



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:16 AM UTC

PDB ID : 7AIW / pdb_00007aiw
Title : Crystal structure of Torpedo Californica acetylcholinesterase in complex with (E)-10-[(3-Chloro-6,7,10,11-tetrahydro-9-methyl-7,11-methanocycloocta[b]quinolin-12-yl)amino]-N-(4-hydroxy-3-methoxybenzyl)-6-decenamide
Authors : Coquelle, N.; Colletier, J.P.
Deposited on : 2020-09-28
Resolution : 1.90 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

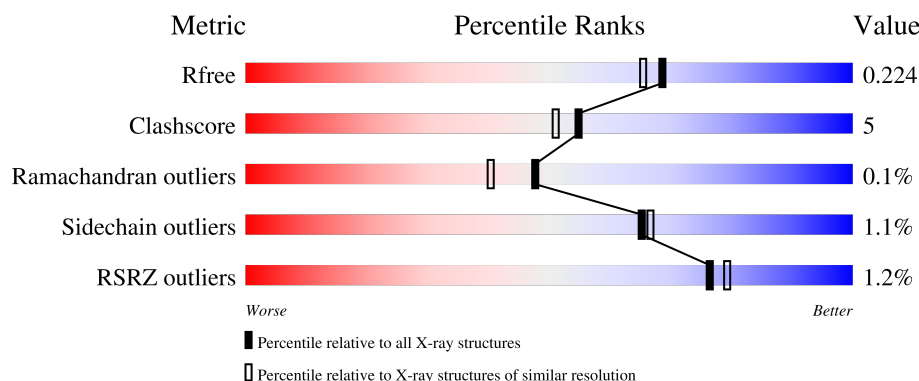
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

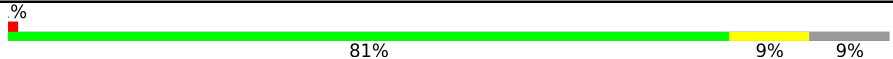
The reported resolution of this entry is 1.90 Å.

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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	586	 % 81% 9% 9%
1	B	586	 % 83% 8% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	8U5	A	601	X	-	-	-
2	8U5	B	601	X	-	-	-

2 Entry composition [i](#)

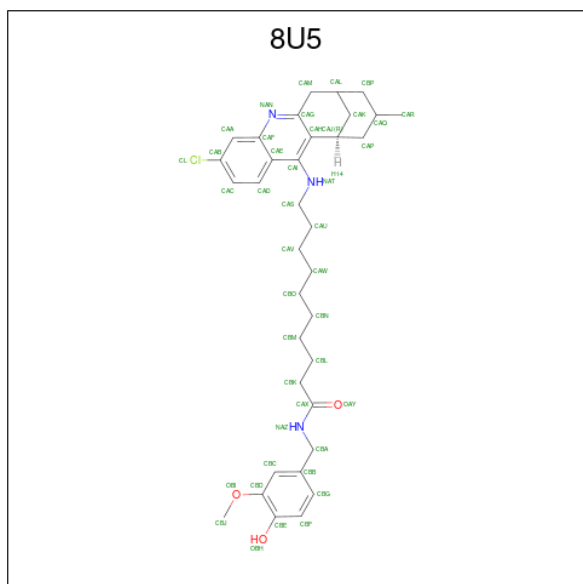
There are 7 unique types of molecules in this entry. The entry contains 9783 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

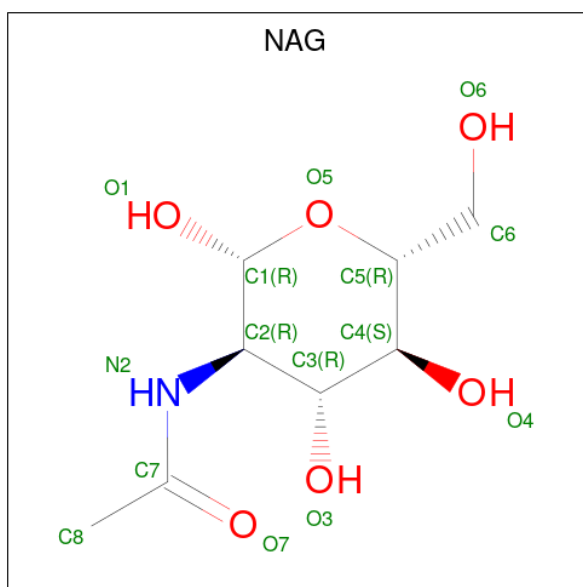
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	1	14	0
			4311	2771	734	782	24			
1	B	532	Total	C	N	O	S	5	10	0
			4283	2752	723	784	24			

- Molecule 2 is E)-10-[(3-Chloro-6,7,10,11-tetrahydro-9-methyl-7,11-methanocycloocta[b]quinolin-12-yl)amino]-N-(4-hydroxy-3-methoxybenzyl)-6-decenamide (CCD ID: 8U5) (formula: $C_{35}H_{46}ClN_3O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			42	35	1	3	3		
2	B	1	Total	C	Cl	N	O	0	0
			42	35	1	3	3		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

