



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 11:28 am BST

PDB ID : 1TXC
Title : Complex crystal structure of SPE16 with ANS
Authors : Wu, F.; Wei, Z.; Zhou, Z.; Gong, W.
Deposited on : 2004-07-02
Resolution : 2.30 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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) : 2.11

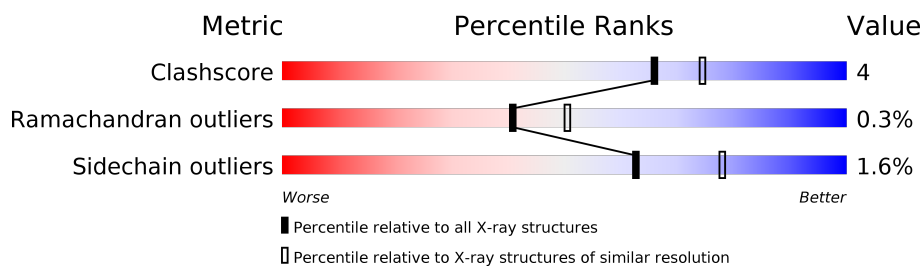
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	157	
1	B	157	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2537 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.

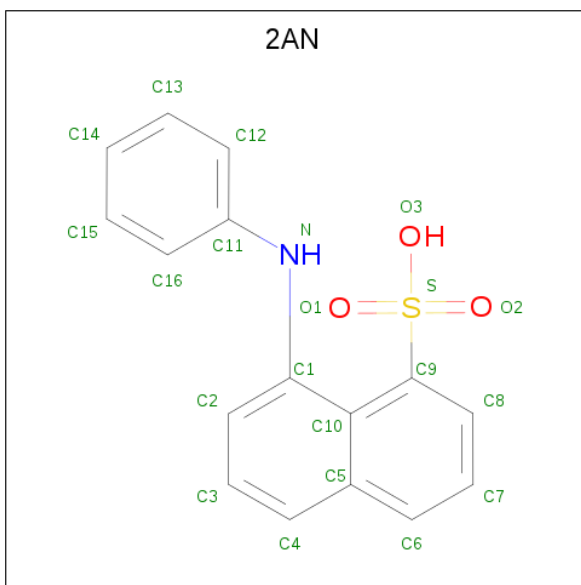
- Molecule 1 is a protein called pathogenesis-related class 10 protein SPE-16.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	0	0	0
			1156	732	187	237			
1	B	157	Total	C	N	O	0	0	0
			1156	732	187	237			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	GLY	-	CLONING ARTIFACT	UNP Q6T6J0
A	149	TYR	-	CLONING ARTIFACT	UNP Q6T6J0
A	150	VAL	-	CLONING ARTIFACT	UNP Q6T6J0
A	151	LEU	-	CLONING ARTIFACT	UNP Q6T6J0
A	152	ALA	-	CLONING ARTIFACT	UNP Q6T6J0
A	153	ASN	-	CLONING ARTIFACT	UNP Q6T6J0
A	154	PRO	-	CLONING ARTIFACT	UNP Q6T6J0
A	155	ALA	-	CLONING ARTIFACT	UNP Q6T6J0
A	156	GLU	-	CLONING ARTIFACT	UNP Q6T6J0
A	157	TYR	-	CLONING ARTIFACT	UNP Q6T6J0
B	148	GLY	-	CLONING ARTIFACT	UNP Q6T6J0
B	149	TYR	-	CLONING ARTIFACT	UNP Q6T6J0
B	150	VAL	-	CLONING ARTIFACT	UNP Q6T6J0
B	151	LEU	-	CLONING ARTIFACT	UNP Q6T6J0
B	152	ALA	-	CLONING ARTIFACT	UNP Q6T6J0
B	153	ASN	-	CLONING ARTIFACT	UNP Q6T6J0
B	154	PRO	-	CLONING ARTIFACT	UNP Q6T6J0
B	155	ALA	-	CLONING ARTIFACT	UNP Q6T6J0
B	156	GLU	-	CLONING ARTIFACT	UNP Q6T6J0
B	157	TYR	-	CLONING ARTIFACT	UNP Q6T6J0

- Molecule 2 is 8-ANILINO-1-NAPHTHALENE SULFONATE (three-letter code: 2AN) (formula: C₁₆H₁₃NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	A	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

- Molecule 3 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		
3	B	58	Total	O	0	0
			58	58		

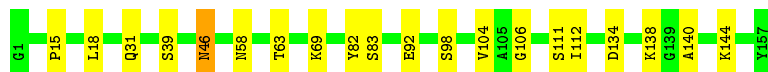
3 Residue-property plots [i](#)

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. 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 was not executed.

