



wwPDB EM Validation Summary Report ⓘ

Oct 27, 2024 – 12:08 AM JST

PDB ID : 9JKQ
EMDB ID : EMD-61567
Title : Cryo-EM structure of the METH-bound hTAAR1-Gs complex
Authors : Lin, Y.; Wang, J.; Shi, F.
Deposited on : 2024-09-16
Resolution : 2.66 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

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

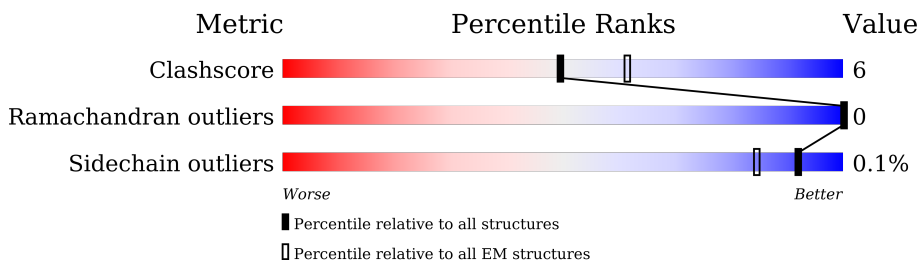
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.66 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	394	
2	B	351	
3	C	71	
4	N	162	
5	R	510	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8386 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 Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	235	Total	C	N	O	S	0	0
			1947	1226	352	362	7		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	ASN	SER	conflict	UNP P63092
A	226	ALA	GLY	conflict	UNP P63092
A	268	ALA	GLU	conflict	UNP P63092
A	271	LYS	ASN	conflict	UNP P63092
A	274	ASP	LYS	conflict	UNP P63092
A	280	LYS	ARG	conflict	UNP P63092
A	284	ASP	THR	conflict	UNP P63092
A	285	THR	ILE	conflict	UNP P63092

- 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	339	Total	C	N	O	S	0	0
			2606	1607	468	510	21		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P62873
B	2	HIS	-	expression tag	UNP P62873
B	3	HIS	-	expression tag	UNP P62873
B	4	HIS	-	expression tag	UNP P62873
B	5	HIS	-	expression tag	UNP P62873
B	6	HIS	-	expression tag	UNP P62873
B	7	HIS	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	8	GLY	-	expression tag	UNP P62873
B	9	SER	-	expression tag	UNP P62873
B	10	LEU	-	expression tag	UNP P62873
B	11	LEU	-	expression tag	UNP P62873
B	12	GLN	-	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
			442	277	78	84	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	68	SER	CYS	conflict	UNP P59768

- Molecule 4 is a protein called Nb35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	128	Total	C	N	O	S	0	0
			973	605	170	192	6		

- Molecule 5 is a protein called Soluble cytochrome b562,Trace amine-associated receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	296	Total	C	N	O	S	0	0
			2407	1611	377	393	26		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-124	MET	-	initiating methionine	UNP P0ABE7
R	-123	LYS	-	expression tag	UNP P0ABE7
R	-122	THR	-	expression tag	UNP P0ABE7
R	-121	ILE	-	expression tag	UNP P0ABE7
R	-120	ILE	-	expression tag	UNP P0ABE7
R	-119	ALA	-	expression tag	UNP P0ABE7
R	-118	LEU	-	expression tag	UNP P0ABE7
R	-117	SER	-	expression tag	UNP P0ABE7

