



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:34 AM UTC

PDB ID : 1E66 / pdb_00001e66
Title : STRUCTURE OF ACETYLCHOLINESTERASE COMPLEXED WITH (-)-HUPRINE X AT 2.1Å RESOLUTION
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Deposited on : 2000-08-08
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 ⓘ 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

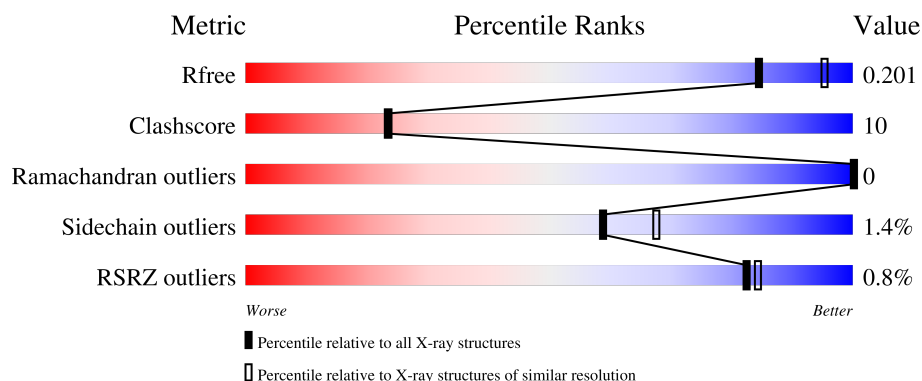
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	543	

2 Entry composition [i](#)

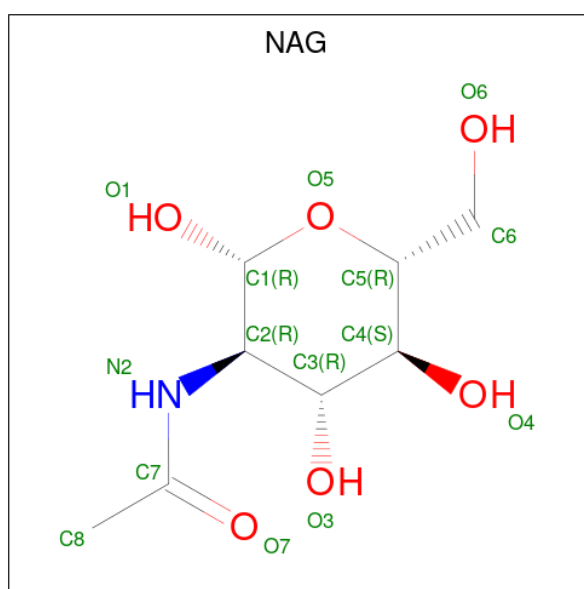
There are 4 unique types of molecules in this entry. The entry contains 4818 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYLCHOLINESTERASE.

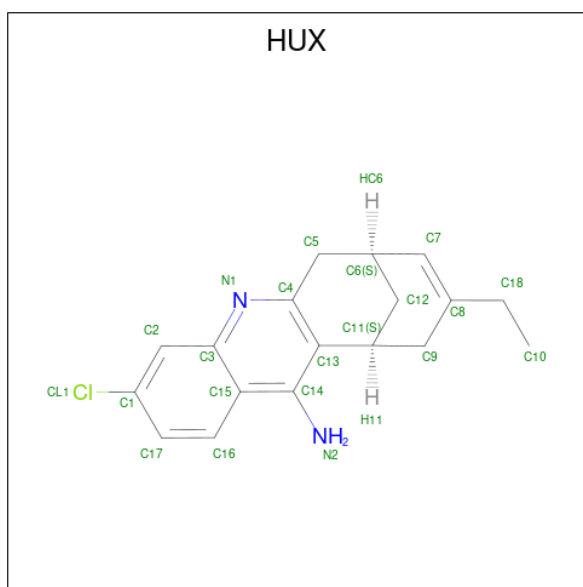
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	14	1
			4272	2747	721	779	25			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 3-CHLORO-9-ETHYL-6,7,8,9,10,11-HEXAHYDRO-7,11-METHANOCYCLO OCTA[B]QUINOLIN-12-AMINE (CCD ID: HUX) (formula: $C_{18}H_{19}ClN_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			21	18	1	2		

