



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:49 AM UTC

PDB ID : 7AIU / pdb_00007aiu
Title : Crystal structure of Torpedo Californica acetylcholinesterase in complex with 8-[(3-Chloro-6,7,10,11-tetrahydro-9-methyl-7,11-methanocycloocta[b]quinolin-12-yl)amino]-N-(4-hydroxy-3-methoxybenzyl)octanamide
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Deposited on : 2020-09-28
Resolution : 2.00 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

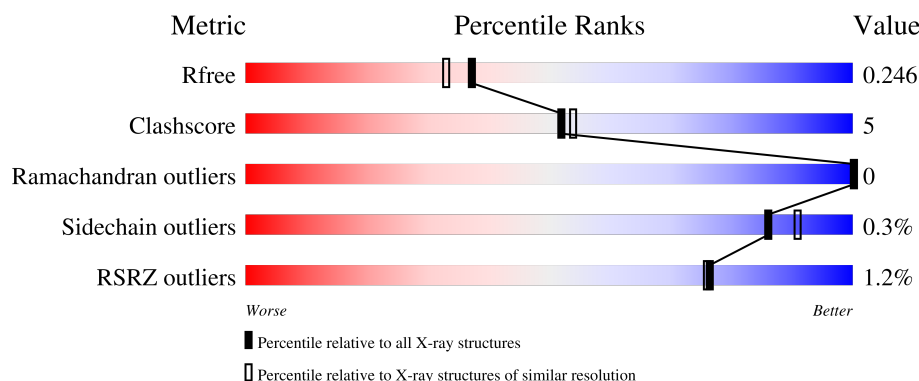
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

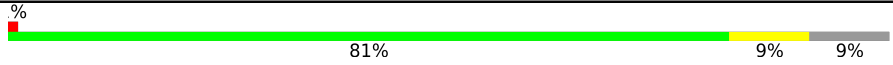
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	
1	B	586	

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
4	8UQ	A	606	X	-	-	-
4	8UQ	B	605[A]	X	-	-	-
4	8UQ	B	605[B]	X	-	-	-

2 Entry composition [i](#)

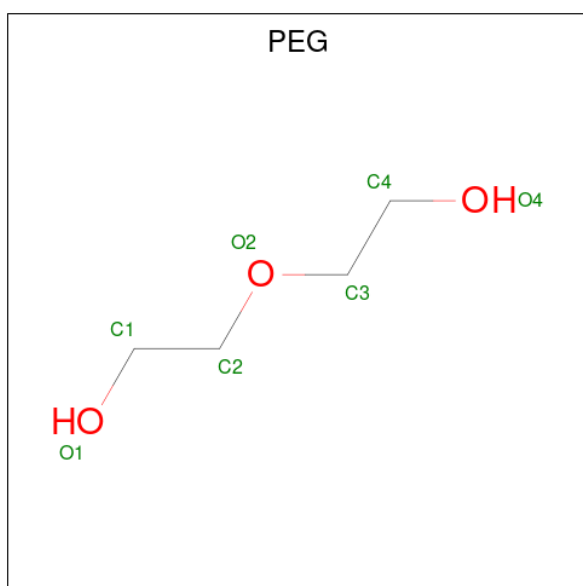
There are 6 unique types of molecules in this entry. The entry contains 9408 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	532	Total	C	N	O	S	0	8	0
			4292	2753	732	785	22			
1	B	532	Total	C	N	O	S	0	6	0
			4275	2745	723	784	23			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



