Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 01:47 am BST

PDB ID	:	1QJ6
Title	:	Novel Covalent Active Site Thrombin Inhibitors
Authors	:	Jhoti, H.; Cleasby, A.
Deposited on	:	1999-06-22
Resolution	:	2.20 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

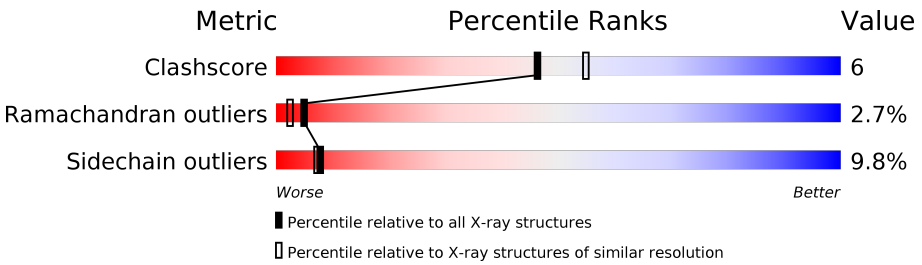
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	36	67% 28% 6%
2	B	259	72% 21% 5% •
3	I	10	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2705 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 THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	36	287	177	48	61	1	0	0	0

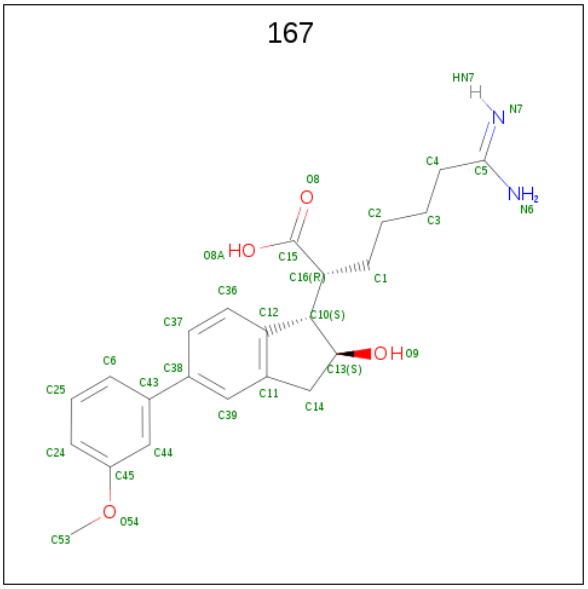
- Molecule 2 is a protein called THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	259	2093	1334	370	375	14	0	0	0

- Molecule 3 is a protein called HIRUGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	10	94	59	10	24	1	0	0	0

- Molecule 4 is 6-CARBAMIMIDOYL-2-[2-HYDROXY-5-(3-METHOXY-PHENYL)-INDAN -1-YL]-HEXANOIC ACID (three-letter code: 167) (formula: $C_{23}H_{28}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	28	23	2	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	34	34	34	0	0
			Total	O		
5	B	163	163	163	0	0
			Total	O		
5	I	6	6	6	0	0

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.

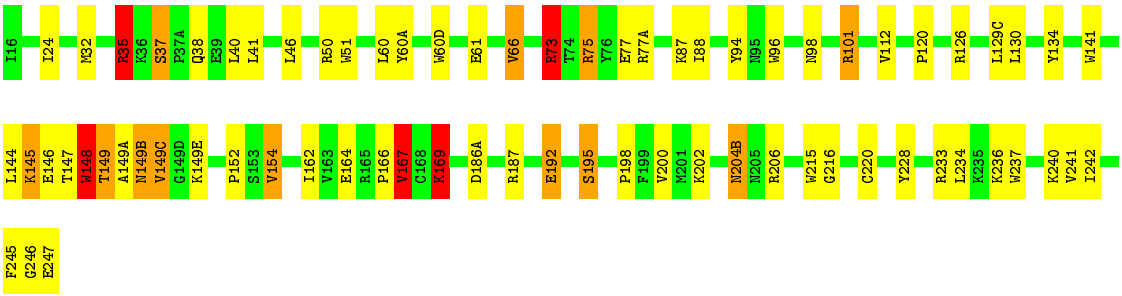
Note EDS was not executed.

- Molecule 1: THROMBIN

Chain A: 67% 28% 6%

- Molecule 2: THROMBIN

Chain B: 72% 21% 5% •



- Molecule 3: HIRUGEN

Chain I: 100%

There are no outlier residues recorded for this chain.

