



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:43 AM UTC

PDB ID : 8TH9 / pdb_00008th9
Title : Structure of mammalian NEIL2 from Monodelphis domestica in complex with THF-containing DNA
Authors : Eckenroth, B.E.; Doubleie, S.
Deposited on : 2023-07-14
Resolution : 2.08 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

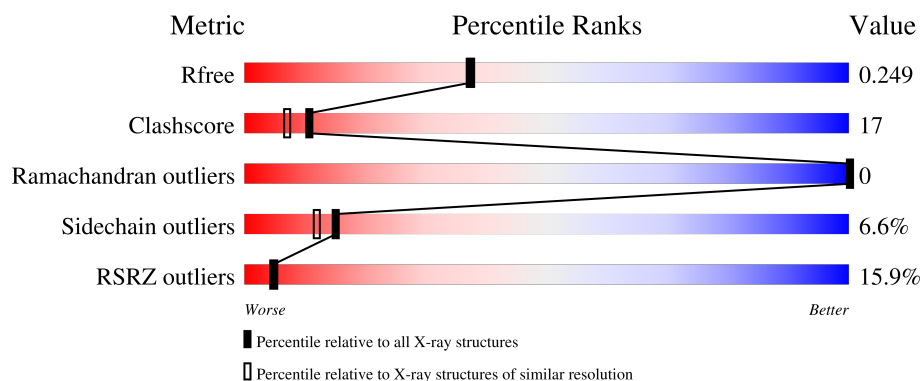
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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}	180053	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	290	15% 53% 30% • 13%
2	C	13	46% 54%
3	D	14	50% 43% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3548 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 DNA-(apurinic or apyrimidinic site) lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	Se	0	125	0
			2946	1914	515	502	10	5			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	GLY	-	linker	UNP F7AMK3
A	122	SER	-	linker	UNP F7AMK3
A	123	GLY	-	linker	UNP F7AMK3
A	124	SER	-	linker	UNP F7AMK3
A	125	GLY	-	linker	UNP F7AMK3
A	337	LEU	-	expression tag	UNP F7AMK3
A	338	GLU	-	expression tag	UNP F7AMK3
A	339	HIS	-	expression tag	UNP F7AMK3
A	340	HIS	-	expression tag	UNP F7AMK3
A	341	HIS	-	expression tag	UNP F7AMK3
A	342	HIS	-	expression tag	UNP F7AMK3
A	343	HIS	-	expression tag	UNP F7AMK3
A	344	HIS	-	expression tag	UNP F7AMK3

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*TP*AP*GP*AP*CP*CP*TP*GP*GP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	13	Total	C	N	O	P	0	0	0
			267	127	53	75	12			

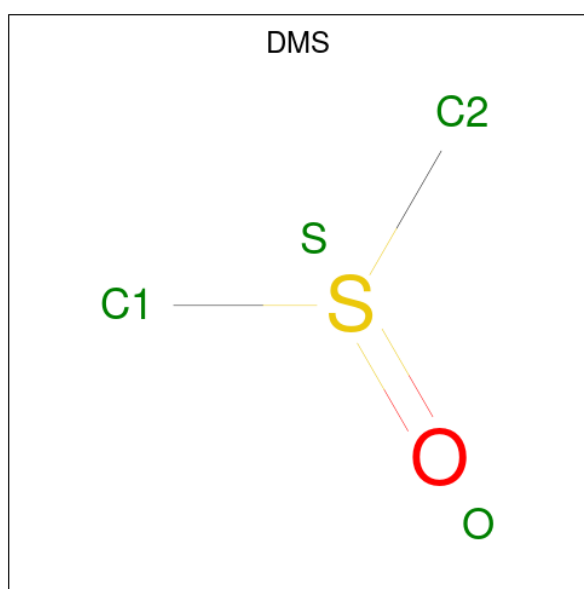
- Molecule 3 is a DNA chain called DNA (5'-D(*GP*CP*GP*TP*CP*CP*AP*(3DR)P*GP*TP*CP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	14	Total	C	N	O	P	0	0	0
			271	130	46	82	13			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



