wwPDB X-ray Structure Validation Summary Report (i)

Oct 11, 2021 – 07:38 AM EDT

PDB ID	:	2Q11
Title	:	Structure of BACE complexed to compound 1
Authors	:	Sharff, A.J.
Deposited on	:	2007-05-23
Resolution	:	2.40 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 following versions of software and data (see references (1)) were used in the production of this report:

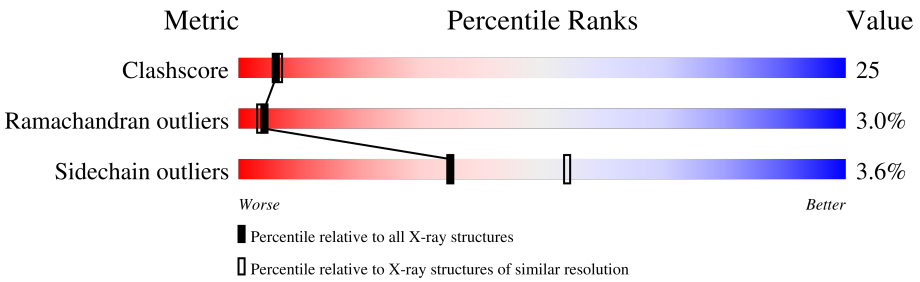
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 was not executed.

Mol	Chain	Length	Quality of chain
1	A	388	66% 31% • •
1	B	388	61% 36% •
1	C	388	56% 40% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9647 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.

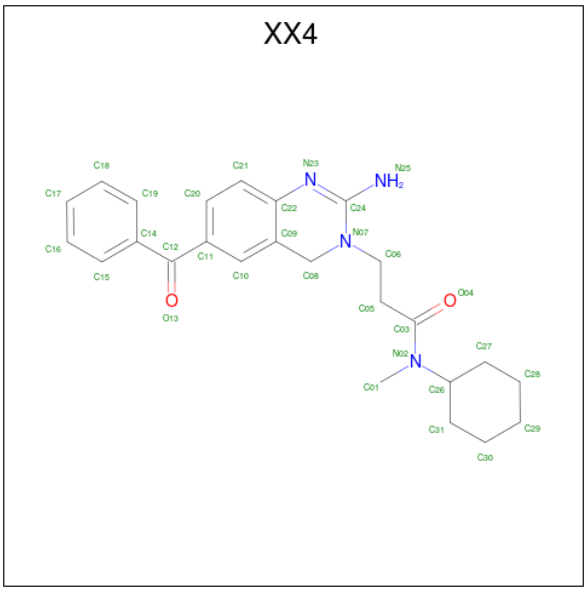
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	3049	1952	505	578	14	164	0	0
1	B	388	3053	1955	506	578	14	164	0	0
1	C	388	3045	1950	504	577	14	164	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	GLN	ASN	engineered mutation	UNP P56817
A	111	GLN	ASN	engineered mutation	UNP P56817
A	162	GLN	ASN	engineered mutation	UNP P56817
A	293	GLN	ASN	engineered mutation	UNP P56817
B	92	GLN	ASN	engineered mutation	UNP P56817
B	111	GLN	ASN	engineered mutation	UNP P56817
B	162	GLN	ASN	engineered mutation	UNP P56817
B	293	GLN	ASN	engineered mutation	UNP P56817
C	92	GLN	ASN	engineered mutation	UNP P56817
C	111	GLN	ASN	engineered mutation	UNP P56817
C	162	GLN	ASN	engineered mutation	UNP P56817
C	293	GLN	ASN	engineered mutation	UNP P56817

- Molecule 2 is 3-(2-AMINO-6-BENZOYLQUINAZOLIN-3(4H)-YL)-N-CYCLOHEXYL-N-METHYLPROPANAMIDE (three-letter code: XX4) (formula: $C_{25}H_{30}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	31	25	4	2	0	0
			Total	C	N	O		
2	B	1	31	25	4	2	0	0
			Total	C	N	O		
2	C	1	31	25	4	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	155	155	155	0	0
			Total	O		
3	B	123	123	123	0	0
			Total	O		
3	C	129	129	129	0	0