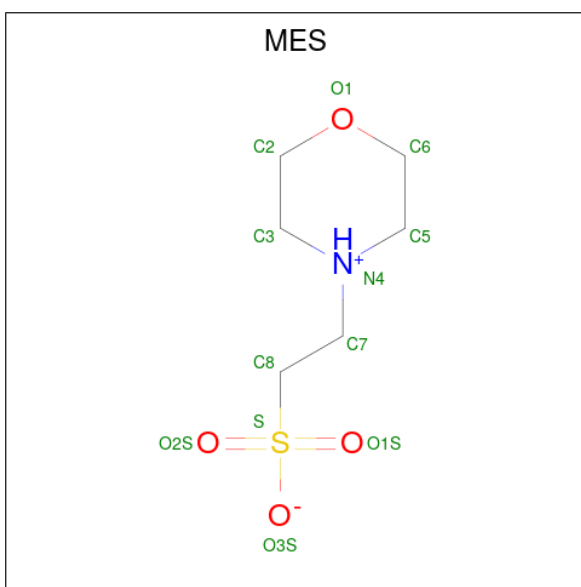


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			15	8	1	6		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

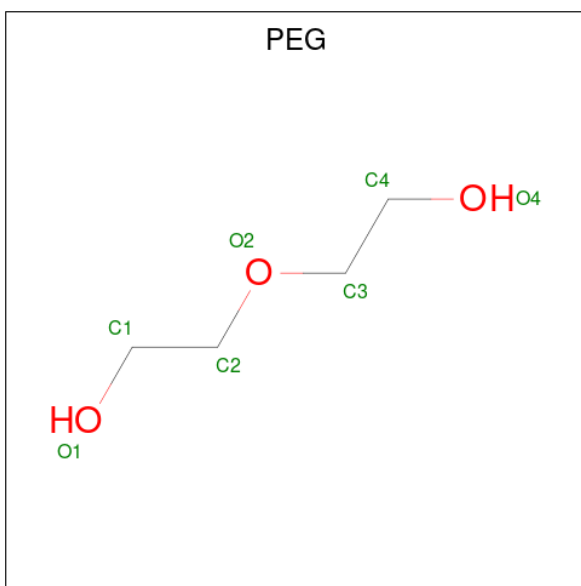
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		

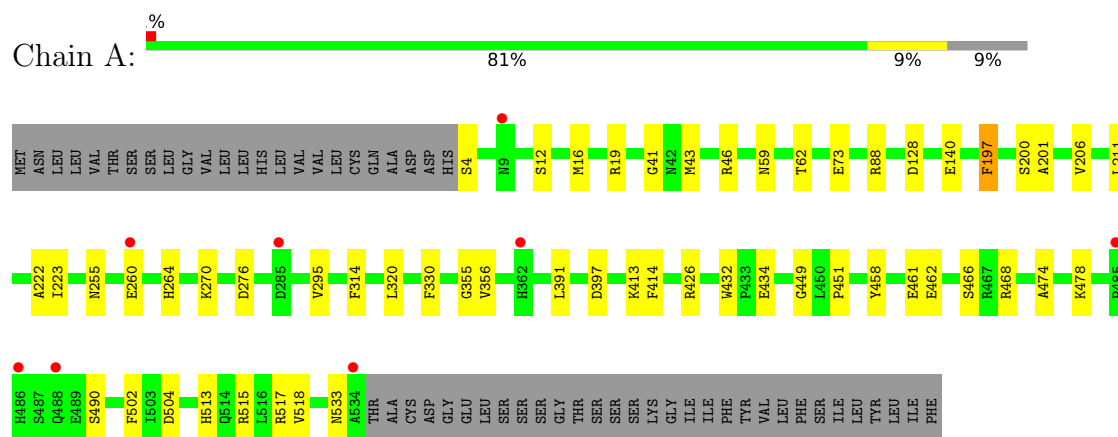
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	502	Total 502	O 502	0	0
7	B	490	Total 490	O 490	0	0

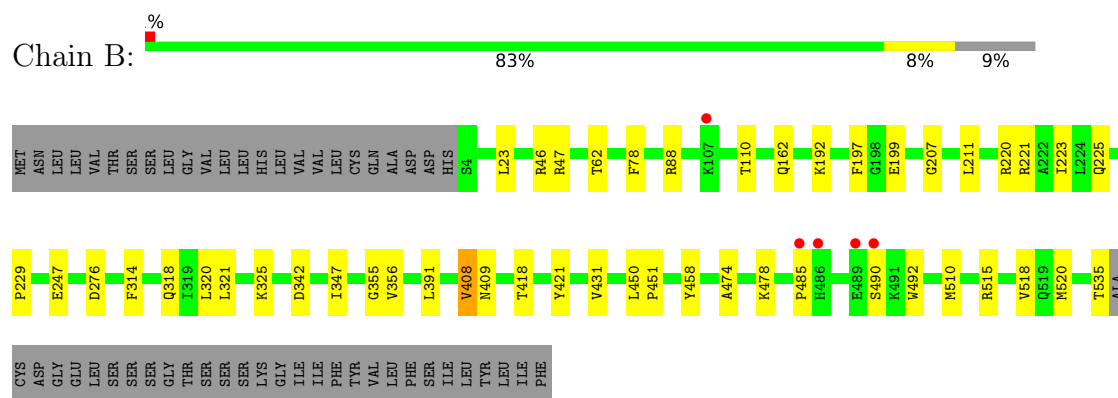
3 Residue-property plots [i](#)