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	71.80Å 72.00Å 73.20Å 90.00° 101.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20	Depositor
% Data completeness (in resolution range)	98.0 (15.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2705	wwPDB-VP
Average B, all atoms (Å^2)	33.0	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: 167, TYS

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	0.94	0/290	1.52	0/384
2	B	1.00	8/2148 (0.4%)	1.60	25/2903 (0.9%)
3	I	1.03	0/79	1.33	0/103
All	All	1.00	8/2517 (0.3%)	1.58	25/3390 (0.7%)

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
2	B	0	3
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	195	SER	CB-OG	-13.67	1.24	1.42
2	B	60(D)	TRP	CD2-CE2	6.30	1.49	1.41
2	B	96	TRP	CD2-CE2	6.18	1.48	1.41
2	B	141	TRP	CD2-CE2	5.97	1.48	1.41
2	B	148	TRP	CD2-CE2	5.44	1.47	1.41
2	B	51	TRP	CD2-CE2	5.27	1.47	1.41
2	B	215	TRP	CD2-CE2	5.24	1.47	1.41
2	B	237	TRP	CD2-CE2	5.06	1.47	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	73	ARG	NE-CZ-NH2	-10.09	115.26	120.30
2	B	73	ARG	NE-CZ-NH1	9.17	124.89	120.30
2	B	77(A)	ARG	NE-CZ-NH1	8.77	124.69	120.30
2	B	94	TYR	CB-CG-CD2	-7.44	116.53	121.00
2	B	134	TYR	CB-CG-CD2	-7.26	116.64	121.00
2	B	77(A)	ARG	NE-CZ-NH2	-7.11	116.75	120.30
2	B	101	ARG	NE-CZ-NH2	-7.04	116.78	120.30
2	B	35	ARG	NE-CZ-NH2	-6.97	116.82	120.30
2	B	187	ARG	NE-CZ-NH1	6.72	123.66	120.30
2	B	77(A)	ARG	C-N-CA	-6.68	105.00	121.70
2	B	206	ARG	NE-CZ-NH2	-6.58	117.01	120.30
2	B	233	ARG	NE-CZ-NH1	6.34	123.47	120.30
2	B	75	ARG	NE-CZ-NH1	6.30	123.45	120.30
2	B	126	ARG	CA-CB-CG	6.02	126.65	113.40
2	B	37	SER	N-CA-CB	5.77	119.15	110.50
2	B	195	SER	CA-CB-OG	5.50	126.04	111.20
2	B	75	ARG	CA-CB-CG	5.47	125.44	113.40
2	B	154	VAL	N-CA-CB	-5.46	99.48	111.50
2	B	169	LYS	CA-CB-CG	5.35	125.18	113.40
2	B	60(A)	TYR	CB-CG-CD2	-5.34	117.79	121.00
2	B	154	VAL	CA-CB-CG1	5.30	118.86	110.90
2	B	167	VAL	CA-CB-CG2	5.27	118.81	110.90
2	B	242	ILE	CA-CB-CG1	5.23	120.94	111.00
2	B	228	TYR	CB-CG-CD2	-5.19	117.88	121.00
2	B	66	VAL	CA-CB-CG1	5.05	118.48	110.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1(E)	SER	Peptide
2	B	246	GLY	Peptide
2	B	35	ARG	Sidechain
2	B	73	ARG	Sidechain

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	287	0	278	6	0
2	B	2093	0	2063	26	0
3	I	94	0	73	0	0
4	B	28	0	25	4	0
5	A	34	0	0	1	0
5	B	163	0	0	0	0
5	I	6	0	0	0	0
All	All	2705	0	2439	31	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 6.

