



Full wwPDB EM Validation Report ⓘ

Jan 7, 2024 – 01:15 AM JST

PDB ID : 8HNN
EMDB ID : EMD-34917
Title : Structure of CXCR3 complexed with antagonist SCH546738
Authors : Jiao, H.Z.; Hu, H.L.
Deposited on : 2022-12-08
Resolution : 3.60 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 : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

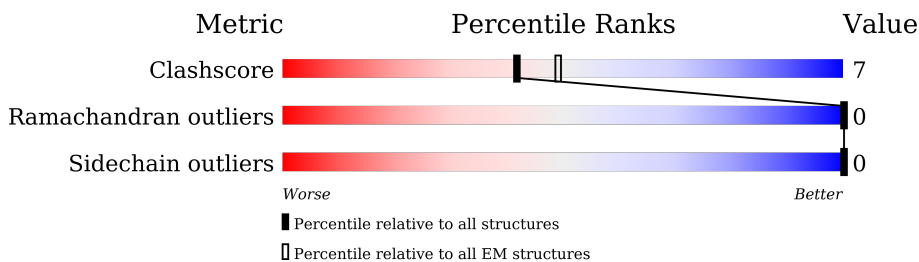
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	N	169	
2	R	507	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3063 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 Nb6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	N	114	852	533	147	168	4	0	0

- Molecule 2 is a protein called Soluble cytochrome b562,C-X-C chemokine receptor type 3,Kappa-type opioid receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	R	278	2150	1410	373	354	13	0	0

There are 35 discrepancies between the modelled and reference sequences:

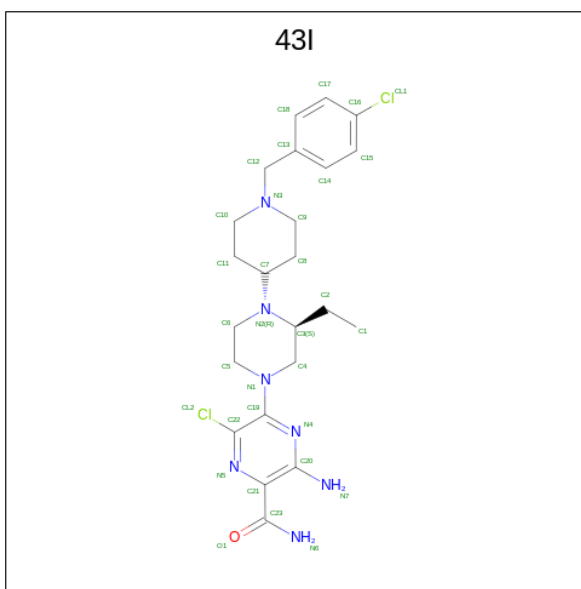
Chain	Residue	Modelled	Actual	Comment	Reference
R	-137	MET	-	initiating methionine	UNP P0ABE7
R	-136	LYS	-	expression tag	UNP P0ABE7
R	-135	THR	-	expression tag	UNP P0ABE7
R	-134	ILE	-	expression tag	UNP P0ABE7
R	-133	ILE	-	expression tag	UNP P0ABE7
R	-132	ALA	-	expression tag	UNP P0ABE7
R	-131	LEU	-	expression tag	UNP P0ABE7
R	-130	SER	-	expression tag	UNP P0ABE7
R	-129	TYR	-	expression tag	UNP P0ABE7
R	-128	ILE	-	expression tag	UNP P0ABE7
R	-127	PHE	-	expression tag	UNP P0ABE7
R	-126	CYS	-	expression tag	UNP P0ABE7
R	-125	LEU	-	expression tag	UNP P0ABE7
R	-124	VAL	-	expression tag	UNP P0ABE7
R	-123	PHE	-	expression tag	UNP P0ABE7
R	-122	ALA	-	expression tag	UNP P0ABE7
R	-121	ASP	-	expression tag	UNP P0ABE7
R	-120	TYR	-	expression tag	UNP P0ABE7
R	-119	LYS	-	expression tag	UNP P0ABE7
R	-118	ASP	-	expression tag	UNP P0ABE7

