



## wwPDB EM Validation Summary Report ⓘ

Jan 2, 2025 – 06:07 PM JST

PDB ID : 8YNT  
EMDB ID : EMD-39430  
Title : Cryo-EM structure of SNAP-94847-bound MCHR1, S2 state  
Authors : Ye, X.; Liu, G.; Li, X.; Liu, H.; Gong, W.  
Deposited on : 2024-03-11  
Resolution : 3.43 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis	: <b>FAILED</b>
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	: <b>FAILED</b>
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.40

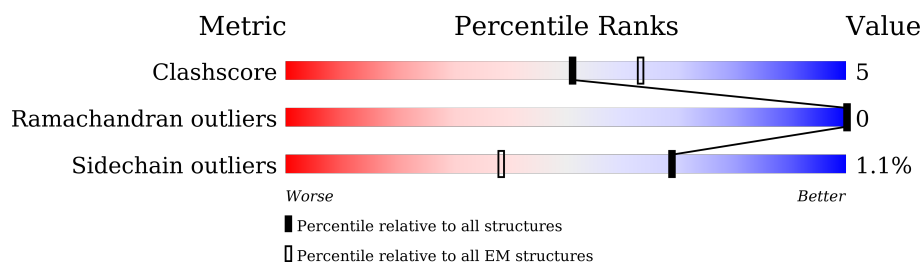
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.43 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  $\geq 3$ , 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	H	238	
2	L	220	
3	N	285	
4	R	585	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7420 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 Antibody 1B3 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	222	Total	C	N	O	S	0	0
			1669	1062	274	327	6		

- Molecule 2 is a protein called Antibody 1B3 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	211	Total	C	N	O	S	0	0
			1610	1010	272	324	4		

- Molecule 3 is a protein called Glue molecule 4-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	146	Total	C	N	O	S	1	0
			1113	691	192	225	5		

- Molecule 4 is a protein called Melanin-concentrating hormone receptor 1, Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	395	Total	C	N	O	S	1	0
			2993	1962	489	525	17		

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-45	ASP	-	expression tag	UNP Q5IFH6
R	-44	TYR	-	expression tag	UNP Q5IFH6
R	-43	LYS	-	expression tag	UNP Q5IFH6
R	-42	ASP	-	expression tag	UNP Q5IFH6
R	-41	ASP	-	expression tag	UNP Q5IFH6
R	-40	ASP	-	expression tag	UNP Q5IFH6
R	-39	ASP	-	expression tag	UNP Q5IFH6
R	-38	MET	-	expression tag	UNP Q5IFH6

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-37	GLY	-	expression tag	UNP Q5IFH6
R	-36	GLN	-	expression tag	UNP Q5IFH6
R	-35	PRO	-	expression tag	UNP Q5IFH6
R	-34	GLY	-	expression tag	UNP Q5IFH6
R	-33	ASN	-	expression tag	UNP Q5IFH6
R	-32	GLY	-	expression tag	UNP Q5IFH6
R	-31	SER	-	expression tag	UNP Q5IFH6
R	-30	ALA	-	expression tag	UNP Q5IFH6
R	-29	PHE	-	expression tag	UNP Q5IFH6
R	-28	LEU	-	expression tag	UNP Q5IFH6
R	-27	LEU	-	expression tag	UNP Q5IFH6
R	-26	ALA	-	expression tag	UNP Q5IFH6
R	-25	PRO	-	expression tag	UNP Q5IFH6
R	-24	ASN	-	expression tag	UNP Q5IFH6
R	-23	GLY	-	expression tag	UNP Q5IFH6
R	-22	SER	-	expression tag	UNP Q5IFH6
R	-21	HIS	-	expression tag	UNP Q5IFH6
R	-20	ALA	-	expression tag	UNP Q5IFH6
R	-19	PRO	-	expression tag	UNP Q5IFH6
R	-18	ASP	-	expression tag	UNP Q5IFH6
R	-17	HIS	-	expression tag	UNP Q5IFH6
R	-16	ASP	-	expression tag	UNP Q5IFH6
R	-15	VAL	-	expression tag	UNP Q5IFH6
R	-14	THR	-	expression tag	UNP Q5IFH6
R	-13	GLN	-	expression tag	UNP Q5IFH6
R	-12	GLN	-	expression tag	UNP Q5IFH6
R	-11	ARG	-	expression tag	UNP Q5IFH6
R	-10	ASP	-	expression tag	UNP Q5IFH6
R	-9	GLU	-	expression tag	UNP Q5IFH6
R	-8	GLU	-	expression tag	UNP Q5IFH6
R	-7	ASN	-	expression tag	UNP Q5IFH6
R	-6	LEU	-	expression tag	UNP Q5IFH6
R	-5	TYR	-	expression tag	UNP Q5IFH6
R	-4	PHE	-	expression tag	UNP Q5IFH6
R	-3	GLN	-	expression tag	UNP Q5IFH6
R	-2	GLY	-	expression tag	UNP Q5IFH6
R	-1	VAL	-	expression tag	UNP Q5IFH6
R	0	ASP	-	expression tag	UNP Q5IFH6
R	32	ASN	ASP	conflict	UNP Q5IFH6
R	305	LYS	-	linker	UNP Q99705
R	306	ARG	-	linker	UNP Q99705
R	307	GLN	-	linker	UNP Q99705