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: Acetylcholinesterase



• Molecule 1: Acetylcholinesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.93Å 106.51Å 150.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.08 – 1.90 46.08 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.5 (46.08-1.90) 97.7 (46.08-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.190 , 0.224 0.191 , 0.224	Depositor DCC
R_{free} test set	5709 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.837	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9783	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.29 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4115e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, CL, 8U5, PEG, MES

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	0.29	0/4476	0.50	0/6070
1	B	0.29	0/4436	0.50	0/6022
All	All	0.29	0/8912	0.50	0/12092

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	4311	0	4211	38	0
1	B	4283	0	4151	37	0
2	A	42	0	0	0	0
2	B	42	0	0	0	0
3	A	57	0	54	9	0
3	B	28	0	26	0	0
4	A	2	0	0	1	0
5	A	12	0	12	1	0
6	A	14	0	20	0	0
7	A	502	0	0	20	3
7	B	490	0	0	13	3
All	All	9783	0	8474	82	3

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 5.

All (82) 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:A:602:NAG:O4	7:A:701:HOH:O	1.85	0.95
1:B:23:LEU:O	7:B:701:HOH:O	1.86	0.92
4:A:607:CL:CL	7:A:1075:HOH:O	2.30	0.86
1:A:413:LYS:HD3	1:A:414:PHE:CE2	2.10	0.86
1:B:192:LYS:NZ	7:B:703:HOH:O	2.14	0.81
3:A:604:NAG:O4	7:A:702:HOH:O	2.03	0.74
1:A:140[A]:GLU:OE2	7:A:705:HOH:O	2.05	0.73
1:B:342:ASP:OD2	7:B:702:HOH:O	2.07	0.71
1:A:128:ASP:OD1	7:A:707:HOH:O	2.11	0.68
3:A:604:NAG:O4	7:A:706:HOH:O	2.10	0.68
1:A:468[B]:ARG:NH1	7:A:714:HOH:O	2.26	0.67
1:B:46:ARG:HD3	7:B:710:HOH:O	1.94	0.67
3:A:603:NAG:O4	7:A:708:HOH:O	2.13	0.66
1:A:355:GLY:HA3	1:A:391:LEU:HD21	1.79	0.64
1:B:62:THR:HG23	1:B:88[B]:ARG:NH2	2.16	0.60
1:A:260:GLU:H	1:A:260:GLU:CD	2.11	0.58
1:A:504:ASP:O	7:A:710:HOH:O	2.18	0.56
3:A:602:NAG:O6	7:A:709:HOH:O	2.17	0.56
1:B:276:ASP:OD2	7:B:705:HOH:O	2.17	0.56
1:B:535:THR:O	7:B:704:HOH:O	2.17	0.56
1:A:478:LYS:NZ	7:A:703:HOH:O	2.04	0.56
1:A:533:ASN:ND2	7:A:721:HOH:O	2.38	0.56
1:A:264:HIS:CE1	3:A:605:NAG:H61	2.41	0.55
1:B:220:ARG:HG3	1:B:221:ARG:HG3	1.88	0.55
1:B:47:ARG:HH21	1:B:162:GLN:HE22	1.55	0.54
1:A:19[B]:ARG:HD3	7:A:704:HOH:O	2.06	0.54
1:A:211:LEU:HD23	1:A:314:PHE:HB3	1.90	0.54
1:A:474:ALA:O	1:A:478:LYS:HG3	2.08	0.53
1:B:62:THR:HG23	1:B:88[B]:ARG:HH22	1.74	0.53
1:B:207:GLY:HA3	1:B:229:PRO:HD3	1.90	0.53
1:B:478:LYS:NZ	7:B:714:HOH:O	2.28	0.53
1:B:355:GLY:HA3	1:B:391:LEU:HD21	1.90	0.52
1:B:211:LEU:HD23	1:B:314:PHE:HB3	1.91	0.51
1:A:264:HIS:ND1	3:A:605:NAG:H61	2.25	0.51