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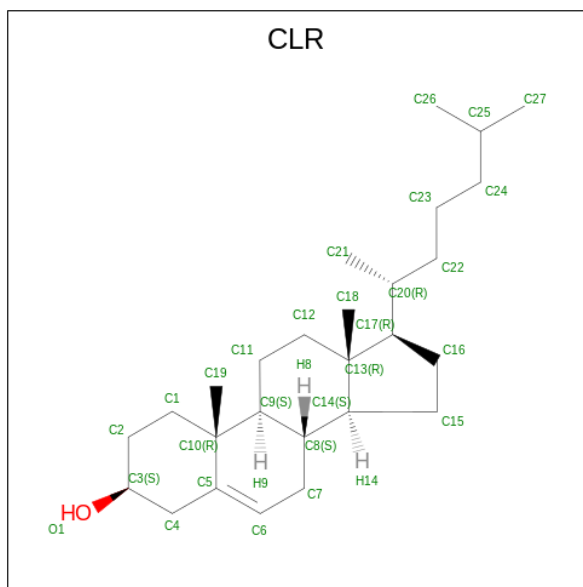
Chain	Residue	Modelled	Actual	Comment	Reference
R	-117	ASP	-	expression tag	UNP P0ABE7
R	-116	ASP	-	expression tag	UNP P0ABE7
R	-115	ASP	-	expression tag	UNP P0ABE7
R	-114	LYS	-	expression tag	UNP P0ABE7
R	-113	GLY	-	expression tag	UNP P0ABE7
R	-112	SER	-	expression tag	UNP P0ABE7
R	-105	TRP	MET	conflict	UNP P0ABE7
R	-10	ILE	HIS	conflict	UNP P0ABE7
R	-6	LEU	-	linker	UNP P0ABE7
R	-5	LEU	-	linker	UNP P0ABE7
R	-4	VAL	-	linker	UNP P0ABE7
R	-3	PRO	-	linker	UNP P0ABE7
R	-2	ARG	-	linker	UNP P0ABE7
R	-1	GLY	-	linker	UNP P0ABE7
R	0	SER	-	linker	UNP P0ABE7

- Molecule 3 is 3-azanyl-6-chloranyl-5-[(3S)-4-[1-[(4-chlorophenyl)methyl]piperidin-4-yl]-3-ethyl-piperazin-1-yl]pyrazine-2-carboxamide (three-letter code: 43I) (formula: C₂₃H₃₁Cl₂N₇O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Cl	N		O
3	R	1	33	23	2	7	1	0

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			AltConf
4	R	1	Total	C	O	0
			28	27	1	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	509297	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 ($e^-/\text{\AA}^2$)	53.43	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
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: 43I, CLR

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	N	0.25	0/866	0.50	0/1173
2	R	0.28	0/2198	0.53	0/3000
All	All	0.27	0/3064	0.52	0/4173

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	N	852	0	792	7	0
2	R	2150	0	2246	39	0
3	R	33	0	0	3	0
4	R	28	0	46	0	0
All	All	3063	0	3084	45	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 7.