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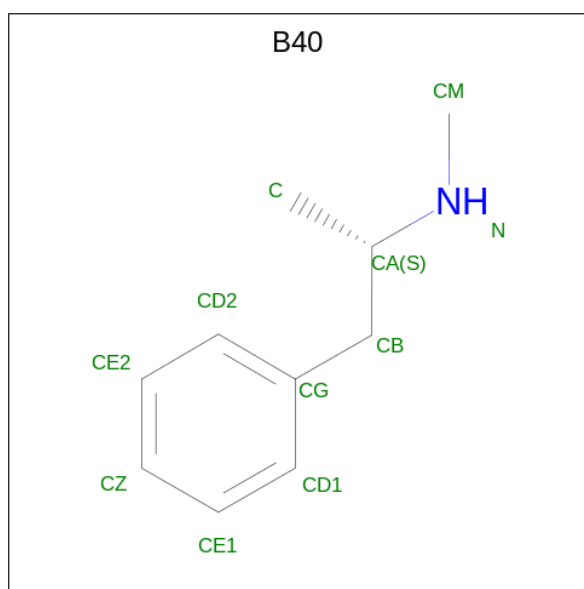
Chain	Residue	Modelled	Actual	Comment	Reference
R	-116	TYR	-	expression tag	UNP P0ABE7
R	-115	ILE	-	expression tag	UNP P0ABE7
R	-114	PHE	-	expression tag	UNP P0ABE7
R	-113	CYS	-	expression tag	UNP P0ABE7
R	-112	LEU	-	expression tag	UNP P0ABE7
R	-111	VAL	-	expression tag	UNP P0ABE7
R	-110	PHE	-	expression tag	UNP P0ABE7
R	-109	ALA	-	expression tag	UNP P0ABE7
R	-108	GLY	-	expression tag	UNP P0ABE7
R	-107	ALA	-	expression tag	UNP P0ABE7
R	-106	PRO	-	expression tag	UNP P0ABE7
R	-99	TRP	MET	conflict	UNP P0ABE7
R	-4	ILE	HIS	conflict	UNP P0ABE7
R	0	LEU	ARG	conflict	UNP P0ABE7
R	63	VAL	HIS	conflict	UNP Q96RJ0
R	112	TRP	PHE	conflict	UNP Q96RJ0
R	340	GLU	-	expression tag	UNP Q96RJ0
R	341	PHE	-	expression tag	UNP Q96RJ0
R	342	LEU	-	expression tag	UNP Q96RJ0
R	343	GLU	-	expression tag	UNP Q96RJ0
R	344	VAL	-	expression tag	UNP Q96RJ0
R	345	LEU	-	expression tag	UNP Q96RJ0
R	346	PHE	-	expression tag	UNP Q96RJ0
R	347	GLN	-	expression tag	UNP Q96RJ0
R	348	GLY	-	expression tag	UNP Q96RJ0
R	349	PRO	-	expression tag	UNP Q96RJ0
R	350	TRP	-	expression tag	UNP Q96RJ0
R	351	SER	-	expression tag	UNP Q96RJ0
R	352	HIS	-	expression tag	UNP Q96RJ0
R	353	PRO	-	expression tag	UNP Q96RJ0
R	354	GLN	-	expression tag	UNP Q96RJ0
R	355	PHE	-	expression tag	UNP Q96RJ0
R	356	GLU	-	expression tag	UNP Q96RJ0
R	357	LYS	-	expression tag	UNP Q96RJ0
R	358	GLY	-	expression tag	UNP Q96RJ0
R	359	GLY	-	expression tag	UNP Q96RJ0
R	360	GLY	-	expression tag	UNP Q96RJ0
R	361	SER	-	expression tag	UNP Q96RJ0
R	362	GLY	-	expression tag	UNP Q96RJ0
R	363	GLY	-	expression tag	UNP Q96RJ0
R	364	GLY	-	expression tag	UNP Q96RJ0
R	365	SER	-	expression tag	UNP Q96RJ0

