Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 03:51 am BST

PDB ID	:	3ZNR
Title	:	HDAC7 bound with inhibitor TMP269
Authors	:	Lobera, m.; madauss, k.; pohlhaus, d.; trump, r.; nolan, m.
Deposited on	:	2013-02-15
Resolution	:	2.40 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 following versions of software and data (see references ⓘ) were used in the production of this report:

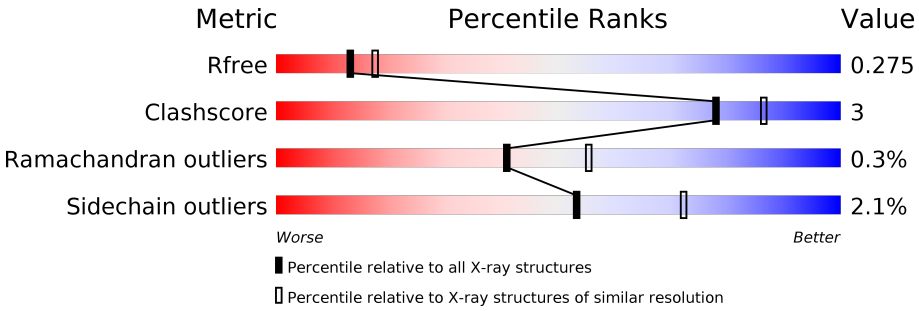
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.40 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))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 on 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	423	79% 8% 13%
1	B	423	82% 8% 10%
1	C	423	77% 7% 15%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8454 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 HISTONE DEACETYLASE 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total 2778	C 1744	N 499	O 516	S 19	0	1	0
1	B	381	Total 2872	C 1801	N 515	O 537	S 19	0	0	0
1	C	359	Total 2712	C 1696	N 493	O 505	S 18	0	1	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	-	expression tag	UNP Q8WUI4
B	481	GLY	-	expression tag	UNP Q8WUI4
C	481	GLY	-	expression tag	UNP Q8WUI4

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Zn 2	0	0
2	A	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	K 2	0	0
3	A	2	Total 2	K 2	0	0

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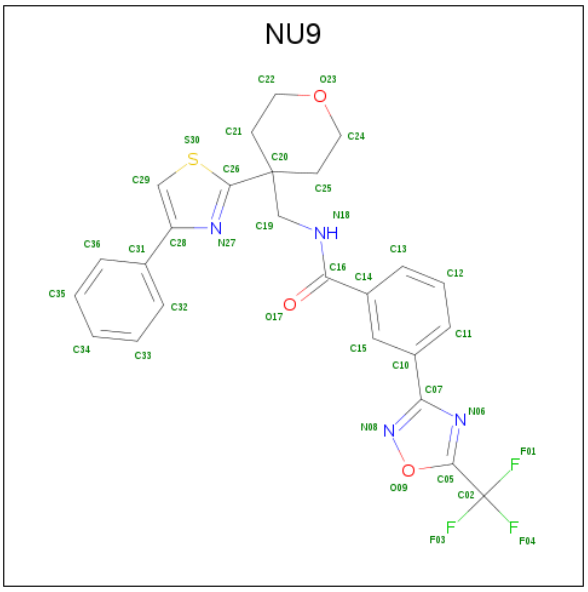
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	2	Total K 2 2	0	0

- Molecule 4 is N-{[4-(4-phenyl-1,3-thiazol-2-yl)tetrahydro-2H-pyran-4-yl]methyl}-3-[5-(trifluoromethyl)-1,2,4-oxadiazol-3-yl]benzamide (three-letter code: NU9) (formula: $C_{25}H_{21}F_3N_4O_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F N O S 36 25 3 4 3 1	0	0

- Molecule 5 is water.