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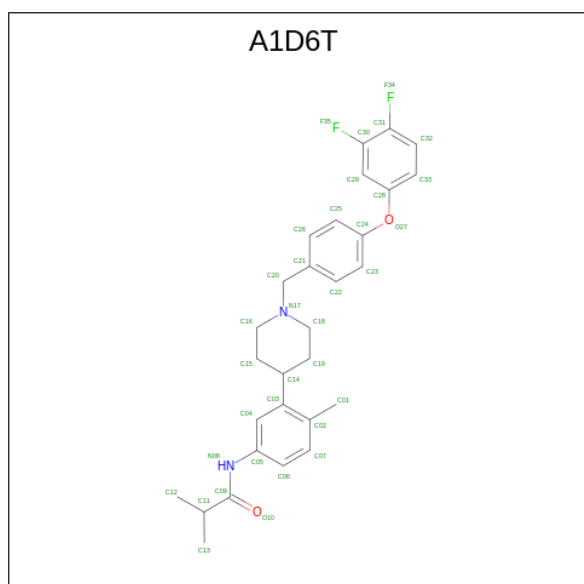
Chain	Residue	Modelled	Actual	Comment	Reference
R	308	LEU	-	linker	UNP Q99705
R	315	TRP	MET	conflict	UNP P0ABE7
R	352	SER	-	linker	UNP P0ABE7
R	353	GLY	-	linker	UNP P0ABE7
R	354	SER	-	linker	UNP P0ABE7
R	355	GLY	-	linker	UNP P0ABE7
R	403	ILE	-	linker	UNP Q8CVG7
R	404	GLN	-	linker	UNP Q8CVG7
R	405	LYS	-	linker	UNP Q8CVG7
R	406	TYR	-	linker	UNP Q8CVG7
R	407	LEU	-	linker	UNP Q8CVG7
R	408	LEU	-	linker	UNP Q8CVG7
R	490	ILE	-	expression tag	UNP Q99705
R	491	ALA	-	expression tag	UNP Q99705
R	492	ALA	-	expression tag	UNP Q99705
R	493	LEU	-	expression tag	UNP Q99705
R	494	LYS	-	expression tag	UNP Q99705
R	495	GLU	-	expression tag	UNP Q99705
R	496	LYS	-	expression tag	UNP Q99705
R	497	ILE	-	expression tag	UNP Q99705
R	498	ALA	-	expression tag	UNP Q99705
R	499	ALA	-	expression tag	UNP Q99705
R	500	LEU	-	expression tag	UNP Q99705
R	501	LYS	-	expression tag	UNP Q99705
R	502	GLU	-	expression tag	UNP Q99705
R	503	LYS	-	expression tag	UNP Q99705
R	504	ILE	-	expression tag	UNP Q99705
R	505	ALA	-	expression tag	UNP Q99705
R	506	ALA	-	expression tag	UNP Q99705
R	507	LEU	-	expression tag	UNP Q99705
R	508	LYS	-	expression tag	UNP Q99705
R	509	GLU	-	expression tag	UNP Q99705
R	510	ALA	-	expression tag	UNP Q99705
R	511	GLU	-	expression tag	UNP Q99705
R	512	GLU	-	expression tag	UNP Q99705
R	513	LYS	-	expression tag	UNP Q99705
R	514	ARG	-	expression tag	UNP Q99705
R	515	ALA	-	expression tag	UNP Q99705
R	516	SER	-	expression tag	UNP Q99705
R	517	ARG	-	expression tag	UNP Q99705
R	518	LEU	-	expression tag	UNP Q99705
R	519	GLU	-	expression tag	UNP Q99705