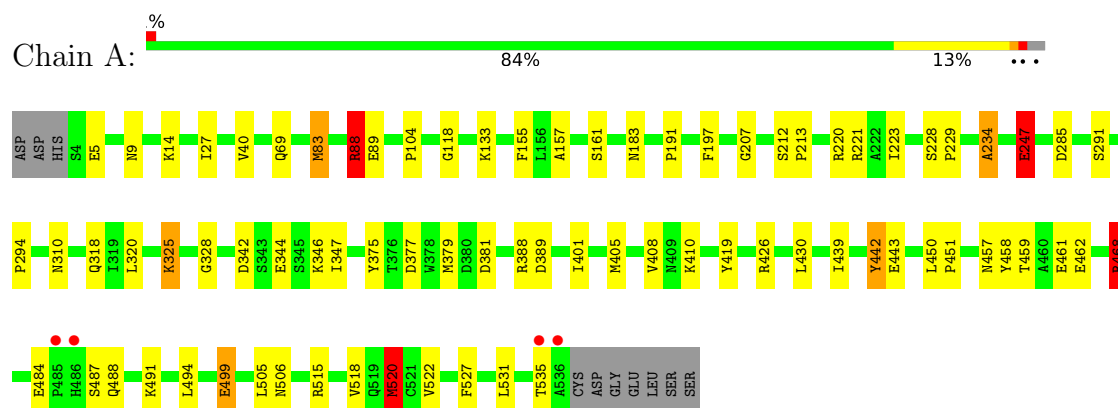
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	497	Total	O	0	0
			497	497		

3 Residue-property plots

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: ACETYLCHOLINESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	112.33Å 112.33Å 138.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.42 – 2.10 29.42 – 2.10	Depositor EDS
% Data completeness (in resolution range)	76.0 (29.42-2.10) 76.0 (29.42-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.177 , 0.205 0.172 , 0.201	Depositor DCC
R_{free} test set	4542 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4818	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: NAG, HUX

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	5.28	27/4395 (0.6%)	2.47	42/5975 (0.7%)

