



Full wwPDB EM Validation Report ⓘ

Nov 11, 2024 – 06:06 PM JST

PDB ID : 8XJK
EMDB ID : EMD-38399
Title : Cloprosetnol bound Prostaglandin F2-alpha receptor-Gq Protein Complex
Authors : Zhang, X.; Li, X.; Liu, G.; Gong, W.
Deposited on : 2023-12-21
Resolution : 2.63 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 : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

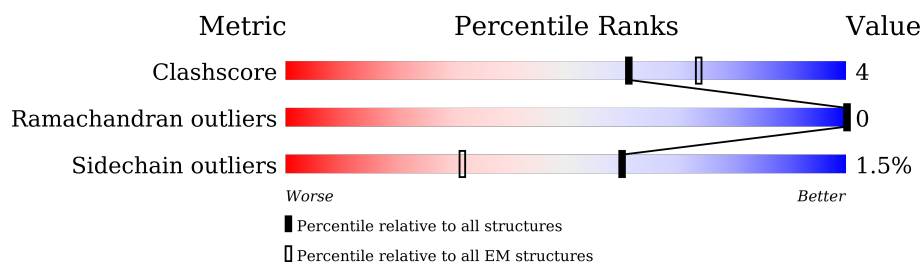
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.63 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	246	
2	B	376	
3	C	71	
4	E	254	
5	R	588	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8850 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 Engineered miniGq.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	224	Total	C	N	O	S	0	0
			1821	1151	325	337	8		

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	342	Total	C	N	O	S	0	0
			2622	1615	471	515	21		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	initiating methionine	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	HIS	-	expression tag	UNP P62873
B	-5	HIS	-	expression tag	UNP P62873
B	-4	HIS	-	expression tag	UNP P62873
B	-3	HIS	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873
B	341	GLY	-	expression tag	UNP P62873
B	342	SER	-	expression tag	UNP P62873
B	343	SER	-	expression tag	UNP P62873
B	344	GLY	-	expression tag	UNP P62873
B	345	GLY	-	expression tag	UNP P62873
B	346	GLY	-	expression tag	UNP P62873
B	347	GLY	-	expression tag	UNP P62873
B	348	SER	-	expression tag	UNP P62873
B	349	GLY	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	350	GLY	-	expression tag	UNP P62873
B	351	GLY	-	expression tag	UNP P62873
B	352	GLY	-	expression tag	UNP P62873
B	353	SER	-	expression tag	UNP P62873
B	354	SER	-	expression tag	UNP P62873
B	355	GLY	-	expression tag	UNP P62873
B	356	VAL	-	expression tag	UNP P62873
B	357	SER	-	expression tag	UNP P62873
B	358	GLY	-	expression tag	UNP P62873
B	359	TRP	-	expression tag	UNP P62873
B	360	ARG	-	expression tag	UNP P62873
B	361	LEU	-	expression tag	UNP P62873
B	362	PHE	-	expression tag	UNP P62873
B	363	LYS	-	expression tag	UNP P62873
B	364	LYS	-	expression tag	UNP P62873
B	365	ILE	-	expression tag	UNP P62873
B	366	SER	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	57	Total	C	N	O	S	0	0
			436	273	77	83	3		

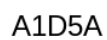
- Molecule 4 is a protein called Antibody fragment scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	230	Total	C	N	O	S	0	0
			1771	1125	293	343	10		