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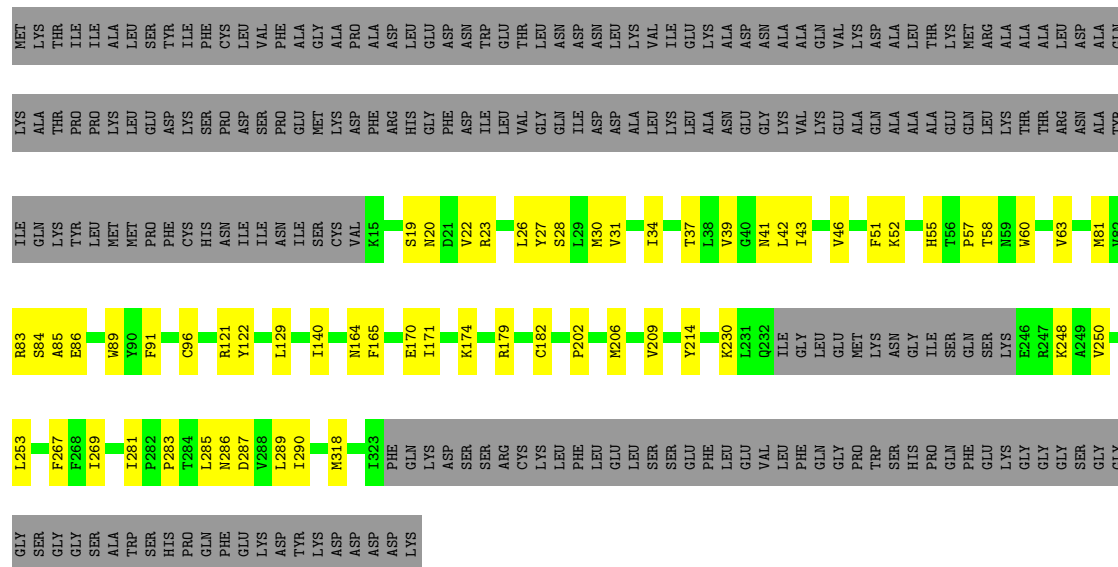
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Chain	Residue	Modelled	Actual	Comment	Reference
R	366	GLY	-	expression tag	UNP Q96RJ0
R	367	GLY	-	expression tag	UNP Q96RJ0
R	368	SER	-	expression tag	UNP Q96RJ0
R	369	ALA	-	expression tag	UNP Q96RJ0
R	370	TRP	-	expression tag	UNP Q96RJ0
R	371	SER	-	expression tag	UNP Q96RJ0
R	372	HIS	-	expression tag	UNP Q96RJ0
R	373	PRO	-	expression tag	UNP Q96RJ0
R	374	GLN	-	expression tag	UNP Q96RJ0
R	375	PHE	-	expression tag	UNP Q96RJ0
R	376	GLU	-	expression tag	UNP Q96RJ0
R	377	LYS	-	expression tag	UNP Q96RJ0
R	378	ASP	-	expression tag	UNP Q96RJ0
R	379	TYR	-	expression tag	UNP Q96RJ0
R	380	LYS	-	expression tag	UNP Q96RJ0
R	381	ASP	-	expression tag	UNP Q96RJ0
R	382	ASP	-	expression tag	UNP Q96RJ0
R	383	ASP	-	expression tag	UNP Q96RJ0
R	384	ASP	-	expression tag	UNP Q96RJ0
R	385	LYS	-	expression tag	UNP Q96RJ0

- Molecule 6 is (2S)-N-methyl-1-phenylpropan-2-amine (three-letter code: B40) (formula: C₁₀H₁₅N) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	R	1	Total	C	N	0
			11	10	1	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	647397	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 ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	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: B40

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	0.25	0/1983	0.49	0/2665
2	B	0.25	0/2653	0.55	0/3597
3	C	0.23	0/448	0.43	0/603
4	N	0.27	0/993	0.53	0/1345
5	R	0.26	0/2480	0.44	0/3366
All	All	0.26	0/8557	0.50	0/11576

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	1947	0	1921	26	0
2	B	2606	0	2510	22	0
3	C	442	0	455	4	0
4	N	973	0	940	10	0
5	R	2407	0	2448	39	0
6	R	11	0	15	1	0
All	All	8386	0	8289	92	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.

The worst 5 of 92 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)
4:N:62:GLY:HA2	4:N:65:LYS:HE3	1.60	0.83
2:B:256:SER:OG	2:B:258:ASP:OD1	2.10	0.70
5:R:83:ARG:HD3	5:R:182:CYS:HB2	1.75	0.66
5:R:23:ARG:NH2	5:R:86:GLU:OE1	2.29	0.65
5:R:57:PRO:HB2	5:R:140:ILE:HG13	1.80	0.63

