Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 07:59 AM EDT

PDB ID	:	6PJ2
Title	:	Crystal structure of HCV NS3/4A D168A protease in complex with P4-P5-4 (AJ-65)
Authors	:	Zephyr, J.; Schiffer, C.A.
Deposited on	:	2019-06-27
Resolution	:	2.10 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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 2999 atoms, of which 1399 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	H	N	O	S			
1	A	197	2734	879	1320	251	276	8	0	2	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	963	MET	-	initiating methionine	UNP A0A0B4WYC6
A	964	GLY	-	expression tag	UNP A0A0B4WYC6
A	965	SER	-	expression tag	UNP A0A0B4WYC6
A	966	SER	-	expression tag	UNP A0A0B4WYC6
A	967	HIS	-	expression tag	UNP A0A0B4WYC6
A	968	HIS	-	expression tag	UNP A0A0B4WYC6
A	969	HIS	-	expression tag	UNP A0A0B4WYC6
A	970	HIS	-	expression tag	UNP A0A0B4WYC6
A	971	HIS	-	expression tag	UNP A0A0B4WYC6
A	972	HIS	-	expression tag	UNP A0A0B4WYC6
A	973	SER	-	expression tag	UNP A0A0B4WYC6
A	974	SER	-	expression tag	UNP A0A0B4WYC6
A	975	GLY	-	expression tag	UNP A0A0B4WYC6
A	976	LEU	-	expression tag	UNP A0A0B4WYC6
A	977	VAL	-	expression tag	UNP A0A0B4WYC6
A	978	PRO	-	expression tag	UNP A0A0B4WYC6
A	979	ARG	-	expression tag	UNP A0A0B4WYC6
A	980	GLY	-	expression tag	UNP A0A0B4WYC6
A	981	SER	-	expression tag	UNP A0A0B4WYC6
A	982	HIS	-	expression tag	UNP A0A0B4WYC6
A	983	MET	-	expression tag	UNP A0A0B4WYC6
A	984	ALA	-	expression tag	UNP A0A0B4WYC6
A	985	SER	-	expression tag	UNP A0A0B4WYC6
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

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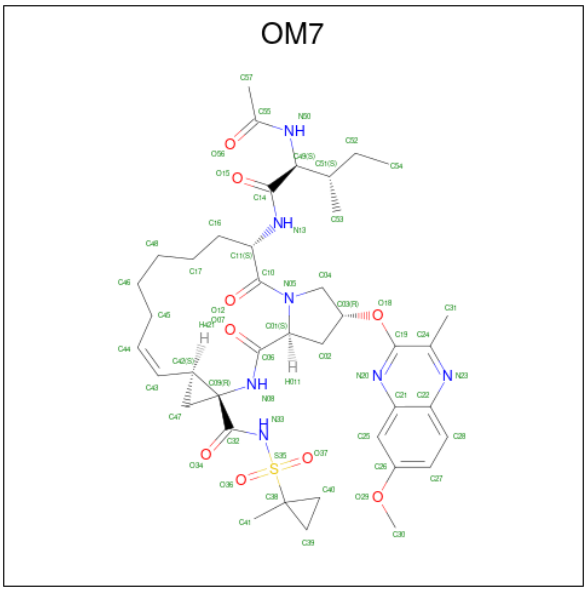
Chain	Residue	Modelled	Actual	Comment	Reference
A	990	GLY	-	expression tag	UNP A0A0B4WYC6
A	991	SER	-	expression tag	UNP A0A0B4WYC6
A	992	VAL	-	expression tag	UNP A0A0B4WYC6
A	993	VAL	-	expression tag	UNP A0A0B4WYC6
A	994	ILE	-	expression tag	UNP A0A0B4WYC6
A	995	VAL	-	expression tag	UNP A0A0B4WYC6
A	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
A	1072	THR	ILE	conflict	UNP A0A0B4WYC6
A	1086	GLN	PRO	conflict	UNP A0A0B4WYC6
A	1159	SER	CYS	conflict	UNP A0A0B4WYC6
A	1168	ALA	ASP	engineered mutation	UNP A0A0B4WYC6
A	1181	SER	-	expression tag	UNP A0A0B4WYC6
A	1182	PRO	-	expression tag	UNP A0A0B4WYC6