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Chain	Residue	Modelled	Actual	Comment	Reference
R	520	GLU	-	expression tag	UNP Q99705
R	521	GLU	-	expression tag	UNP Q99705
R	522	LEU	-	expression tag	UNP Q99705
R	523	ARG	-	expression tag	UNP Q99705
R	524	ARG	-	expression tag	UNP Q99705
R	525	ARG	-	expression tag	UNP Q99705
R	526	LEU	-	expression tag	UNP Q99705
R	527	THR	-	expression tag	UNP Q99705
R	528	GLU	-	expression tag	UNP Q99705
R	529	ALA	-	expression tag	UNP Q99705
R	530	ALA	-	expression tag	UNP Q99705
R	531	ALA	-	expression tag	UNP Q99705
R	532	HIS	-	expression tag	UNP Q99705
R	533	HIS	-	expression tag	UNP Q99705
R	534	HIS	-	expression tag	UNP Q99705
R	535	HIS	-	expression tag	UNP Q99705
R	536	HIS	-	expression tag	UNP Q99705
R	537	HIS	-	expression tag	UNP Q99705
R	538	HIS	-	expression tag	UNP Q99705
R	539	HIS	-	expression tag	UNP Q99705

- Molecule 5 is {N}-[3-[1-[[4-[3,4-bis(fluoranyl)phenoxy]phenyl]methyl]piperidin-4-yl]-4-methyl-phenyl]-2-methyl-propanamide (three-letter code: A1D6T) (formula: C<sub>29</sub>H<sub>32</sub>F<sub>2</sub>N<sub>2</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

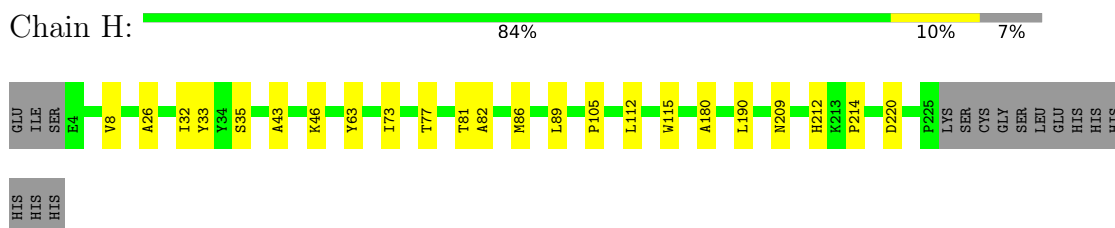


Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	N	O	
5	R	1	35	29	2	2	2	0

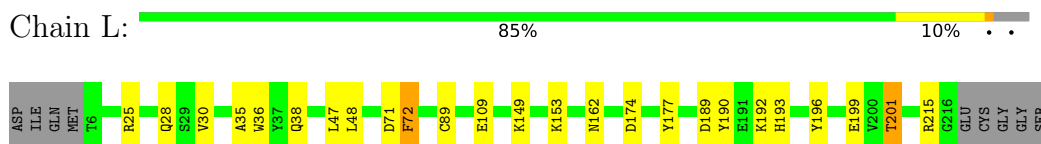
### 3 Residue-property plots

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.

