



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:15 PM UTC

PDB ID : 1JJB / pdb_00001jjb
Title : A neutral molecule in cation-binding site: Specific binding of PEG-SH to Acetylcholinesterase from Torpedo californica
Authors : Koellner, G.; Steiner, T.; Millard, C.B.; Silman, I.; Sussman, J.L.
Deposited on : 2001-07-04
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

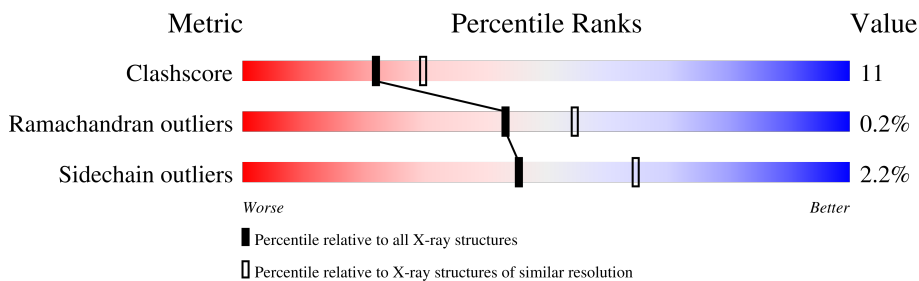
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	532	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4874 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 ACETYLCHOLINESTERASE.

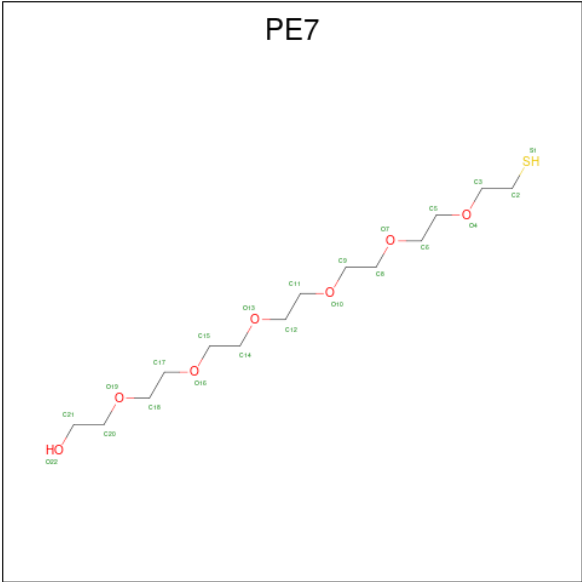
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4201	2702	708	769	22			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 1-DEOXY-1-THIO-HEPTAETHYLENE GLYCOL (CCD ID: PE7) (formula: $C_{14}H_{30}O_7S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			22	14	7	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	623	Total	O	0	0
			623	623		

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.20 Å 111.20 Å 137.12 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.89 – 2.30	Depositor
% Data completeness (in resolution range)	94.1 (19.89-2.30)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.178 , 0.224	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4874	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, PE7

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	0.37	1/4324 (0.0%)	0.93	20/5877 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	MET	SD-CE	-5.59	1.65	1.79

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	439	ILE	N-CA-C	7.62	119.94	109.80
1	A	291	SER	N-CA-C	7.58	119.23	110.97
1	A	443	GLU	N-CA-C	-7.33	104.48	113.50
1	A	401	ILE	N-CA-C	7.07	117.16	110.30
1	A	527	PHE	N-CA-C	6.64	118.41	111.03
1	A	285	ASP	N-CA-C	-6.39	98.77	108.67
1	A	328	GLY	N-CA-C	6.20	122.35	114.66
1	A	360	VAL	CA-C-N	6.20	125.88	119.56
1	A	360	VAL	C-N-CA	6.20	125.88	119.56
1	A	457	ASN	N-CA-C	5.80	119.69	111.92
1	A	101	VAL	N-CA-C	5.71	114.41	107.61
1	A	329	SER	N-CA-C	5.53	118.02	111.33
1	A	286	SER	N-CA-C	5.49	116.31	108.74
1	A	342	ASP	N-CA-C	5.44	118.92	112.72
1	A	164	ALA	CA-C-N	5.39	125.00	119.56
1	A	164	ALA	C-N-CA	5.39	125.00	119.56
1	A	300	PHE	N-CA-C	-5.37	105.43	111.28
1	A	157	ALA	N-CA-C	5.28	117.25	108.02
1	A	379	MET	N-CA-C	-5.24	106.88	113.28
1	A	234	ALA	N-CA-C	5.09	119.34	113.18