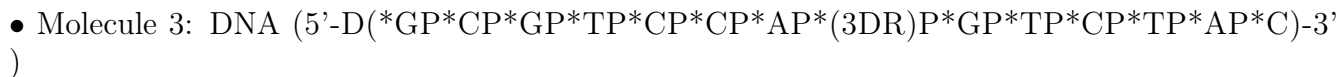
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	32	Total	O	0	0
			32	32		
6	C	16	Total	O	0	0
			16	16		
6	D	11	Total	O	0	0
			11	11		

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- Molecule 1: DNA-(apurinic or apyrimidinic site) lyase



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.43Å 121.43Å 117.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.40 – 2.08 38.40 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.40-2.08) 99.9 (38.40-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.222 , 0.244 0.228 , 0.249	Depositor DCC
R_{free} test set	2638 reflections (8.79%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 74.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h 0.013 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3548	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DMS, 3DR, ZN

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	0.31	0/3030	0.47	0/4107
2	C	0.45	0/300	0.62	0/462
3	D	0.44	0/289	0.62	0/441
All	All	0.34	0/3619	0.50	0/5010

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	2946	0	2898	101	0
2	C	267	0	147	10	0
3	D	271	0	156	11	0
4	A	1	0	0	0	0
5	A	4	0	6	0	0
6	A	32	0	0	7	0
6	C	16	0	0	2	0
6	D	11	0	0	1	0
All	All	3548	0	3207	110	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 17.

