



Full wwPDB EM Validation Report ⓘ

Dec 17, 2024 – 02:07 PM JST

PDB ID : 8KEX
EMDB ID : EMD-37191
Title : CryoEM structure of Gq coupled MRGPRX4 with agonist DCA-3P, local
Authors : Yang, J.; Fan, J.P.; Lei, X.G.
Deposited on : 2023-08-14
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 : 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) : 2.40

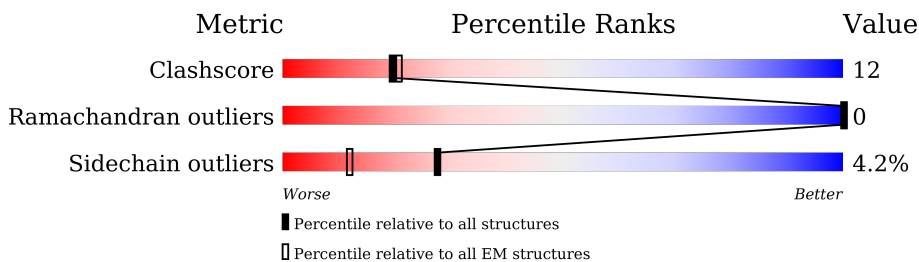
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	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	E	710	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1988 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 Soluble cytochrome b562,Mas-related G-protein coupled receptor member X4,Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	255	Total	C	N	O	S	0	0
			1956	1304	314	322	16		

There are 63 discrepancies between the modelled and reference sequences:

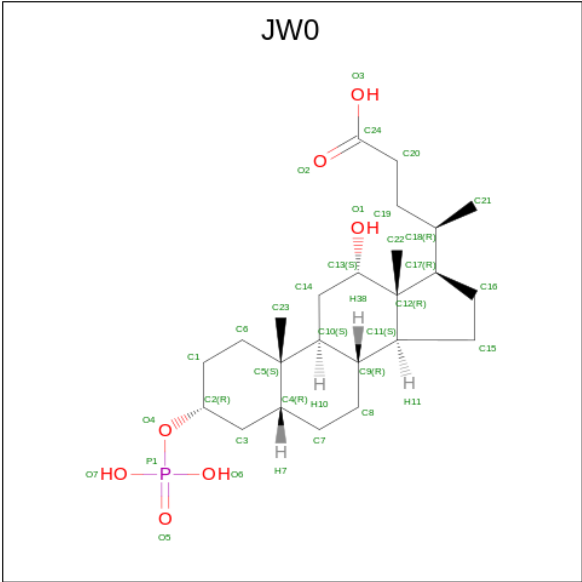
Chain	Residue	Modelled	Actual	Comment	Reference
E	-115	ASP	-	expression tag	UNP P0ABE7
E	-114	TYR	-	expression tag	UNP P0ABE7
E	-113	LYS	-	expression tag	UNP P0ABE7
E	-112	ASP	-	expression tag	UNP P0ABE7
E	-111	ASP	-	expression tag	UNP P0ABE7
E	-110	ASP	-	expression tag	UNP P0ABE7
E	-109	ASP	-	expression tag	UNP P0ABE7
E	-108	LYS	-	expression tag	UNP P0ABE7
E	-107	GLU	-	expression tag	UNP P0ABE7
E	-106	PHE	-	expression tag	UNP P0ABE7
E	-99	TRP	MET	conflict	UNP P0ABE7
E	-4	ILE	HIS	conflict	UNP P0ABE7
E	0	LEU	ARG	conflict	UNP P0ABE7
E	323	LEU	-	linker	UNP Q96LA9
E	324	GLU	-	linker	UNP Q96LA9
E	325	LEU	-	linker	UNP Q96LA9
E	326	GLU	-	linker	UNP Q96LA9
E	327	VAL	-	linker	UNP Q96LA9
E	328	LEU	-	linker	UNP Q96LA9
E	329	PHE	-	linker	UNP Q96LA9
E	330	GLN	-	linker	UNP Q96LA9
E	331	GLY	-	linker	UNP Q96LA9
E	332	PRO	-	linker	UNP Q96LA9
E	361	ARG	SER	conflict	UNP P42212
E	370	ASN	TYR	conflict	UNP P42212
E	395	LEU	PHE	conflict	UNP P42212
E	396	THR	SER	conflict	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	411	ARG	GLN	conflict	UNP P42212
E	430	SER	PHE	conflict	UNP P42212
E	436	THR	ASN	conflict	UNP P42212
E	476	PHE	TYR	conflict	UNP P42212
E	484	THR	MET	conflict	UNP P42212
E	494	ALA	VAL	conflict	UNP P42212
E	502	VAL	ILE	conflict	UNP P42212
E	537	VAL	ALA	conflict	UNP P42212
E	567	TRP	-	expression tag	UNP P42212
E	568	SER	-	expression tag	UNP P42212
E	569	HIS	-	expression tag	UNP P42212
E	570	PRO	-	expression tag	UNP P42212
E	571	GLN	-	expression tag	UNP P42212
E	572	PHE	-	expression tag	UNP P42212
E	573	GLU	-	expression tag	UNP P42212
E	574	LYS	-	expression tag	UNP P42212
E	575	GLY	-	expression tag	UNP P42212
E	576	GLY	-	expression tag	UNP P42212
E	577	GLY	-	expression tag	UNP P42212
E	578	SER	-	expression tag	UNP P42212
E	579	GLY	-	expression tag	UNP P42212
E	580	GLY	-	expression tag	UNP P42212
E	581	GLY	-	expression tag	UNP P42212
E	582	SER	-	expression tag	UNP P42212
E	583	GLY	-	expression tag	UNP P42212
E	584	GLY	-	expression tag	UNP P42212
E	585	SER	-	expression tag	UNP P42212
E	586	ALA	-	expression tag	UNP P42212
E	587	TRP	-	expression tag	UNP P42212
E	588	SER	-	expression tag	UNP P42212
E	589	HIS	-	expression tag	UNP P42212
E	590	PRO	-	expression tag	UNP P42212
E	591	GLN	-	expression tag	UNP P42212
E	592	PHE	-	expression tag	UNP P42212
E	593	GLU	-	expression tag	UNP P42212
E	594	LYS	-	expression tag	UNP P42212

