



wwPDB X-ray Structure Validation Summary Report

Oct 2, 2023 – 05:10 AM EDT

PDB ID : 6N4N
Title : Crystal structure of the designed protein DNCR2/danoprevir/NS3a complex
Authors : Wang, Z.; Foight, G.W.; Baker, D.; Maly, D.J.
Deposited on : 2018-11-19
Resolution : 2.29 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

<https://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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

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 2.29 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6161 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 NS3 protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	195	1448	894	266	282	6	0	0	0
1	B	195	1448	894	266	282	6	0	0	0

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	MET	-	expression tag	UNP A0A0B4WYC6
A	987	LYS	-	expression tag	UNP A0A0B4WYC6
A	988	LYS	-	expression tag	UNP A0A0B4WYC6
A	989	LYS	-	expression tag	UNP A0A0B4WYC6
A	990	GLY	-	expression tag	UNP A0A0B4WYC6
A	991	SER	-	expression tag	UNP A0A0B4WYC6
A	992	VAL	-	expression tag	UNP A0A0B4WYC6
A	993	VAL	-	expression tag	UNP A0A0B4WYC6
A	994	ILE	-	expression tag	UNP A0A0B4WYC6
A	995	VAL	-	expression tag	UNP A0A0B4WYC6
A	996	GLY	-	expression tag	UNP A0A0B4WYC6
A	997	ARG	-	expression tag	UNP A0A0B4WYC6
A	998	ILE	-	expression tag	UNP A0A0B4WYC6
A	999	ASN	-	expression tag	UNP A0A0B4WYC6
A	1000	LEU	-	expression tag	UNP A0A0B4WYC6
A	1001	SER	-	expression tag	UNP A0A0B4WYC6
A	1002	GLY	-	expression tag	UNP A0A0B4WYC6
A	1003	ASP	-	expression tag	UNP A0A0B4WYC6
A	1013	GLU	LEU	conflict	UNP A0A0B4WYC6
A	1014	GLU	LEU	conflict	UNP A0A0B4WYC6
A	1017	GLN	ILE	conflict	UNP A0A0B4WYC6
A	1018	GLU	ILE	conflict	UNP A0A0B4WYC6
A	1021	GLN	LEU	conflict	UNP A0A0B4WYC6
A	1047	SER	CYS	conflict	UNP A0A0B4WYC6
A	1052	LEU	CYS	conflict	UNP A0A0B4WYC6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1072	THR	ILE	conflict	UNP A0A0B4WYC6
A	1086	GLN	PRO	conflict	UNP A0A0B4WYC6
A	1139	ALA	SER	conflict	UNP A0A0B4WYC6
A	1159	SER	CYS	conflict	UNP A0A0B4WYC6
B	986	MET	-	expression tag	UNP A0A0B4WYC6
B	987	LYS	-	expression tag	UNP A0A0B4WYC6
B	988	LYS	-	expression tag	UNP A0A0B4WYC6
B	989	LYS	-	expression tag	UNP A0A0B4WYC6
B	990	GLY	-	expression tag	UNP A0A0B4WYC6
B	991	SER	-	expression tag	UNP A0A0B4WYC6
B	992	VAL	-	expression tag	UNP A0A0B4WYC6
B	993	VAL	-	expression tag	UNP A0A0B4WYC6
B	994	ILE	-	expression tag	UNP A0A0B4WYC6
B	995	VAL	-	expression tag	UNP A0A0B4WYC6
B	996	GLY	-	expression tag	UNP A0A0B4WYC6
B	997	ARG	-	expression tag	UNP A0A0B4WYC6
B	998	ILE	-	expression tag	UNP A0A0B4WYC6
B	999	ASN	-	expression tag	UNP A0A0B4WYC6
B	1000	LEU	-	expression tag	UNP A0A0B4WYC6
B	1001	SER	-	expression tag	UNP A0A0B4WYC6
B	1002	GLY	-	expression tag	UNP A0A0B4WYC6
B	1003	ASP	-	expression tag	UNP A0A0B4WYC6
B	1013	GLU	LEU	conflict	UNP A0A0B4WYC6
B	1014	GLU	LEU	conflict	UNP A0A0B4WYC6
B	1017	GLN	ILE	conflict	UNP A0A0B4WYC6
B	1018	GLU	ILE	conflict	UNP A0A0B4WYC6
B	1021	GLN	LEU	conflict	UNP A0A0B4WYC6
B	1047	SER	CYS	conflict	UNP A0A0B4WYC6
B	1052	LEU	CYS	conflict	UNP A0A0B4WYC6
B	1072	THR	ILE	conflict	UNP A0A0B4WYC6
B	1086	GLN	PRO	conflict	UNP A0A0B4WYC6
B	1139	ALA	SER	conflict	UNP A0A0B4WYC6
B	1159	SER	CYS	conflict	UNP A0A0B4WYC6