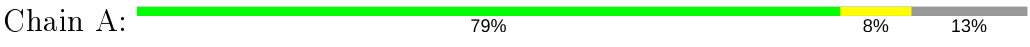
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	16	Total O 16 16	0	0
5	B	21	Total O 21 21	0	0
5	C	7	Total O 7 7	0	0

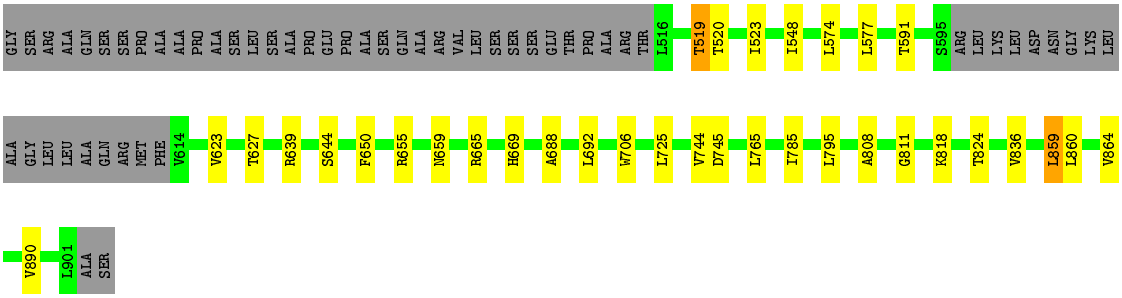
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: HISTONE DEACETYLASE 7

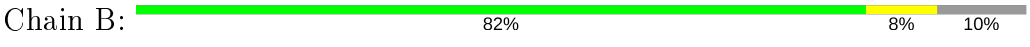
Chain A:

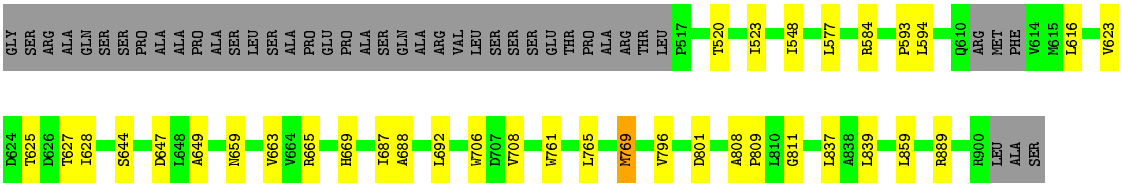




- Molecule 1: HISTONE DEACETYLASE 7

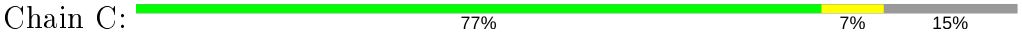
Chain B:

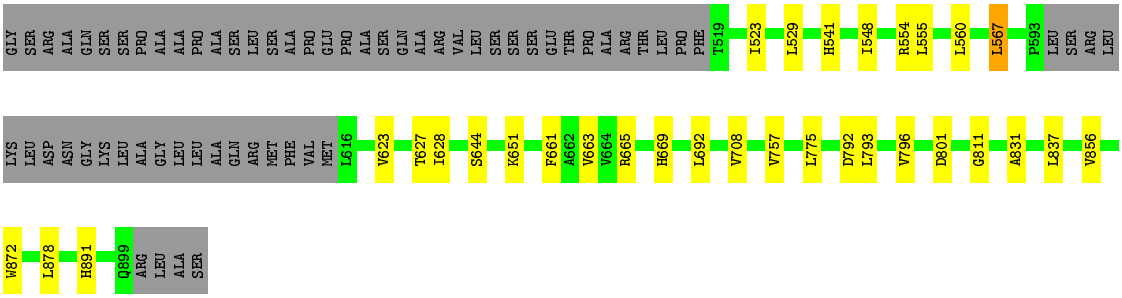




- Molecule 1: HISTONE DEACETYLASE 7

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	81.39Å 81.39Å 149.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	70.49 – 2.40 27.50 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (70.49-2.40) 99.4 (27.50-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.212 , 0.241 0.254 , 0.275	Depositor DCC
R_{free} test set	2165 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	45.6	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 24.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l 0.043 for h,-h-k,-l 0.025 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8454	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, K, NU9

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	0.27	0/2849	0.43	0/3869
1	B	0.28	0/2939	0.44	0/3988
1	C	0.28	0/2781	0.43	0/3778
All	All	0.28	0/8569	0.43	0/11635

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

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	2778	0	2657	16	0
1	B	2872	0	2753	16	0
1	C	2712	0	2583	15	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	36	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	16	0	0	0	0
5	B	21	0	0	0	0
5	C	7	0	0	0	0
All	All	8454	0	8014	47	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 3.