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	4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	468[A]	ARG	CZ-NH2	193.72	3.85	1.33
1	A	468[B]	ARG	CZ-NH2	193.72	3.85	1.33
1	A	88[A]	ARG	CZ-NH2	135.30	3.09	1.33
1	A	88[B]	ARG	CZ-NH2	135.30	3.09	1.33
1	A	468[A]	ARG	CZ-NH1	39.15	1.87	1.32
1	A	468[B]	ARG	CZ-NH1	39.15	1.87	1.32
1	A	325[A]	LYS	CE-NZ	28.40	2.34	1.49
1	A	325[B]	LYS	CE-NZ	28.40	2.34	1.49
1	A	247[A]	GLU	CD-OE2	22.55	1.68	1.25
1	A	247[B]	GLU	CD-OE2	22.55	1.68	1.25
1	A	88[A]	ARG	CZ-NH1	22.15	1.63	1.32
1	A	88[B]	ARG	CZ-NH1	22.15	1.63	1.32
1	A	88[A]	ARG	CG-CD	-21.03	0.89	1.52
1	A	88[B]	ARG	CG-CD	-21.03	0.89	1.52
1	A	247[A]	GLU	CD-OE1	-16.63	0.93	1.25
1	A	247[B]	GLU	CD-OE1	-16.63	0.93	1.25
1	A	83[A]	MET	CB-CG	-14.45	1.09	1.52
1	A	83[B]	MET	CB-CG	-14.45	1.09	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83[A]	MET	SD-CE	-8.79	1.57	1.79
1	A	83[B]	MET	SD-CE	-8.79	1.57	1.79
1	A	520[A]	MET	SD-CE	6.59	1.96	1.79
1	A	520[B]	MET	SD-CE	6.59	1.96	1.79
1	A	228[A]	SER	CA-CB	-5.82	1.45	1.54
1	A	228[B]	SER	CA-CB	-5.82	1.45	1.54
1	A	535	THR	C-N	-5.52	1.25	1.33
1	A	191[A]	PRO	CA-CB	5.11	1.61	1.53
1	A	191[B]	PRO	CA-CB	5.11	1.61	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	468[A]	ARG	NH1-CZ-NH2	-69.80	28.55	119.30
1	A	468[B]	ARG	NH1-CZ-NH2	-69.80	28.55	119.30
1	A	88[A]	ARG	NH1-CZ-NH2	-61.42	39.46	119.30
1	A	88[B]	ARG	NH1-CZ-NH2	-61.42	39.46	119.30
1	A	88[A]	ARG	NE-CZ-NH1	-49.21	72.29	121.50
1	A	88[B]	ARG	NE-CZ-NH1	-49.21	72.29	121.50
1	A	468[A]	ARG	NE-CZ-NH2	-44.59	79.07	119.20
1	A	468[B]	ARG	NE-CZ-NH2	-44.59	79.07	119.20
1	A	247[A]	GLU	OE1-CD-OE2	-30.47	49.78	122.90
1	A	247[B]	GLU	OE1-CD-OE2	-30.47	49.78	122.90
1	A	88[A]	ARG	NE-CZ-NH2	-17.41	103.53	119.20
1	A	88[B]	ARG	NE-CZ-NH2	-17.41	103.53	119.20
1	A	468[A]	ARG	NE-CZ-NH1	-14.50	107.00	121.50
1	A	468[B]	ARG	NE-CZ-NH1	-14.50	107.00	121.50
1	A	88[A]	ARG	CB-CG-CD	-11.44	85.00	111.30
1	A	88[B]	ARG	CB-CG-CD	-11.44	85.00	111.30
1	A	247[A]	GLU	CG-CD-OE1	-10.88	93.37	118.40
1	A	247[B]	GLU	CG-CD-OE1	-10.88	93.37	118.40
1	A	247[A]	GLU	CG-CD-OE2	10.17	141.80	118.40
1	A	247[B]	GLU	CG-CD-OE2	10.17	141.80	118.40
1	A	439	ILE	N-CA-C	9.35	122.23	109.80
1	A	291	SER	N-CA-C	8.08	119.71	111.07
1	A	401	ILE	N-CA-C	7.53	117.60	110.30
1	A	443	GLU	N-CA-C	-7.36	104.11	113.23
1	A	457	ASN	N-CA-C	7.24	121.41	112.58
1	A	285	ASP	N-CA-C	-6.70	98.29	108.67
1	A	328	GLY	N-CA-C	6.42	122.62	114.66
1	A	484	GLU	CA-C-N	6.33	127.75	119.84
1	A	484	GLU	C-N-CA	6.33	127.75	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	ILE	N-CA-C	5.96	116.88	108.36
1	A	442	TYR	N-CA-C	5.54	119.67	113.02
1	A	379	MET	N-CA-C	-5.42	106.71	113.38
1	A	522	VAL	N-CA-C	-5.42	105.25	110.72
1	A	381	ASP	N-CA-C	5.41	118.98	112.38
1	A	183	ASN	N-CA-C	5.31	121.50	114.12
1	A	234	ALA	N-CA-C	5.28	119.56	113.18
1	A	342	ASP	N-CA-C	5.26	119.39	112.92
1	A	69	GLN	N-CA-C	5.23	116.80	108.79
1	A	527	PHE	N-CA-C	5.18	116.78	111.03
1	A	157	ALA	N-CA-C	5.08	117.06	108.02
1	A	155	PHE	N-CA-C	5.05	121.17	113.19
1	A	40	VAL	N-CA-C	5.04	116.44	109.29

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	247[A]	GLU	Sidechain
1	A	442	TYR	Sidechain
1	A	468[A]	ARG	Sidechain
1	A	88[A]	ARG	Sidechain

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	4272	0	4052	81	0
2	A	28	0	26	5	0
3	A	21	0	19	1	0
4	A	497	0	0	5	0
All	All	4818	0	4097	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 10.