All (110) 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:D:8:3DR:O4'	3:D:8:3DR:C4'	1.66	1.25
1:A:22[A]:VAL:O	1:A:39[A]:MSE:N	2.06	0.87
1:A:168[B]:ARG:NH2	6:A:501:HOH:O	2.10	0.82
1:A:24[A]:THR:HG23	1:A:172[A]:HIS:HB2	1.63	0.81
1:A:33[A]:ASN:HB3	1:A:36[A]:MSE:HE2	1.65	0.78
3:D:9:DG:OP1	6:D:101:HOH:O	2.09	0.71
1:A:141[A]:LEU:HB3	3:D:9:DG:C2	2.26	0.71
1:A:57[B]:GLY:HA3	1:A:131[B]:SER:HA	1.73	0.70
2:C:4:DG:N3	6:C:101:HOH:O	2.26	0.68
1:A:168[A]:ARG:HH11	1:A:168[A]:ARG:HG3	1.60	0.67
1:A:146[B]:ARG:NH2	2:C:8:DT:OP2	2.28	0.67
2:C:12:DC:H2'	2:C:13:DG:C8	2.32	0.65
1:A:56[B]:PHE:HB2	1:A:133[B]:LEU:HD22	1.80	0.63
1:A:48[B]:HIS:CE1	1:A:198[B]:ASP:HB2	2.34	0.62
1:A:135[B]:LEU:HB3	1:A:185[B]:ILE:HD11	1.82	0.62
1:A:168[A]:ARG:HH11	1:A:168[A]:ARG:CG	2.13	0.61
1:A:155[A]:LYS:O	2:C:7:DC:N4	2.32	0.59
1:A:6[B]:SER:HA	1:A:278:LYS:HE2	1.85	0.58
1:A:197[A]:SER:HB2	1:A:227:ARG:O	2.03	0.58
1:A:142[B]:PHE:HE2	2:C:8:DT:N3	2.02	0.57
1:A:24[A]:THR:HG23	1:A:172[A]:HIS:CB	2.35	0.57
1:A:2[B]:PRO:HG2	1:A:139[B]:PHE:HB2	1.85	0.57
1:A:3[B]:GLU:HG2	1:A:233:GLY:HA3	1.87	0.57
1:A:33[A]:ASN:OD1	1:A:35[A]:ASN:HB2	2.06	0.56
1:A:165[B]:PRO:HB3	2:C:7:DC:C2'	2.35	0.56
1:A:48[A]:HIS:CD2	1:A:194[A]:LYS:H	2.23	0.56
1:A:326:GLU:OE1	6:A:502:HOH:O	2.18	0.56
1:A:245:ARG:NH2	6:A:505:HOH:O	2.41	0.54
1:A:36[A]:MSE:CE	1:A:187[A]:TRP:HZ2	2.20	0.54
1:A:44[B]:ASP:OD1	1:A:45[B]:SER:N	2.40	0.54
1:A:6[B]:SER:HA	1:A:278:LYS:CE	2.38	0.53
1:A:54[B]:LEU:HB3	1:A:56[B]:PHE:CE1	2.43	0.53
1:A:213:LEU:O	1:A:252:GLY:HA3	2.08	0.53
1:A:211:GLU:OE1	1:A:214[B]:LYS:HD2	2.09	0.53
1:A:10[B]:PHE:CD1	1:A:145[B]:VAL:HG12	2.44	0.52
1:A:25[A]:VAL:HG21	1:A:37[A]:LEU:HB2	1.92	0.52
1:A:134[A]:TRP:CH2	1:A:191[A]:PRO:HG3	2.43	0.52
2:C:7:DC:H1'	6:C:105:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20[B]:GLN:OE1	1:A:175[B]:LYS:HG2	2.11	0.51
1:A:289:TYR:CE1	1:A:290:GLN:HG3	2.47	0.50
1:A:36[A]:MSE:SE	1:A:187[A]:TRP:CZ2	3.15	0.50
1:A:48[A]:HIS:HB2	1:A:193[A]:VAL:HA	1.93	0.50
1:A:156[B]:ALA:HB2	1:A:162[B]:TRP:CD1	2.47	0.50
1:A:46[A]:GLN:HB3	1:A:193[A]:VAL:HG21	1.94	0.49
1:A:55[A]:ASN:ND2	1:A:133[A]:LEU:O	2.44	0.49
1:A:25[B]:VAL:HG23	1:A:38[B]:GLU:HG2	1.95	0.49
1:A:20[B]:GLN:HE22	1:A:175[B]:LYS:HE3	1.77	0.49
1:A:49[A]:GLY:HA3	1:A:230:ALA:HB1	1.93	0.49
1:A:43[A]:GLN:NE2	1:A:55[A]:ASN:OD1	2.37	0.49
1:A:136[B]:CYS:HB2	1:A:188[B]:CYS:SG	2.53	0.49
1:A:141[B]:LEU:HD21	3:D:7:DA:C4	2.47	0.48
1:A:36[A]:MSE:HE3	1:A:187[A]:TRP:HZ2	1.78	0.48
1:A:198[A]:ASP:HA	1:A:230:ALA:HB3	1.95	0.48
1:A:43[B]:GLN:NE2	1:A:131[B]:SER:OG	2.40	0.48
1:A:211:GLU:O	1:A:214[B]:LYS:HD3	2.13	0.48
