



wwPDB EM Validation Summary Report ⓘ

Nov 14, 2024 – 10:07 PM JST

PDB ID : 8XVK
EMDB ID : EMD-38707
Title : Cryo-EM structure of ETAR bound with Ambrisentan
Authors : Hou, J.Y.; Liu, S.H.; Wu, L.J.; Liu, Z.J.; Hua, T.
Deposited on : 2024-01-15
Resolution : 3.21 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

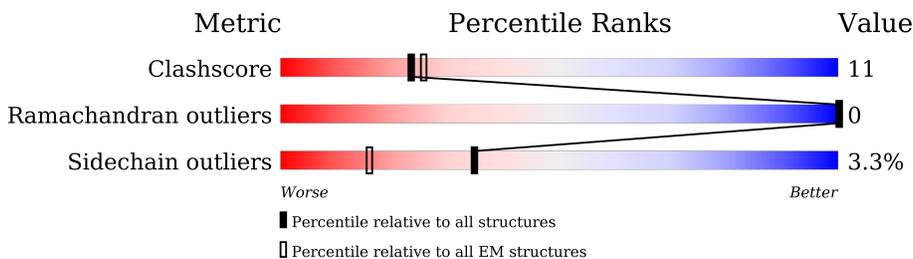
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.21 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	H	266	61% 23% 15%
2	K	136	57% 29% 12%
3	L	235	74% 15% 10%
4	R	783	38% 12% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7388 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 anti-BRIL Fab Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	H	225	1682	1069	279	329	5	0	0

- Molecule 2 is a protein called anti-Fab Nanobody.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	K	120	921	571	162	184	4	0	0

- Molecule 3 is a protein called anti-BRIL Fab Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	212	1624	1019	270	330	5	0	0

- Molecule 4 is a protein called Endoglucanase H,Endothelin-1 receptor,Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	R	392	3133	2044	519	546	24	0	0

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-276	MET	-	initiating methionine	UNP P16218
R	-275	LYS	-	expression tag	UNP P16218
R	-274	THR	-	expression tag	UNP P16218
R	-273	ILE	-	expression tag	UNP P16218
R	-272	ILE	-	expression tag	UNP P16218
R	-271	ALA	-	expression tag	UNP P16218
R	-270	LEU	-	expression tag	UNP P16218
R	-269	SER	-	expression tag	UNP P16218