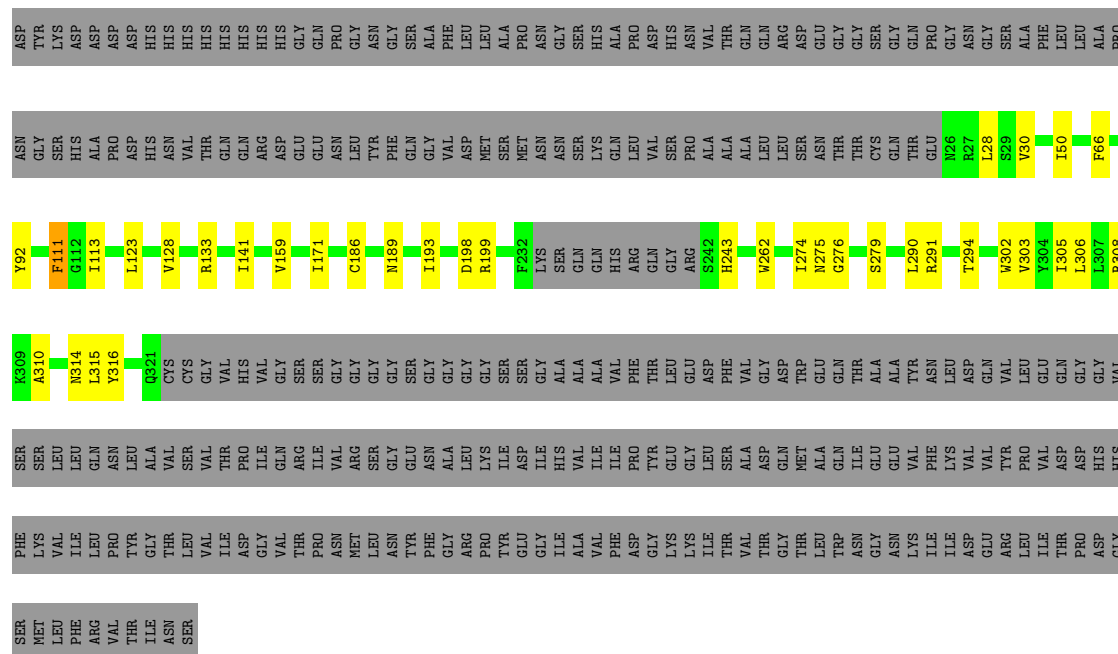
- Molecule 5 is a protein called Fusion tag,Prostaglandin F2-alpha receptor,LgBiT.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	287	Total	C	N	O	S	0	0
			2171	1440	347	364	20		

- Molecule 6 is Cloprostenol (three-letter code: A1D5A) (formula: C₂₂H₂₉ClO₆) (labeled as "Ligand of Interest" by depositor).



Chain R: 43% 6% 51%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88851	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 ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

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: A1D5A

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	0.23	0/1853	0.46	0/2493
2	B	0.24	0/2669	0.51	0/3618
3	C	0.23	0/442	0.40	0/597
4	E	0.25	0/1815	0.48	0/2461
5	R	0.24	0/2219	0.39	0/3020
All	All	0.24	0/8998	0.46	0/12189

