



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:37 PM EDT

PDB ID : 4C2X / pdb_00004c2x
Title : Human N-myristoyltransferase isoform 2 (NMT2)
Authors : Thinon, E.; Serwa, R.A.; Brannigan, J.A.; Brassat, U.; Wright, M.H.; Heal, W.P.; Wilkinson, A.J.; Mann, D.J.; Tate, E.W.
Deposited on : 2013-08-20
Resolution : 2.33 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

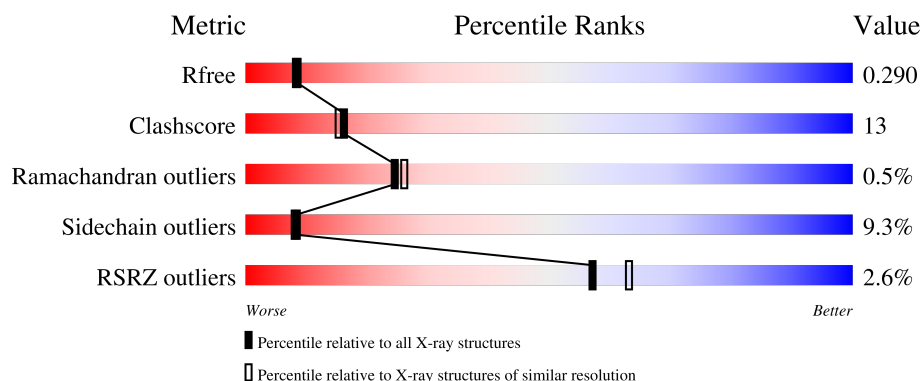
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

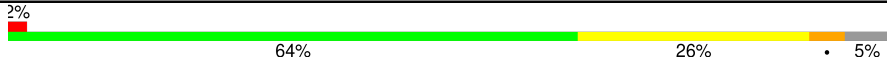
The reported resolution of this entry is 2.33 Å.

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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	410	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3345 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 GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	4	0
			3212	2081	544	572	15			

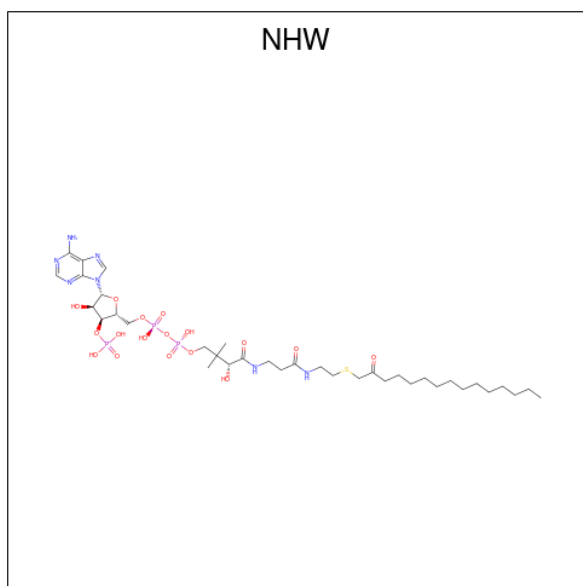
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	MET	-	expression tag	UNP O60551
A	88	GLY	-	expression tag	UNP O60551
A	89	SER	-	expression tag	UNP O60551
A	90	SER	-	expression tag	UNP O60551
A	91	HIS	-	expression tag	UNP O60551
A	92	HIS	-	expression tag	UNP O60551
A	93	HIS	-	expression tag	UNP O60551
A	94	HIS	-	expression tag	UNP O60551
A	95	HIS	-	expression tag	UNP O60551
A	96	HIS	-	expression tag	UNP O60551
A	97	SER	-	expression tag	UNP O60551
A	98	SER	-	expression tag	UNP O60551
A	99	GLY	-	expression tag	UNP O60551
A	100	LEU	-	expression tag	UNP O60551
A	101	GLU	-	expression tag	UNP O60551
A	102	VAL	-	expression tag	UNP O60551
A	103	LEU	-	expression tag	UNP O60551
A	104	PHE	-	expression tag	UNP O60551
A	105	GLN	-	expression tag	UNP O60551
A	106	GLY	-	expression tag	UNP O60551
A	107	PRO	-	expression tag	UNP O60551
A	108	HIS	-	expression tag	UNP O60551
A	109	MET	-	expression tag	UNP O60551
A	304	LYS	ARG	variant	UNP O60551