All (45) 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:R:401:43I:C4	3:R:401:43I:CL2	2.43	1.03
2:R:116:GLN:HE21	2:R:201:THR:H	1.33	0.77
2:R:194:HIS:HA	2:R:201:THR:HG22	1.76	0.67
1:N:92:THR:HA	1:N:119:VAL:O	1.97	0.64
1:N:100:GLU:HG2	1:N:111:ASP:HB3	1.81	0.61
2:R:164:PRO:HG2	2:R:167:ARG:HB2	1.83	0.61
2:R:88:THR:HG23	2:R:145:ILE:HD11	1.83	0.61
2:R:158:GLN:O	2:R:162:ARG:NH1	2.32	0.60
2:R:253:GLU:O	2:R:257:ASN:ND2	2.35	0.59
2:R:155:HIS:HB3	2:R:157:THR:HG22	1.84	0.59
2:R:133:ILE:HG13	2:R:179:CYS:HB3	1.86	0.57
2:R:56:LEU:HD23	2:R:59:LEU:HD21	1.88	0.56
2:R:108:LEU:HD21	2:R:123:LEU:HD12	1.88	0.56
1:N:102:ARG:NH2	2:R:246:ARG:O	2.42	0.53
2:R:239:LEU:HD21	3:R:401:43I:N7	2.24	0.52
2:R:280:HIS:HA	2:R:283:VAL:HG12	1.90	0.52
2:R:197:ARG:HB2	2:R:200:ALA:HB3	1.92	0.52
2:R:221:VAL:O	2:R:225:LEU:HB2	2.10	0.51
2:R:111:VAL:HG21	2:R:119:PHE:HE1	1.76	0.51
1:N:108:GLU:HB2	2:R:256:ARG:HD3	1.92	0.50
2:R:130:LEU:HA	2:R:133:ILE:HG22	1.94	0.50
2:R:239:LEU:HD11	3:R:401:43I:C20	2.43	0.49
2:R:125:LYS:NZ	2:R:190:LEU:O	2.27	0.49
2:R:220:LEU:HD12	2:R:283:VAL:HG13	1.94	0.49
1:N:9:SER:OG	1:N:23:SER:OG	2.29	0.49
2:R:115:VAL:HG23	2:R:116:GLN:H	1.78	0.48
2:R:159:LEU:HD12	2:R:162:ARG:HG3	1.95	0.47
2:R:273:ALA:O	2:R:277:THR:OG1	2.21	0.46
2:R:220:LEU:HD11	2:R:284:LEU:HB2	1.98	0.46
1:N:32:ARG:HH11	1:N:34:TYR:HE1	1.64	0.45
2:R:171:THR:O	2:R:175:VAL:HG13	2.17	0.45
2:R:167:ARG:O	2:R:170:LEU:HG	2.17	0.44
2:R:94:HIS:HA	2:R:97:VAL:HG12	2.00	0.44
2:R:296:ARG:NH1	2:R:301:GLU:OE2	2.51	0.44
1:N:111:ASP:OD1	1:N:111:ASP:N	2.47	0.43
2:R:102:LEU:O	2:R:105:THR:HG22	2.18	0.43
2:R:325:LEU:HD23	2:R:328:PHE:CE1	2.53	0.43
2:R:116:GLN:NE2	2:R:201:THR:H	2.09	0.43
2:R:151:LEU:HD23	2:R:151:LEU:HA	1.86	0.42
2:R:88:THR:O	2:R:92:LEU:HD23	2.20	0.42
2:R:159:LEU:HG	2:R:163:GLY:HA3	2.02	0.41
2:R:117:TRP:HE1	2:R:120:GLY:H	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:284:LEU:HA	2:R:287:ILE:HG22	2.03	0.41
2:R:263:ARG:O	2:R:267:VAL:HG13	2.21	0.40
2:R:216:ARG:HD3	2:R:216:ARG:HA	1.90	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	N	110/169 (65%)	107 (97%)	3 (3%)	0	100	100
2	R	276/507 (54%)	255 (92%)	21 (8%)	0	100	100
All	All	386/676 (57%)	362 (94%)	24 (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	N	84/138 (61%)	84 (100%)	0	100	100
2	R	228/427 (53%)	228 (100%)	0	100	100
All	All	312/565 (55%)	312 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	R	116	GLN
2	R	318	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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
3	43I	R	401	-	35,36,36	0.65	0	41,51,51	0.97	2 (4%)
4	CLR	R	402	-	31,31,31	0.36	0	48,48,48	0.69	1 (2%)

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
3	43I	R	401	-	-	4/14/41/41	1/4/4/4
4	CLR	R	402	-	-	4/10/68/68	0/4/4/4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	401	43I	C8-C7-N2	3.00	123.35	113.42
3	R	401	43I	C21-C20-N7	-2.14	120.33	122.84
4	R	402	CLR	C17-C13-C14	2.06	102.51	100.07

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	R	401	43I	C1-C2-C3-C4
3	R	401	43I	C1-C2-C3-N2
3	R	401	43I	C13-C12-N3-C9
4	R	402	CLR	C20-C22-C23-C24
4	R	402	CLR	C22-C23-C24-C25
4	R	402	CLR	C23-C24-C25-C26
4	R	402	CLR	C23-C24-C25-C27
3	R	401	43I	C13-C12-N3-C10