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

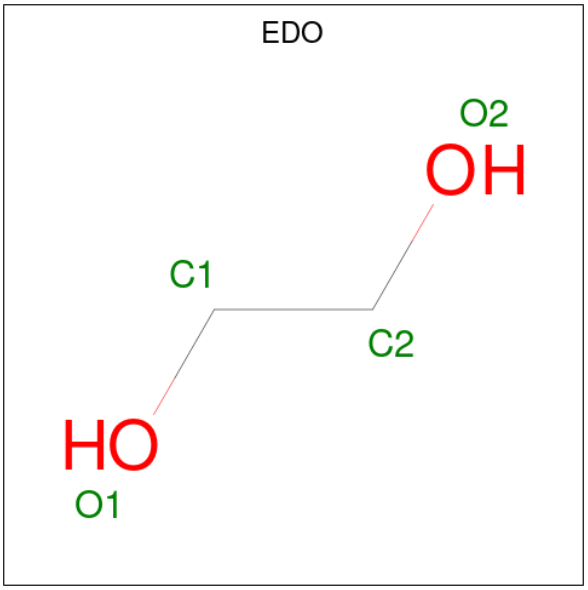
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0

- Molecule 3 is (2R,6S,12Z,13aS,14aR,16aS)-6-[(N-acetyl-L-isoleucyl)amino]-2-[(7-methoxy-3-methylquinoxalin-2-yl)oxy]-N-[(1-methylcyclo propyl)sulfonyl]-5,16-dioxo-1,2,3,6,7,8,9,10,11,13a,14,15,16,16a-tetradecahydrocyclopropa[e]pyrrolo[1,2-a][1,4]diazacycl opentadecine-14a(5H)-carboxamide (three-letter code: OM7) (formula: $C_{40}H_{55}N_7O_9S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
3	A	1	112	40	55	7	9	1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	10	2	6	2	0	0
			Total	C	H	O		
4	A	1	10	2	6	2	0	0
			Total	C	H	O		
4	A	1	10	2	6	2	0	0

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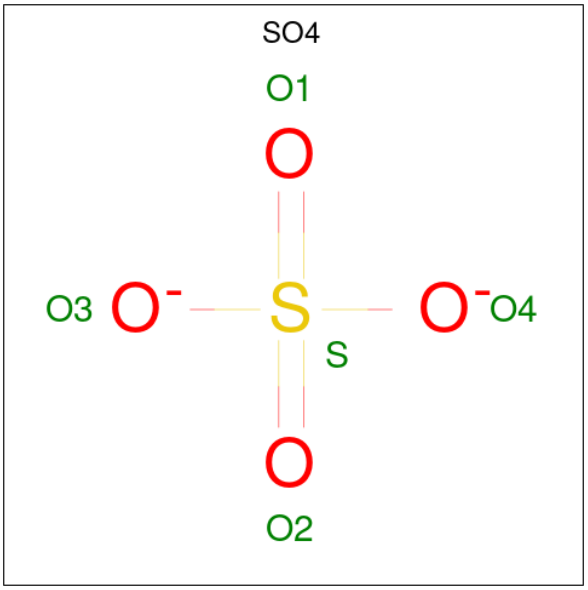
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	10	2	6	2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	107	107	107	0	0