- Molecule 1: pathogenesis-related class 10 protein SPE-16

Chain A: 



- Molecule 1: pathogenesis-related class 10 protein SPE-16

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.90 Å 65.09 Å 78.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.99 – 2.30	Depositor
% Data completeness (in resolution range)	95.2 (28.99-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.182 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2537	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2AN

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	0.35	0/1173	0.57	0/1582
1	B	0.33	0/1173	0.59	0/1582
All	All	0.34	0/2346	0.58	0/3164

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	1156	0	1160	12	0
1	B	1156	0	1160	6	0
2	A	42	0	26	1	0
2	B	63	0	39	2	0
3	A	62	0	0	1	0
3	B	58	0	0	0	0
All	All	2537	0	2385	19	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 4.

All (19) 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:134:ASP:OD1	1:A:138:LYS:HE2	1.90	0.70
1:A:15:PRO:HG3	1:A:111:SER:HB3	1.78	0.66
1:A:58:ASN:OD1	1:A:63:THR:HG22	1.97	0.64
1:A:92:GLU:HG3	3:A:763:HOH:O	1.98	0.63
1:A:83:SER:HB3	1:A:98:SER:HA	1.80	0.62
2:A:715:2AN:H4	2:A:716:2AN:O3	2.02	0.59
1:B:8:GLU:HG2	1:B:114:LYS:HG2	1.86	0.56
1:A:104:VAL:HG23	1:A:112:ILE:HB	1.90	0.54
1:B:83:SER:HB3	1:B:98:SER:HA	1.90	0.52
1:A:104:VAL:CG2	1:A:112:ILE:HB	2.40	0.51
1:A:31:GLN:HE21	1:A:39:SER:HA	1.79	0.48
1:B:135:ALA:HB1	2:B:718:2AN:H14	1.94	0.48
1:A:69:LYS:O	1:A:82:TYR:HB2	2.14	0.47
1:B:90:LEU:HD12	1:B:91:PRO:HD2	1.97	0.46
1:A:46:ASN:HD22	1:A:46:ASN:C	2.20	0.45
1:B:27:ASP:HA	1:B:40:ILE:HD12	2.00	0.44
1:A:140:ALA:O	1:A:144:LYS:HG2	2.19	0.43
1:B:69:LYS:HE2	2:B:719:2AN:O3	2.21	0.41
1:A:106:GLY:N	1:A:111:SER:HA	2.36	0.41

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	155/157 (99%)	155 (100%)	0	0	100	100
1	B	155/157 (99%)	148 (96%)	6 (4%)	1 (1%)	25	31
All	All	310/314 (99%)	303 (98%)	6 (2%)	1 (0%)	41	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	123	GLY

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	122/122 (100%)	120 (98%)	2 (2%)	62	78
1	B	122/122 (100%)	120 (98%)	2 (2%)	62	78
All	All	244/244 (100%)	240 (98%)	4 (2%)	62	78

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	46	ASN
1	B	18	LEU
1	B	59	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	46	ASN
1	B	58	ASN
1	B	77	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

5 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	2AN	B	717	-	22,23,23	3.99	16 (72%)	29,33,33	1.33	3 (10%)
2	2AN	A	715	-	22,23,23	3.98	16 (72%)	29,33,33	1.48	4 (13%)
2	2AN	B	719	-	22,23,23	4.04	16 (72%)	29,33,33	1.50	5 (17%)
2	2AN	B	718	-	22,23,23	3.90	16 (72%)	29,33,33	1.61	6 (20%)
2	2AN	A	716	-	22,23,23	4.09	16 (72%)	29,33,33	1.53	4 (13%)

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	2AN	B	717	-	-	0/10/10/10	0/3/3/3
2	2AN	A	715	-	-	2/10/10/10	0/3/3/3
2	2AN	B	719	-	-	0/10/10/10	0/3/3/3
2	2AN	B	718	-	-	0/10/10/10	0/3/3/3
2	2AN	A	716	-	-	0/10/10/10	0/3/3/3