- Molecule 2 is (4 {R})-4-[(3 {R},5 {R},8 {R},9 {S},10 {S},12 {S},13 {R},14 {S},17 {R})-10,13-dimethyl-12-oxidanyl-3-phosphonooxy-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1 {H}-cyclopenta[a]phenanthren-17-yl]pentanoic acid (three-letter code: JW0) (formula: C₂₄H₄₁O₇P) (labeled as "Ligand of Interest" by depositor).

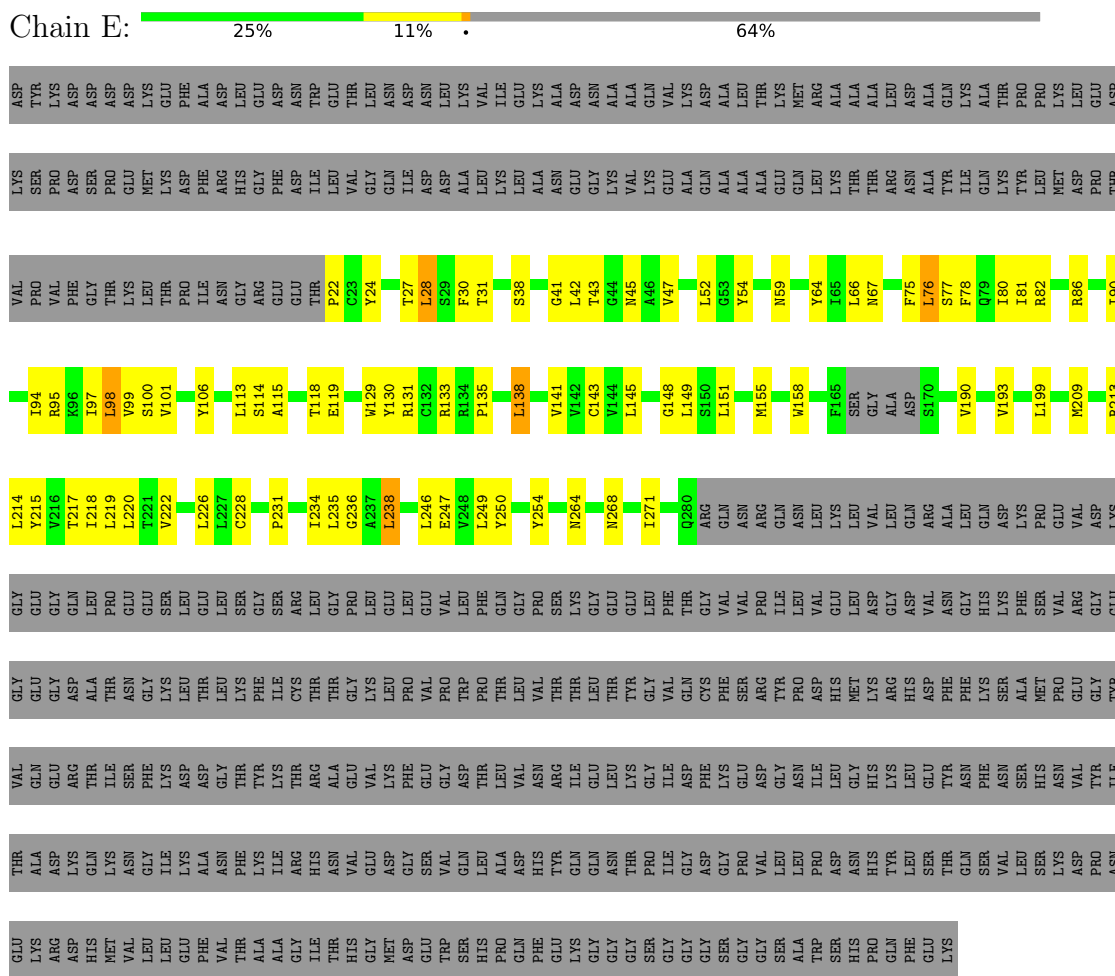


Mol	Chain	Residues	Atoms				AltConf
2	E	1	Total	C	O	P	0
			32	24	7	1	

3 Residue-property plots

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: Soluble cytochrome b562,Mas-related G-protein coupled receptor member X4,Green fluorescent protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	451859	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k 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: JW0

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	E	0.26	0/2003	0.57	4/2744 (0.1%)

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	E	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	98	LEU	CA-CB-CG	8.57	135.02	115.30
1	E	42	LEU	CA-CB-CG	6.21	129.58	115.30
1	E	138	LEU	CA-CB-CG	5.40	127.71	115.30
1	E	76	LEU	CA-CB-CG	5.13	127.09	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	209	MET	Peptide

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	E	1956	0	1986	49	0
2	E	32	0	0	7	0
All	All	1988	0	1986	49	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 12.

All (49) 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:E:100:SER:HG	1:E:158:TRP:HE1	1.05	0.97
1:E:67:ASN:ND2	1:E:143:CYS:SG	2.55	0.79
1:E:75:PHE:HE2	1:E:106:TYR:HB2	1.46	0.79
1:E:38:SER:HA	1:E:76:LEU:HD12	1.66	0.76
1:E:247:GLU:HG3	1:E:249:LEU:H	1.50	0.75
1:E:94:ILE:O	1:E:98:LEU:HD12	1.93	0.69
1:E:228:CYS:HB3	1:E:264:ASN:HB2	1.75	0.68
1:E:135:PRO:HG2	1:E:138:LEU:HB2	1.79	0.64