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

3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.36Å 59.64Å 58.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.29 – 2.10	Depositor
% Data completeness (in resolution range)	99.1 (26.29-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.28 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.12-2829	Depositor
R, R_{free}	0.182 , 0.214	Depositor
Wilson B-factor (Å^2)	21.8	Xtriage
Anisotropy	0.379	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,l,k	Xtriage
Total number of atoms	2999	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	OM7	A	9202	-	58,62,62	4.71	29 (50%)	80,93,93	2.17	16 (20%)
4	EDO	A	9204	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	A	9206	-	3,3,3	0.45	0	2,2,2	0.33	0
4	EDO	A	9205	-	3,3,3	0.41	0	2,2,2	0.42	0
5	SO4	A	9207	-	4,4,4	0.13	0	6,6,6	0.11	0
4	EDO	A	9203	-	3,3,3	0.45	0	2,2,2	0.38	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	OM7	A	9202	-	-	8/62/95/95	0/5/6/6
4	EDO	A	9204	-	-	0/1/1/1	-
4	EDO	A	9206	-	-	0/1/1/1	-
4	EDO	A	9205	-	-	1/1/1/1	-
4	EDO	A	9203	-	-	1/1/1/1	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	9202	OM7	C24-N23	11.28	1.46	1.32
3	A	9202	OM7	C02-C03	-10.00	1.30	1.52
3	A	9202	OM7	C25-C26	9.63	1.54	1.37
3	A	9202	OM7	C25-C21	9.16	1.56	1.41
3	A	9202	OM7	C28-C22	8.55	1.56	1.41
3	A	9202	OM7	C28-C27	8.44	1.54	1.36
3	A	9202	OM7	C04-C03	8.31	1.66	1.52
3	A	9202	OM7	C27-C26	8.02	1.54	1.38
3	A	9202	OM7	C04-N05	-7.81	1.34	1.47
3	A	9202	OM7	S35-N33	7.75	1.72	1.60
3	A	9202	OM7	C10-N05	7.29	1.51	1.34
3	A	9202	OM7	C22-N23	7.02	1.49	1.37
3	A	9202	OM7	C14-N13	6.99	1.49	1.34
3	A	9202	OM7	C06-N08	6.84	1.48	1.34
3	A	9202	OM7	C21-N20	6.69	1.48	1.37
3	A	9202	OM7	C19-N20	6.30	1.46	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	9202	OM7	C01-N05	5.72	1.58	1.47
3	A	9202	OM7	C01-C06	-5.12	1.40	1.52
3	A	9202	OM7	C42-C43	4.89	1.55	1.49
3	A	9202	OM7	C22-C21	4.78	1.52	1.42
3	A	9202	OM7	C55-N50	3.95	1.47	1.34
3	A	9202	OM7	O18-C19	2.71	1.43	1.36
3	A	9202	OM7	C02-C01	2.64	1.58	1.53
3	A	9202	OM7	C47-C09	2.52	1.53	1.51
3	A	9202	OM7	C31-C24	2.29	1.54	1.50
3	A	9202	OM7	C38-S35	2.27	1.83	1.81
3	A	9202	OM7	C57-C55	2.26	1.55	1.50
3	A	9202	OM7	O36-S35	2.25	1.47	1.43
3	A	9202	OM7	O37-S35	2.07	1.47	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	9202	OM7	O37-S35-O36	-9.22	101.86	120.57
3	A	9202	OM7	C47-C09-N08	5.56	125.26	117.80
3	A	9202	OM7	O36-S35-C38	5.09	111.69	107.60
3	A	9202	OM7	C02-C01-C06	4.80	120.91	111.32
3	A	9202	OM7	O37-S35-C38	4.42	111.15	107.60
3	A	9202	OM7	C42-C09-C32	-4.29	107.71	116.80
3	A	9202	OM7	C32-N33-S35	-4.20	117.30	124.08
3	A	9202	OM7	C09-C32-N33	4.13	122.84	115.70
3	A	9202	OM7	C06-C01-N05	-4.10	101.28	112.56
3	A	9202	OM7	C04-N05-C01	-3.86	106.12	111.70
3	A	9202	OM7	C19-O18-C03	-3.24	113.90	118.56
3	A	9202	OM7	C57-C55-N50	2.72	120.71	116.10
3	A	9202	OM7	C47-C42-C43	2.60	126.59	120.03
3	A	9202	OM7	C47-C09-C32	-2.58	108.80	117.37
3	A	9202	OM7	C51-C49-C14	2.06	115.49	111.62
3	A	9202	OM7	O18-C03-C04	-2.02	103.30	108.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	9202	OM7	C14-C49-C51-C52
3	A	9202	OM7	C14-C49-C51-C53
3	A	9202	OM7	N50-C49-C51-C52
3	A	9202	OM7	N50-C49-C51-C53