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	716	2AN	O2-S	7.59	1.81	1.43
2	B	717	2AN	O2-S	7.45	1.81	1.43
2	B	719	2AN	O2-S	7.45	1.81	1.43
2	A	715	2AN	O2-S	7.42	1.80	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	718	2AN	O2-S	7.41	1.80	1.43
2	B	718	2AN	O3-S	6.65	1.79	1.45
2	B	717	2AN	O3-S	6.55	1.78	1.45
2	B	719	2AN	O3-S	6.53	1.78	1.45
2	A	715	2AN	O3-S	6.40	1.78	1.45
2	A	716	2AN	O3-S	6.38	1.77	1.45
2	A	716	2AN	C8-C9	6.35	1.45	1.37
2	B	719	2AN	C8-C9	6.33	1.45	1.37
2	B	717	2AN	O1-S	6.12	1.74	1.43
2	A	716	2AN	O1-S	6.10	1.74	1.43
2	A	715	2AN	O1-S	5.98	1.73	1.43
2	B	718	2AN	O1-S	5.96	1.73	1.43
2	B	719	2AN	O1-S	5.92	1.73	1.43
2	A	716	2AN	C9-C10	5.82	1.51	1.43
2	B	717	2AN	C8-C9	5.81	1.44	1.37
2	A	715	2AN	C8-C9	5.71	1.44	1.37
2	B	718	2AN	C8-C9	5.67	1.44	1.37
2	A	715	2AN	C9-C10	5.13	1.50	1.43
2	B	719	2AN	C9-C10	4.96	1.50	1.43
2	A	716	2AN	C10-C5	4.91	1.52	1.42
2	A	715	2AN	C16-C11	4.89	1.47	1.39
2	B	718	2AN	C10-C5	4.86	1.52	1.42
2	B	719	2AN	C10-C5	4.85	1.52	1.42
2	B	718	2AN	C9-C10	4.81	1.50	1.43
2	A	716	2AN	C16-C11	4.79	1.47	1.39
2	A	715	2AN	C10-C5	4.75	1.52	1.42
2	B	717	2AN	C2-C1	4.72	1.48	1.38
2	B	717	2AN	C16-C11	4.72	1.47	1.39
2	A	716	2AN	C2-C1	4.71	1.48	1.38
2	B	718	2AN	C2-C1	4.71	1.48	1.38
2	B	719	2AN	C16-C11	4.67	1.47	1.39
2	B	719	2AN	C2-C1	4.65	1.48	1.38
2	A	715	2AN	C2-C1	4.50	1.47	1.38
2	B	718	2AN	C16-C11	4.48	1.46	1.39
2	B	717	2AN	C9-C10	4.46	1.49	1.43
2	B	717	2AN	C12-C11	4.46	1.46	1.39
2	B	719	2AN	C12-C11	4.44	1.46	1.39
2	A	715	2AN	C1-C10	4.42	1.49	1.42
2	A	716	2AN	C12-C11	4.28	1.46	1.39
2	B	717	2AN	C10-C5	4.17	1.51	1.42
2	B	717	2AN	C1-C10	4.13	1.48	1.42
2	B	718	2AN	C12-C11	4.12	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	716	2AN	C1-C10	4.07	1.48	1.42
2	A	715	2AN	C12-C11	3.82	1.45	1.39
2	B	717	2AN	C3-C4	3.69	1.45	1.36
2	A	715	2AN	C13-C12	3.62	1.46	1.38
2	B	719	2AN	C13-C12	3.58	1.46	1.38
2	B	717	2AN	C13-C12	3.48	1.46	1.38
2	B	719	2AN	C1-C10	3.47	1.47	1.42
2	B	718	2AN	C3-C4	3.40	1.44	1.36
2	A	715	2AN	C3-C4	3.32	1.44	1.36
2	A	716	2AN	C3-C4	3.23	1.44	1.36
2	B	719	2AN	C3-C4	3.22	1.44	1.36
2	A	716	2AN	C13-C12	3.19	1.45	1.38
2	B	718	2AN	C13-C12	3.12	1.45	1.38
2	B	717	2AN	C14-C13	2.97	1.45	1.38
2	B	717	2AN	C15-C16	2.91	1.45	1.38
2	B	719	2AN	C14-C13	2.86	1.45	1.38
2	B	719	2AN	C15-C16	2.84	1.44	1.38
2	A	716	2AN	C14-C13	2.83	1.45	1.38
2	A	715	2AN	C15-C16	2.77	1.44	1.38
2	B	719	2AN	C7-C6	2.68	1.42	1.36
2	B	718	2AN	C14-C13	2.67	1.45	1.38
2	B	718	2AN	C7-C8	2.65	1.44	1.38
2	A	715	2AN	C14-C13	2.59	1.44	1.38
2	B	718	2AN	C15-C16	2.58	1.44	1.38
2	B	719	2AN	C7-C8	2.56	1.44	1.38
2	A	716	2AN	C7-C6	2.56	1.42	1.36
2	A	716	2AN	C15-C16	2.47	1.44	1.38
2	B	718	2AN	C1-C10	2.45	1.46	1.42
2	B	718	2AN	C7-C6	2.42	1.42	1.36
2	B	717	2AN	C7-C6	2.39	1.42	1.36
2	A	715	2AN	C7-C8	2.37	1.43	1.38
2	A	716	2AN	C7-C8	2.32	1.43	1.38
2	A	715	2AN	C7-C6	2.29	1.41	1.36
2	B	717	2AN	C7-C8	2.13	1.43	1.38

