Full wwPDB EM Validation Report ⓘ

Dec 25, 2023 – 11:07 PM JST

PDB ID	:	8JJL
EMDB ID	:	EMD-36360
Title	:	cryo-EM structure of the beta2-AR-mBRIL/1b3 Fab/Glue complex with a full agonist
Authors	:	He, B.B.; Zhong, Y.X.; Guo, Q.; Tao, Y.Y.
Deposited on	:	2023-05-30
Resolution	:	3.20 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

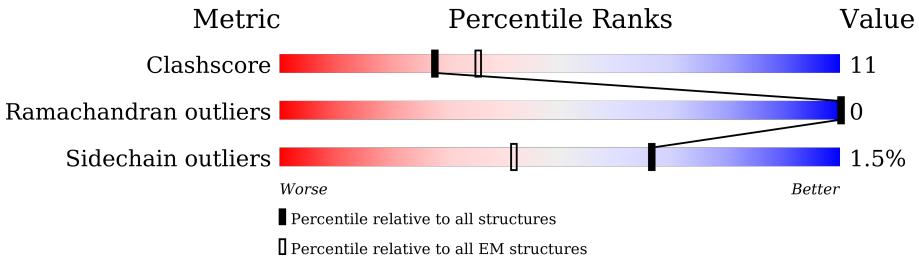
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	A	453	62% 20% • 17%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3026 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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-2 adrenergic receptor,Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	375	2998	1965	486	527	20	0	0

There are 87 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MET	-	initiating methionine	UNP P07550
A	6	LYS	-	expression tag	UNP P07550
A	7	THR	-	expression tag	UNP P07550
A	8	ILE	-	expression tag	UNP P07550
A	9	ILE	-	expression tag	UNP P07550
A	10	ALA	-	expression tag	UNP P07550
A	11	LEU	-	expression tag	UNP P07550
A	12	SER	-	expression tag	UNP P07550
A	13	TYR	-	expression tag	UNP P07550
A	14	ILE	-	expression tag	UNP P07550
A	15	PHE	-	expression tag	UNP P07550
A	16	CYS	-	expression tag	UNP P07550
A	17	LEU	-	expression tag	UNP P07550
A	18	VAL	-	expression tag	UNP P07550
A	19	PHE	-	expression tag	UNP P07550
A	20	ALA	-	expression tag	UNP P07550
A	21	ASP	-	expression tag	UNP P07550
A	22	TYR	-	expression tag	UNP P07550
A	23	LYS	-	expression tag	UNP P07550
A	24	ASP	-	expression tag	UNP P07550
A	25	ASP	-	expression tag	UNP P07550
A	26	ASP	-	expression tag	UNP P07550
A	27	ASP	-	expression tag	UNP P07550
A	28	LYS	-	expression tag	UNP P07550
A	187	GLU	ASN	conflict	UNP P07550
A	237	TRP	MET	conflict	UNP P0ABE7
A	274	SER	THR	linker	UNP P0ABE7
A	275	GLY	PRO	linker	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	276	SER	PRO	linker	UNP P0ABE7
A	277	GLY	LYS	linker	UNP P0ABE7
A	?	-	LEU	deletion	UNP P0ABE7
A	?	-	GLU	deletion	UNP P0ABE7
A	?	-	ASP	deletion	UNP P0ABE7
A	?	-	LYS	deletion	UNP P0ABE7
A	325	ILE	HIS	conflict	UNP P0ABE7
A	329	LEU	ARG	conflict	UNP P0ABE7
A	394	SER	CYS	conflict	UNP P07550
A	408	LYS	-	expression tag	UNP P07550
A	409	ILE	-	expression tag	UNP P07550
A	410	ALA	-	expression tag	UNP P07550
A	411	ALA	-	expression tag	UNP P07550
A	412	LEU	-	expression tag	UNP P07550
A	413	LYS	-	expression tag	UNP P07550
A	414	GLU	-	expression tag	UNP P07550
A	415	LYS	-	expression tag	UNP P07550
A	416	ILE	-	expression tag	UNP P07550
A	417	ALA	-	expression tag	UNP P07550
A	418	ALA	-	expression tag	UNP P07550
A	419	LEU	-	expression tag	UNP P07550
A	420	LYS	-	expression tag	UNP P07550
A	421	GLU	-	expression tag	UNP P07550
A	422	LYS	-	expression tag	UNP P07550
A	423	ILE	-	expression tag	UNP P07550
A	424	ALA	-	expression tag	UNP P07550
A	425	ALA	-	expression tag	UNP P07550
A	426	LEU	-	expression tag	UNP P07550
A	427	LYS	-	expression tag	UNP P07550
A	428	GLU	-	expression tag	UNP P07550
A	429	ALA	-	expression tag	UNP P07550
A	430	GLU	-	expression tag	UNP P07550
A	431	GLU	-	expression tag	UNP P07550
A	432	LYS	-	expression tag	UNP P07550
A	433	ARG	-	expression tag	UNP P07550
A	434	ALA	-	expression tag	UNP P07550
A	435	SER	-	expression tag	UNP P07550
A	436	ARG	-	expression tag	UNP P07550
A	437	LEU	-	expression tag	UNP P07550
A	438	GLU	-	expression tag	UNP P07550
A	439	GLU	-	expression tag	UNP P07550
A	440	GLU	-	expression tag	UNP P07550