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 [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	1821	0	1804	17	0
2	B	2622	0	2523	26	0
3	C	436	0	448	3	0
4	E	1771	0	1710	14	0
5	R	2171	0	2181	22	0
6	R	29	0	0	0	0
All	All	8850	0	8666	73	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 (73) 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)
5:R:291:ARG:O	5:R:294:THR:HG22	1.51	1.11
5:R:303:VAL:O	5:R:308:ARG:NH2	2.23	0.70
4:E:21:CYS:HB3	4:E:78:LEU:HB3	1.73	0.70
1:A:244:ASN:HD22	5:R:243:HIS:HB3	1.58	0.68
5:R:302:TRP:HA	5:R:306:LEU:HB2	1.77	0.67
2:B:294:CYS:HB3	2:B:308:LEU:HB2	1.77	0.66
5:R:291:ARG:O	5:R:294:THR:CG2	2.38	0.65
1:A:52:GLN:NE2	1:A:218:ALA:O	2.29	0.64
5:R:28:LEU:HA	5:R:291:ARG:HH22	1.63	0.64
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.80	0.63
3:C:20:LYS:O	3:C:24:ASN:ND2	2.27	0.62
1:A:69:ILE:HD11	2:B:117:LEU:HB3	1.80	0.61
2:B:220:GLN:NE2	2:B:258:ASP:OD1	2.35	0.60
1:A:101:ASN:HB3	2:B:57:LYS:HE3	1.82	0.60
4:E:90:THR:HG23	4:E:117:THR:HA	1.85	0.59
2:B:51:LEU:HB2	2:B:336:LEU:HB2	1.85	0.58
4:E:13:PRO:HD3	4:E:119:SER:HB2	1.86	0.57
1:A:69:ILE:HD12	1:A:86:VAL:HG22	1.86	0.57
2:B:210:LEU:HD22	2:B:255:LEU:HD22	1.89	0.54
5:R:291:ARG:C	5:R:294:THR:HG22	2.26	0.54
2:B:96:ARG:NH1	2:B:138:GLU:OE2	2.41	0.54
2:B:149:CYS:O	2:B:150:ARG:NH1	2.41	0.54
1:A:146:GLN:HG3	1:A:215:PHE:HB3	1.91	0.53
1:A:235:ILE:HD12	5:R:141:ILE:HG12	1.89	0.53
2:B:48:ARG:HH22	2:B:342:SER:HB3	1.74	0.52
5:R:193:ILE:HD11	5:R:276:GLY:HA2	1.92	0.50
4:E:19:LEU:HD12	4:E:80:LEU:HD23	1.94	0.50
2:B:228:ASP:N	2:B:228:ASP:OD1	2.44	0.50
1:A:36:LEU:HD13	1:A:107:ILE:HD11	1.95	0.49
1:A:244:ASN:ND2	5:R:243:HIS:HB3	2.26	0.49
5:R:199:ARG:NH2	5:R:274:ILE:O	2.46	0.49
2:B:260:GLU:OE2	2:B:263:THR:OG1	2.31	0.49
1:A:94:ARG:NE	2:B:228:ASP:OD2	2.37	0.48
2:B:250:CYS:HB2	2:B:264:TYR:HB2	1.96	0.48
2:B:112:VAL:HG13	2:B:126:LEU:HD11	1.95	0.48
2:B:79:LEU:HB3	2:B:93:ILE:HB	1.96	0.48
2:B:256:ARG:NH2	3:C:36:ASP:OD2	2.43	0.47
1:A:94:ARG:HH21	2:B:204:CYS:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:30:VAL:HG22	5:R:92:TYR:HB3	1.98	0.46
5:R:113:ILE:HD11	5:R:171:ILE:HG13	1.98	0.46
2:B:296:VAL:O	2:B:305:ALA:N	2.49	0.46
2:B:274:THR:HG21	2:B:314:ARG:HD3	1.98	0.46
5:R:128:VAL:HG21	5:R:159:VAL:HG21	1.98	0.45
3:C:59:ASN:O	3:C:62:ARG:HG3	2.16	0.45
4:E:7:GLY:O	4:E:17:ARG:NE	2.49	0.45
2:B:254:ASP:HB2	2:B:261:LEU:HD11	1.98	0.45
5:R:111:PHE:HB3	5:R:186:CYS:HB2	1.99	0.45
2:B:249:THR:HG22	2:B:265:SER:HB3	2.00	0.44
4:E:82:MET:HB3	4:E:85:LEU:HD21	2.00	0.44
2:B:66:ASP:OD1	2:B:66:ASP:N	2.47	0.44
5:R:310:ALA:O	5:R:314:ASN:ND2	2.40	0.44
4:E:1:VAL:HG13	4:E:26:PHE:CD1	2.52	0.43
4:E:39:ALA:HB3	4:E:42:LYS:HB2	2.01	0.43
1:A:93:ARG:NH2	1:A:124:ASP:OD1	2.52	0.43
5:R:275:ASN:HB2	5:R:279:SER:HB3	2.00	0.43
1:A:246:VAL:HG11	5:R:305:ILE:HD12	2.01	0.42
2:B:30:LEU:HD23	2:B:262:MET:HB2	2.01	0.42
5:R:66:PHE:CD1	5:R:133:ARG:HD3	2.54	0.42
4:E:232:HIS:HA	4:E:237:LEU:HD22	2.00	0.42
1:A:112:SER:HA	1:A:118:LEU:HD21	2.00	0.42
2:B:245:SER:HB3	2:B:247:ASP:OD1	2.19	0.42
4:E:201:ASP:N	4:E:201:ASP:OD1	2.53	0.42
4:E:178:LEU:HD13	4:E:227:TYR:CZ	2.54	0.42
1:A:38:LEU:HG	1:A:46:LYS:HD2	2.02	0.42
1:A:167:PHE:O	1:A:188:ARG:NH2	2.53	0.41
4:E:18:LYS:HE2	4:E:79:PHE:HB3	2.01	0.41
5:R:189:ASN:ND2	5:R:198:ASP:OD2	2.51	0.41
5:R:123:LEU:HD21	5:R:262:TRP:CD1	2.55	0.41
2:B:118:ASP:O	2:B:120:ILE:HG12	2.21	0.41
4:E:31:PHE:CD2	4:E:99:ILE:HB	2.56	0.41
4:E:72:ASP:HB2	4:E:79:PHE:HE2	1.86	0.40
1:A:71:GLU:HG2	1:A:84:PHE:HD1	1.87	0.40
5:R:50:ILE:HD11	5:R:315:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	218/246 (89%)	216 (99%)	2 (1%)	0	100	100
2	B	340/376 (90%)	334 (98%)	6 (2%)	0	100	100
3	C	55/71 (78%)	55 (100%)	0	0	100	100
4	E	226/254 (89%)	221 (98%)	5 (2%)	0	100	100
5	R	283/588 (48%)	281 (99%)	2 (1%)	0	100	100
All	All	1122/1535 (73%)	1107 (99%)	15 (1%)	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	196/213 (92%)	195 (100%)	1 (0%)	86	93
2	B	284/306 (93%)	277 (98%)	7 (2%)	42	63
3	C	46/58 (79%)	46 (100%)	0	100	100
4	E	195/207 (94%)	192 (98%)	3 (2%)	60	77
5	R	227/498 (46%)	224 (99%)	3 (1%)	65	80
All	All	948/1282 (74%)	934 (98%)	14 (2%)	60	77