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	716	2AN	C7-C8-C9	3.67	124.16	120.37
2	B	718	2AN	C7-C8-C9	3.66	124.15	120.37
2	A	715	2AN	C7-C8-C9	3.58	124.06	120.37
2	B	718	2AN	C11-N-C1	3.53	135.48	126.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	719	2AN	C7-C8-C9	3.36	123.84	120.37
2	B	719	2AN	C11-N-C1	3.18	134.61	126.71
2	B	717	2AN	C7-C8-C9	3.12	123.59	120.37
2	B	718	2AN	C8-C9-C10	-2.70	115.99	120.16
2	A	716	2AN	C6-C5-C4	-2.57	117.17	123.19
2	A	715	2AN	C6-C5-C4	-2.55	117.22	123.19
2	B	718	2AN	C9-C10-C5	2.50	118.81	116.29
2	A	716	2AN	C11-N-C1	2.43	132.75	126.71
2	B	718	2AN	C6-C5-C4	-2.41	117.55	123.19
2	B	719	2AN	C6-C5-C4	-2.38	117.62	123.19
2	A	716	2AN	C8-C9-C10	-2.29	116.62	120.16
2	B	717	2AN	C6-C5-C4	-2.29	117.83	123.19
2	B	718	2AN	O1-S-C9	2.26	113.17	106.43
2	B	717	2AN	C11-N-C1	2.21	132.19	126.71
2	B	719	2AN	C8-C9-C10	-2.18	116.78	120.16
2	A	715	2AN	C2-C1-N	-2.14	118.08	123.92
2	A	715	2AN	C8-C9-C10	-2.10	116.91	120.16
2	B	719	2AN	C2-C1-C10	-2.04	118.12	120.27

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	715	2AN	C2-C1-N-C11
2	A	715	2AN	C10-C1-N-C11