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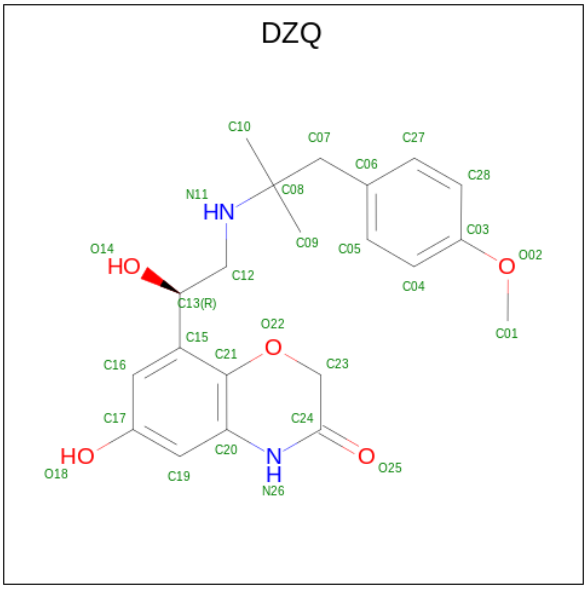
Chain	Residue	Modelled	Actual	Comment	Reference
A	441	LEU	-	expression tag	UNP P07550
A	442	ARG	-	expression tag	UNP P07550
A	443	ARG	-	expression tag	UNP P07550
A	444	ARG	-	expression tag	UNP P07550
A	445	LEU	-	expression tag	UNP P07550
A	446	THR	-	expression tag	UNP P07550
A	447	GLU	-	expression tag	UNP P07550
A	448	GLY	-	expression tag	UNP P07550
A	449	SER	-	expression tag	UNP P07550
A	450	HIS	-	expression tag	UNP P07550
A	451	HIS	-	expression tag	UNP P07550
A	452	HIS	-	expression tag	UNP P07550
A	453	HIS	-	expression tag	UNP P07550
A	454	HIS	-	expression tag	UNP P07550
A	455	HIS	-	expression tag	UNP P07550
A	456	HIS	-	expression tag	UNP P07550
A	457	HIS	-	expression tag	UNP P07550

- Molecule 2 is Olodaterol (three-letter code: DZQ) (formula: $C_{21}H_{26}N_2O_5$) (labeled as "Ligand of Interest" by depositor).