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	HIS
2	B	57	LYS
2	B	59	TYR
2	B	105	TYR
2	B	135	VAL
2	B	146	LEU
2	B	228	ASP
2	B	234	PHE
4	E	62	THR
4	E	137	ASP
4	E	218	ARG
5	R	111	PHE
5	R	290	LEU
5	R	316	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	HIS
1	A	244	ASN
2	B	91	HIS
2	B	176	GLN
4	E	112	GLN
4	E	171	ASN
4	E	183	GLN
5	R	143	HIS

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 oligosaccharides 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
6	A1D5A	R	601	-	30,30,30	3.99	8 (26%)	31,39,39	1.06	2 (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
6	A1D5A	R	601	-	-	10/19/35/35	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	601	A1D5A	C10-C11	-16.30	1.32	1.53
6	R	601	A1D5A	C15-C14	-9.71	1.34	1.55
6	R	601	A1D5A	C15-C10	7.56	1.69	1.55
6	R	601	A1D5A	C13-C11	3.50	1.62	1.52
6	R	601	A1D5A	C13-C14	2.30	1.59	1.52
6	R	601	A1D5A	O20-C21	2.18	1.42	1.37
6	R	601	A1D5A	O28-C18	-2.13	1.39	1.43
6	R	601	A1D5A	C25-CL27	2.12	1.79	1.74

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	601	A1D5A	C09-C08-C07	-2.34	117.71	126.40
6	R	601	A1D5A	C18-C17-C16	-2.02	119.81	125.09

There are no chirality outliers.