1:A:41:GLY:HA2	3:A:605:NAG:H83	1.93	0.51
1:A:62:THR:HG23	1:A:88[B]:ARG:NH2	2.26	0.50
1:A:397:ASP:OD1	1:A:517:ARG:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:PHE:HB3	1:A:223:ILE:HB	1.93	0.50
1:A:200:SER:OG	1:A:201:ALA:N	2.46	0.49
1:B:451:PRO:HA	1:B:458:TYR:CD1	2.46	0.49
1:A:515:ARG:HB3	1:A:518:VAL:HB	1.95	0.49
1:B:110:THR:OG1	1:B:478:LYS:HG2	2.12	0.49
1:A:426[B]:ARG:NH1	1:A:434:GLU:OE1	2.46	0.48
1:A:19[B]:ARG:NH1	7:A:704:HOH:O	2.04	0.48
1:A:223:ILE:HA	1:A:320:LEU:O	2.14	0.48
1:B:223:ILE:HA	1:B:320:LEU:O	2.14	0.48
1:A:426[A]:ARG:NH2	1:A:432:TRP:O	2.46	0.47
1:B:409:ASN:OD1	7:B:707:HOH:O	2.21	0.47
1:A:461:GLU:HG3	1:A:462:GLU:N	2.30	0.47
1:A:270[A]:LYS:HD3	7:A:814:HOH:O	2.15	0.46
1:B:197:PHE:CB	1:B:223:ILE:HB	2.46	0.46
1:A:43[A]:MET:HA	1:A:46[A]:ARG:HD2	1.97	0.46
1:B:47:ARG:NH1	7:B:734:HOH:O	2.48	0.46
1:B:47:ARG:NH1	7:B:737:HOH:O	2.49	0.46
1:A:276:ASP:OD2	7:A:711:HOH:O	2.20	0.45
1:B:221:ARG:HD3	1:B:318:GLN:OE1	2.16	0.45
1:B:515:ARG:HB3	1:B:518:VAL:HB	1.99	0.45
1:A:4:SER:N	7:A:734:HOH:O	2.49	0.44
1:B:199:GLU:HA	1:B:225:GLN:O	2.17	0.44
1:B:247:GLU:OE2	7:B:706:HOH:O	2.20	0.44
1:B:321:LEU:HD21	1:B:408:VAL:HG23	1.99	0.44
5:A:608:MES:H81	5:A:608:MES:H51	1.64	0.44
1:A:451:PRO:HA	1:A:458:TYR:CD1	2.53	0.43
1:B:421:TYR:HB3	1:B:492:TRP:CZ2	2.54	0.43
1:A:197:PHE:CB	1:A:223:ILE:HB	2.48	0.43
1:A:73[A]:GLU:OE1	7:A:712:HOH:O	2.21	0.43
1:A:206:VAL:CG1	1:A:222:ALA:HB1	2.49	0.43
1:A:43[A]:MET:HE2	7:A:1034:HOH:O	2.19	0.43
1:B:408:VAL:HG22	1:B:418:THR:HG21	2.00	0.43
1:B:474:ALA:O	1:B:478:LYS:HG3	2.19	0.43
1:B:391:LEU:HD12	1:B:391:LEU:HA	1.89	0.42
1:B:325:LYS:HE2	7:B:749:HOH:O	2.19	0.42
1:B:47:ARG:HH21	1:B:162:GLN:NE2	2.18	0.42
1:B:78:PHE:CZ	1:B:431:VAL:HG12	2.55	0.42
1:B:347:ILE:HD13	1:B:347:ILE:HA	1.87	0.41
1:A:59:ASN:HD22	3:A:602:NAG:H83	1.84	0.41
1:B:46:ARG:NE	7:B:740:HOH:O	2.52	0.41
1:B:490:SER:HB2	1:B:510:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:GLY:HA2	1:A:466:SER:OG	2.20	0.41
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.56	0.41
1:A:255:ASN:HB2	7:A:936:HOH:O	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:829:HOH:O	7:B:770:HOH:O[4_576]	1.77	0.43
7:A:829:HOH:O	7:B:967:HOH:O[4_576]	1.98	0.22
7:A:952:HOH:O	7:B:703:HOH:O[4_576]	2.17	0.03

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	543/586 (93%)	527 (97%)	16 (3%)	0	100	100
1	B	540/586 (92%)	518 (96%)	21 (4%)	1 (0%)	43	36
All	All	1083/1172 (92%)	1045 (96%)	37 (3%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	485	PRO

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	475/513 (93%)	468 (98%)	7 (2%)	57	56
1	B	470/513 (92%)	467 (99%)	3 (1%)	78	81
All	All	945/1026 (92%)	935 (99%)	10 (1%)	65	67