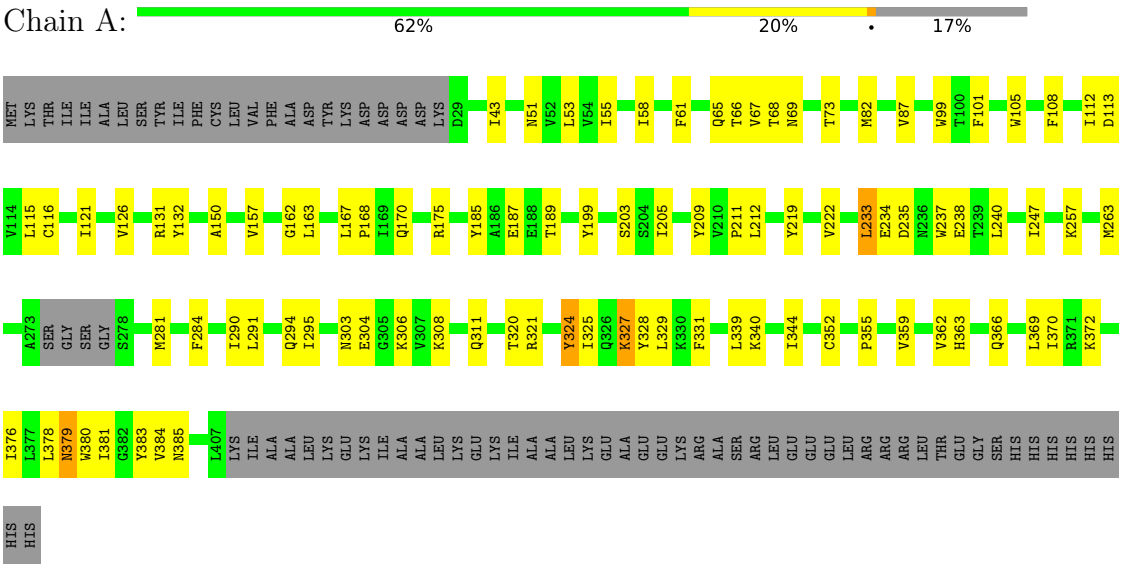
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			28	21	2	5	

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.

- Molecule 1: Beta-2 adrenergic receptor,Soluble cytochrome b562

Chain A:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	785234	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.28	0/3065	0.48	0/4162

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	2998	0	3045	65	0
2	A	28	0	0	1	0
All	All	3026	0	3045	65	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 11.