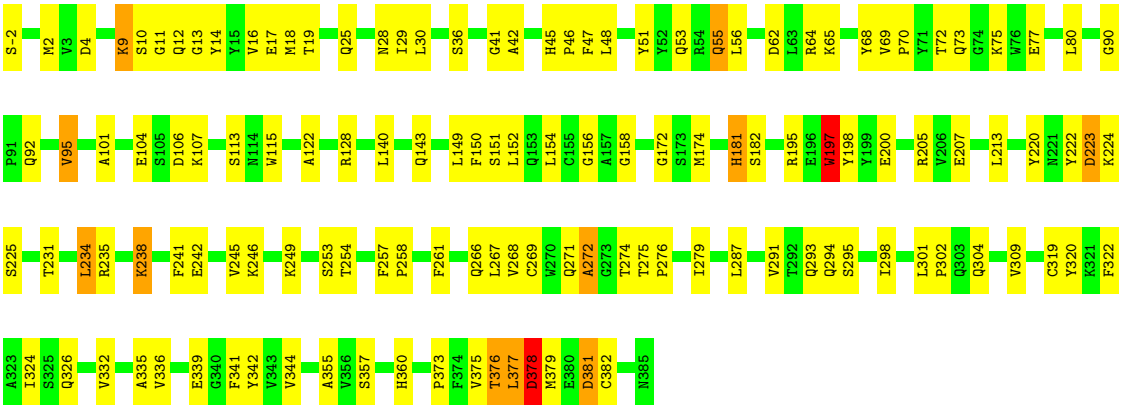
3 Residue-property plots (i)

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 was not executed.