All (47) 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:C:523:ILE:HG21	1:C:644:SER:HB3	1.66	0.77
1:C:623:VAL:HG22	1:C:627:THR:HB	1.74	0.69
1:B:623:VAL:HG22	1:B:627:THR:HB	1.77	0.66
1:A:623:VAL:HG22	1:A:627:THR:HB	1.77	0.65
1:B:523:ILE:HG21	1:B:644:SER:HB3	1.79	0.64
1:A:523:ILE:HG21	1:A:644:SER:HB3	1.80	0.64
1:C:661:PHE:CE2	1:C:663:VAL:HG22	2.33	0.63
1:C:692:LEU:HD21	1:C:793:LEU:HD13	1.82	0.61
1:C:555:LEU:HD23	1:C:560:LEU:HD12	1.84	0.59
1:A:744:VAL:HG12	1:A:890:VAL:HG21	1.86	0.58
1:A:520:THR:HG23	1:A:860:LEU:HD23	1.86	0.57
1:B:520:THR:HG22	1:B:659:ASN:OD1	2.06	0.56
1:B:808:ALA:HB3	1:B:809:PRO:HD3	1.87	0.55
1:A:519:THR:HG22	1:A:520:THR:H	1.71	0.55
1:A:824:THR:HG21	1:A:859:LEU:HD13	1.89	0.53
1:B:548:ILE:HD13	1:B:665:ARG:HG2	1.91	0.51
1:C:567:LEU:HD11	1:C:651:LYS:HE3	1.93	0.50
1:C:548:ILE:HD13	1:C:665:ARG:HG2	1.94	0.50
1:A:765:LEU:HD11	1:A:808:ALA:HB2	1.93	0.50
1:C:757:VAL:HG22	1:C:891:HIS:CE1	2.47	0.50
1:A:795:LEU:HD23	1:A:836:VAL:HB	1.95	0.49
1:C:529:LEU:HD23	1:C:548:ILE:HD11	1.95	0.48
1:A:650:PHE:CE1	1:A:692:LEU:HD12	2.49	0.47
1:B:649:ALA:HB1	1:B:692:LEU:HD21	1.97	0.47
1:C:796:VAL:HB	1:C:837:LEU:HD23	1.97	0.46
1:C:555:LEU:HD21	1:C:856:VAL:HG21	1.98	0.45
1:A:577:LEU:HD11	1:A:639:ARG:HG2	1.97	0.45
1:A:520:THR:HG22	1:A:659:ASN:OD1	2.15	0.45
1:C:541:HIS:CE1	1:C:628:ILE:HD11	2.52	0.45
1:A:548:ILE:HD13	1:A:665:ARG:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:LEU:HD23	1:B:687:ILE:HD13	1.98	0.45
1:B:796:VAL:HB	1:B:837:LEU:HD22	1.99	0.44
1:A:725:LEU:HD21	1:A:785:ILE:HG22	2.00	0.44
1:B:659:ASN:HB2	1:B:859:LEU:HD22	2.01	0.43
1:C:708:VAL:HG12	1:C:801:ASP:CG	2.39	0.43
1:B:548:ILE:HB	1:B:663:VAL:HG12	2.01	0.42
1:C:792:ASP:O	1:C:831:ALA:HB1	2.20	0.42
1:C:775:LEU:HD11	1:C:872:TRP:CD2	2.55	0.41
1:B:628:ILE:HD12	1:B:628:ILE:C	2.41	0.41
1:A:688:ALA:O	1:A:692:LEU:HD13	2.21	0.41
1:B:616:LEU:HD22	1:B:625:THR:HA	2.01	0.41
1:B:708:VAL:HG12	1:B:801:ASP:CG	2.41	0.41
1:A:574:LEU:HD21	1:A:591:THR:HG22	2.03	0.40
1:B:688:ALA:O	1:B:692:LEU:HD13	2.21	0.40
1:B:761:TRP:CE3	1:B:769:MET:CE	3.04	0.40
1:B:593:PRO:HA	1:B:594:LEU:HA	1.80	0.40
1:A:818:LYS:HE2	1:A:864:VAL:HG13	2.03	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 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	365/423 (86%)	354 (97%)	10 (3%)	1 (0%)	41	55
1	B	377/423 (89%)	365 (97%)	11 (3%)	1 (0%)	41	55
1	C	356/423 (84%)	343 (96%)	12 (3%)	1 (0%)	41	55
All	All	1098/1269 (86%)	1062 (97%)	33 (3%)	3 (0%)	41	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	811	GLY
1	B	811	GLY
1	C	811	GLY