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:83[B]:MET:CB	1:A:83[B]:MET:CG	1.95	1.40
1:A:468[A]:ARG:NH1	1:A:468[A]:ARG:CZ	1.87	1.37
1:A:247[A]:GLU:OE2	1:A:247[A]:GLU:CD	1.68	1.36
1:A:83[A]:MET:CE	1:A:83[A]:MET:SD	1.11	1.19
1:A:468[B]:ARG:CZ	1:A:468[B]:ARG:NH1	2.08	1.16
1:A:520[A]:MET:CE	1:A:520[A]:MET:SD	1.07	1.16
1:A:468[B]:ARG:NH2	1:A:468[B]:ARG:HH11	1.47	1.12
1:A:83[A]:MET:SD	1:A:83[A]:MET:HE3	1.70	1.07
1:A:520[A]:MET:SD	1:A:520[A]:MET:HE1	1.66	1.07
1:A:520[A]:MET:SD	1:A:520[A]:MET:HE3	1.66	1.06
1:A:520[A]:MET:SD	1:A:520[A]:MET:HE2	1.66	1.05
1:A:83[A]:MET:SD	1:A:83[A]:MET:HE1	1.70	1.04
1:A:468[A]:ARG:HH11	1:A:468[A]:ARG:HD2	1.19	1.03
1:A:83[A]:MET:SD	1:A:83[A]:MET:HE2	1.70	1.03
1:A:88[B]:ARG:CD	1:A:88[B]:ARG:CG	2.42	0.98
1:A:88[A]:ARG:NH1	1:A:88[A]:ARG:HD2	1.82	0.95
1:A:88[B]:ARG:NH2	1:A:88[B]:ARG:HH11	1.66	0.94
1:A:468[A]:ARG:HH11	1:A:468[A]:ARG:NH2	1.67	0.91
1:A:325[A]:LYS:CE	1:A:325[A]:LYS:NZ	2.34	0.90
1:A:468[A]:ARG:NH1	1:A:468[A]:ARG:CD	2.35	0.90
1:A:83[A]:MET:CE	1:A:83[A]:MET:CG	2.51	0.89
1:A:468[A]:ARG:NH1	1:A:468[A]:ARG:HD2	1.85	0.88
1:A:247[B]:GLU:OE2	1:A:247[B]:GLU:HG3	1.73	0.87
1:A:88[A]:ARG:NH1	1:A:88[A]:ARG:CD	2.43	0.81
1:A:88[A]:ARG:NH1	1:A:88[A]:ARG:NH2	2.29	0.80
1:A:468[A]:ARG:HH11	1:A:468[A]:ARG:CD	1.90	0.80
1:A:468[A]:ARG:NH1	1:A:468[A]:ARG:NH2	2.28	0.80
1:A:88[B]:ARG:NH2	1:A:88[B]:ARG:NH1	2.30	0.79
1:A:468[B]:ARG:NH1	1:A:468[B]:ARG:NH2	2.30	0.78
1:A:468[A]:ARG:NH1	1:A:468[A]:ARG:NE	2.33	0.77
2:A:801:NAG:H3	2:A:801:NAG:H82	1.69	0.75
1:A:88[B]:ARG:NH2	1:A:88[B]:ARG:HE	1.84	0.75
1:A:88[A]:ARG:NH1	1:A:88[A]:ARG:HH21	1.91	0.68
2:A:801:NAG:H82	2:A:801:NAG:C3	2.24	0.67
1:A:520[A]:MET:HG2	4:A:1113:HOH:O	1.94	0.67
1:A:88[B]:ARG:CD	1:A:88[B]:ARG:CB	2.74	0.66
1:A:247[B]:GLU:OE2	1:A:247[B]:GLU:CG	2.45	0.65
1:A:310:ASN:HD21	1:A:410:LYS:NZ	1.97	0.63
1:A:221:ARG:HD3	1:A:318:GLN:OE1	2.00	0.62
1:A:468[A]:ARG:HD2	1:A:468[A]:ARG:NH2	2.16	0.61
1:A:247[B]:GLU:OE2	1:A:247[B]:GLU:OE1	2.20	0.60
1:A:83[B]:MET:CG	1:A:83[B]:MET:CA	2.77	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247[A]:GLU:OE2	1:A:247[A]:GLU:OE1	2.19	0.59