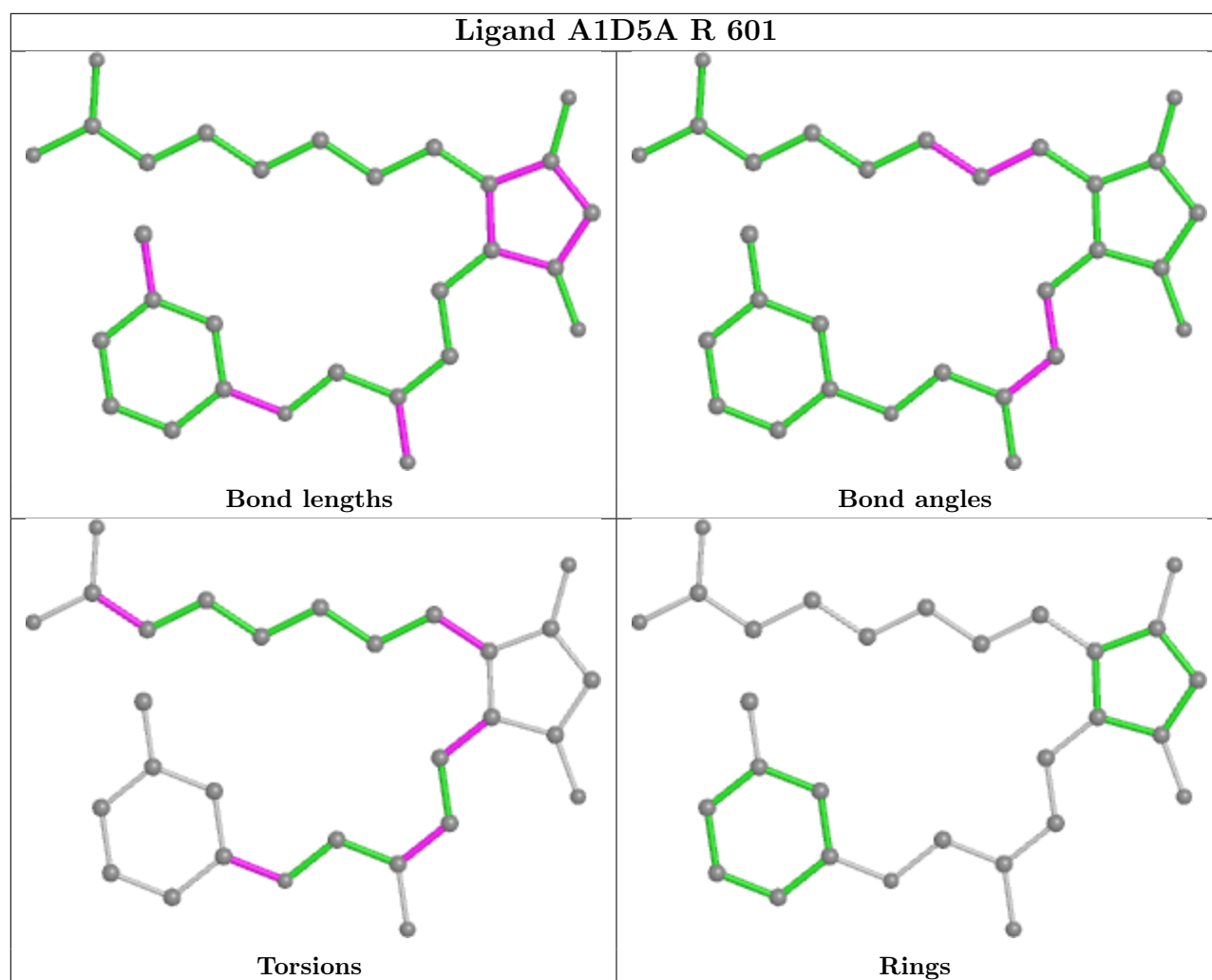
All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	601	A1D5A	C08-C09-C10-C15
6	R	601	A1D5A	C16-C17-C18-C19
6	R	601	A1D5A	C10-C15-C16-C17
6	R	601	A1D5A	C14-C15-C16-C17
6	R	601	A1D5A	C22-C21-O20-C19
6	R	601	A1D5A	C26-C21-O20-C19
6	R	601	A1D5A	C16-C17-C18-O28
6	R	601	A1D5A	C08-C09-C10-C11
6	R	601	A1D5A	O03-C02-C04-C05
6	R	601	A1D5A	O01-C02-C04-C05

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.



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.