All (31) 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)
2:B:75:ARG:HD2	2:B:77:GLU:HG2	1.49	0.95
1:A:1(C):GLU:HA	1:A:1(B):ALA:HB3	1.66	0.76
2:B:166:PRO:HA	2:B:169:LYS:HD2	1.71	0.73
2:B:130:LEU:HD23	2:B:162:ILE:HD13	1.77	0.66
2:B:35:ARG:HG2	2:B:41:LEU:HD21	1.79	0.64
2:B:148:TRP:CZ3	2:B:220:CYS:SG	2.93	0.62
2:B:32:MET:HG3	2:B:40:LEU:HD12	1.81	0.60
2:B:147:THR:HA	2:B:149(A):ALA:HA	1.83	0.60
1:A:14(G):LEU:HD21	2:B:202:LYS:HD3	1.91	0.52
1:A:1(C):GLU:HG2	2:B:120:PRO:HG3	1.92	0.52
2:B:146:GLU:O	2:B:149(B):ASN:HB2	2.08	0.52
1:A:1(C):GLU:HA	1:A:1(B):ALA:CB	2.37	0.51
2:B:164:GLU:HB2	2:B:167:VAL:HG13	1.91	0.51
2:B:73:ARG:HD3	2:B:152:PRO:O	2.12	0.50
2:B:204(B):ASN:HD22	2:B:204(B):ASN:C	2.16	0.49
2:B:240:LYS:HB2	2:B:240:LYS:NZ	2.28	0.49
2:B:145:LYS:HB3	2:B:149(B):ASN:HB3	1.96	0.48
2:B:148:TRP:NE1	2:B:192:GLU:HG3	2.29	0.47
2:B:148:TRP:CZ2	4:B:1248:167:H11	2.52	0.45
2:B:101:ARG:HG2	2:B:234:LEU:HD21	1.97	0.45
4:B:1248:167:H11	4:B:1248:167:H36	1.98	0.44
2:B:144:LEU:HD21	2:B:152:PRO:HB3	1.99	0.43
2:B:35:ARG:O	2:B:38:GLN:HA	2.18	0.42
2:B:198:PRO:HB2	2:B:200:VAL:HG13	2.00	0.42
2:B:87:LYS:HD3	2:B:88:ILE:N	2.34	0.42
1:A:14(K):ILE:HA	5:A:2028:HOH:O	2.20	0.42
2:B:61:GLU:HG3	2:B:88:ILE:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:ASN:HA	4:B:1248:167:H533	2.03	0.41
2:B:24:ILE:HG21	2:B:24:ILE:HD13	1.89	0.41
2:B:216:GLY:O	4:B:1248:167:H37	2.21	0.41
1:A:14(J):TYR:O	1:A:14(K):ILE:HG13	2.21	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	34/36 (94%)	25 (74%)	5 (15%)	4 (12%)	0 0
2	B	257/259 (99%)	242 (94%)	11 (4%)	4 (2%)	9 7
3	I	7/10 (70%)	7 (100%)	0	0	100 100
All	All	298/305 (98%)	274 (92%)	16 (5%)	8 (3%)	5 2

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14(L)	ASP
2	B	37	SER
2	B	149	THR
2	B	149(E)	LYS
1	A	1(B)	ALA
2	B	149(C)	VAL
1	A	1(G)	PHE
1	A	1(F)	GLY

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	31/31 (100%)	27 (87%)	4 (13%)	4 3
2	B	225/225 (100%)	203 (90%)	22 (10%)	8 7
3	I	9/9 (100%)	9 (100%)	0	100 100
All	All	265/265 (100%)	239 (90%)	26 (10%)	8 7

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1(H)	THR
1	A	1(C)	GLU
1	A	14	ASP
1	A	14(D)	ARG
2	B	46	LEU
2	B	50	ARG
2	B	60	LEU
2	B	66	VAL
2	B	112	VAL
2	B	129(C)	LEU
2	B	145	LYS
2	B	148	TRP
2	B	149	THR
2	B	149(B)	ASN
2	B	149(C)	VAL
2	B	154	VAL
2	B	167	VAL
2	B	169	LYS
2	B	186(A)	ASP
2	B	192	GLU
2	B	195	SER
2	B	204(B)	ASN
2	B	236	LYS
2	B	241	VAL
2	B	245	PHE
2	B	247	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	62	ASN
2	B	78	ASN
2	B	204(B)	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	TYS	I	63	3	11,15,17	0.84	1 (9%)	12,19,24	1.16	1 (8%)

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	TYS	I	63	3	-	0/7/10/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	63	TYS	OH-CZ	2.55	1.46	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	63	TYS	CB-CA-C	-2.45	106.87	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
4	167	B	1248	2	29,30,31	1.00	1 (3%)	34,41,43	2.27	11 (32%)