1:A:468[B]:ARG:NH2	1:A:468[B]:ARG:HD3	2.19	0.57
1:A:520[A]:MET:HE2	1:A:520[A]:MET:HA	1.86	0.56
1:A:89:GLU:CG	4:A:1372:HOH:O	2.54	0.54
1:A:310:ASN:HD21	1:A:410:LYS:HZ1	1.52	0.54
1:A:344:GLU:OE2	1:A:346:LYS:HE3	2.08	0.54
1:A:223:ILE:HA	1:A:320:LEU:O	2.07	0.54
1:A:5:GLU:OE2	1:A:104:PRO:HA	2.09	0.52
1:A:499:GLU:HG3	4:A:1296:HOH:O	2.09	0.52
1:A:88[B]:ARG:HD3	1:A:88[B]:ARG:HA	1.92	0.51
1:A:9[A]:ASN:ND2	1:A:14:LYS:HG2	2.26	0.51
1:A:375:TYR:CZ	1:A:520[B]:MET:SD	3.04	0.51
1:A:468[A]:ARG:NH2	1:A:468[A]:ARG:CD	2.74	0.51
1:A:405:MET:HA	1:A:408:VAL:HG12	1.92	0.50
1:A:197:PHE:CB	1:A:223:ILE:HB	2.41	0.50
2:A:801:NAG:C3	2:A:801:NAG:C8	2.87	0.50
1:A:451:PRO:HA	1:A:458:TYR:CD1	2.46	0.50
1:A:531:LEU:C	1:A:531:LEU:HD23	2.37	0.50
1:A:459:THR:OG1	1:A:462:GLU:HG3	2.12	0.50
1:A:419:TYR:CZ	1:A:494:LEU:HD13	2.46	0.50
1:A:88[B]:ARG:CD	1:A:88[B]:ARG:HA	2.44	0.48
1:A:310:ASN:ND2	1:A:410:LYS:NZ	2.62	0.47
1:A:488:GLN:CG	4:A:1263:HOH:O	2.63	0.47
1:A:247[A]:GLU:OE1	1:A:247[A]:GLU:HB2	2.15	0.46
1:A:515:ARG:HB3	1:A:518:VAL:HB	1.96	0.46
1:A:88[B]:ARG:NH2	1:A:88[B]:ARG:NE	2.57	0.46
1:A:118:GLY:HA2	3:A:803:HUX:C8	2.46	0.46
1:A:491:LYS:HA	1:A:491:LYS:HD3	1.79	0.45
1:A:220:ARG:HG3	1:A:221:ARG:HG3	1.98	0.45
1:A:88[A]:ARG:NH1	1:A:88[A]:ARG:HD3	2.27	0.45
1:A:197:PHE:HB3	1:A:223:ILE:HB	1.99	0.45
1:A:207:GLY:HA3	1:A:229:PRO:HD3	1.99	0.45
1:A:388:ARG:HD2	1:A:389:ASP:OD1	2.16	0.45
1:A:506:ASN:HB2	4:A:1115:HOH:O	2.17	0.44
1:A:426:ARG:CZ	1:A:430:LEU:HD23	2.47	0.44
1:A:212:SER:HA	1:A:213:PRO:HD3	1.88	0.44
1:A:27:ILE:HD11	1:A:133:LYS:HB2	2.00	0.43
1:A:468[B]:ARG:NH1	1:A:468[B]:ARG:HD3	2.34	0.42
1:A:461:GLU:OE1	1:A:461:GLU:N	2.41	0.41
2:A:801:NAG:C8	2:A:801:NAG:O3	2.68	0.41
1:A:377:ASP:OD1	1:A:377:ASP:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ALA:O	1:A:294:PRO:HD2	2.21	0.41
1:A:450:LEU:N	1:A:451:PRO:CD	2.84	0.40
2:A:801:NAG:H82	2:A:801:NAG:O3	2.21	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	545/543 (100%)	520 (95%)	25 (5%)	0	100 100