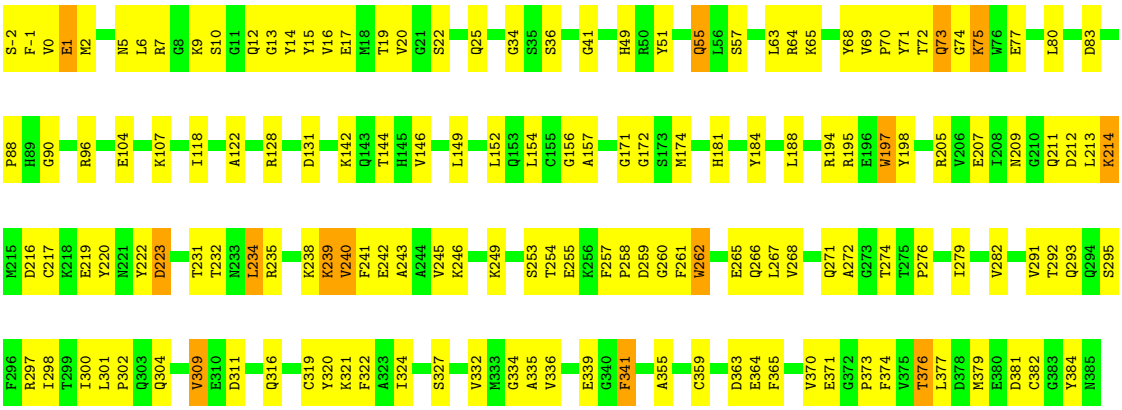
• Molecule 1: Beta-secretase 1

Chain A: 66% 31%



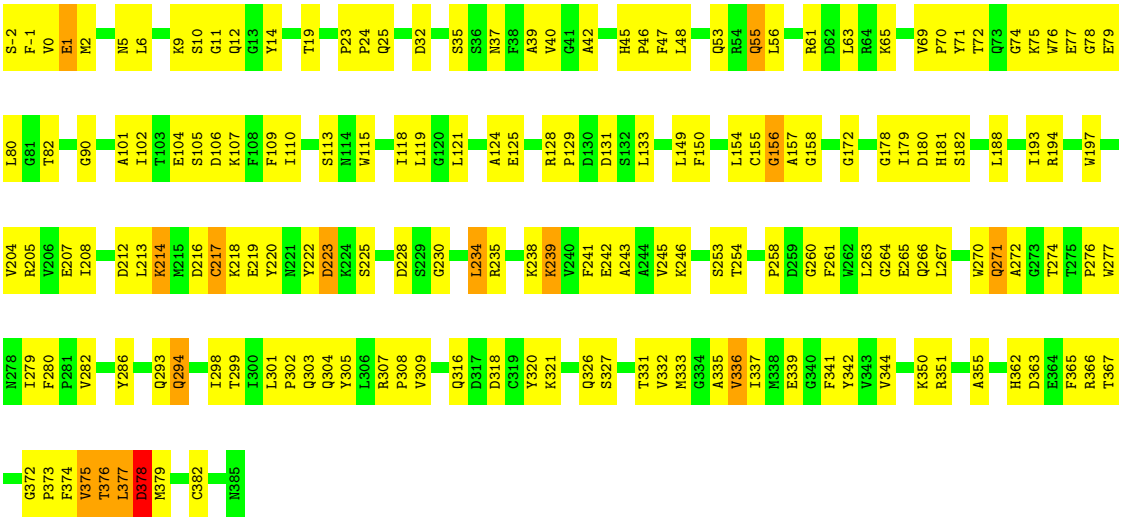
• Molecule 1: Beta-secretase 1

Chain B: 61% 36%



• Molecule 1: Beta-secretase 1

Chain C: 56% 40%


S-2 F-1 V0 E1 M2 N5 L6 K9 S10 G11 Q12 G13 Y14 T19 P23 P24 Q25 D32 S35 S36 N37 F38 A39 V40 G41 A42 H45 P46 F47 L48 Q53 R54 Q55 L56 R61 D62 L63 R64 K65 V69 P70 Y71 T72 G73 G74 K75 W76 E77 G78 E79
L80 G81 T82 G90 A101 I102 T103 E104 S105 D106 K107 F108 F109 I110 S113 N114 W115 I118 L119 G120 L121 A124 E125 R128 P129 D130 D131 S132 L133 L149 F150 L154 C155 G156 A157 G158 G172 G178 I179 D180 H181 S182 L188 I193 R194 W197
V204 R205 V206 E207 I208 D212 L213 K214 M215 D216 C217 K218 E219 Y220 N221 Y222 D223 K224 S225 D228 S229 G230 L234 R235 K238 K239 V240 F241 E242 A243 A244 V245 K246 S253 T254 P258 D259 G260 F261 W262 L263 G264 E265 Q266 L267 W270 Q271 A272 G273 T274 T275 P276 W277
N278 I279 F280 P281 V282 Y286 Q293 Q294 I298 T299 I300 L301 P302 Q303 Q304 Y305 L306 R307 P308 V309 Q316 D317 D318 C319 Y320 K321 Q326 S327 T331 V332 M333 G334 A335 V336 I337 M338 E339 G340 F341 Y342 V343 V344 K350 R351 A355 H362 D363 E364 F365 R366 T367
G372 P373 F374 V375 T376 L377 D378 M379 C382 M385

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	235.90Å 108.50Å 63.10Å 90.00° 102.94° 90.00°	Depositor
Resolution (Å)	500.00 – 2.40	Depositor
% Data completeness (in resolution range)	97.9 (500.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.278 , 0.337	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9647	wwPDB-VP
Average B, all atoms ($Å^2$)	52.0	wwPDB-VP

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: XX4

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	0.41	0/3127	0.68	2/4251 (0.0%)
1	B	0.37	0/3131	0.64	0/4255
1	C	0.39	0/3123	0.63	1/4246 (0.0%)
All	All	0.39	0/9381	0.65	3/12752 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	342	TYR	N-CA-C	-5.28	96.74	111.00
1	A	342	TYR	N-CA-C	-5.20	96.95	111.00
1	A	197	TRP	N-CA-C	-5.13	97.14	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	3049	0	2956	124	0
1	B	3053	0	2967	145	0
1	C	3045	0	2950	161	0
2	A	31	0	30	4	0
2	B	31	0	30	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	31	0	30	6	0
3	A	155	0	0	5	0
3	B	123	0	0	8	0
3	C	129	0	0	7	0
All	All	9647	0	8963	424	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 25.