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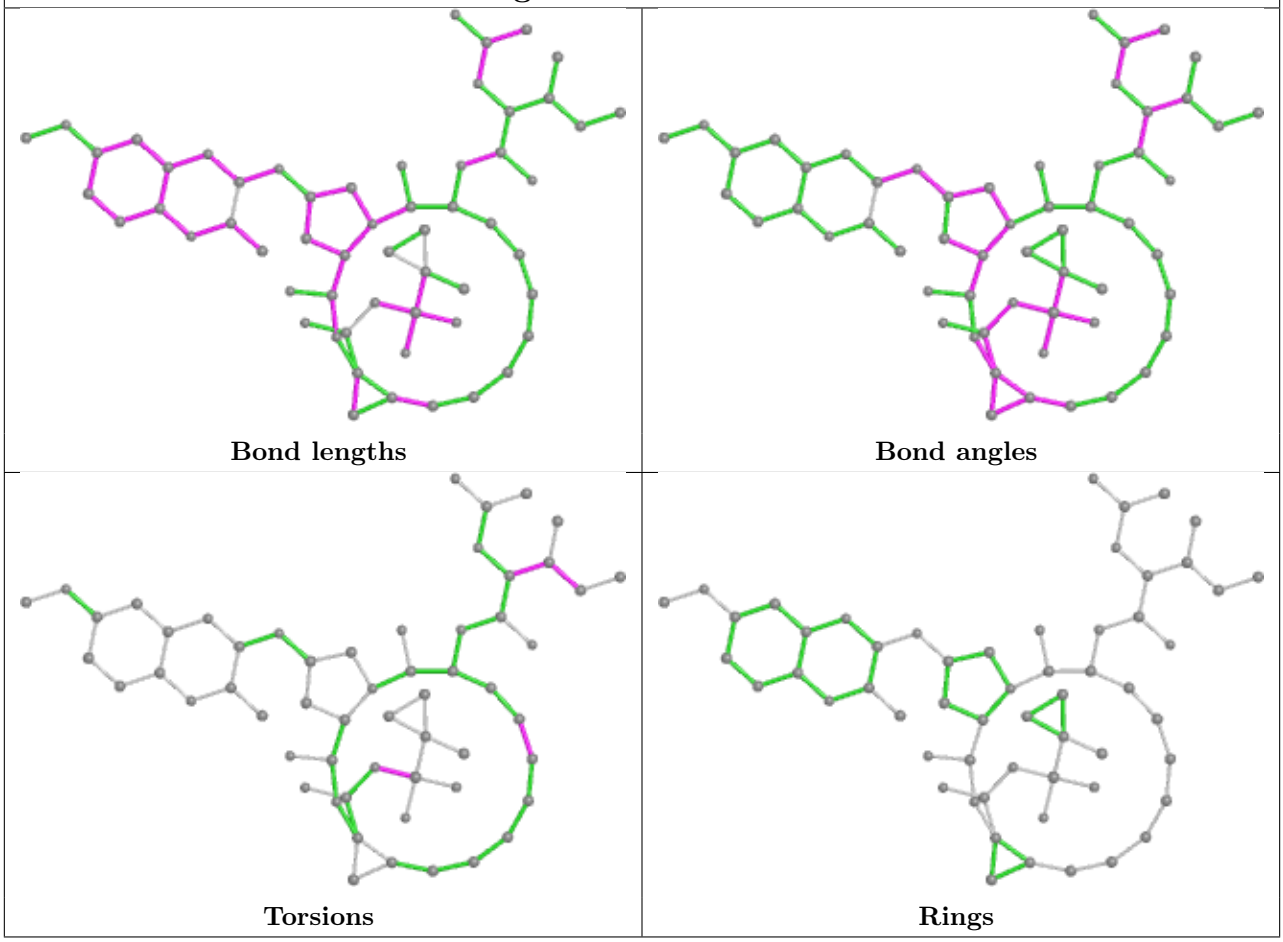
Mol	Chain	Res	Type	Atoms
3	A	9202	OM7	C32-N33-S35-C38
3	A	9202	OM7	C16-C17-C48-C46
3	A	9202	OM7	C49-C51-C52-C54
3	A	9202	OM7	C53-C51-C52-C54
4	A	9203	EDO	O1-C1-C2-O2
4	A	9205	EDO	O1-C1-C2-O2

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 then 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.

Ligand OM7 A 9202



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.