There are no Ramachandran outliers to report.

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	451/474 (95%)	443 (98%)	8 (2%)	51 60

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88[A]	ARG
1	A	88[B]	ARG
1	A	161	SER

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Mol	Chain	Res	Type
1	A	487	SER
1	A	499	GLU
1	A	505	LEU
1	A	520[A]	MET
1	A	520[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	65	ASN
1	A	68	GLN
1	A	251	ASN
1	A	280	ASN
1	A	310	ASN
1	A	409	ASN
1	A	500	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are 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	HUX	A	803	-	23,24,24	4.07	13 (56%)	24,36,36	3.86	15 (62%)
2	NAG	A	802	1	14,14,15	0.73	0	17,19,21	0.78	1 (5%)
2	NAG	A	801	1	14,14,15	1.09	1 (7%)	17,19,21	1.22	3 (17%)

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	HUX	A	803	-	-	0/2/22/22	0/5/4/4
2	NAG	A	802	1	-	2/6/23/26	0/1/1/1
2	NAG	A	801	1	-	3/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	HUX	C5-C4	10.88	1.62	1.51
3	A	803	HUX	C17-C1	7.13	1.51	1.38
3	A	803	HUX	C2-C1	6.81	1.48	1.36
3	A	803	HUX	C6-C7	5.88	1.67	1.51
3	A	803	HUX	C3-N1	5.65	1.46	1.37
3	A	803	HUX	C12-C11	4.81	1.59	1.53
3	A	803	HUX	C16-C15	4.52	1.51	1.42
2	A	801	NAG	C1-C2	3.63	1.57	1.52
3	A	803	HUX	C1-CL1	-3.25	1.66	1.74
3	A	803	HUX	C13-C4	-3.17	1.38	1.42
3	A	803	HUX	C15-C3	-2.94	1.37	1.42
3	A	803	HUX	C4-N1	2.64	1.35	1.32
3	A	803	HUX	C14-C13	2.41	1.50	1.41
3	A	803	HUX	C2-C3	-2.12	1.38	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	HUX	C13-C4-N1	8.06	127.19	123.65
3	A	803	HUX	C2-C3-C15	7.83	128.32	119.58
3	A	803	HUX	C9-C11-C13	-6.60	104.42	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	HUX	C14-C15-C3	6.34	121.77	118.23
3	A	803	HUX	C2-C3-N1	-5.12	111.29	118.78
3	A	803	HUX	C1-C2-C3	-4.96	115.38	119.47
3	A	803	HUX	C17-C1-C2	-4.30	117.28	122.00
3	A	803	HUX	C16-C17-C1	4.29	123.79	119.22
3	A	803	HUX	C11-C9-C8	3.19	118.56	112.78
3	A	803	HUX	C13-C14-N2	-3.17	117.11	121.11
3	A	803	HUX	C2-C1-CL1	3.03	123.29	119.65
2	A	801	NAG	C1-C2-N2	2.72	114.71	110.43
3	A	803	HUX	C12-C11-C13	2.66	114.96	111.52
3	A	803	HUX	C17-C16-C15	-2.57	117.55	121.15
3	A	803	HUX	C15-C3-N1	-2.30	120.37	122.80
2	A	801	NAG	C8-C7-N2	2.29	119.92	116.12
2	A	802	NAG	C2-N2-C7	-2.28	119.84	122.90
2	A	801	NAG	O7-C7-C8	-2.25	118.06	122.05
3	A	803	HUX	C5-C4-N1	-2.07	113.07	116.39