1:E:246:LEU:HD21	2:E:601:JW0:C2	2.28	0.63
1:E:94:ILE:HA	1:E:97:ILE:HG12	1.85	0.57
1:E:95:ARG:HB3	2:E:601:JW0:O7	2.06	0.56
1:E:113:LEU:HD21	1:E:268:ASN:HD21	1.69	0.56
1:E:28:LEU:H	1:E:28:LEU:HD23	1.71	0.56
1:E:235:LEU:HD21	1:E:254:TYR:HD1	1.71	0.56
1:E:246:LEU:HD21	2:E:601:JW0:C1	2.36	0.55
1:E:222:VAL:O	1:E:226:LEU:HG	2.07	0.55
1:E:27:THR:O	1:E:31:THR:HG22	2.09	0.53
1:E:77:SER:O	1:E:81:ILE:HG13	2.09	0.53
1:E:119:GLU:OE1	1:E:130:TYR:HE1	1.92	0.52
1:E:148:GLY:HA2	1:E:151:LEU:HG	1.92	0.52
1:E:97:ILE:O	1:E:101:VAL:HG12	2.12	0.50
1:E:41:GLY:O	1:E:45:ASN:ND2	2.44	0.49
1:E:129:TRP:HA	1:E:133:ARG:HG3	1.94	0.49
1:E:199:LEU:HD21	1:E:218:ILE:HG21	1.96	0.48
1:E:59:ASN:OD1	1:E:59:ASN:N	2.47	0.47
1:E:43:THR:O	1:E:47:VAL:HG12	2.13	0.47
1:E:95:ARG:O	1:E:99:VAL:HG22	2.14	0.47
1:E:82:ARG:NH2	2:E:601:JW0:O5	2.49	0.46
1:E:220:LEU:HD23	1:E:271:ILE:HG12	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:PRO:HD3	1:E:86:ARG:HE	1.81	0.45
1:E:115:ALA:O	1:E:119:GLU:HB2	2.16	0.45
1:E:246:LEU:HD11	2:E:601:JW0:C3	2.47	0.44
1:E:219:LEU:HD12	1:E:219:LEU:HA	1.82	0.44
1:E:76:LEU:O	1:E:80:ILE:HG13	2.18	0.44
1:E:52:LEU:HD22	1:E:66:LEU:HB2	1.99	0.44
1:E:141:VAL:O	1:E:145:LEU:HG	2.18	0.43
1:E:213:ARG:O	1:E:217:THR:HG22	2.18	0.43
1:E:234:ILE:O	1:E:238:LEU:HD22	2.18	0.43
1:E:236:GLY:HA2	2:E:601:JW0:C22	2.48	0.43
1:E:64:TYR:CE2	1:E:119:GLU:HG3	2.54	0.42
1:E:90:ILE:HA	1:E:95:ARG:HH21	1.83	0.42
1:E:190:VAL:HA	1:E:193:VAL:HG12	2.00	0.42
1:E:155:MET:SD	1:E:155:MET:N	2.93	0.42
1:E:214:LEU:HD23	1:E:215:TYR:HD1	1.83	0.42
1:E:114:SER:O	1:E:118:THR:HG22	2.20	0.42
1:E:100:SER:OG	1:E:158:TRP:NE1	2.17	0.42
1:E:129:TRP:CD1	1:E:133:ARG:HB2	2.56	0.40
1:E:231:PRO:HA	1:E:234:ILE:HG12	2.03	0.40
1:E:236:GLY:HA3	2:E:601:JW0:C18	2.52	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	E	251/710 (35%)	228 (91%)	23 (9%)	0	100	100