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 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	289/336 (86%)	283 (98%)	6 (2%)	53 72
1	B	298/336 (89%)	290 (97%)	8 (3%)	44 65
1	C	281/336 (84%)	277 (99%)	4 (1%)	67 82
All	All	868/1008 (86%)	850 (98%)	18 (2%)	53 72

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	519	THR
1	A	655	ARG
1	A	669	HIS
1	A	706	TRP
1	A	745	ASP
1	A	859	LEU
1	B	584	ARG
1	B	647	ASP
1	B	669	HIS
1	B	706	TRP
1	B	765	LEU
1	B	769	MET
1	B	839	LEU
1	B	889	ARG
1	C	554	ARG
1	C	567	LEU
1	C	669	HIS
1	C	878	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	636	ASN
1	A	673	HIS
1	A	879	ASN
1	A	899	GLN
1	B	610	GLN
1	B	636	ASN
1	B	825	GLN
1	B	879	ASN
1	B	899	GLN
1	C	636	ASN
1	C	695	GLN
1	C	756	ASN
1	C	879	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 12 are monoatomic - leaving 1 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	$\#\|Z\|>2$
4	NU9	A	1000	2	34,40,40	2.58	7 (20%)	44,58,58	1.91	11 (25%)

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	NU9	A	1000	2	-	5/23/40/40	1/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1000	NU9	C28-N27	8.36	1.63	1.37
4	A	1000	NU9	C26-S30	-6.12	1.54	1.73
4	A	1000	NU9	C31-C28	-5.85	1.39	1.48
4	A	1000	NU9	C29-S30	-5.51	1.61	1.70
4	A	1000	NU9	C16-N18	4.22	1.43	1.33
4	A	1000	NU9	C07-N06	3.51	1.40	1.35
4	A	1000	NU9	C10-C07	-3.49	1.39	1.48

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1000	NU9	C10-C07-N08	5.77	126.63	119.12
4	A	1000	NU9	C05-N06-C07	4.89	108.30	101.38
4	A	1000	NU9	C21-C20-C26	3.85	118.20	110.51
4	A	1000	NU9	C02-C05-N06	3.43	125.76	122.41
4	A	1000	NU9	C25-C20-C19	-3.31	102.65	109.31
4	A	1000	NU9	C21-C20-C19	-2.88	103.52	109.31
4	A	1000	NU9	C28-C29-S30	-2.87	108.27	111.79
4	A	1000	NU9	C25-C20-C26	2.82	116.14	110.51
4	A	1000	NU9	C31-C28-N27	2.18	124.45	120.78
4	A	1000	NU9	C20-C19-N18	2.14	117.09	114.12
4	A	1000	NU9	O23-C22-C21	2.08	113.77	111.56