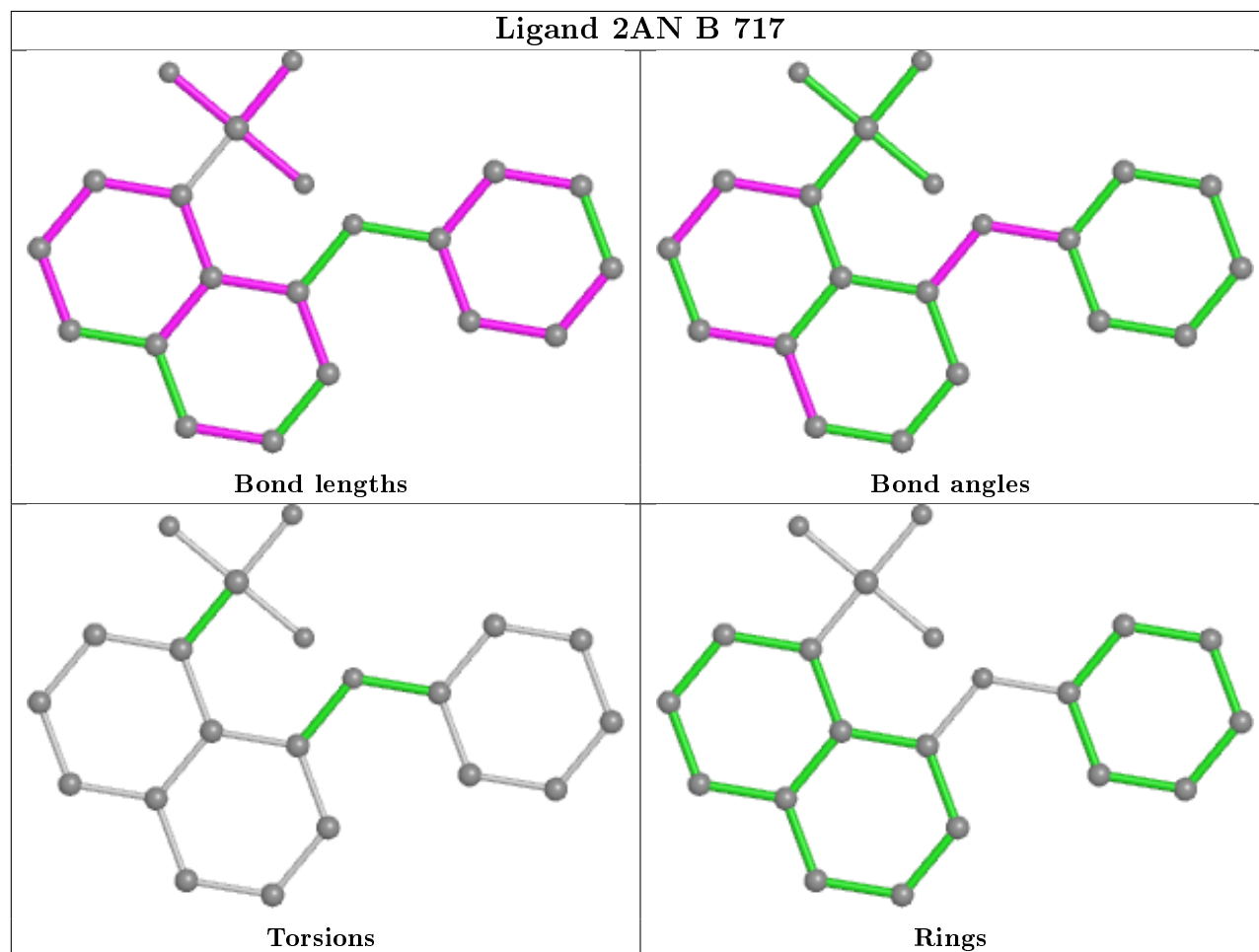
There are no ring outliers.

4 monomers are involved in 3 short contacts:

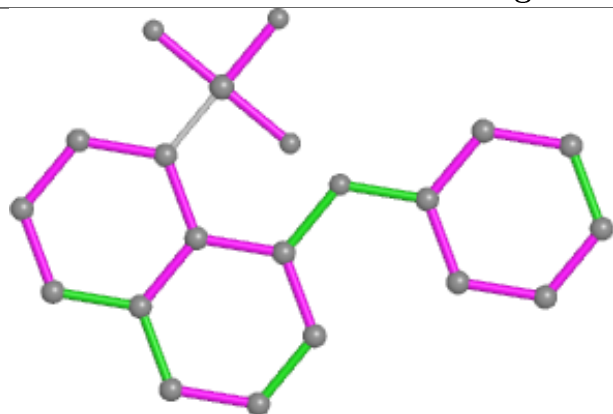
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	715	2AN	1	0
2	B	719	2AN	1	0
2	B	718	2AN	1	0
2	A	716	2AN	1	0

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 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

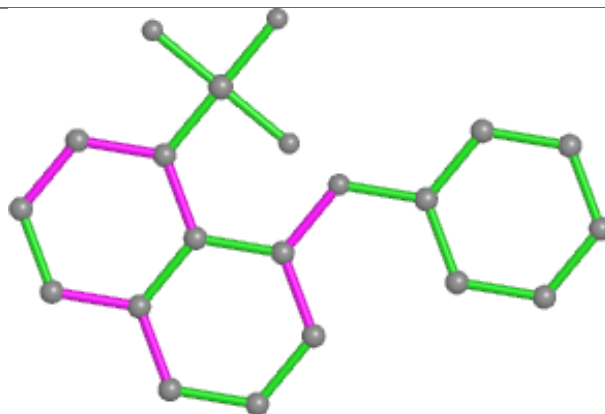
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