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	229/394 (58%)	225 (98%)	4 (2%)	0	100	100
2	B	337/351 (96%)	325 (96%)	12 (4%)	0	100	100
3	C	55/71 (78%)	54 (98%)	1 (2%)	0	100	100
4	N	126/162 (78%)	126 (100%)	0	0	100	100
5	R	292/510 (57%)	279 (96%)	13 (4%)	0	100	100
All	All	1039/1488 (70%)	1009 (97%)	30 (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	A	210/349 (60%)	209 (100%)	1 (0%)	86	94
2	B	282/293 (96%)	282 (100%)	0	100	100
3	C	47/58 (81%)	47 (100%)	0	100	100
4	N	106/130 (82%)	106 (100%)	0	100	100
5	R	268/446 (60%)	268 (100%)	0	100	100
All	All	913/1276 (72%)	912 (100%)	1 (0%)	92	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	HIS

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

Mol	Chain	Res	Type
4	N	1	GLN

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 [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
6	B40	R	401	-	11,11,11	0.67	0	12,13,13	0.81	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
6	B40	R	401	-	-	0/6/6/6	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	401	B40	C-CA-CB	-2.04	107.70	111.91

There are no chirality outliers.

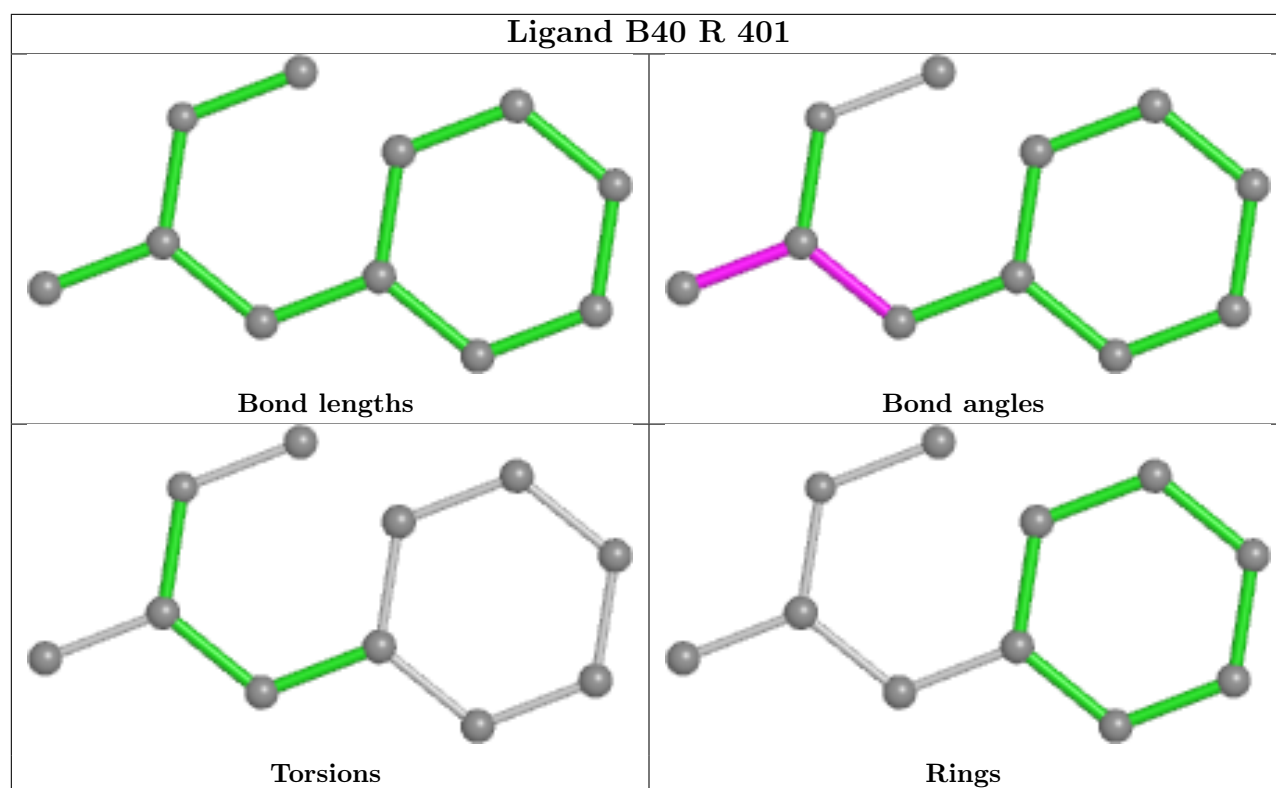
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	401	B40	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 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.