There are no chirality outliers.

There are no planarity outliers.

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	A	4201	0	4017	88	0
2	A	28	0	26	2	0
3	A	22	0	30	0	0
4	A	623	0	0	12	2
All	All	4874	0	4073	89	2

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.

All (89) 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:A:36:ALA:HB2	1:A:175:MET:HE3	1.49	0.92
1:A:190:ASP:OD1	1:A:192:LYS:HG2	1.78	0.83
1:A:48:PRO:HB2	1:A:175:MET:CE	2.20	0.71
1:A:454:LYS:HA	1:A:454:LYS:HE2	1.72	0.70
1:A:485:PRO:HA	4:A:1446:HOH:O	1.91	0.69
1:A:260:GLU:H	1:A:260:GLU:CD	2.02	0.68
1:A:383:ASN:C	1:A:383:ASN:HD22	1.99	0.68
1:A:36:ALA:CB	1:A:175:MET:HE3	2.24	0.68
1:A:132:GLY:HA3	1:A:143:LEU:HD22	1.76	0.67
1:A:455:GLU:CD	1:A:455:GLU:H	2.04	0.66
2:A:9010:NAG:O7	2:A:9010:NAG:H3	1.96	0.64
1:A:484:GLU:OE1	1:A:485:PRO:HD2	1.97	0.64
1:A:36:ALA:HB2	1:A:175:MET:CE	2.24	0.64
1:A:48:PRO:HB2	1:A:175:MET:HE2	1.82	0.60
1:A:48:PRO:HB2	1:A:175:MET:HE1	1.83	0.60
1:A:207:GLY:HA3	1:A:229:PRO:HD3	1.85	0.58
1:A:46:ARG:HD2	4:A:1417:HOH:O	2.04	0.58
1:A:161:SER:HB2	4:A:1441:HOH:O	2.04	0.57
1:A:4:SER:HA	4:A:1509:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:GLY:HA3	1:A:391:LEU:HD21	1.87	0.56
1:A:353:MET:HA	1:A:356:VAL:HG12	1.86	0.56
1:A:5:GLU:OE2	1:A:104:PRO:HA	2.05	0.56
1:A:531:LEU:C	1:A:531:LEU:HD23	2.31	0.55
1:A:197:PHE:CB	1:A:223:ILE:HB	2.37	0.55
1:A:515:ARG:HB3	1:A:518:VAL:HB	1.89	0.54
1:A:353:MET:HA	1:A:356:VAL:CG1	2.38	0.53
1:A:299:GLU:HB3	4:A:1450:HOH:O	2.09	0.53
1:A:413:LYS:HE3	1:A:414:PHE:CE2	2.44	0.52
1:A:452:LEU:CD2	1:A:463:GLU:HG3	2.39	0.52
1:A:204:ALA:O	1:A:208:MET:HG3	2.10	0.51
1:A:316:LYS:HE3	1:A:414:PHE:HB3	1.92	0.51
1:A:36:ALA:CB	1:A:175:MET:CE	2.88	0.51
1:A:223:ILE:HA	1:A:320:LEU:O	2.10	0.51
1:A:197:PHE:HB3	1:A:223:ILE:HB	1.92	0.51
1:A:132:GLY:HA3	1:A:143:LEU:CD2	2.40	0.51
1:A:453:VAL:HG23	1:A:455:GLU:OE1	2.12	0.50
1:A:373:LEU:HD12	1:A:378:TRP:HE1	1.77	0.49
1:A:228:SER:HB2	1:A:229:PRO:HD2	1.94	0.49
1:A:236:VAL:HG23	1:A:295:VAL:HG12	1.95	0.49
1:A:132:GLY:CA	1:A:143:LEU:HD22	2.40	0.49
1:A:59:ASN:OD1	2:A:9010:NAG:H2	2.13	0.49
1:A:405:MET:HA	1:A:408:VAL:HG12	1.94	0.49