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is 2-oxopentadecyl-CoA (CCD ID: NHW) (formula: $C_{36}H_{64}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		

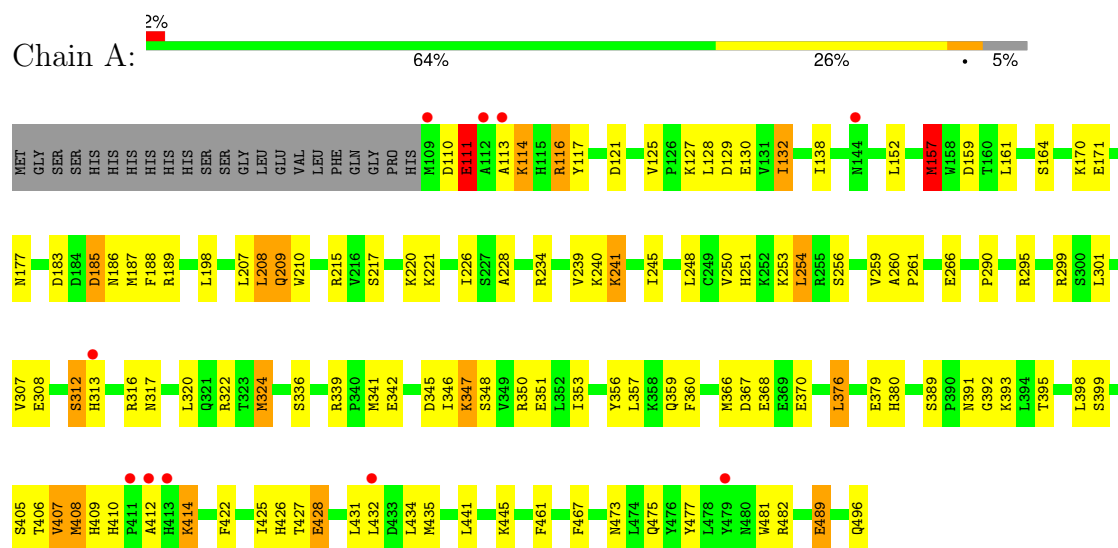
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total	O	0	0
			68	68		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.70Å 72.32Å 114.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.17 – 2.33 61.17 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.8 (61.17-2.33) 99.8 (61.17-2.33)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0033	Depositor
R, R_{free}	0.218 , 0.288 0.221 , 0.290	Depositor DCC
R_{free} test set	940 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3345	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: NHW, MG

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	0.84	1/3312 (0.0%)	1.07	5/4493 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	342	GLU	N-CA	5.06	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	LEU	N-CA-C	-5.94	106.57	113.88
1	A	407	VAL	CB-CA-C	-5.77	105.00	111.23
1	A	339	ARG	N-CA-C	5.67	113.12	108.07
1	A	157	MET	N-CA-C	5.67	118.01	109.23
1	A	187	MET	N-CA-C	-5.63	106.40	113.72

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	A	312	SER	Peptide

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	3212	0	3227	85	0
2	A	1	0	0	0	0
3	A	64	0	60	6	0
4	A	68	0	0	0	0
All	All	3345	0	3287	86	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 13.