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAG	C3-C2-N2-C7
2	A	801	NAG	C8-C7-N2-C2
2	A	801	NAG	O7-C7-N2-C2
2	A	802	NAG	O5-C5-C6-O6
2	A	802	NAG	C4-C5-C6-O6

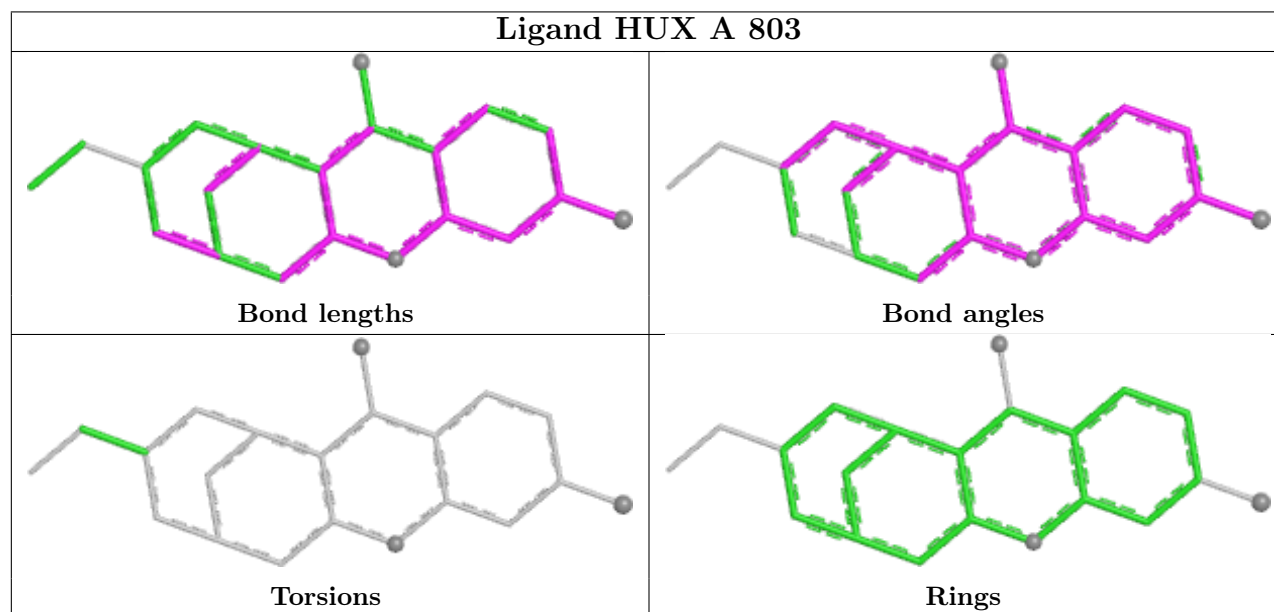
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	HUX	1	0
2	A	801	NAG	5	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	533/543 (98%)	-0.40	4 (0%) 82 84	11, 31, 46, 70	14 (2%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	486	HIS	3.8
1	A	485	PRO	3.1
1	A	536	ALA	2.8
1	A	535	THR	2.6

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](#)