1:A:515:ARG:NE	4:A:1389:HOH:O	2.45	0.48
1:A:211:LEU:HD23	1:A:314:PHE:HB3	1.93	0.48
1:A:455:GLU:CD	1:A:455:GLU:N	2.71	0.48
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.49	0.48
1:A:375:TYR:CE2	1:A:520:MET:HE3	2.49	0.48
1:A:528:LEU:HB3	1:A:529:PRO:HD3	1.94	0.47
1:A:408:VAL:HG23	1:A:418:THR:HG21	1.96	0.47
1:A:26:HIS:HD2	4:A:1340:HOH:O	1.97	0.47
1:A:347:ILE:HG22	1:A:348:SER:O	2.15	0.47
1:A:103:SER:HA	1:A:104:PRO:C	2.40	0.46
1:A:206:VAL:CG1	1:A:222:ALA:HB1	2.45	0.46
1:A:185:GLN:HA	1:A:189:GLY:O	2.16	0.46
1:A:451:PRO:HA	1:A:458:TYR:CD1	2.51	0.46
1:A:83:MET:HE3	1:A:442:TYR:OH	2.16	0.45
1:A:430:LEU:CD1	1:A:432:TRP:HB2	2.47	0.45
1:A:450:LEU:O	1:A:453:VAL:HG12	2.16	0.45
1:A:452:LEU:HD22	1:A:463:GLU:HG3	1.98	0.45
1:A:383:ASN:HD22	1:A:384:GLY:N	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LEU:O	1:A:457:ASN:HB2	2.18	0.44
1:A:83:MET:HE2	4:A:1401:HOH:O	2.16	0.44
1:A:325:LYS:HD3	4:A:1302:HOH:O	2.16	0.44
1:A:221:ARG:CD	1:A:480:GLY:HA2	2.48	0.43
1:A:449:GLY:HA2	1:A:466:SER:OG	2.18	0.43
1:A:383:ASN:HB3	1:A:386:LYS:HB2	2.01	0.43
1:A:119:GLY:O	1:A:120:PHE:HB2	2.18	0.43
1:A:221:ARG:HD3	1:A:480:GLY:HA2	2.00	0.43
1:A:350:GLU:H	1:A:350:GLU:CD	2.26	0.43
1:A:450:LEU:N	1:A:451:PRO:CD	2.82	0.43
1:A:439:ILE:HG22	1:A:440:HIS:N	2.34	0.42
1:A:146:LEU:C	1:A:146:LEU:HD12	2.45	0.42
1:A:383:ASN:ND2	1:A:385:ILE:H	2.17	0.42
1:A:135:LEU:HD23	1:A:143:LEU:HD13	2.01	0.42
1:A:413:LYS:HE2	4:A:1034:HOH:O	2.19	0.42
1:A:453:VAL:HG13	1:A:456:LEU:HD12	2.02	0.42
1:A:430:LEU:HD13	1:A:432:TRP:H	1.84	0.41
1:A:497:THR:HG22	4:A:1097:HOH:O	2.20	0.41
1:A:404:LEU:C	1:A:404:LEU:HD23	2.45	0.41
1:A:459:THR:OG1	1:A:461:GLU:HG2	2.20	0.41
1:A:401:ILE:HG21	1:A:517:ARG:HD3	2.02	0.41
1:A:212:SER:HA	1:A:213:PRO:HD3	1.92	0.41
1:A:153:PHE:HZ	1:A:271:PRO:HA	1.85	0.41
1:A:184:ILE:HD12	1:A:184:ILE:HA	1.95	0.41
1:A:47:ARG:NH1	1:A:171:LEU:HD11	2.36	0.41
1:A:63:TYR:CD1	1:A:126:THR:HG22	2.56	0.41
1:A:321:LEU:HD23	1:A:321:LEU:N	2.35	0.41
1:A:452:LEU:HD11	1:A:470:MET:HE1	2.03	0.41
1:A:242:ARG:HD3	4:A:1369:HOH:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1563:HOH:O	4:A:1563:HOH:O[4_556]	1.92	0.28
4:A:1465:HOH:O	4:A:1465:HOH:O[5_675]	2.05	0.15