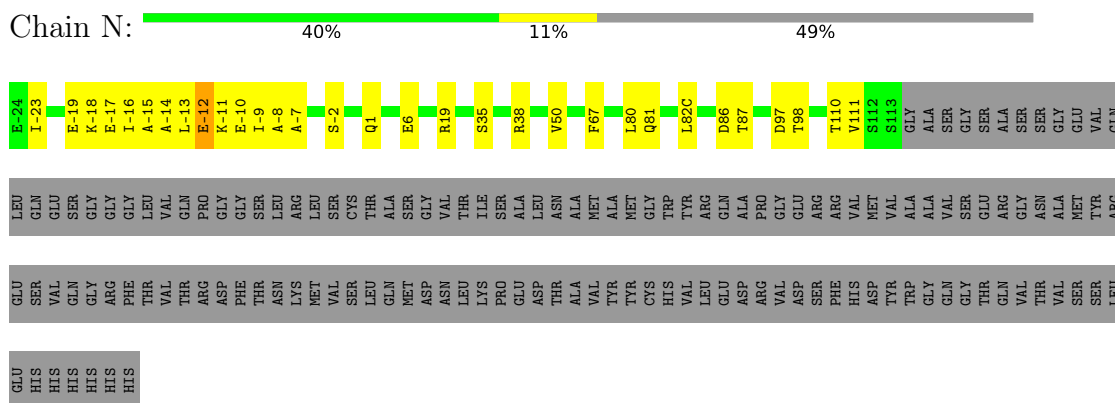
- Molecule 1: Antibody 1B3 Fab heavy chain



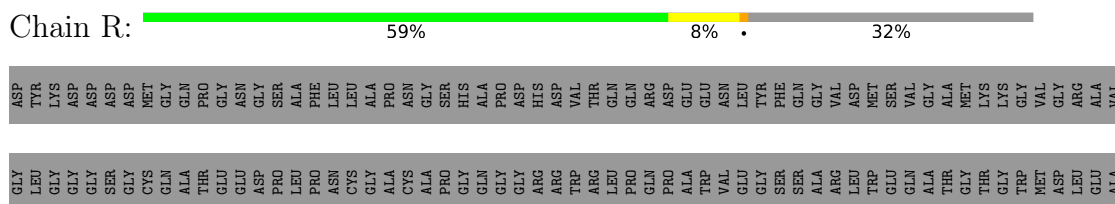
- Molecule 2: Antibody 1B3 Fab light chain



- Molecule 3: Glue molecule 4-9



- Molecule 4: Melanin-concentrating hormone receptor 1, Soluble cytochrome b562







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	268193	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: A1D6T

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	H	0.26	0/1718	0.46	0/2350
2	L	0.26	0/1647	0.47	0/2239
3	N	0.25	0/1135	0.50	0/1531
4	R	0.24	0/3056	0.39	0/4169
All	All	0.25	0/7556	0.44	0/10289

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	H	1669	0	1608	13	0
2	L	1610	0	1570	14	0
3	N	1113	0	1072	23	0
4	R	2993	0	3002	28	0
5	R	35	0	0	0	0
All	All	7420	0	7252	77	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 5.

The worst 5 of 77 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:L:193:HIS:O	2:L:215:ARG:NH1	2.27	0.68
4:R:315:TRP:HE1	4:R:399:ARG:HG3	1.57	0.67
3:N:-11:LYS:HA	3:N:-8:ALA:HB3	1.78	0.64
3:N:-17:GLU:O	3:N:-13:LEU:N	2.27	0.63
3:N:-13:LEU:HB3	4:R:497:ILE:HG21	1.82	0.62

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	H	220/238 (92%)	215 (98%)	5 (2%)	0	100	100
2	L	209/220 (95%)	205 (98%)	4 (2%)	0	100	100
3	N	145/285 (51%)	139 (96%)	6 (4%)	0	100	100
4	R	392/585 (67%)	381 (97%)	11 (3%)	0	100	100
All	All	966/1328 (73%)	940 (97%)	26 (3%)	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	H	185/200 (92%)	185 (100%)	0	100	100
2	L	184/191 (96%)	182 (99%)	2 (1%)	70	82
3	N	115/227 (51%)	113 (98%)	2 (2%)	56	75
4	R	303/482 (63%)	298 (98%)	5 (2%)	56	75
All	All	787/1100 (72%)	778 (99%)	9 (1%)	69	82

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	R	480	PHE
4	R	493	LEU
3	N	-12	GLU
4	R	112	MET
4	R	280	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
4	R	281	GLN
4	R	307	GLN
4	R	469	ASN
4	R	441	GLN
4	R	465	ASN