All (86) 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:341:MET:HE2	1:A:376:LEU:HD13	1.28	1.13
1:A:234:ARG:NH2	1:A:360:PHE:O	1.88	1.06
1:A:116:ARG:NE	1:A:116:ARG:HA	1.65	1.06
1:A:116:ARG:HA	1:A:116:ARG:HE	1.26	0.93
1:A:132:ILE:HD13	1:A:482:ARG:HD2	1.62	0.80
1:A:183:ASP:O	1:A:186:ASN:ND2	2.17	0.78
1:A:322:ARG:HH11	1:A:322:ARG:HG2	1.52	0.73
1:A:171:GLU:OE1	1:A:215:ARG:NH2	2.16	0.72
1:A:312:SER:HA	1:A:313:HIS:ND1	2.06	0.70
1:A:157:MET:HE2	1:A:217:SER:HA	1.75	0.68
1:A:410:HIS:NE2	1:A:412:ALA:HB3	2.10	0.66
1:A:307:VAL:HA	1:A:312:SER:O	1.96	0.65
1:A:347:LYS:O	1:A:351:GLU:HG3	1.97	0.65
1:A:435:MET:HG3	1:A:461:PHE:CE2	2.32	0.65
1:A:295:ARG:HD3	1:A:473:ASN:OD1	1.97	0.64
1:A:248:LEU:HG	3:A:1000:NHW:H14	1.82	0.60
1:A:414:LYS:HD3	1:A:414:LYS:H	1.67	0.59
1:A:398:LEU:HD23	1:A:434:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:HIS:CD2	1:A:412:ALA:H	2.21	0.58
1:A:240:LYS:HE2	1:A:481:TRP:CZ3	2.39	0.58
1:A:441:LEU:O	1:A:445:LYS:HG3	2.04	0.57
1:A:171:GLU:CD	1:A:215:ARG:HH22	2.08	0.56
1:A:379:GLU:HG2	1:A:380:HIS:CE1	2.41	0.56
1:A:240:LYS:HE2	1:A:481:TRP:HZ3	1.71	0.55
1:A:251:HIS:CE1	1:A:253:LYS:HG2	2.41	0.55
1:A:113:ALA:O	1:A:114:LYS:HD3	2.07	0.55
1:A:295:ARG:CD	1:A:473:ASN:OD1	2.54	0.55
1:A:395:THR:HB	1:A:428:GLU:HB2	1.89	0.53
1:A:116:ARG:HD3	1:A:121:ASP:OD2	2.08	0.53
1:A:410:HIS:CD2	1:A:412:ALA:N	2.76	0.53
1:A:367:ASP:OD1	1:A:367:ASP:C	2.52	0.51
1:A:266:GLU:HA	1:A:266:GLU:OE1	2.11	0.51
1:A:350:ARG:HE	1:A:368:GLU:HG3	1.76	0.51
1:A:209:GLN:H	1:A:209:GLN:CD	2.19	0.51
1:A:322:ARG:HH11	1:A:322:ARG:CG	2.23	0.50
1:A:414:LYS:HD3	1:A:414:LYS:N	2.26	0.50
1:A:260:ALA:HB2	3:A:1000:NHW:H12A	1.93	0.50
1:A:312:SER:HA	1:A:313:HIS:CG	2.47	0.49
1:A:260:ALA:HB3	1:A:261:PRO:HD3	1.95	0.49
1:A:366:MET:HA	1:A:370:GLU:OE1	2.12	0.49
1:A:250:VAL:HG23	3:A:1000:NHW:H14B	1.94	0.49
1:A:152:LEU:HD12	1:A:157:MET:HA	1.95	0.49
1:A:353:ILE:HG12	1:A:357:LEU:CD1	2.44	0.48
1:A:254:LEU:HD13	1:A:259:VAL:HG21	1.96	0.48