There are no Ramachandran outliers to report.

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 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	E	212/621 (34%)	203 (96%)	9 (4%)	25 58

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	24	TYR
1	E	28	LEU
1	E	30	PHE
1	E	54	TYR
1	E	78	PHE
1	E	131	ARG
1	E	149	LEU
1	E	238	LEU
1	E	250	TYR

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

Mol	Chain	Res	Type
1	E	67	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

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
2	JW0	E	601	-	35,35,35	2.15	11 (31%)	56,56,56	3.06	22 (39%)

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	JW0	E	601	-	-	9/14/76/76	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	JW0	C12-C17	-5.32	1.46	1.55
2	E	601	JW0	P1-O4	5.12	1.69	1.59
2	E	601	JW0	O1-C13	-4.42	1.36	1.43
2	E	601	JW0	C14-C10	-4.18	1.46	1.53
2	E	601	JW0	C6-C5	-3.90	1.47	1.54
2	E	601	JW0	C12-C11	-2.95	1.50	1.55
2	E	601	JW0	C16-C15	2.62	1.61	1.54
2	E	601	JW0	C9-C11	-2.53	1.48	1.53
2	E	601	JW0	C9-C10	-2.20	1.49	1.53
2	E	601	JW0	C5-C4	-2.07	1.52	1.55
2	E	601	JW0	C8-C7	-2.03	1.47	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	JW0	C12-C11-C9	-10.94	102.64	114.71
2	E	601	JW0	C12-C17-C18	-7.54	110.49	119.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	JW0	C11-C9-C10	-6.59	100.27	109.09
2	E	601	JW0	C22-C12-C13	6.37	115.55	109.07
2	E	601	JW0	C16-C17-C12	-5.31	98.35	103.55
2	E	601	JW0	C22-C12-C11	-5.25	103.00	111.21
2	E	601	JW0	C14-C10-C5	-5.17	108.40	113.73
2	E	601	JW0	C11-C12-C13	4.25	111.36	107.40
2	E	601	JW0	C15-C11-C9	-4.17	112.21	119.08
2	E	601	JW0	C8-C9-C10	3.56	114.91	110.49
2	E	601	JW0	C17-C12-C13	-3.54	114.44	117.67
2	E	601	JW0	C6-C5-C10	-3.32	106.14	111.35
2	E	601	JW0	O1-C13-C12	-3.31	105.43	111.03
2	E	601	JW0	C21-C18-C17	-3.05	108.26	112.92
2	E	601	JW0	C10-C5-C4	2.76	112.46	108.58
2	E	601	JW0	C6-C1-C2	-2.74	105.65	110.33
2	E	601	JW0	C8-C9-C11	-2.70	107.47	112.08
2	E	601	JW0	C16-C15-C11	-2.56	100.06	105.13
2	E	601	JW0	C23-C5-C10	-2.46	107.80	111.18
2	E	601	JW0	C3-C4-C7	-2.03	108.01	111.74
2	E	601	JW0	C15-C11-C12	-2.02	101.58	103.55
2	E	601	JW0	C20-C19-C18	-2.00	110.86	114.52

There are no chirality outliers.