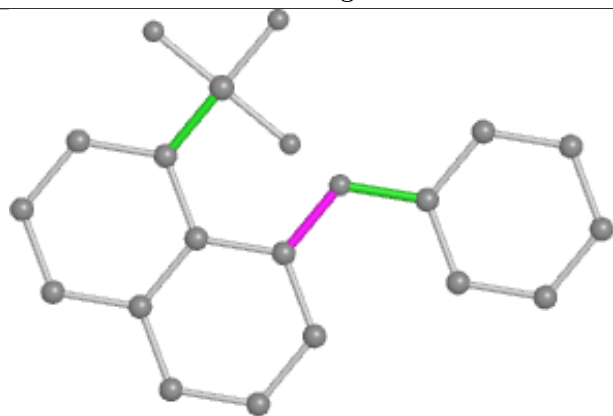
Ligand 2AN A 715



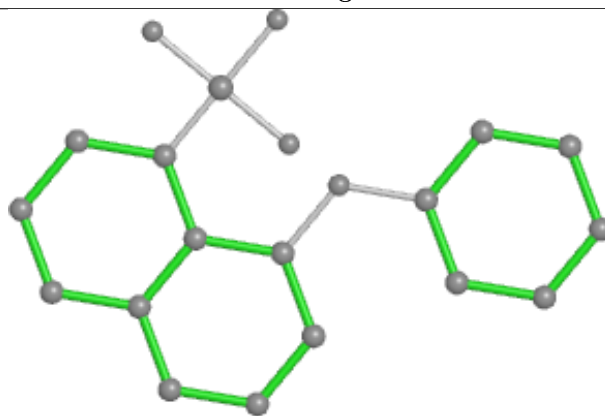
Bond lengths



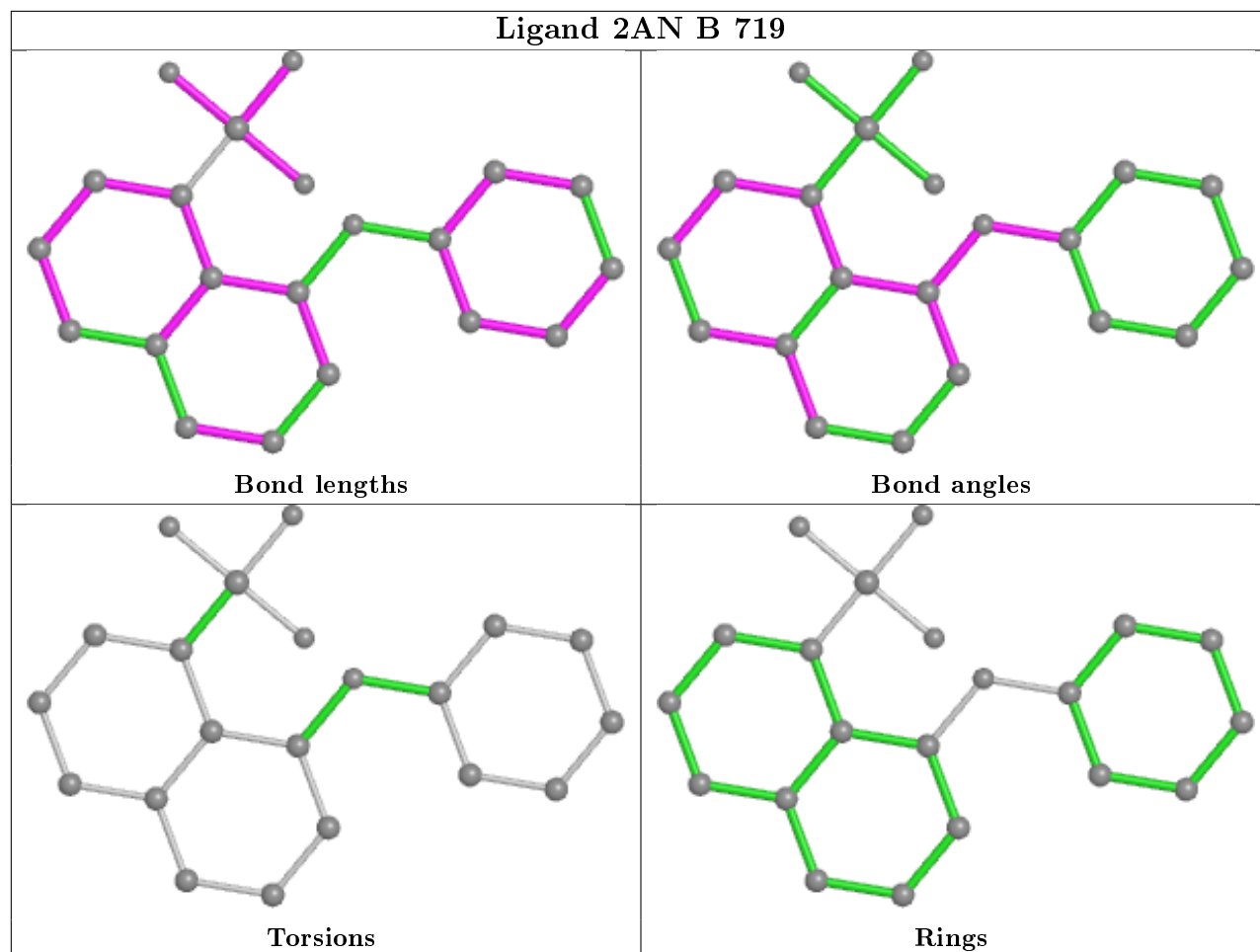
Bond angles