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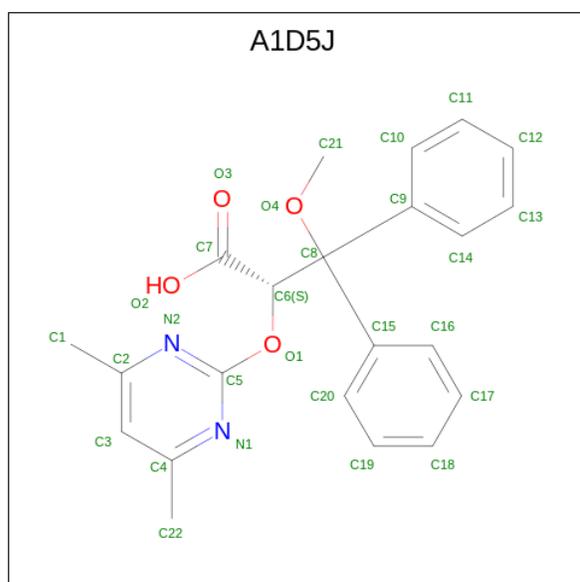
Chain	Residue	Modelled	Actual	Comment	Reference
R	-268	TYR	-	expression tag	UNP P16218
R	-267	ILE	-	expression tag	UNP P16218
R	-266	PHE	-	expression tag	UNP P16218
R	-265	CYS	-	expression tag	UNP P16218
R	-264	LEU	-	expression tag	UNP P16218
R	-263	VAL	-	expression tag	UNP P16218
R	-262	PHE	-	expression tag	UNP P16218
R	-261	ALA	-	expression tag	UNP P16218
R	-260	ASP	-	expression tag	UNP P16218
R	-259	TYR	-	expression tag	UNP P16218
R	-258	LYS	-	expression tag	UNP P16218
R	-257	ASP	-	expression tag	UNP P16218
R	-256	ASP	-	expression tag	UNP P16218
R	-255	ASP	-	expression tag	UNP P16218
R	-254	ASP	-	expression tag	UNP P16218
R	-253	ALA	-	expression tag	UNP P16218
R	-252	HIS	-	expression tag	UNP P16218
R	-251	HIS	-	expression tag	UNP P16218
R	-250	HIS	-	expression tag	UNP P16218
R	-249	HIS	-	expression tag	UNP P16218
R	-248	HIS	-	expression tag	UNP P16218
R	-247	HIS	-	expression tag	UNP P16218
R	-246	HIS	-	expression tag	UNP P16218
R	-245	HIS	-	expression tag	UNP P16218
R	-244	HIS	-	expression tag	UNP P16218
R	-243	HIS	-	expression tag	UNP P16218
R	-242	GLY	-	expression tag	UNP P16218
R	-241	ARG	-	expression tag	UNP P16218
R	-240	ALA	-	expression tag	UNP P16218
R	-239	MET	-	expression tag	UNP P16218
R	-238	ALA	-	expression tag	UNP P16218
R	-237	SER	-	expression tag	UNP P16218
R	-131	ALA	GLU	conflict	UNP P16218
R	43	GLU	-	linker	UNP P16218
R	44	ASN	-	linker	UNP P16218
R	45	LEU	-	linker	UNP P16218
R	46	TYR	-	linker	UNP P16218
R	47	PHE	-	linker	UNP P16218
R	48	GLN	-	linker	UNP P16218
R	49	GLY	-	linker	UNP P16218
R	281	GLU	-	linker	UNP P25101
R	1001	ALA	-	linker	UNP P25101

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Chain	Residue	Modelled	Actual	Comment	Reference
R	1002	ARG	-	linker	UNP P25101
R	1003	ARG	-	linker	UNP P25101
R	1004	GLN	-	linker	UNP P25101
R	1005	LEU	-	linker	UNP P25101
R	1012	TRP	MET	conflict	UNP P0ABE7
R	1107	ILE	HIS	conflict	UNP P0ABE7
R	1111	LEU	-	linker	UNP P0ABE7
R	1112	GLU	-	linker	UNP P0ABE7
R	1113	ARG	-	linker	UNP P0ABE7
R	1114	ALA	-	linker	UNP P0ABE7
R	1115	ARG	-	linker	UNP P0ABE7
R	1116	SER	-	linker	UNP P0ABE7
R	1117	THR	-	linker	UNP P0ABE7

- Molecule 5 is Ambrisentan (three-letter code: A1D5J) (formula: C₂₂H₂₂N₂O₄).

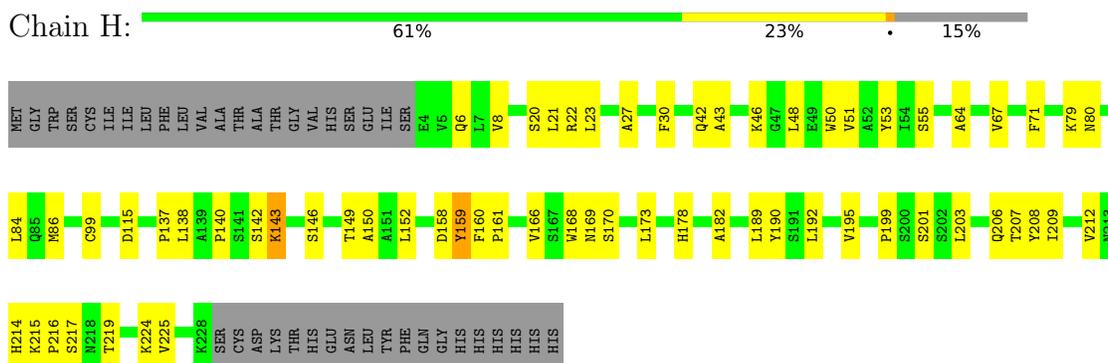


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	R	1	28	22	2	4	0

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.