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
4	167	B	1248	2	-	7/19/31/33	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1248	167	C16-C15	3.59	1.56	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1248	167	C12-C10-C16	7.27	127.19	112.77
4	B	1248	167	C11-C12-C10	-5.80	106.41	110.72
4	B	1248	167	O9-C13-C10	3.22	116.95	110.29
4	B	1248	167	C11-C14-C13	-3.05	100.57	103.50
4	B	1248	167	C39-C11-C12	2.98	123.85	120.80
4	B	1248	167	C38-C39-C11	-2.67	117.90	121.90
4	B	1248	167	C4-C5-N6	2.57	124.02	117.15
4	B	1248	167	C37-C36-C12	-2.52	116.87	121.13
4	B	1248	167	C53-O54-C45	-2.50	112.08	117.51
4	B	1248	167	C36-C12-C10	2.40	134.26	129.60
4	B	1248	167	C14-C11-C39	-2.01	124.83	129.32

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1248	167	C2-C1-C16-C10
4	B	1248	167	C3-C4-C5-N6
4	B	1248	167	C3-C4-C5-N7
4	B	1248	167	C12-C10-C16-C1
4	B	1248	167	C24-C45-O54-C53
4	B	1248	167	C44-C45-O54-C53
4	B	1248	167	C13-C10-C16-C1

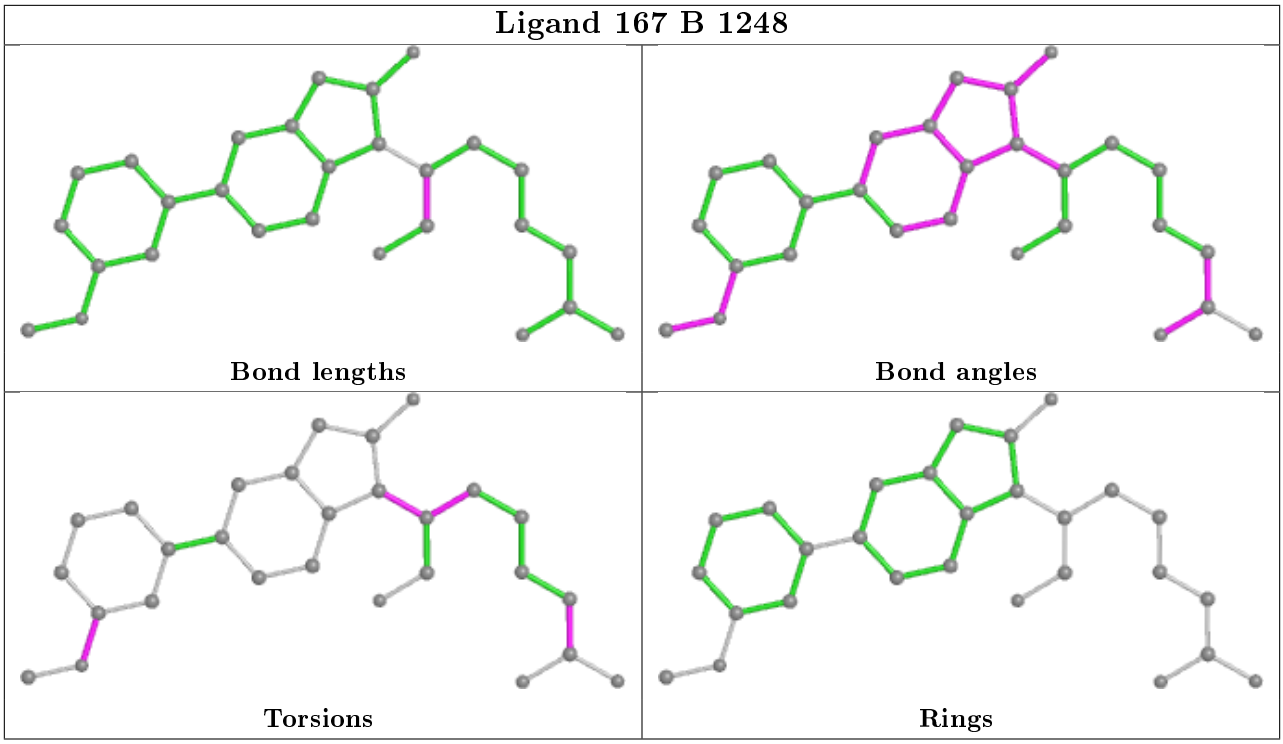
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1248	167	4	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.



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.