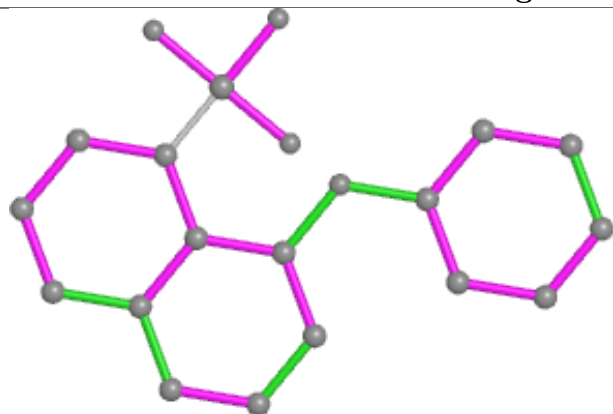
Torsions



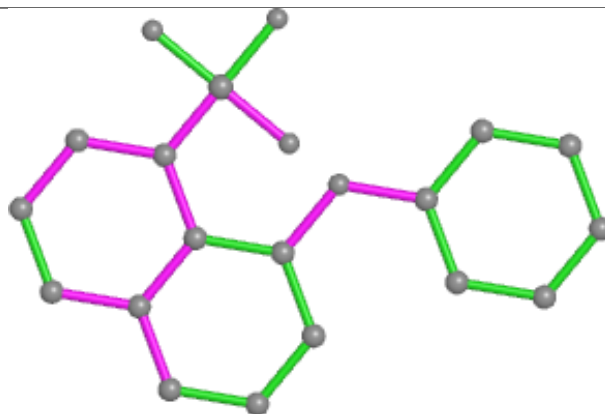
Rings



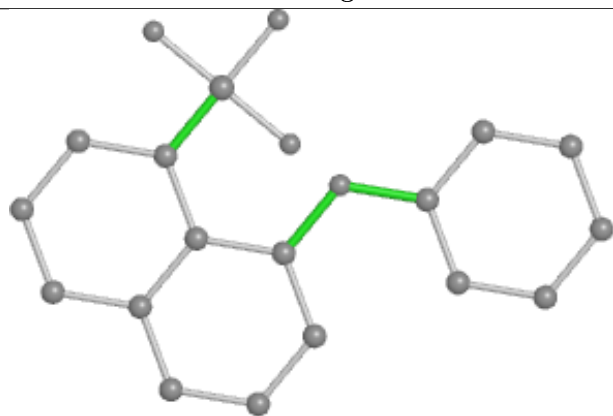
Ligand 2AN B 718



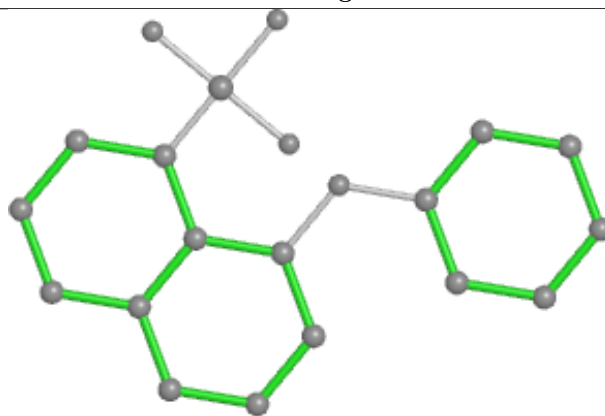