1:A:135[B]:LEU:HB3	1:A:185[B]:ILE:CD1	2.44	0.48
1:A:135[B]:LEU:HD13	1:A:185[B]:ILE:HD11	1.96	0.47
1:A:36[B]:MSE:HE1	1:A:135[B]:LEU:HD21	1.96	0.47
1:A:43[A]:GLN:OE1	1:A:59[A]:THR:HG22	2.15	0.47
1:A:7[A]:LEU:HD11	6:A:506:HOH:O	2.13	0.47
2:C:1:DG:H2'	2:C:2:DT:C6	2.50	0.47
1:A:140[A]:GLY:CA	3:D:10:DT:H5'	2.45	0.47
1:A:140[A]:GLY:HA2	3:D:9:DG:O4'	2.15	0.47
1:A:210:LEU:HD11	1:A:261:GLU:OE1	2.15	0.47
1:A:11[B]:HIS:HB2	1:A:47[B]:VAL:HG11	1.97	0.46
1:A:5[B]:PRO:HG2	1:A:274:TRP:CE3	2.50	0.46
1:A:134[A]:TRP:CD1	1:A:190[A]:GLY:HA2	2.50	0.46
6:A:527:HOH:O	3:D:8:3DR:H5'	2.16	0.46
1:A:49[A]:GLY:CA	1:A:230:ALA:HB1	2.46	0.45
1:A:55[A]:ASN:HA	1:A:133[A]:LEU:O	2.16	0.45
1:A:55[B]:ASN:HB2	1:A:134[B]:TRP:CH2	2.51	0.45
1:A:3[B]:GLU:HA	1:A:50[B]:LYS:HG2	1.98	0.45
1:A:212:ALA:O	1:A:215:GLN:HG2	2.17	0.45
1:A:22[A]:VAL:HG12	1:A:38[A]:GLU:HA	1.98	0.45
1:A:140[A]:GLY:HA2	3:D:9:DG:C1'	2.46	0.44
1:A:136[B]:CYS:O	1:A:185[B]:ILE:HA	2.17	0.44
1:A:138[A]:HIS:HE1	6:A:528:HOH:O	2.00	0.44
1:A:50[B]:LYS:HG3	1:A:231:GLY:HA2	2.00	0.44
1:A:145[B]:VAL:HA	1:A:179[B]:ALA:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57[A]:GLY:C	1:A:58[A]:LEU:HG	2.43	0.44
1:A:143[A]:GLY:HA2	1:A:182[A]:ASN:HB3	1.99	0.43
1:A:191[A]:PRO:HB2	1:A:193[A]:VAL:HG23	2.00	0.43
3:D:6:DC:H4'	3:D:7:DA:OP1	2.18	0.43
1:A:263:LEU:O	1:A:267:VAL:HG23	2.19	0.43
1:A:168[B]:ARG:N	1:A:180[B]:PHE:O	2.52	0.43
1:A:43[A]:GLN:CD	1:A:59[A]:THR:HG22	2.44	0.43
1:A:142[B]:PHE:HE2	2:C:8:DT:C4	2.36	0.42
1:A:36[A]:MSE:CE	1:A:187[A]:TRP:CZ2	3.02	0.42
1:A:36[A]:MSE:HE3	1:A:36[A]:MSE:HB2	1.89	0.42
1:A:57[A]:GLY:O	1:A:58[A]:LEU:HG	2.19	0.42
1:A:195[B]:PRO:C	1:A:197[B]:SER:H	2.27	0.42
1:A:2[B]:PRO:O	1:A:6[B]:SER:HB2	2.19	0.42
3:D:11:DC:H2'	3:D:12:DT:H71	2.02	0.42
1:A:10[A]:PHE:O	1:A:14[A]:VAL:HG23	2.20	0.42
1:A:139[B]:PHE:CD1	1:A:183[B]:CYS:HB3	2.54	0.41
1:A:10[B]:PHE:CG	1:A:145[B]:VAL:HG12	2.55	0.41
1:A:33[A]:ASN:CB	1:A:36[A]:MSE:HE2	2.43	0.41
1:A:196[A]:THR:HA	1:A:203:GLU:O	2.20	0.41
1:A:140[A]:GLY:HA2	3:D:9:DG:H1'	2.03	0.41
1:A:156[A]:ALA:HB2	1:A:162[A]:TRP:CD1	2.56	0.41
1:A:29[A]:SER:HB3	1:A:168[A]:ARG:O	2.21	0.41
1:A:2[A]:PRO:HD2	6:A:506:HOH:O	2.21	0.41
1:A:162[A]:TRP:CD1	1:A:162[A]:TRP:N	2.88	0.41
1:A:168[A]:ARG:HH11	1:A:168[A]:ARG:HB3	1.86	0.41
1:A:134[A]:TRP:CG	1:A:190[A]:GLY:HA2	2.56	0.41
1:A:156[B]:ALA:HA	2:C:7:DC:H42	1.85	0.40
1:A:223:LEU:HD23	1:A:223:LEU:HA	1.92	0.40
1:A:7[A]:LEU:HD23	1:A:47[A]:VAL:HG23	2.04	0.40
1:A:8[B]:ARG:HB2	1:A:275:LEU:HD13	2.03	0.40
1:A:18[A]:VAL:HA	1:A:42[A]:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