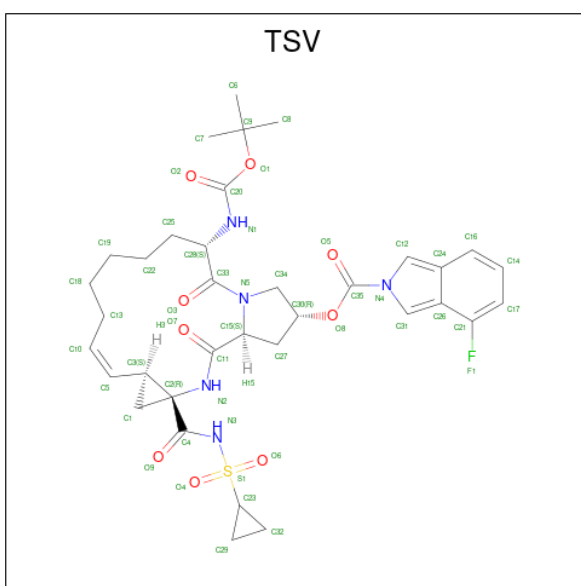
- Molecule 2 is a protein called Rosetta-designed danoprevir/NS3a complex reader 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	C	184	Total	C	N	O	S	0	0	0
			1432	872	260	299	1			
2	F	191	Total	C	N	O	S	0	0	0
			1490	904	275	310	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is (2R,6S,12Z,13aS,14aR,16aS)-6-[(tert-butoxycarbonyl)amino]-14a-[(cyclopropylsulfonyl)carbamoyl]-5,16-dioxo-1,2,3,5,6,7,8,9,10,11,13a,14,14a,15,16,16a-hexadecahydrocyclopropa[e]pyrrolo[1,2-a][1,4]diazacyclopentadecin-2-yl 4-fluoro-2H-isoindole-2-carboxylate (three-letter code: TSV) (formula: C₃₅H₄₄FN₅O₉S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	F	N	O	S	0	0
			51	35	1	5	9	1		
4	B	1	Total	C	F	N	O	S	0	0
			51	35	1	5	9	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	65	Total	O	0	0
			65	65		
6	B	63	Total	O	0	0
			63	63		
6	C	37	Total	O	0	0
			37	37		
6	F	44	Total	O	0	0
			44	44		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.84Å 69.26Å 99.34Å 90.00° 108.59° 90.00°	Depositor
Resolution (Å)	94.16 – 2.29	Depositor
% Data completeness (in resolution range)	98.3 (94.16-2.29)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.203 , 0.241	Depositor
Wilson B-factor (Å ²)	33.4	Xtrriage
Anisotropy	0.040	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtrriage
Total number of atoms	6161	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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	SO4	B	1204	-	4,4,4	0.34	0	6,6,6	0.07	0
5	SO4	A	1204	-	4,4,4	0.36	0	6,6,6	0.09	0
5	SO4	C	301	-	4,4,4	0.33	0	6,6,6	0.09	0
4	TSV	A	1202	-	50,56,56	2.52	14 (28%)	62,85,85	2.85	15 (24%)
5	SO4	F	301	-	4,4,4	0.35	0	6,6,6	0.12	0
5	SO4	A	1203	-	4,4,4	0.30	0	6,6,6	0.30	0
5	SO4	B	1203	-	4,4,4	0.28	0	6,6,6	0.22	0
4	TSV	B	1202	-	50,56,56	2.59	13 (26%)	62,85,85	3.05	14 (22%)

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
4	TSV	B	1202	-	-	5/55/83/83	0/5/6/6
4	TSV	A	1202	-	-	6/55/83/83	0/5/6/6

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1202	TSV	C12-N4	8.09	1.48	1.39
4	A	1202	TSV	C12-N4	8.03	1.48	1.39
4	B	1202	TSV	C31-N4	7.84	1.48	1.39
4	A	1202	TSV	C31-N4	7.39	1.47	1.39
4	B	1202	TSV	O1-C20	5.84	1.46	1.34

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1202	TSV	O6-S1-O4	-13.60	109.04	119.24
4	B	1202	TSV	C17-C21-C26	-12.84	118.48	123.48
4	A	1202	TSV	C17-C21-C26	-12.63	118.57	123.48
4	A	1202	TSV	O6-S1-O4	-11.06	110.94	119.24
4	B	1202	TSV	C4-C2-N2	8.10	124.77	116.06

There are no chirality outliers.