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	530/532 (100%)	511 (96%)	18 (3%)	1 (0%)	43	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	VAL

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	450/465 (97%)	440 (98%)	10 (2%)	45	65

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	LEU
1	A	330	PHE
1	A	356	VAL
1	A	358	LEU
1	A	383	ASN
1	A	430	LEU
1	A	453	VAL
1	A	461	GLU
1	A	497	THR
1	A	505	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	74	GLN
1	A	162	GLN
1	A	257	ASN
1	A	374	GLN
1	A	383	ASN
1	A	409	ASN
1	A	457	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 [i](#)

3 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	PE7	A	999	-	21,21,21	0.32	0	19,20,20	0.16	0
2	NAG	A	9020	1	14,14,15	0.58	0	17,19,21	0.71	1 (5%)
2	NAG	A	9010	1	14,14,15	0.73	0	17,19,21	0.54	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
3	PE7	A	999	-	-	8/19/19/19	-
2	NAG	A	9020	1	-	2/6/23/26	0/1/1/1
2	NAG	A	9010	1	-	3/6/23/26	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(°)
2	A	9020	NAG	C2-N2-C7	-2.15	120.02	122.90

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	9010	NAG	C3-C2-N2-C7
2	A	9020	NAG	O5-C5-C6-O6
3	A	999	PE7	O7-C8-C9-O10
2	A	9020	NAG	C4-C5-C6-O6
2	A	9010	NAG	C4-C5-C6-O6
3	A	999	PE7	C14-C15-O16-C17
3	A	999	PE7	C18-C17-O16-C15
3	A	999	PE7	C17-C18-O19-C20
2	A	9010	NAG	O5-C5-C6-O6
3	A	999	PE7	O16-C17-C18-O19
3	A	999	PE7	C5-C6-O7-C8
3	A	999	PE7	C8-C9-O10-C11
3	A	999	PE7	C21-C20-O19-C18

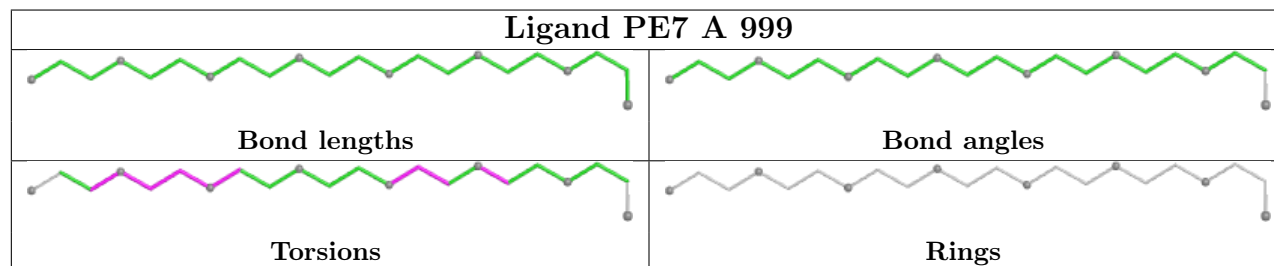
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9010	NAG	2	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.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.