All (9) torsion outliers are listed below:

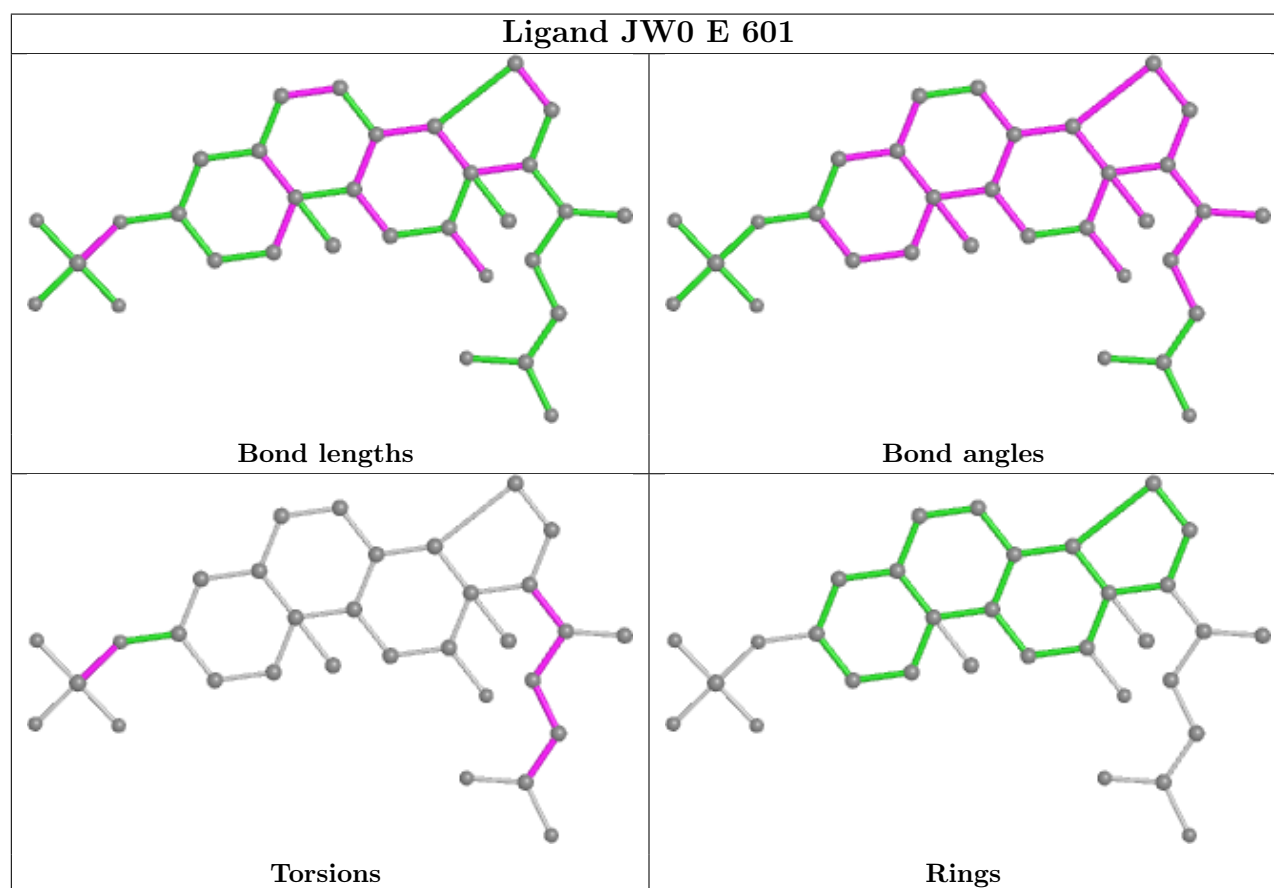
Mol	Chain	Res	Type	Atoms
2	E	601	JW0	C12-C17-C18-C19
2	E	601	JW0	C16-C17-C18-C21
2	E	601	JW0	C12-C17-C18-C21
2	E	601	JW0	C16-C17-C18-C19
2	E	601	JW0	C18-C19-C20-C24
2	E	601	JW0	C21-C18-C19-C20
2	E	601	JW0	C2-O4-P1-O5
2	E	601	JW0	C19-C20-C24-O3
2	E	601	JW0	C19-C20-C24-O2

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	601	JW0	7	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.



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.