The worst 5 of 424 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:C:267:LEU:HD22	1:C:309:VAL:HG21	1.32	1.09
1:B:301:LEU:H	1:B:304:GLN:NE2	1.70	0.89
1:B:276:PRO:O	1:B:279:ILE:HG12	1.77	0.84
1:C:75:LYS:HA	2:C:503:XX4:H18	1.60	0.83
1:A:9:LYS:HE2	1:A:11:GLY:H	1.43	0.82

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	386/388 (100%)	343 (89%)	37 (10%)	6 (2%)	9 13
1	B	386/388 (100%)	328 (85%)	42 (11%)	16 (4%)	3 2
1	C	386/388 (100%)	340 (88%)	33 (8%)	13 (3%)	3 3
All	All	1158/1164 (100%)	1011 (87%)	112 (10%)	35 (3%)	4 3

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASP
1	A	377	LEU
1	B	157	ALA
1	B	223	ASP
1	B	240	VAL

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	330/331 (100%)	319 (97%)	11 (3%)	38	57
1	B	331/331 (100%)	321 (97%)	10 (3%)	41	61
1	C	329/331 (99%)	314 (95%)	15 (5%)	27	43
All	All	990/993 (100%)	954 (96%)	36 (4%)	35	54

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	254	THR
1	C	378	ASP
1	C	271	GLN
1	C	327	SER
1	B	49	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	304	GLN
1	C	304	GLN
1	B	362	HIS
1	C	362	HIS
1	C	55	GLN

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)

3 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	XX4	B	502	-	34,34,34	1.83	9 (26%)	43,47,47	1.14	3 (6%)
2	XX4	A	501	-	34,34,34	1.83	9 (26%)	43,47,47	1.10	3 (6%)
2	XX4	C	503	-	34,34,34	1.69	8 (23%)	43,47,47	1.22	3 (6%)

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	XX4	B	502	-	-	7/21/41/41	0/4/4/4
2	XX4	A	501	-	-	11/21/41/41	0/4/4/4
2	XX4	C	503	-	-	9/21/41/41	0/4/4/4

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	XX4	C22-C09	4.08	1.46	1.40
2	B	502	XX4	C10-C11	4.00	1.45	1.39
2	B	502	XX4	C03-N02	3.87	1.41	1.35
2	C	503	XX4	C08-N07	3.74	1.52	1.46
2	A	501	XX4	C24-N07	3.61	1.42	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	503	XX4	C22-N23-C24	5.70	123.38	117.92
2	B	502	XX4	N07-C24-N23	-4.10	120.02	125.50
2	A	501	XX4	C22-N23-C24	3.94	121.70	117.92
2	A	501	XX4	N07-C24-N23	-3.59	120.70	125.50
2	B	502	XX4	C22-N23-C24	3.48	121.26	117.92

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	XX4	C27-C26-N02-C01
2	A	501	XX4	C31-C26-N02-C01
2	A	501	XX4	C27-C26-N02-C03
2	A	501	XX4	C03-C05-C06-N07
2	B	502	XX4	C27-C26-N02-C01

There are no ring outliers.