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	367/290 (127%)	350 (95%)	17 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	313/250 (125%)	287 (92%)	26 (8%)	10	7

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7[A]	LEU
1	A	7[B]	LEU
1	A	24[A]	THR
1	A	24[B]	THR
1	A	28[A]	ASN
1	A	28[B]	ASN
1	A	29[A]	SER
1	A	29[B]	SER
1	A	42[A]	LEU
1	A	42[B]	LEU
1	A	133[A]	LEU
1	A	133[B]	LEU
1	A	157[A]	ASN
1	A	157[B]	ASN
1	A	162[A]	TRP
1	A	162[B]	TRP
1	A	168[A]	ARG
1	A	168[B]	ARG
1	A	175[A]	LYS
1	A	175[B]	LYS
1	A	192[A]	THR

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Mol	Chain	Res	Type
1	A	192[B]	THR
1	A	196[A]	THR
1	A	196[B]	THR
1	A	278	LYS
1	A	280	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	A	259	ASN
1	A	285	HIS
1	A	312	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	3DR	D	8	3	8,11,12	5.94	4 (50%)	7,14,17	1.00	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	3DR	D	8	3	-	2/3/15/16	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	8	3DR	O4'-C4'	13.72	1.66	1.44
3	D	8	3DR	C3'-C4'	-7.62	1.33	1.53
3	D	8	3DR	O4'-C1'	-3.89	1.31	1.43
3	D	8	3DR	C2'-C1'	3.81	1.61	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	8	3DR	O4'-C4'-C5'-O5'
3	D	8	3DR	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	8	3DR	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is 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	$\# Z > 2$
5	DMS	A	402	-	3,3,3	0.67	0	3,3,3	0.56	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/290 (86%)	1.03	44 (17%) 4 4	19, 50, 97, 138	123 (49%)
2	C	13/13 (100%)	-0.09	0 100 100	67, 79, 128, 131	0
3	D	13/14 (92%)	-0.00	0 100 100	60, 86, 130, 139	0
All	All	276/317 (87%)	0.93	44 (15%) 5 5	19, 55, 112, 139	123 (44%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33[A]	ASN	6.0
1	A	189[A]	LEU	5.9
1	A	2[A]	PRO	5.4
1	A	131[A]	SER	4.8
1	A	59[A]	THR	4.6
1	A	37[A]	LEU	4.5
1	A	193[A]	VAL	4.4
1	A	58[A]	LEU	4.4
1	A	31[A]	LYS	4.2
1	A	133[A]	LEU	4.1
1	A	30[A]	LYS	4.0
1	A	192[A]	THR	3.9
1	A	32[A]	ILE	3.8
1	A	40[A]	LEU	3.6
1	A	309	GLY	3.6
1	A	156[A]	ALA	3.6
1	A	138[A]	HIS	3.4
1	A	28[A]	ASN	3.3
1	A	187[A]	TRP	3.3
1	A	166[A]	ILE	3.2
1	A	153[A]	ALA	3.1
1	A	162[A]	TRP	3.1
1	A	3[A]	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	308	PRO	2.8
1	A	158[A]	LYS	2.6
1	A	307	PRO	2.6
1	A	50[A]	LYS	2.5
1	A	178[A]	LEU	2.5
1	A	150[A]	LEU	2.5
1	A	279	LEU	2.4
1	A	132[A]	GLY	2.4
1	A	327	GLU	2.4
1	A	163[A]	LYS	2.4
1	A	57[A]	GLY	2.4
1	A	35[A]	ASN	2.4
1	A	274	TRP	2.3
1	A	188[A]	CYS	2.3
1	A	34[A]	PRO	2.2
1	A	168[A]	ARG	2.1
1	A	53[A]	TYR	2.1
1	A	195[A]	PRO	2.1
1	A	165[A]	PRO	2.0
1	A	157[A]	ASN	2.0
1	A	186[A]	TYR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	3DR	D	8	11/12	0.95	0.12	59,64,70,75	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