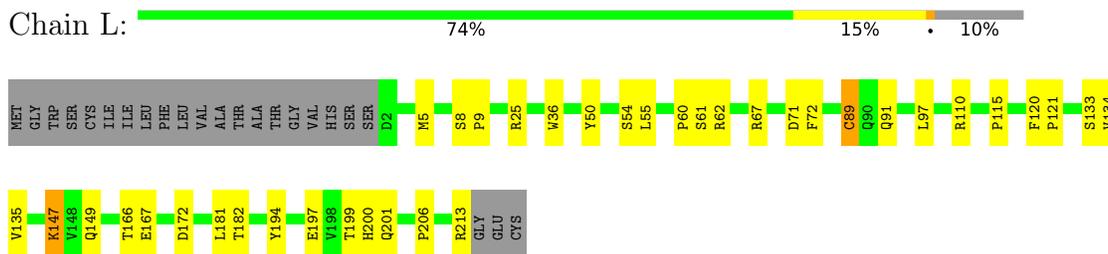
- Molecule 1: anti-BRIL Fab Heavy chain



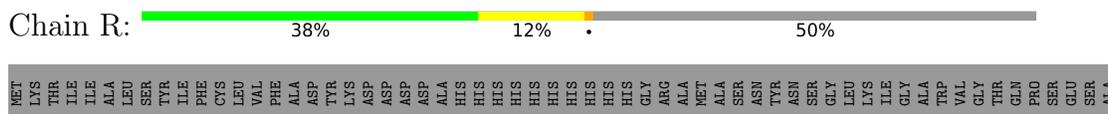
- Molecule 2: anti-Fab Nanobody



- Molecule 3: anti-BRIL Fab Light chain



- Molecule 4: Endoglucanase H,Endothelin-1 receptor,Soluble cytochrome b562



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	568027	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k 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: A1D5J

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	0.27	0/1730	0.50	0/2365
2	K	0.28	0/940	0.57	0/1272
3	L	0.28	0/1659	0.50	0/2256
4	R	0.28	0/3199	0.48	1/4330 (0.0%)
All	All	0.28	0/7528	0.50	1/10223 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	219	PRO	CA-N-CD	-5.19	104.23	111.50

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	1682	0	1619	44	0
2	K	921	0	862	31	0
3	L	1624	0	1573	24	0
4	R	3133	0	3211	61	0
5	R	28	0	0	0	0
All	All	7388	0	7265	158	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.

The worst 5 of 158 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)
3:L:97:LEU:HD12	3:L:97:LEU:O	1.60	1.00
2:K:34:MET:HG2	2:K:79:VAL:HG11	1.63	0.80
1:H:158:ASP:HA	1:H:189:LEU:HD13	1.70	0.73
4:R:115:PRO:HG3	4:R:183:ARG:HH22	1.57	0.68
4:R:226:MET:HG2	4:R:239:CYS:HB3	1.76	0.67

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	223/266 (84%)	206 (92%)	17 (8%)	0	100	100
2	K	118/136 (87%)	109 (92%)	9 (8%)	0	100	100
3	L	210/235 (89%)	195 (93%)	15 (7%)	0	100	100
4	R	386/783 (49%)	372 (96%)	14 (4%)	0	100	100
All	All	937/1420 (66%)	882 (94%)	55 (6%)	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	185/222 (83%)	179 (97%)	6 (3%)	34	63
2	K	95/110 (86%)	93 (98%)	2 (2%)	48	72
3	L	186/206 (90%)	183 (98%)	3 (2%)	58	78
4	R	340/671 (51%)	324 (95%)	16 (5%)	22	53
All	All	806/1209 (67%)	779 (97%)	27 (3%)	35	62

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	R	139	PHE
4	R	182	ASP
4	R	306	LYS
4	R	163	PHE
4	R	224	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	6	GLN
1	H	214	HIS
3	L	201	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
5	A1D5J	R	1201	-	29,30,30	0.75	0	32,42,42	0.51	0

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	A1D5J	R	1201	-	-	7/29/29/29	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