All (65) 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:121:ILE:HG13	1:A:211:PRO:HB2	1.68	0.76
1:A:233:LEU:HD13	1:A:328:TYR:CE2	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ILE:HA	1:A:209:TYR:HD2	1.60	0.67
1:A:233:LEU:HD22	1:A:328:TYR:CE1	2.32	0.64
1:A:101:PHE:HB3	1:A:105:TRP:HE3	1.64	0.62
1:A:257:LYS:NZ	1:A:303:ASN:OD1	2.28	0.61
1:A:327:LYS:NZ	1:A:327:LYS:HB2	2.17	0.59
1:A:187:GLU:HG3	1:A:189:THR:HG22	1.87	0.56
1:A:321:ARG:O	1:A:325:ILE:HG23	2.05	0.56
1:A:219:TYR:OH	1:A:339:LEU:O	2.19	0.56
1:A:366:GLN:HE22	1:A:369:LEU:H	1.54	0.55
1:A:66:THR:HG23	1:A:69:ASN:H	1.73	0.54
1:A:113:ASP:OD2	1:A:383:TYR:OH	2.17	0.54
1:A:87:VAL:HG13	1:A:380:TRP:CZ3	2.42	0.54
1:A:295:ILE:H	1:A:295:ILE:HD12	1.73	0.54
1:A:324:TYR:C	1:A:324:TYR:CD2	2.80	0.54
1:A:379:ASN:C	1:A:379:ASN:HD22	2.12	0.54
1:A:237:TRP:CZ2	1:A:324:TYR:CE2	2.96	0.53
1:A:199:TYR:O	1:A:203:SER:CB	2.57	0.53
1:A:58:ILE:O	1:A:65:GLN:NE2	2.42	0.53
1:A:43:ILE:HG21	1:A:384:VAL:HG12	1.91	0.52
1:A:82:MET:HB2	1:A:116:CYS:HB3	1.91	0.52
1:A:234:GLU:O	1:A:238:GLU:N	2.43	0.52
1:A:359:VAL:HB	1:A:370:ILE:HD13	1.92	0.51
1:A:113:ASP:OD2	2:A:501:DZQ:N11	2.44	0.51
1:A:359:VAL:HA	1:A:362:VAL:HG22	1.93	0.51
1:A:199:TYR:O	1:A:203:SER:HB3	2.11	0.50
1:A:58:ILE:HG21	1:A:73:THR:OG1	2.11	0.50
1:A:340:LYS:O	1:A:344:ILE:HG12	2.10	0.50
1:A:175:ARG:HD2	1:A:185:TYR:CE2	2.47	0.50
1:A:363:HIS:HB2	1:A:370:ILE:HD12	1.94	0.50
1:A:126:VAL:HG21	1:A:157:VAL:HG21	1.93	0.49
1:A:240:LEU:HD12	1:A:263:MET:HG2	1.93	0.48
1:A:325:ILE:O	1:A:329:LEU:HG	2.14	0.48
1:A:304:GLU:HG2	1:A:306:LYS:HE2	1.95	0.48
1:A:290:ILE:O	1:A:294:GLN:HG2	2.14	0.48
1:A:328:TYR:O	1:A:329:LEU:C	2.52	0.48
1:A:355:PRO:HB2	1:A:378:LEU:HD22	1.96	0.47
1:A:281:MET:HA	1:A:284:PHE:HB2	1.97	0.46
1:A:68:THR:OG1	1:A:131:ARG:NH1	2.44	0.46
1:A:67:VAL:HG13	1:A:150:ALA:HB2	1.97	0.45
1:A:372:LYS:O	1:A:376:ILE:HG12	2.16	0.45
1:A:115:LEU:HD13	1:A:162:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PHE:O	1:A:112:ILE:HG12	2.15	0.45
1:A:381:ILE:HA	1:A:384:VAL:HG22	1.98	0.45
1:A:308:LYS:HA	1:A:308:LYS:HE2	1.99	0.45
1:A:366:GLN:NE2	1:A:369:LEU:H	2.15	0.45
1:A:61:PHE:O	1:A:65:GLN:NE2	2.49	0.44
1:A:237:TRP:CE2	1:A:324:TYR:CE2	3.06	0.44
1:A:237:TRP:CE2	1:A:240:LEU:HD23	2.53	0.43
1:A:163:LEU:HA	1:A:167:LEU:HD23	2.00	0.43
1:A:170:GLN:HA	1:A:170:GLN:OE1	2.18	0.43
1:A:247:ILE:HG22	1:A:311:GLN:OE1	2.19	0.42
1:A:340:LYS:O	1:A:344:ILE:N	2.45	0.42
1:A:234:GLU:O	1:A:235:ASP:C	2.58	0.42
1:A:352:CYS:HB2	1:A:385:ASN:HD22	1.83	0.42
1:A:291:LEU:HD13	1:A:320:THR:HG21	2.01	0.41
1:A:53:LEU:HD12	1:A:53:LEU:HA	1.96	0.41
1:A:209:TYR:HA	1:A:212:LEU:HB3	2.02	0.41
1:A:359:VAL:O	1:A:363:HIS:HB3	2.21	0.41
1:A:51:ASN:O	1:A:55:ILE:HG12	2.21	0.40
1:A:99:TRP:NE1	1:A:101:PHE:HB2	2.36	0.40
1:A:168:PRO:HB2	1:A:199:TYR:HE1	1.86	0.40
1:A:132:TYR:HA	1:A:222:VAL:HG22	2.04	0.40
1:A:327:LYS:HB2	1:A:327:LYS:HZ2	1.84	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 PDB entries followed by that with respect to all EM entries.

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	371/453 (82%)	356 (96%)	15 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	323/388 (83%)	318 (98%)	5 (2%)	65 85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	LEU
1	A	324	TYR
1	A	327	LYS
1	A	331	PHE
1	A	379	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	366	GLN

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
2	DZQ	A	501	-	28,30,30	1.97	6 (21%)	36,43,43	1.50	3 (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
2	DZQ	A	501	-	-	8/17/26/26	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	DZQ	C24-N26	6.09	1.41	1.35
2	A	501	DZQ	O22-C21	5.28	1.46	1.37
2	A	501	DZQ	C20-N26	3.05	1.45	1.39
2	A	501	DZQ	C08-N11	-2.63	1.46	1.49
2	A	501	DZQ	O25-C24	-2.18	1.18	1.23
2	A	501	DZQ	C15-C13	2.02	1.53	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	DZQ	C12-N11-C08	-6.01	109.74	116.36
2	A	501	DZQ	C20-N26-C24	-3.55	120.10	124.49
2	A	501	DZQ	O22-C21-C15	2.99	120.96	116.75