All (1) ring outliers are listed below:

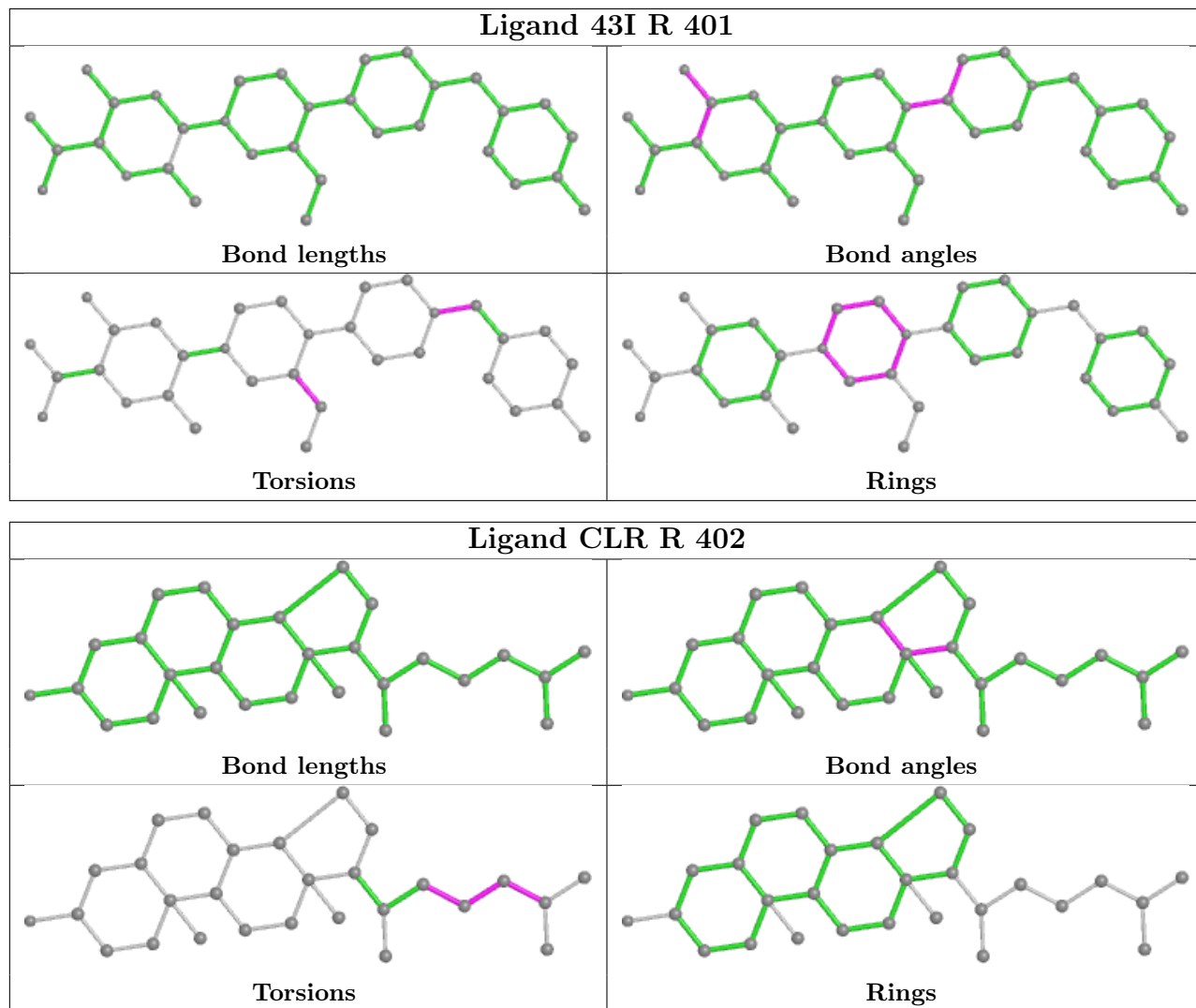
Mol	Chain	Res	Type	Atoms
3	R	401	43I	C3-C4-C5-C6-N1-N2

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	401	43I	3	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.