### 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
5	A1D6T	R	601	-	38,38,38	2.98	9 (23%)	53,53,53	1.21	5 (9%)

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
5	A1D6T	R	601	-	-	7/20/30/30	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	601	A1D6T	C20-N17	-13.42	1.21	1.47
5	R	601	A1D6T	C09-N08	7.37	1.52	1.35
5	R	601	A1D6T	C03-C14	4.50	1.60	1.52
5	R	601	A1D6T	C20-C21	4.08	1.58	1.51
5	R	601	A1D6T	C05-N08	3.35	1.48	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	601	A1D6T	C28-O27-C24	-3.95	109.57	118.80
5	R	601	A1D6T	C19-C14-C03	-3.30	105.69	112.26
5	R	601	A1D6T	C05-N08-C09	-3.01	120.19	127.40
5	R	601	A1D6T	C18-N17-C16	2.22	113.83	108.83
5	R	601	A1D6T	C11-C09-N08	2.05	119.75	114.60

There are no chirality outliers.

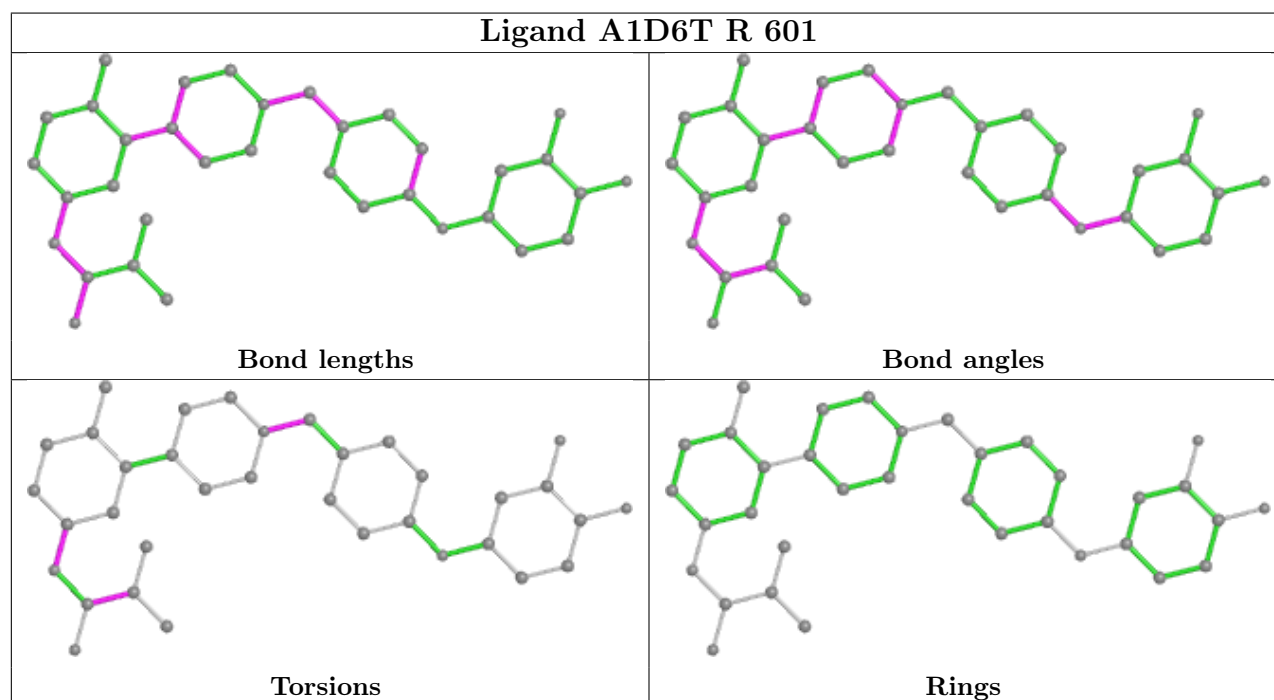
5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	R	601	A1D6T	C04-C05-N08-C09
5	R	601	A1D6T	C06-C05-N08-C09
5	R	601	A1D6T	N08-C09-C11-C13
5	R	601	A1D6T	O10-C09-C11-C13
5	R	601	A1D6T	N08-C09-C11-C12

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.