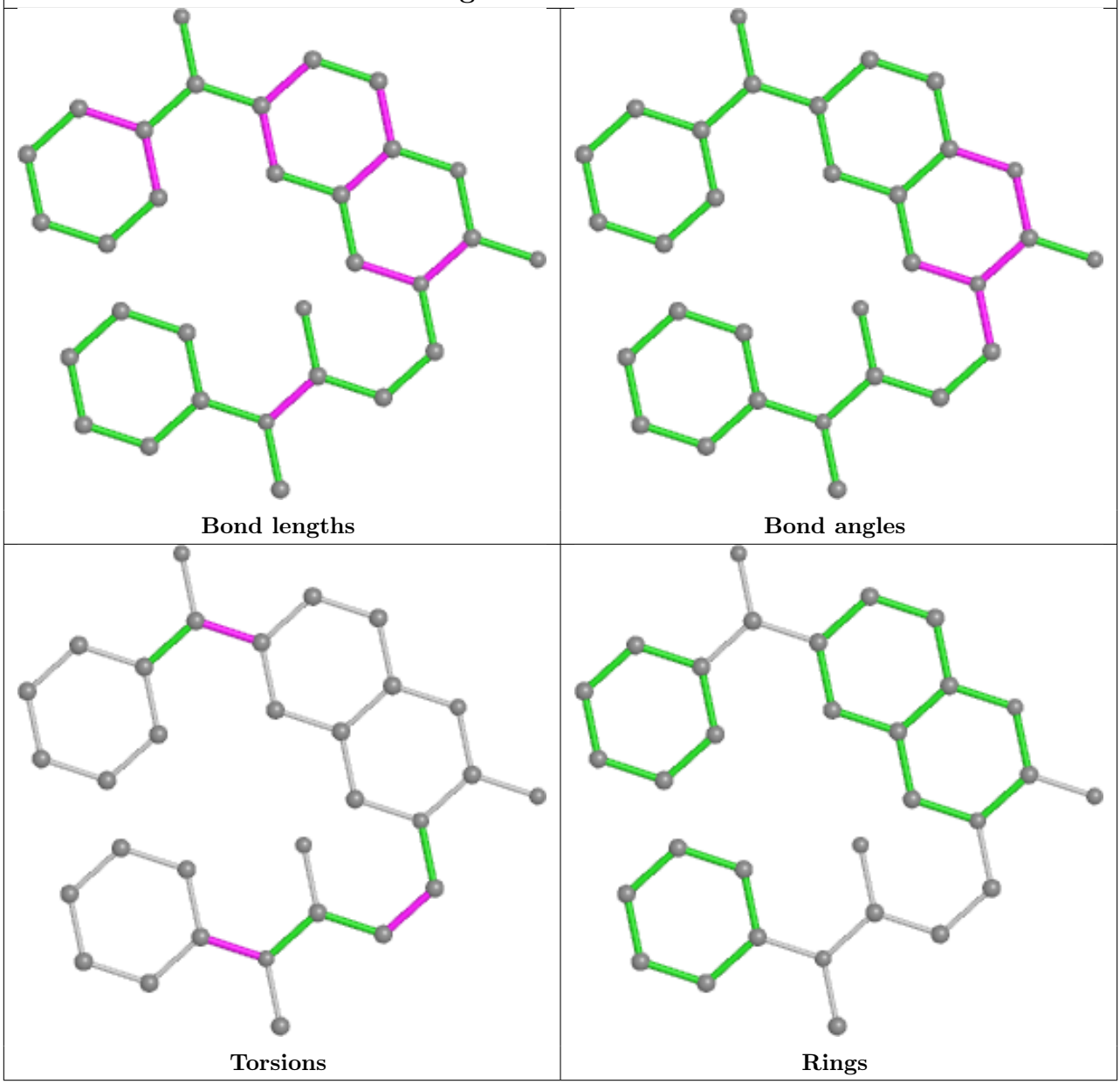
3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	XX4	6	0
2	A	501	XX4	4	0
2	C	503	XX4	6	0

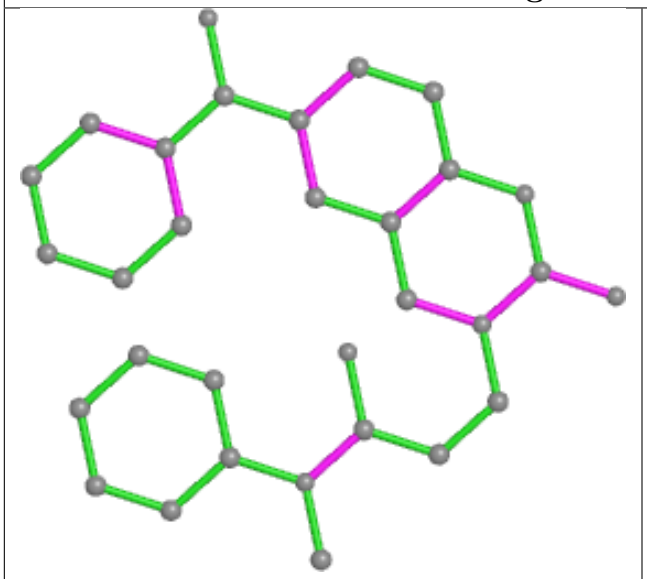
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