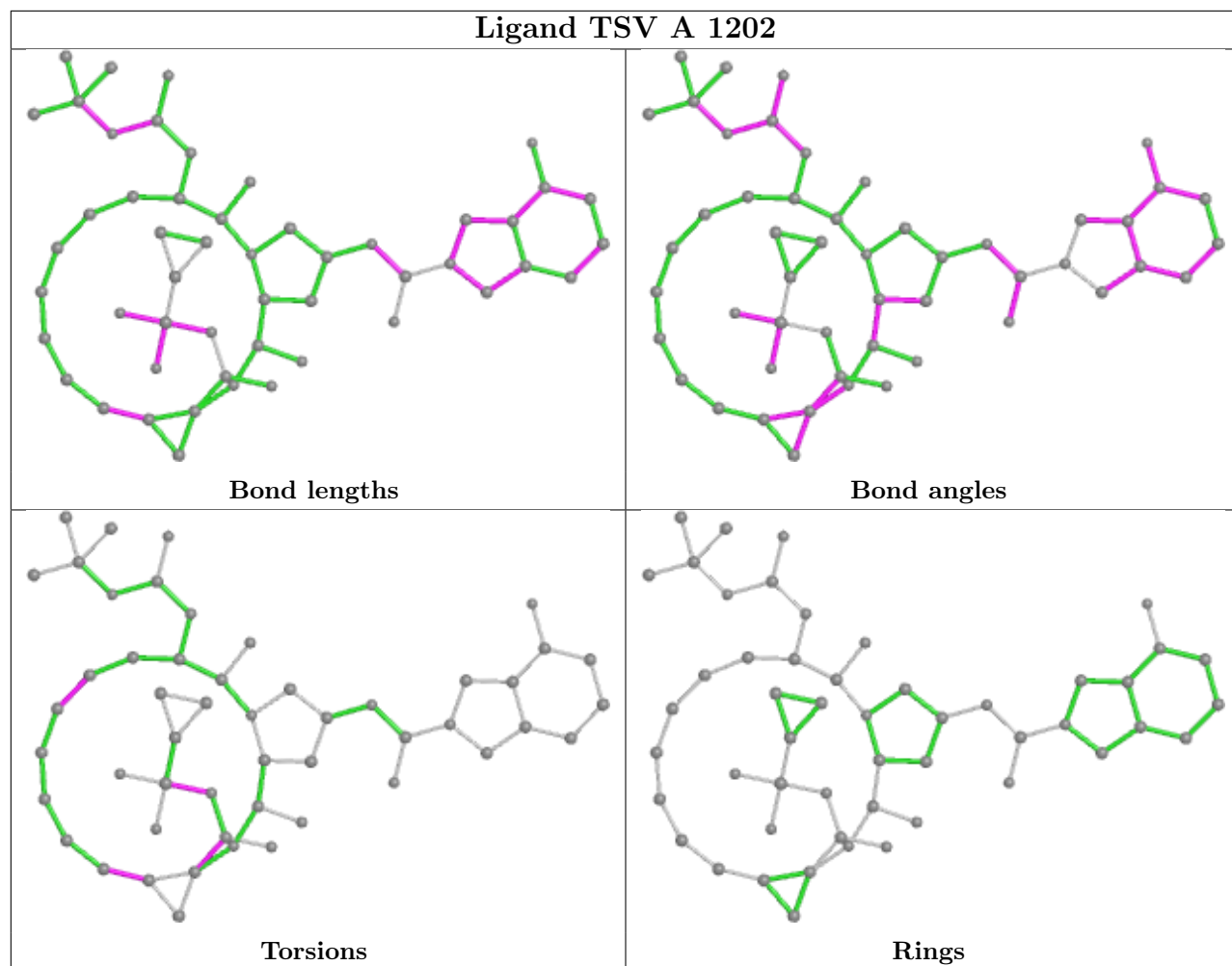
5 of 11 torsion outliers are listed below:

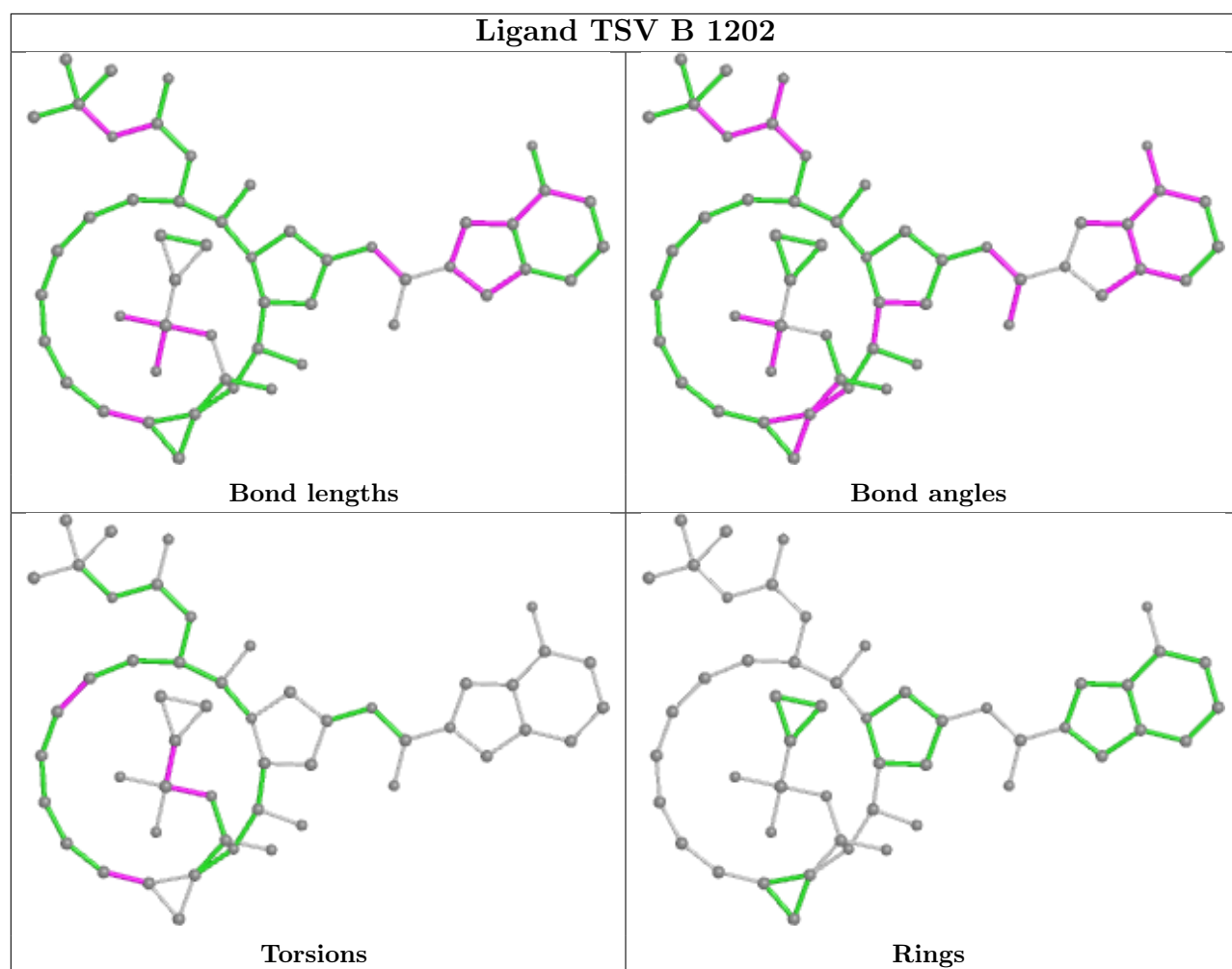
Mol	Chain	Res	Type	Atoms
4	A	1202	TSV	C4-N3-S1-O6
4	A	1202	TSV	C4-N3-S1-C23
4	B	1202	TSV	C4-N3-S1-C23
4	A	1202	TSV	C18-C19-C22-C25
4	B	1202	TSV	C18-C19-C22-C25

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.





4.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.