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	16	MET
1	A	197	PHE
1	A	295	VAL
1	A	330	PHE
1	A	356	VAL
1	A	490	SER
1	B	356	VAL
1	B	408	VAL
1	B	450	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	HIS
1	A	253	ASN
1	A	257	ASN
1	B	42	ASN
1	B	162	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	NAG	B	603	1	14,14,15	0.35	0	17,19,21	0.41	0
3	NAG	B	602	1	14,14,15	0.42	0	17,19,21	0.52	0
3	NAG	A	604	1	14,14,15	0.55	0	17,19,21	0.46	0
6	PEG	A	610	-	6,6,6	0.48	0	5,5,5	0.31	0
3	NAG	A	602	1	14,14,15	0.29	0	17,19,21	0.56	0
5	MES	A	608	-	12,12,12	2.28	1 (8%)	15,16,16	2.41	5 (33%)
6	PEG	A	609	-	6,6,6	0.49	0	5,5,5	0.25	0
2	8U5	B	601	-	46,46,46	2.31	12 (26%)	55,63,63	3.04	15 (27%)
2	8U5	A	601	-	46,46,46	2.18	9 (19%)	55,63,63	3.10	13 (23%)
3	NAG	A	605	-	15,15,15	0.69	1 (6%)	21,21,21	0.57	0
3	NAG	A	603	1	14,14,15	0.26	0	17,19,21	0.47	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	NAG	B	603	1	-	0/6/23/26	0/1/1/1
3	NAG	B	602	1	-	2/6/23/26	0/1/1/1
3	NAG	A	604	1	-	2/6/23/26	0/1/1/1
6	PEG	A	610	-	-	2/4/4/4	-
3	NAG	A	602	1	-	2/6/23/26	0/1/1/1
5	MES	A	608	-	-	4/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	A	609	-	-	4/4/4/4	-
2	8U5	B	601	-	2/2/4/6	8/20/40/40	0/6/5/5
2	8U5	A	601	-	2/2/4/6	9/20/40/40	0/6/5/5
3	NAG	A	605	-	-	0/6/26/26	0/1/1/1
3	NAG	A	603	1	-	1/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	608	MES	C8-S	-7.52	1.67	1.77
2	B	601	8U5	CAM-CAG	-6.73	1.44	1.51
2	A	601	8U5	CBP-CAL	-6.53	1.34	1.52
2	B	601	8U5	CBP-CAL	-6.22	1.35	1.52
2	B	601	8U5	CBA-CBB	-5.72	1.38	1.51
2	A	601	8U5	CAM-CAG	-5.62	1.45	1.51
2	B	601	8U5	CBP-CAQ	-5.51	1.40	1.53
2	A	601	8U5	CBP-CAQ	-5.45	1.41	1.53
2	A	601	8U5	CBA-CBB	-5.33	1.39	1.51
2	B	601	8U5	CAH-CAJ	-4.98	1.43	1.51
2	A	601	8U5	CAH-CAJ	-4.82	1.44	1.51
2	A	601	8U5	CAR-CAQ	-3.80	1.40	1.52
2	B	601	8U5	CAP-CAJ	3.69	1.58	1.53
2	B	601	8U5	CAR-CAQ	-3.52	1.41	1.52
2	A	601	8U5	CAP-CAQ	-3.26	1.45	1.53
2	A	601	8U5	CAP-CAJ	2.96	1.57	1.53
2	B	601	8U5	CAP-CAQ	-2.93	1.46	1.53
3	A	605	NAG	C1-C2	2.45	1.55	1.52
2	A	601	8U5	CAG-NAN	2.28	1.34	1.32
2	B	601	8U5	CAF-NAN	-2.14	1.34	1.37
2	B	601	8U5	CAK-CAL	-2.11	1.47	1.52
2	B	601	8U5	CAG-NAN	2.08	1.34	1.32
2	B	601	8U5	CAS-NAT	2.02	1.49	1.45

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	8U5	CAH-CAG-NAN	-13.03	117.93	123.65
2	B	601	8U5	CAH-CAG-NAN	-9.10	119.66	123.65
2	A	601	8U5	CAP-CAQ-CBP	8.62	122.62	110.02
2	B	601	8U5	CBB-CBA-NAZ	-8.27	95.64	113.07
2	B	601	8U5	CAP-CAQ-CBP	8.09	121.85	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	8U5	CBP-CAL-CAK	6.68	122.38	109.69
2	B	601	8U5	CAG-CAM-CAL	-6.43	99.44	111.77
2	A	601	8U5	CBP-CAL-CAK	6.40	121.85	109.69
2	A	601	8U5	CAG-CAM-CAL	-6.40	99.50	111.77
2	A	601	8U5	CAG-NAN-CAF	5.38	124.04	117.67
2	B	601	8U5	CAR-CAQ-CAP	5.12	119.68	111.17
5	A	608	MES	C5-N4-C3	5.00	119.62	108.84
2	A	601	8U5	CAK-CAL-CAM	4.99	114.62	109.37
2	B	601	8U5	CBJ-OBI-CBD	-4.99	110.20	117.51
2	B	601	8U5	CAJ-CAK-CAL	-4.88	93.49	110.60
2	A	601	8U5	CAJ-CAK-CAL	-4.85	93.59	110.60
2	B	601	8U5	CAG-NAN-CAF	4.55	123.06	117.67
2	A	601	8U5	CAR-CAQ-CBP	4.52	118.67	111.17
2	A	601	8U5	CAR-CAQ-CAP	4.47	118.59	111.17
2	B	601	8U5	CAR-CAQ-CBP	4.37	118.43	111.17
5	A	608	MES	C6-C5-N4	-4.36	103.49	110.12
2	A	601	8U5	CBJ-OBI-CBD	-4.35	111.14	117.51
2	B	601	8U5	CAK-CAL-CAM	4.12	113.70	109.37
2	A	601	8U5	CAH-CAI-NAT	-4.01	112.95	119.47
2	B	601	8U5	CBA-NAZ-CAX	3.80	128.59	122.42
5	A	608	MES	O1S-S-C8	3.43	111.91	106.73
5	A	608	MES	C7-N4-C5	3.35	120.18	111.24
2	B	601	8U5	CAP-CAJ-CAK	-3.33	105.65	109.55
2	B	601	8U5	CBG-CBF-CBE	-2.72	117.78	120.50
2	A	601	8U5	CAM-CAG-NAN	2.67	120.67	116.39
5	A	608	MES	C7-N4-C3	2.58	118.11	111.24
2	B	601	8U5	CBA-CBB-CBG	-2.26	116.32	120.94
2	A	601	8U5	CAP-CAJ-CAK	-2.15	107.03	109.55