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	DZQ	C12-C13-C15-C16
2	A	501	DZQ	O14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
2	A	501	DZQ	C28-C03-O02-C01
2	A	501	DZQ	C04-C03-O02-C01
2	A	501	DZQ	C06-C07-C08-C10
2	A	501	DZQ	C13-C12-N11-C08
2	A	501	DZQ	O14-C13-C15-C21
2	A	501	DZQ	C12-C13-C15-C21

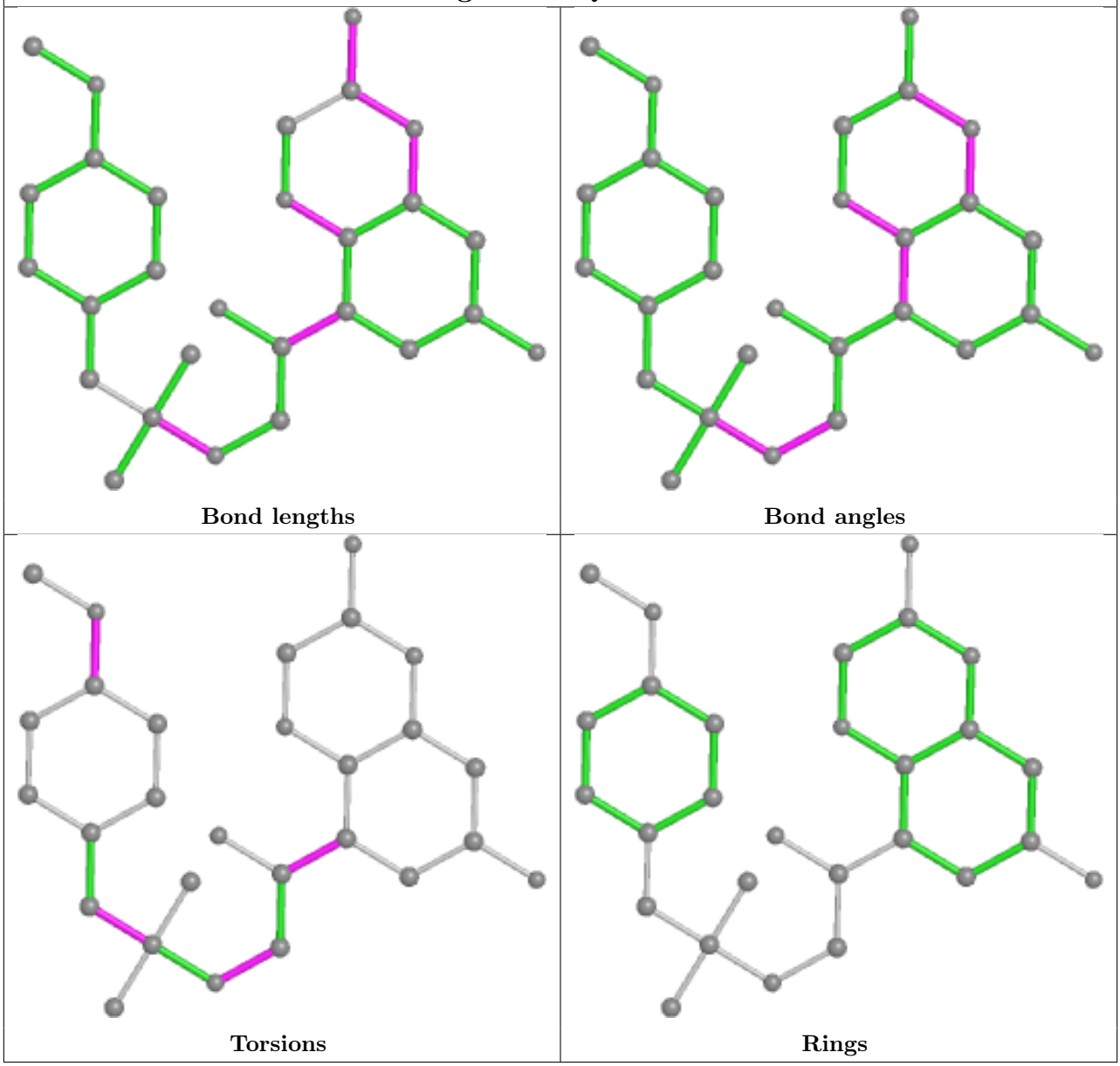
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	DZQ	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 DZQ A 501



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.