Bond lengths



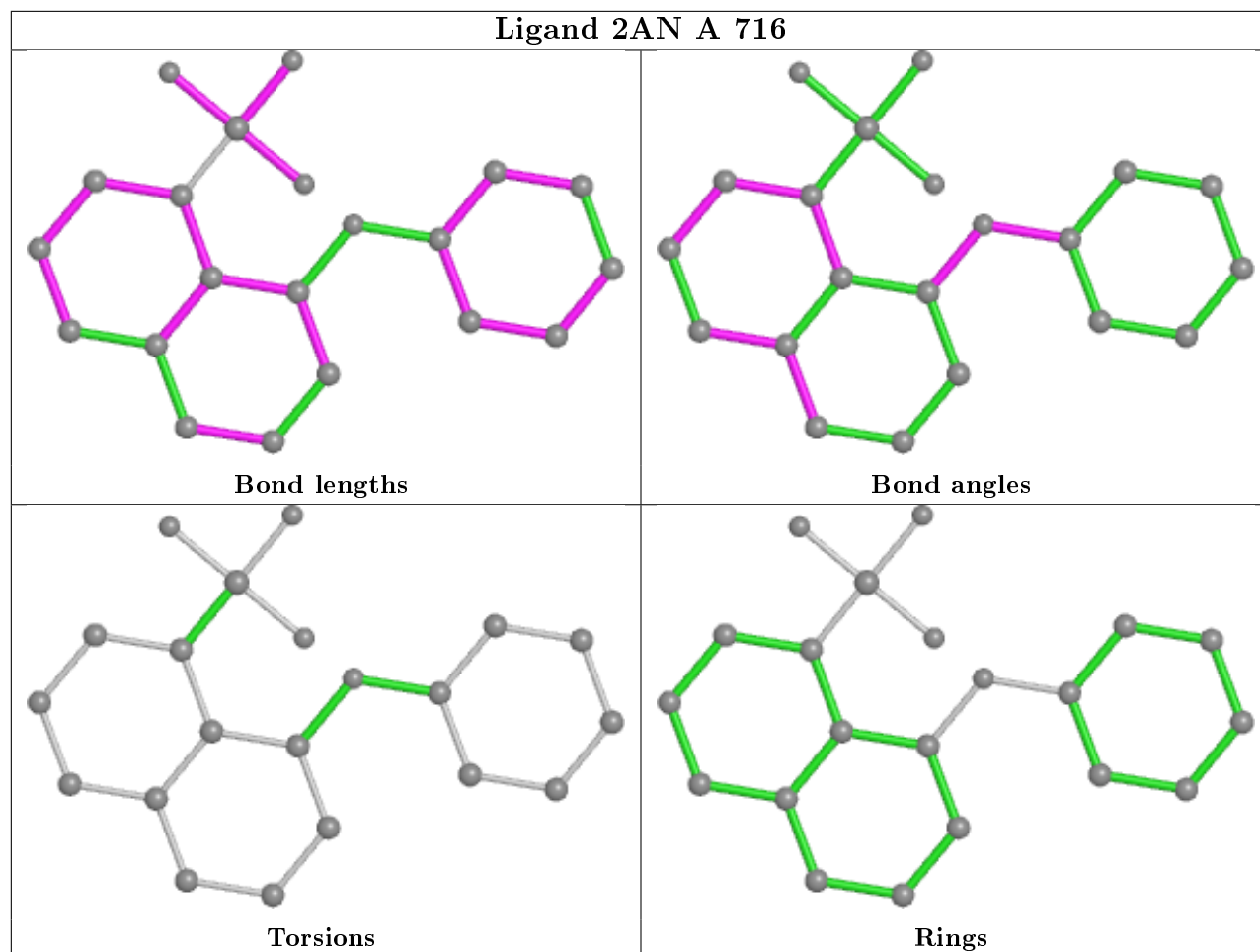
Bond angles



Torsions



Rings



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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.