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	8U5	CAQ
2	A	601	8U5	CAL
2	B	601	8U5	CAQ
2	B	601	8U5	CAL

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	608	MES	C8-C7-N4-C5
5	A	608	MES	C7-C8-S-O2S

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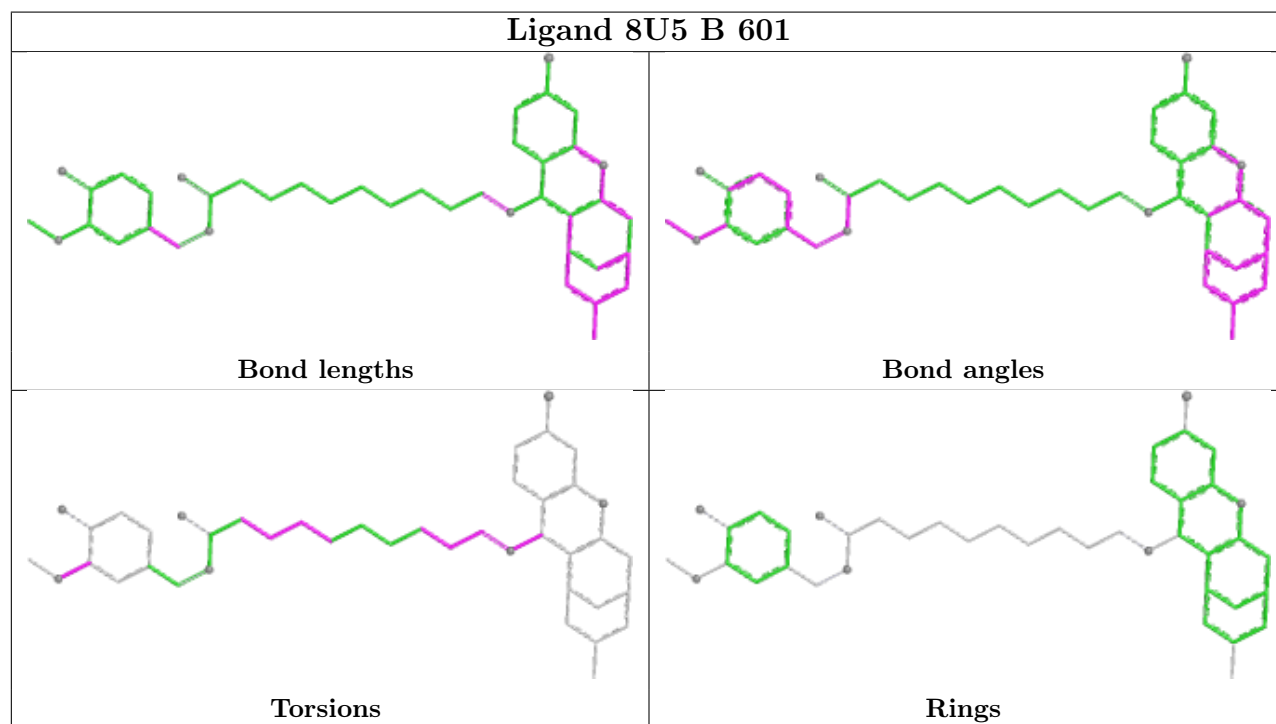
Mol	Chain	Res	Type	Atoms
5	A	608	MES	C7-C8-S-O3S
2	A	601	8U5	CBE-CBD-OBI-CBJ
3	B	602	NAG	O5-C5-C6-O6
3	A	604	NAG	O5-C5-C6-O6
3	A	604	NAG	C4-C5-C6-O6
2	A	601	8U5	NAT-CAS-CAU-CAV
2	A	601	8U5	CBC-CBD-OBI-CBJ
3	B	602	NAG	C4-C5-C6-O6
3	A	602	NAG	C8-C7-N2-C2
3	A	602	NAG	O7-C7-N2-C2
6	A	609	PEG	O1-C1-C2-O2
6	A	609	PEG	O2-C3-C4-O4
6	A	610	PEG	O2-C3-C4-O4
2	A	601	8U5	CBK-CBL-CBM-CBN
2	A	601	8U5	CAU-CAV-CAW-CBO
2	B	601	8U5	NAT-CAS-CAU-CAV
2	B	601	8U5	CAU-CAS-NAT-CAI
2	B	601	8U5	CAX-CBK-CBL-CBM
5	A	608	MES	C7-C8-S-O1S
6	A	609	PEG	C4-C3-O2-C2
6	A	609	PEG	C1-C2-O2-C3
2	A	601	8U5	OAY-CAX-CBK-CBL
6	A	610	PEG	C4-C3-O2-C2
2	A	601	8U5	NAZ-CAX-CBK-CBL
2	B	601	8U5	CBL-CBM-CBN-CBO
2	A	601	8U5	CAS-CAU-CAV-CAW
2	B	601	8U5	CAH-CAI-NAT-CAS
2	B	601	8U5	CBE-CBD-OBI-CBJ
2	B	601	8U5	CBK-CBL-CBM-CBN
2	B	601	8U5	CAS-CAU-CAV-CAW
3	A	603	NAG	C4-C5-C6-O6
2	A	601	8U5	CBM-CBN-CBO-CAW