1:A:356:TYR:O	1:A:359:GLN:HG2	2.14	0.47
1:A:395:THR:O	1:A:427:THR:OG1	2.21	0.47
1:A:316:ARG:HD2	1:A:317:ASN:HA	1.96	0.46
1:A:475[A]:GLN:HB2	1:A:477:TYR:CE2	2.51	0.46
1:A:186:ASN:O	1:A:408:MET:HE2	2.17	0.45
3:A:1000:NHW:O9	3:A:1000:NHW:H6	2.16	0.45
1:A:350:ARG:HD3	1:A:368:GLU:HG3	1.98	0.45
1:A:313:HIS:O	1:A:313:HIS:CD2	2.69	0.45
1:A:320:LEU:O	1:A:324:MET:HG2	2.17	0.45
1:A:389:SER:O	1:A:391:ASN:N	2.50	0.45
1:A:260:ALA:CB	3:A:1000:NHW:H12A	2.47	0.44
1:A:157:MET:HE1	1:A:220:LYS:CD	2.48	0.44
1:A:117:TYR:O	1:A:121:ASP:HB2	2.17	0.44
1:A:241:LYS:HD2	1:A:241:LYS:HA	1.62	0.44
1:A:125:VAL:HA	1:A:138:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LEU:C	1:A:210:TRP:H	2.26	0.43
1:A:496:GLN:H	1:A:496:GLN:CD	2.26	0.43
1:A:399:SER:OG	1:A:422:PHE:HB3	2.18	0.43
1:A:290:PRO:HB3	1:A:475[A]:GLN:HE21	1.83	0.43
1:A:157:MET:CE	1:A:220:LYS:HD2	2.49	0.43
1:A:316:ARG:HA	1:A:317:ASN:HA	1.44	0.43
1:A:345:ASP:O	1:A:346:ILE:C	2.61	0.43
1:A:308:GLU:O	1:A:410:HIS:CE1	2.72	0.43
1:A:215:ARG:NH1	1:A:220:LYS:O	2.49	0.42
1:A:110:ASP:OD1	1:A:111:GLU:N	2.52	0.42
1:A:350:ARG:HE	1:A:368:GLU:CG	2.33	0.42
1:A:127:LYS:HE2	1:A:127:LYS:HB3	1.87	0.42
1:A:159:ASP:OD2	1:A:161:LEU:HD23	2.20	0.42
1:A:207:LEU:HB3	1:A:209:GLN:NE2	2.35	0.42
1:A:299:ARG:HB2	1:A:467:PHE:CE2	2.55	0.41
1:A:350:ARG:NE	1:A:368:GLU:HG3	2.35	0.41
1:A:188:PHE:HA	1:A:406:THR:O	2.20	0.41
1:A:322:ARG:CG	1:A:322:ARG:NH1	2.83	0.41
1:A:185:ASP:OD1	1:A:185:ASP:N	2.54	0.41
1:A:226:ILE:HD12	1:A:248:LEU:HD13	2.03	0.41
1:A:261:PRO:HD3	3:A:1000:NHW:O5X	2.21	0.41
1:A:426:HIS:CD2	1:A:431:LEU:HD13	2.56	0.41
1:A:489:GLU:H	1:A:489:GLU:HG3	1.54	0.41
1:A:228:ALA:HB2	1:A:245:ILE:HD13	2.02	0.41
1:A:316:ARG:HD2	1:A:316:ARG:HA	1.86	0.41
1:A:177:ASN:O	1:A:189:ARG:HD2	2.20	0.40
1:A:312:SER:HA	1:A:313:HIS:HD1	1.84	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	390/410 (95%)	357 (92%)	31 (8%)	2 (0%)	24 26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	GLU
1	A	392	GLY