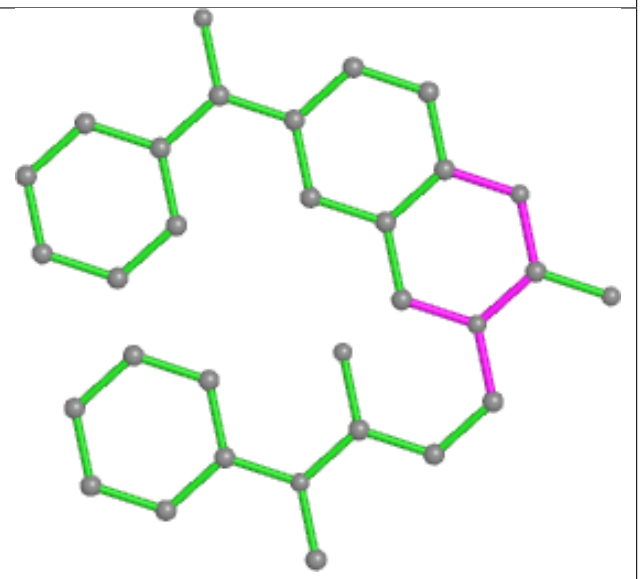
Ligand XX4 B 502



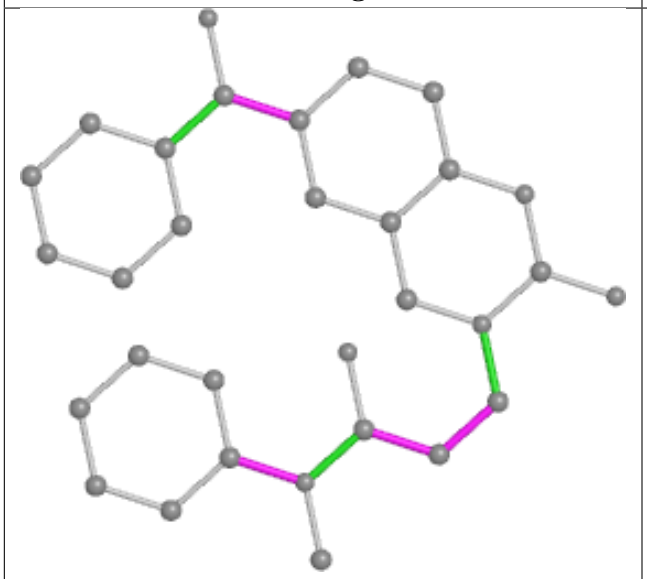
Ligand XX4 A 501



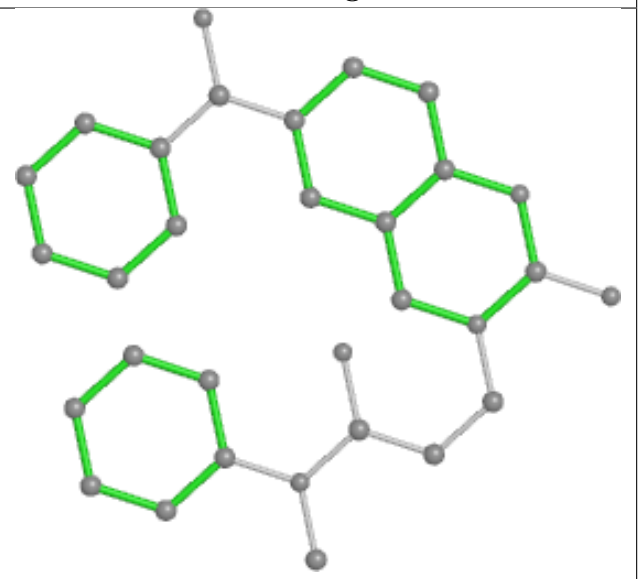
Bond lengths



Bond angles