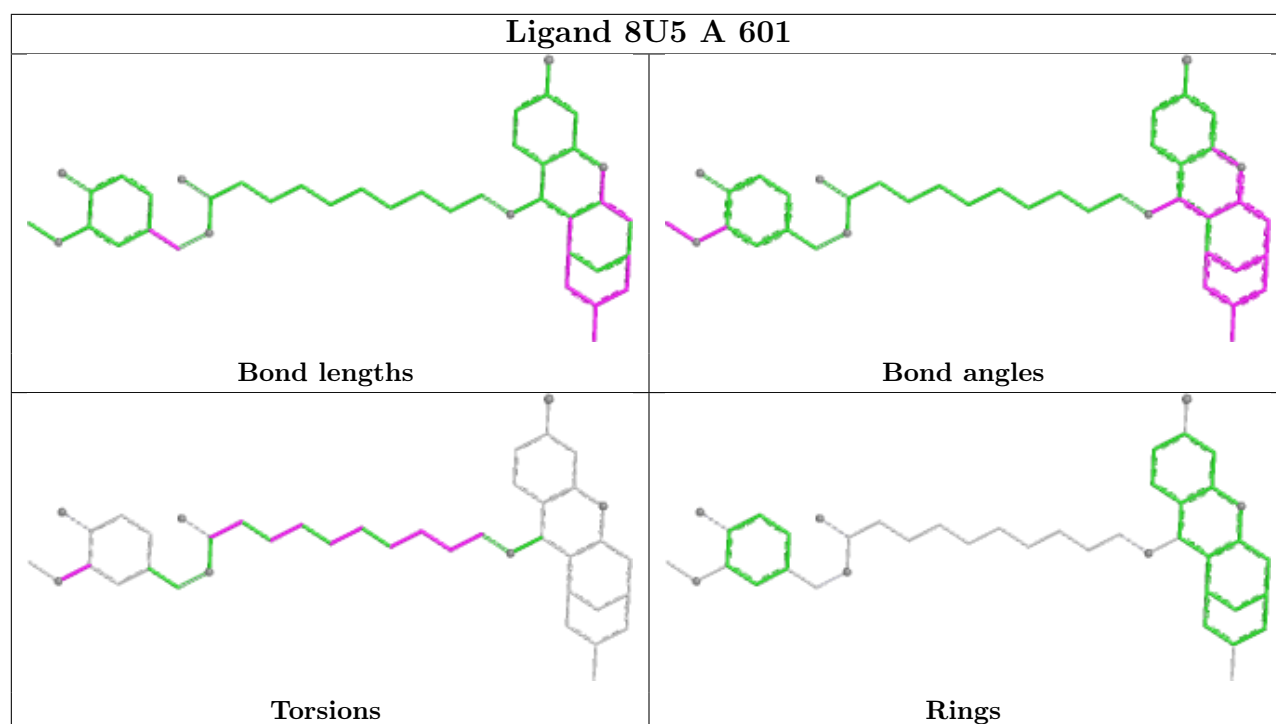
There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	NAG	2	0
3	A	602	NAG	3	0
5	A	608	MES	1	0
3	A	605	NAG	3	0
3	A	603	NAG	1	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	531/586 (90%)	0.07	8 (1%) 72 75	15, 29, 45, 66	16 (3%)
1	B	532/586 (90%)	0.01	5 (0%) 81 83	15, 29, 45, 73	12 (2%)
All	All	1063/1172 (90%)	0.04	13 (1%) 76 79	15, 29, 45, 73	28 (2%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	486	HIS	2.9
1	A	534	ALA	2.9
1	B	485	PRO	2.9
1	A	488	GLN	2.8
1	A	486	HIS	2.8
1	A	362	HIS	2.7
1	B	107	LYS	2.7
1	A	485	PRO	2.6
1	A	285	ASP	2.5
1	B	490	SER	2.5
1	B	489	GLU	2.2
1	A	260	GLU	2.0
1	A	9	ASN	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