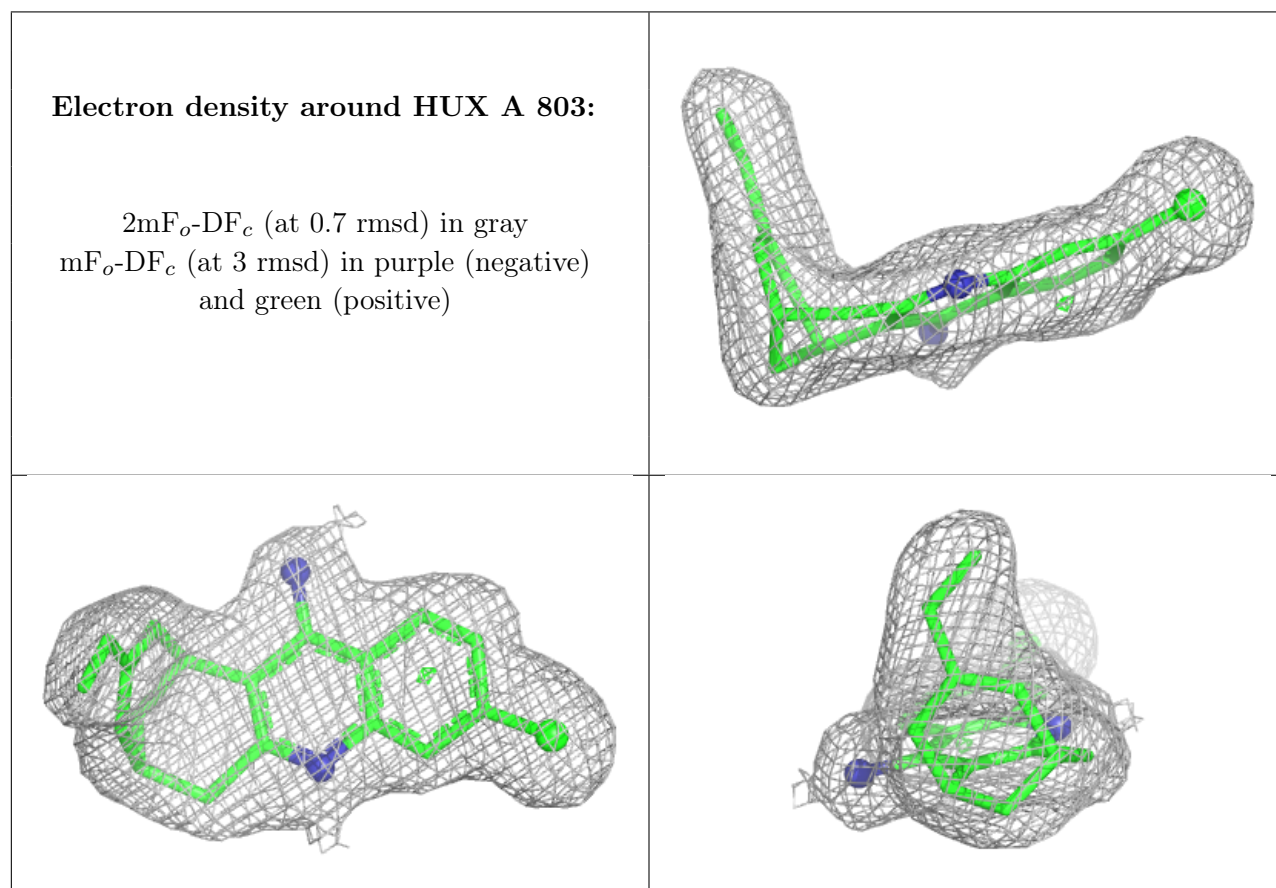
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
2	NAG	A	801	14/15	0.61	0.16	67,72,74,74	0
2	NAG	A	802	14/15	0.87	0.10	46,49,53,54	0
3	HUX	A	803	21/21	0.98	0.06	24,26,27,28	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.