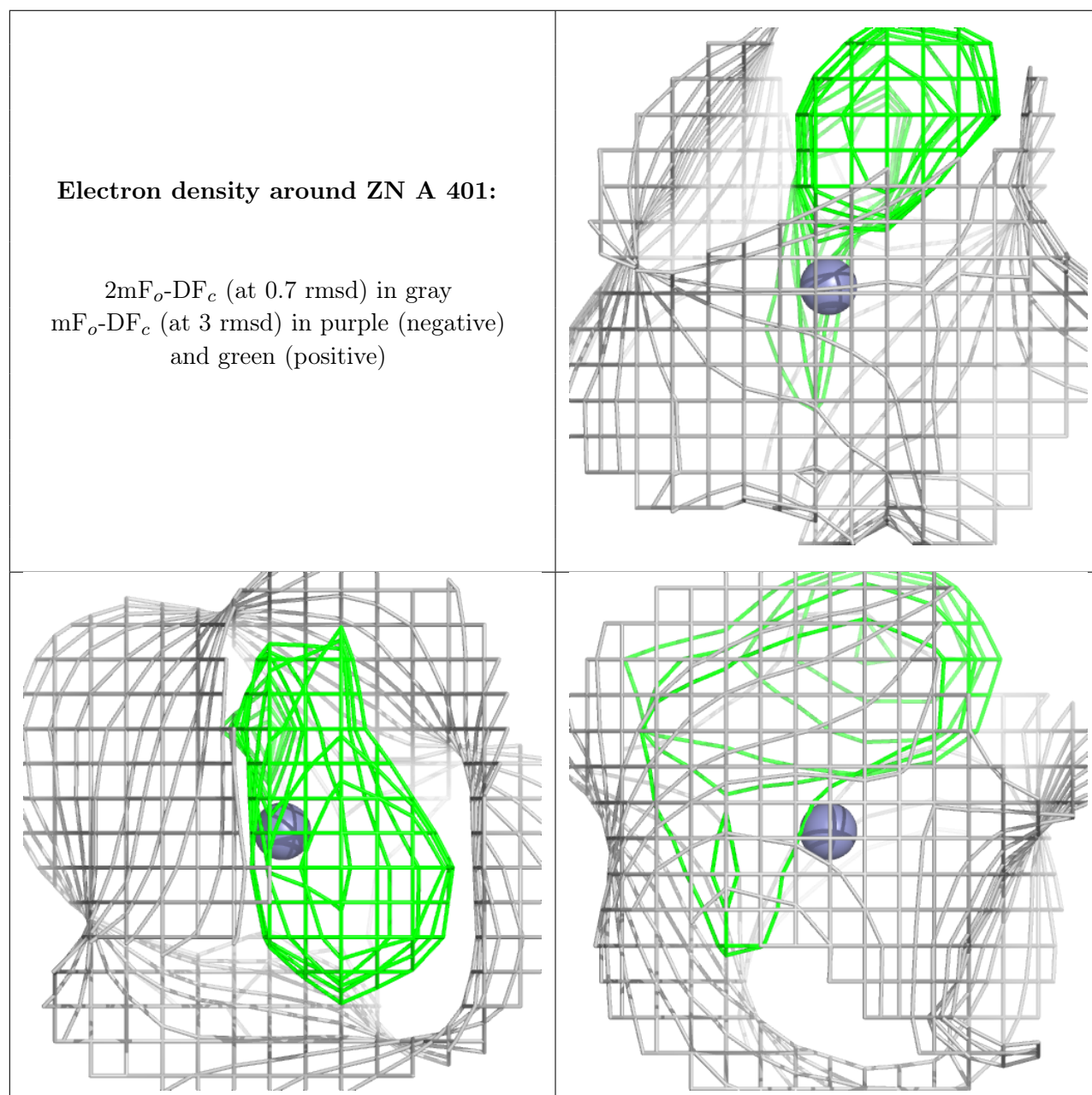
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DMS	A	402	4/4	0.93	0.14	65,70,91,91	0
4	ZN	A	401	1/1	0.97	0.06	70,70,70,70	0

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.



6.5 Other polymers [i](#)

There are no such residues in this entry.