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	358/373 (96%)	325 (91%)	33 (9%)	8 8

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	GLU
1	A	114	LYS
1	A	116	ARG
1	A	128	LEU
1	A	130	GLU
1	A	132	ILE
1	A	157	MET
1	A	164	SER
1	A	170	LYS
1	A	185	ASP
1	A	198	LEU
1	A	208	LEU
1	A	209	GLN
1	A	221	LYS
1	A	239	VAL
1	A	241	LYS
1	A	254	LEU
1	A	256	SER
1	A	324	MET

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Mol	Chain	Res	Type
1	A	336	SER
1	A	347	LYS
1	A	348	SER
1	A	376	LEU
1	A	393	LYS
1	A	405	SER
1	A	407	VAL
1	A	408	MET
1	A	409	HIS
1	A	414	LYS
1	A	425	ILE
1	A	428	GLU
1	A	432	LEU
1	A	489	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	HIS
1	A	186	ASN
1	A	232	ASN
1	A	302	ASN
1	A	410	HIS
1	A	426	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

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
3	NHW	A	1000	2	64,66,66	1.39	4 (6%)	87,92,92	1.57	11 (12%)

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	NHW	A	1000	2	-	10/65/81/81	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	NHW	P1A-O3A	-5.60	1.53	1.59
3	A	1000	NHW	P3X-O3X	4.91	1.68	1.59
3	A	1000	NHW	C5A-N7A	-3.19	1.33	1.39
3	A	1000	NHW	C8A-N9A	-2.78	1.32	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1000	NHW	C5A-C4A-N3A	-5.48	119.17	126.72
3	A	1000	NHW	N3A-C2A-N1A	-4.76	121.37	128.58
3	A	1000	NHW	N3A-C4A-N9A	3.70	133.46	127.17
3	A	1000	NHW	C13-C11-C10	3.65	114.98	108.77
3	A	1000	NHW	C6-C7-N8	-3.62	104.29	112.00
3	A	1000	NHW	C2A-N3A-C4A	3.40	120.15	111.83
3	A	1000	NHW	N9A-C8A-N7A	-2.89	109.84	113.94
3	A	1000	NHW	C5A-N7A-C8A	2.56	107.48	103.45
3	A	1000	NHW	C4A-C5A-N7A	-2.56	107.65	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1000	NHW	O4X-C4X-C5X	-2.44	101.53	109.33
3	A	1000	NHW	C7-C6-C5	-2.18	108.77	112.39

There are no chirality outliers.

All (10) torsion outliers are listed below:

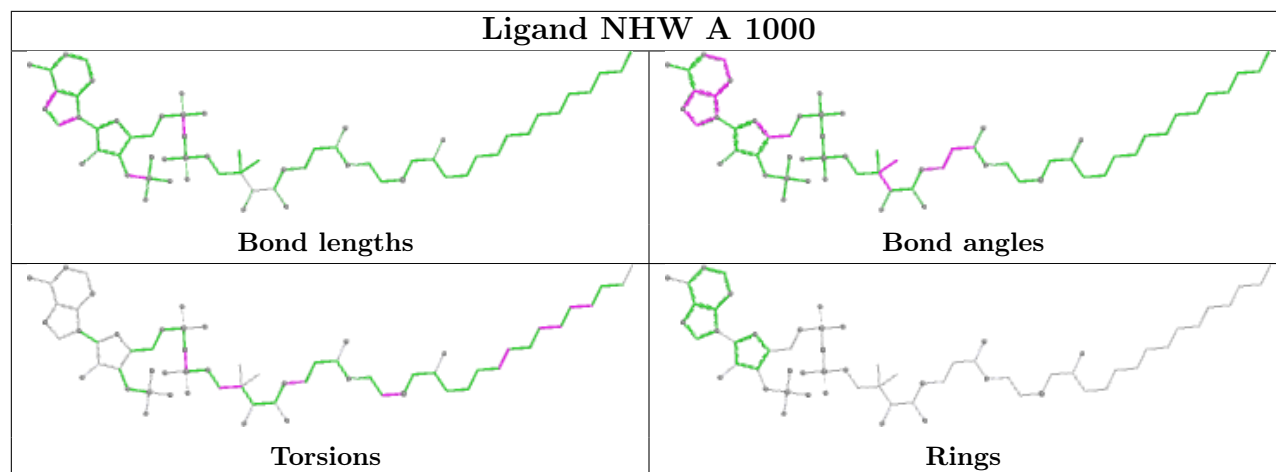
Mol	Chain	Res	Type	Atoms
3	A	1000	NHW	C9M-CAM-CBM-CCM
3	A	1000	NHW	C7M-C8M-C9M-CAM
3	A	1000	NHW	C6-C7-N8-C9
3	A	1000	NHW	P1A-O3A-P2A-O5A
3	A	1000	NHW	C14-C11-C12-O6A
3	A	1000	NHW	C4M-C5M-C6M-C7M
3	A	1000	NHW	C10-C11-C12-O6A
3	A	1000	NHW	P1A-O3A-P2A-O4A
3	A	1000	NHW	C3-C2-S1-CP
3	A	1000	NHW	C13-C11-C12-O6A

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	NHW	6	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 [i](#)

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

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	388/410 (94%)	0.26	10 (2%) 57 63	27, 53, 84, 124	8 (2%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	412	ALA	4.7
1	A	113	ALA	3.6
1	A	112	ALA	3.2
1	A	144	ASN	3.1
1	A	109	MET	2.8
1	A	411	PRO	2.7
1	A	432	LEU	2.4
1	A	479	TYR	2.2
1	A	413	HIS	2.2
1	A	313	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