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1000	NU9	C13-C14-C16-N18

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Mol	Chain	Res	Type	Atoms
4	A	1000	NU9	C13-C14-C16-O17
4	A	1000	NU9	C15-C14-C16-N18
4	A	1000	NU9	C15-C14-C16-O17
4	A	1000	NU9	C21-C20-C26-N27

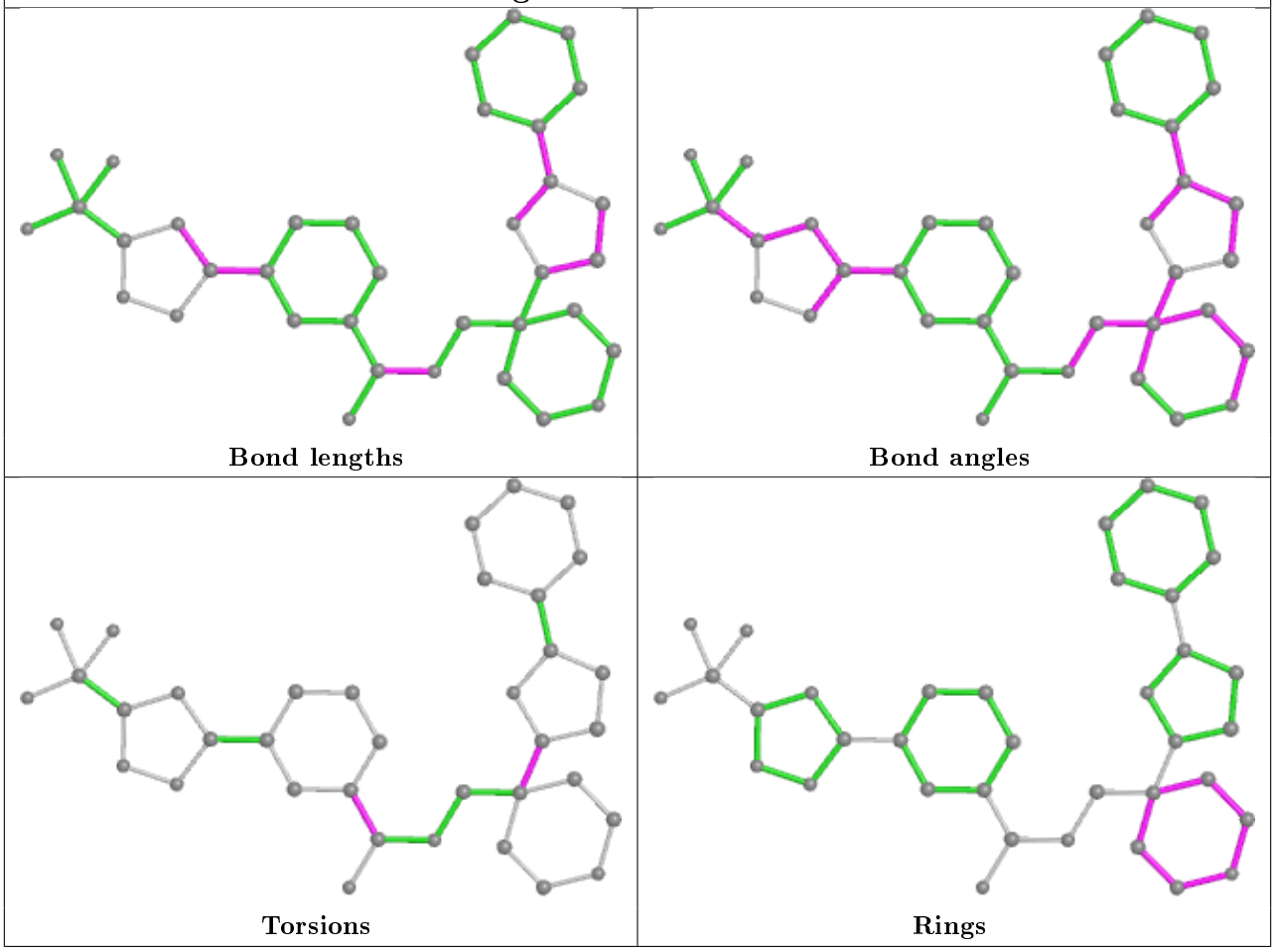
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1000	NU9	C20-C21-C22-C24-C25-O23

