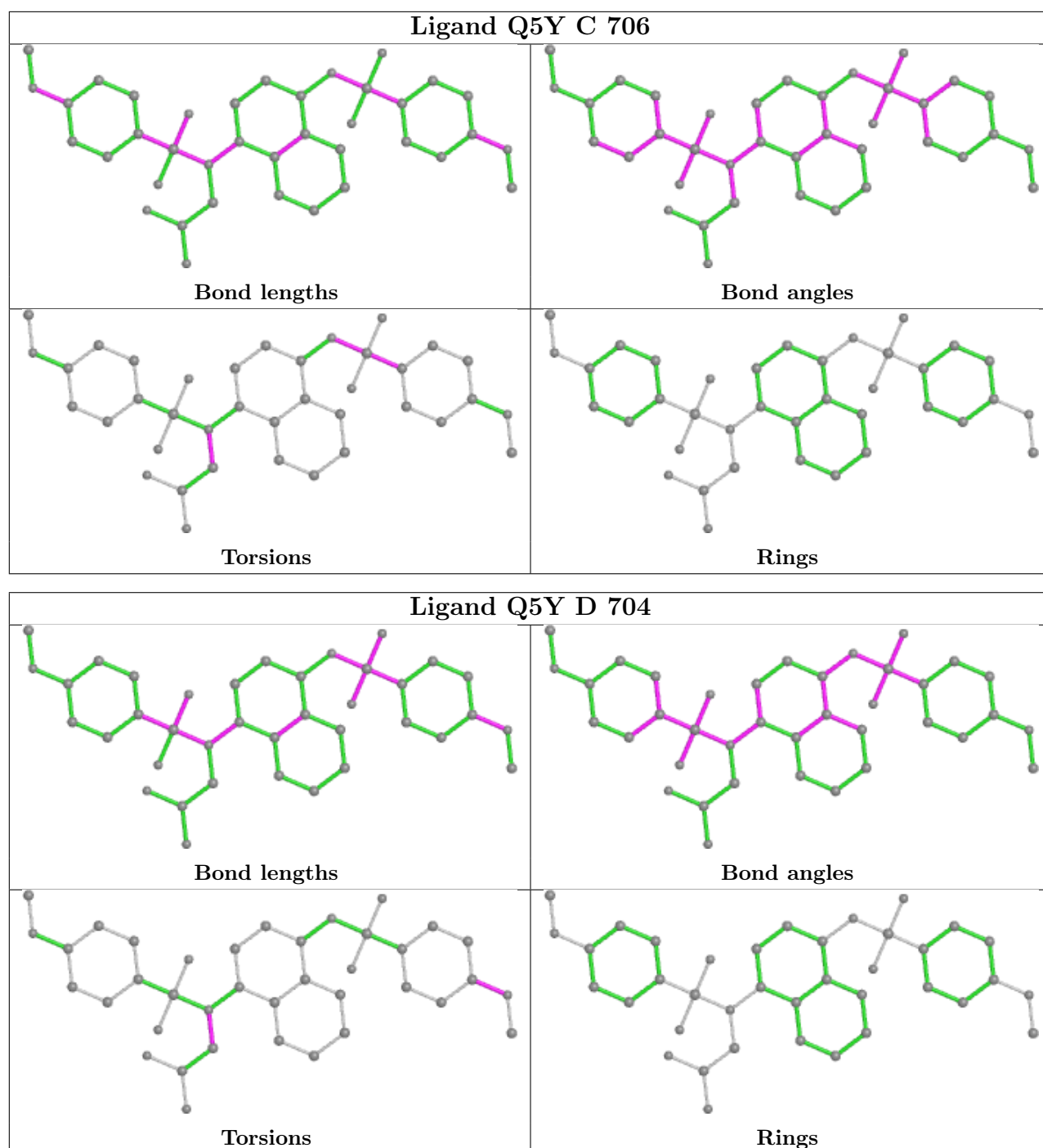
There are no ring outliers.

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.





4.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

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

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.3 Carbohydrates [i](#)

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

5.4 Ligands [i](#)

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

5.5 Other polymers [i](#)

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