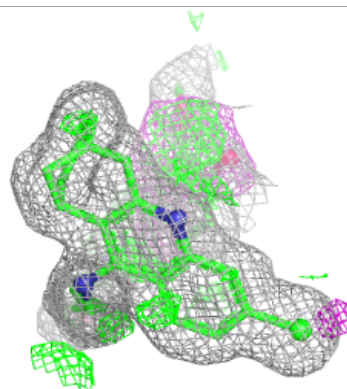
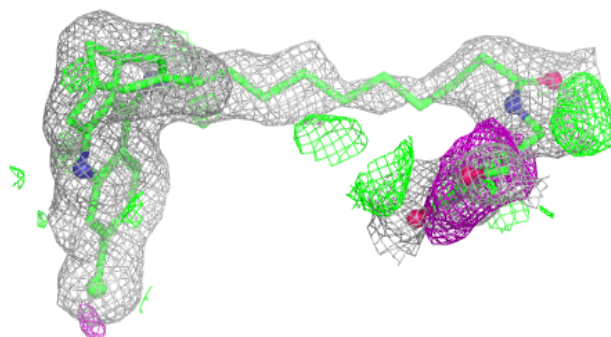
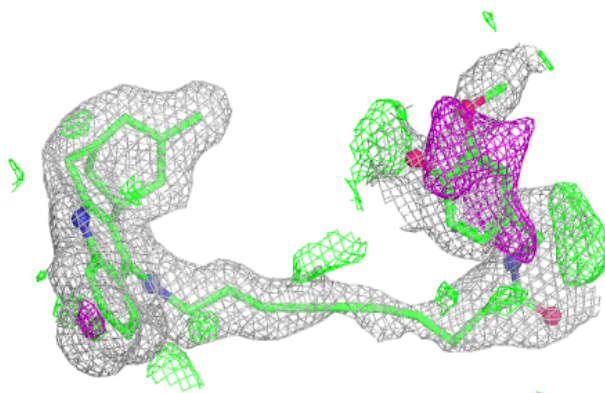
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAG	A	604	14/15	0.52	0.17	65,70,77,80	0
3	NAG	B	602	14/15	0.64	0.15	46,57,69,74	0
3	NAG	A	605	15/15	0.72	0.18	53,60,70,70	0
5	MES	A	608	12/12	0.73	0.18	51,61,64,78	0
6	PEG	A	609	7/7	0.78	0.16	42,54,61,63	0
3	NAG	A	602	14/15	0.80	0.12	38,51,60,63	0
3	NAG	B	603	14/15	0.87	0.11	38,44,59,62	0
3	NAG	A	603	14/15	0.89	0.10	30,36,50,52	0
6	PEG	A	610	7/7	0.89	0.13	37,43,51,60	0
2	8U5	B	601	42/42	0.90	0.14	19,29,55,57	0
2	8U5	A	601	42/42	0.93	0.12	19,35,57,69	0
4	CL	A	607	1/1	0.95	0.09	47,47,47,47	0
4	CL	A	606	1/1	0.96	0.12	59,59,59,59	0

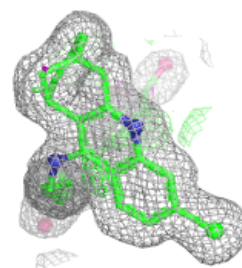
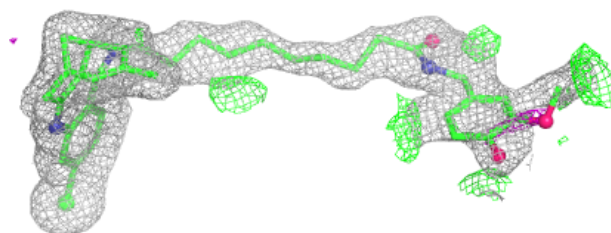
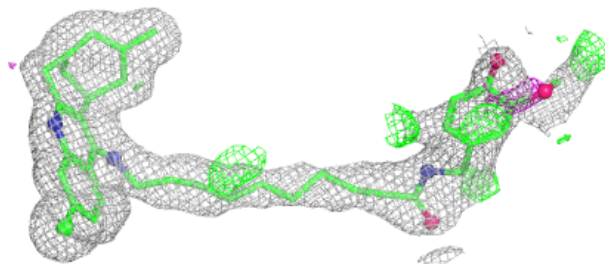
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8U5 B 601:

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

**Electron density around 8U5 A 601:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.