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 NU9 A 1000



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

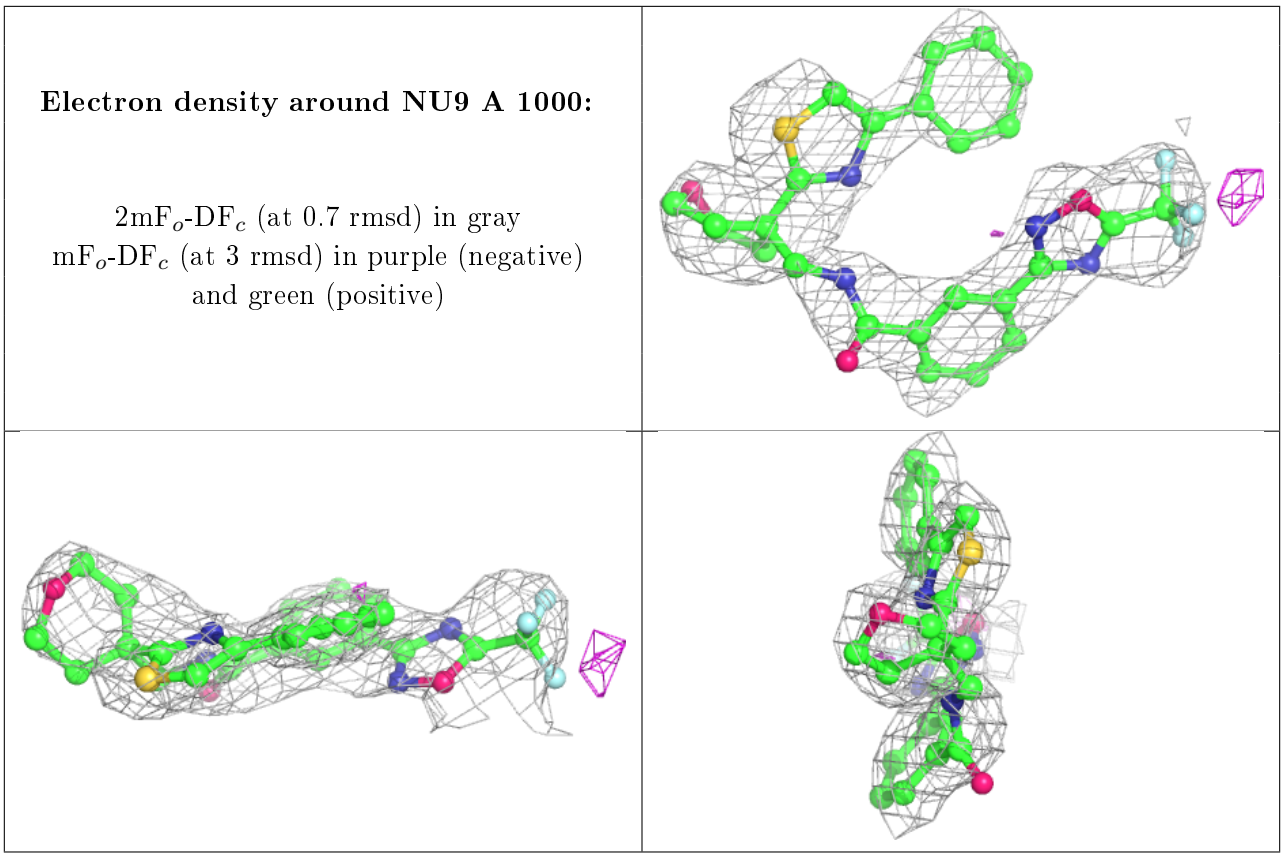
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NU9 A 1000:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.