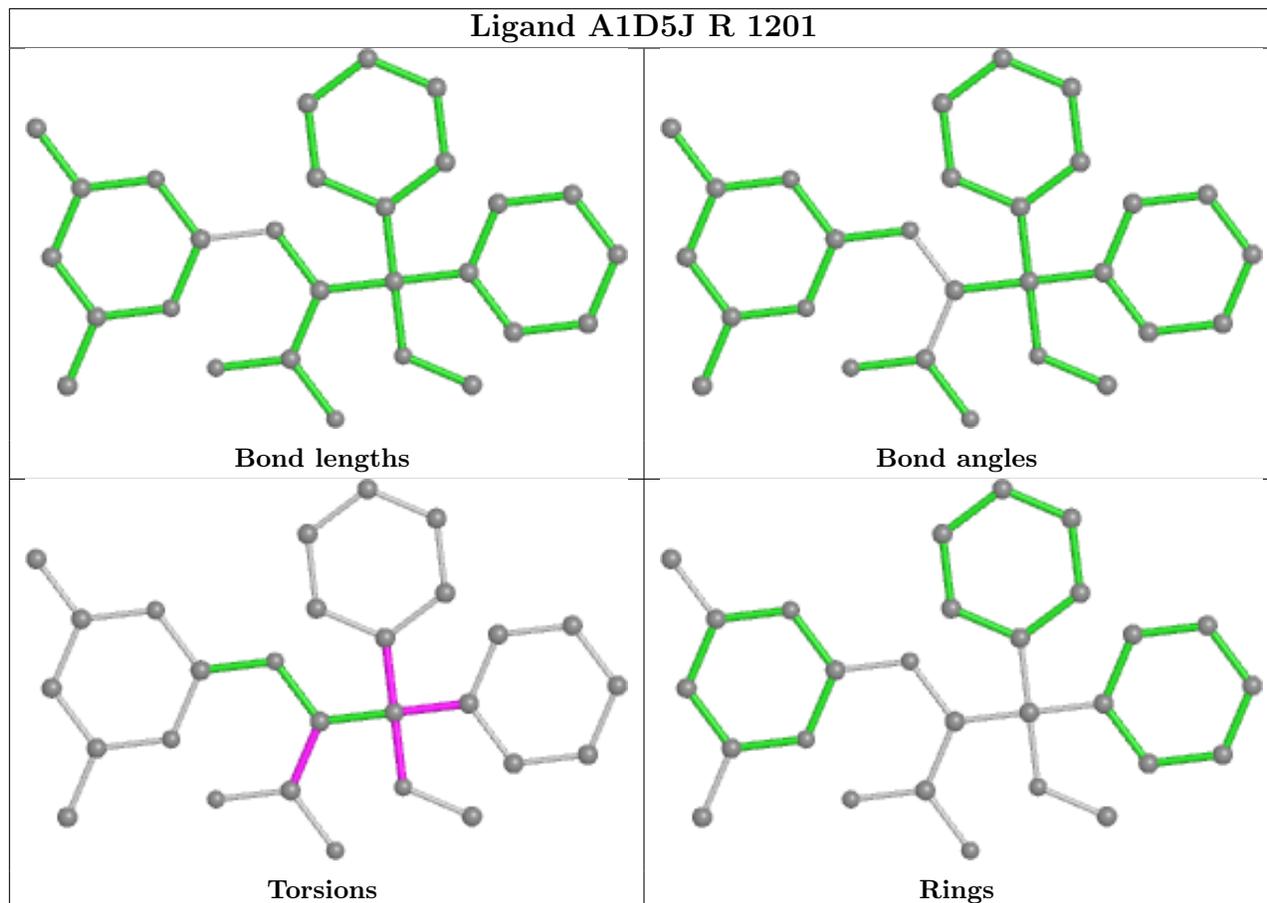
Mol	Chain	Res	Type	Atoms
5	R	1201	A1D5J	C8-C6-C7-O2
5	R	1201	A1D5J	C6-C8-O4-C21
5	R	1201	A1D5J	C16-C15-C8-C9
5	R	1201	A1D5J	C20-C15-C8-C6
5	R	1201	A1D5J	C20-C15-C8-C9

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.