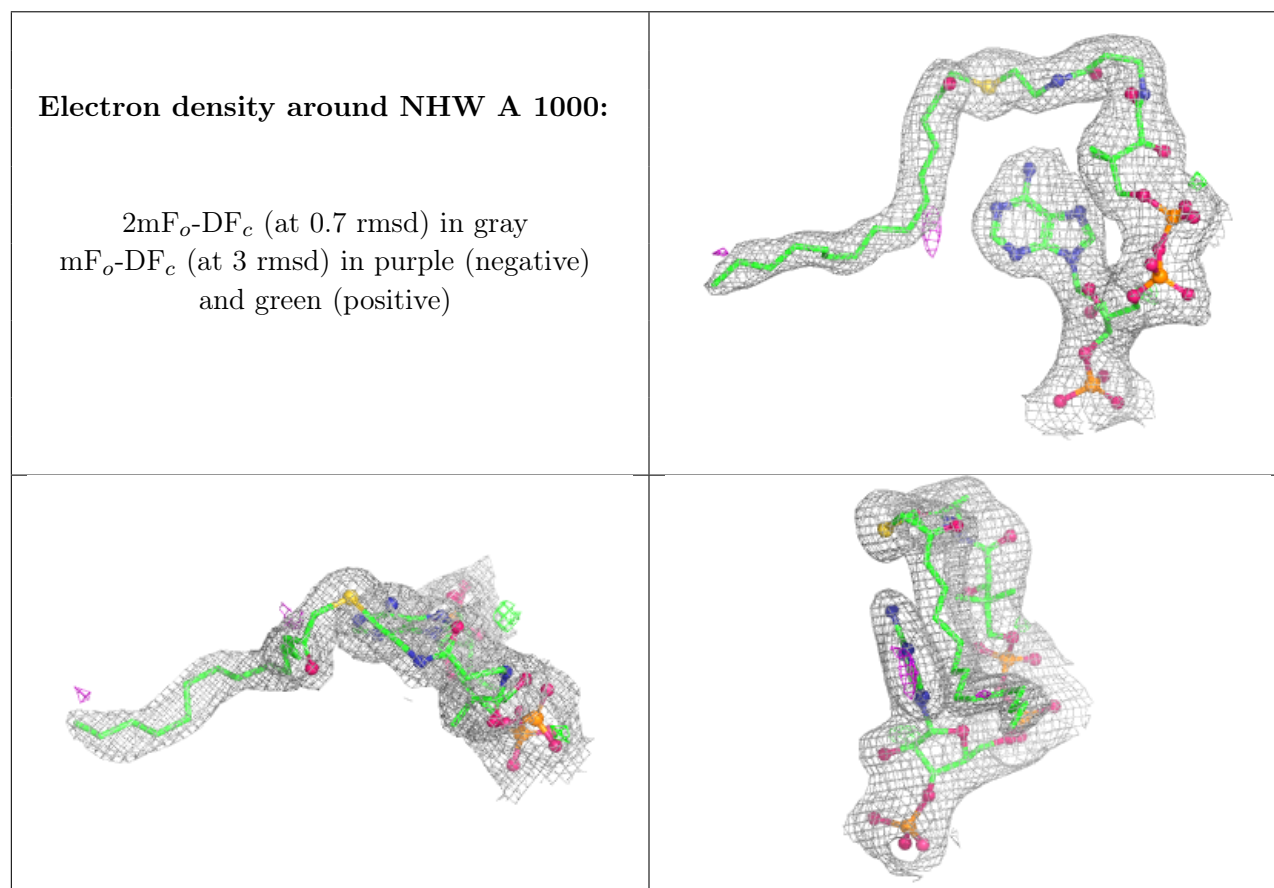
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
2	MG	A	999	1/1	0.95	0.11	65,65,65,65	0
3	NHW	A	1000	64/64	0.95	0.09	30,45,52,58	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 ⓘ

There are no such residues in this entry.