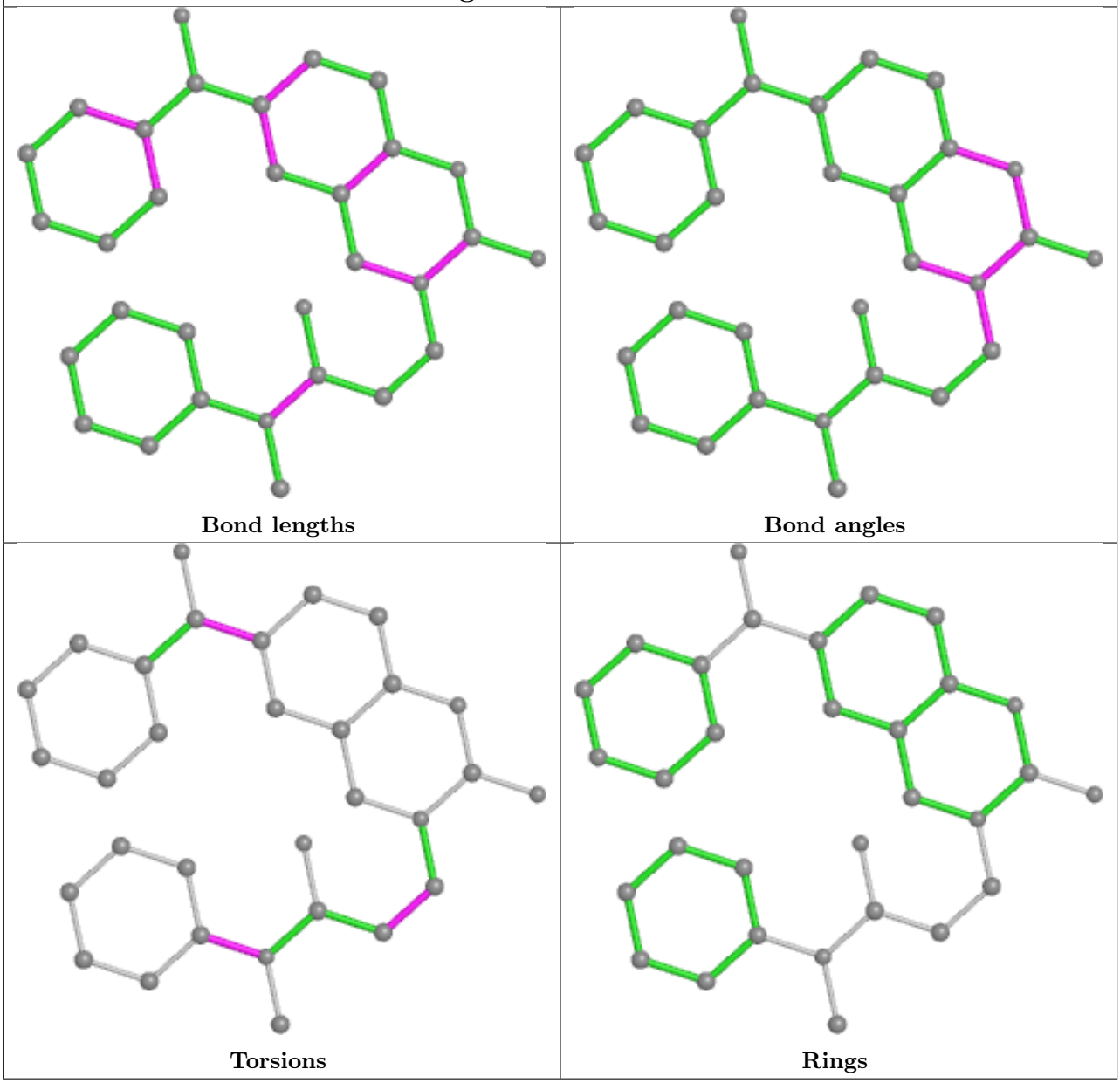


Torsions



Rings

Ligand XX4 C 503



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 was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.