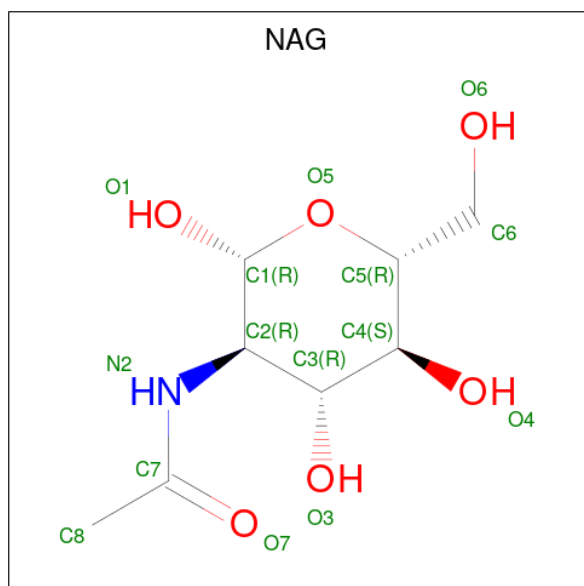
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		

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

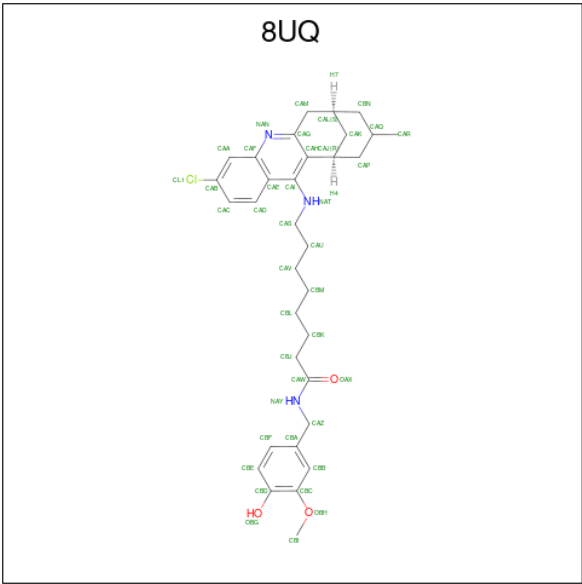
- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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	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 8-[(3-Chloro-6,7,10,11-tetrahydro-9-methyl-7,11-methanocycloocta[b]quin

olin-12-yl)amino]-N-(4-hydroxy-3-methoxybenzyl)octanamide (CCD ID: 8UQ) (formula: C₃₃H₄₂ClN₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 40	C 33	Cl 1	N 3	O 3	0	0
4	B	1	Total 80	C 66	Cl 2	N 6	O 6	0	1

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		
5	B	1	Total	Cl	0	0
			1	1		

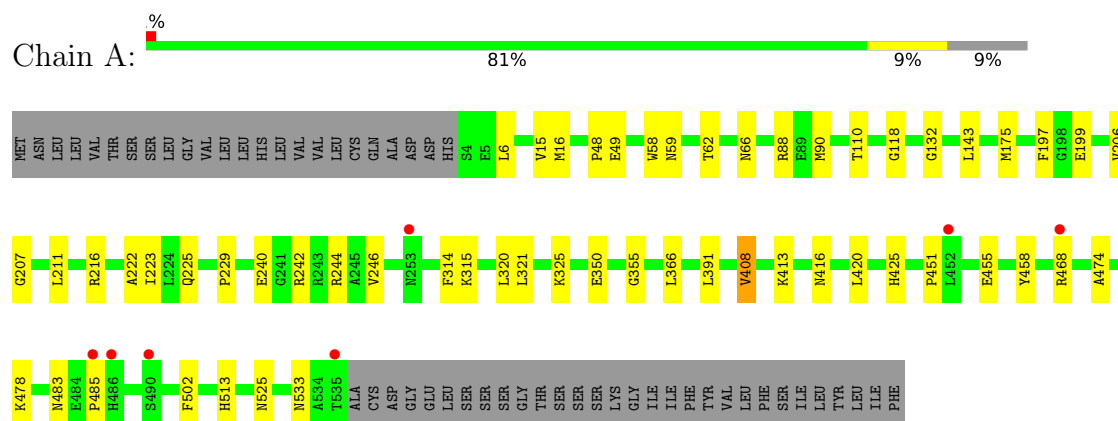
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	287	Total	O	0	0
			287	287		
6	B	298	Total	O	0	0
			298	298		

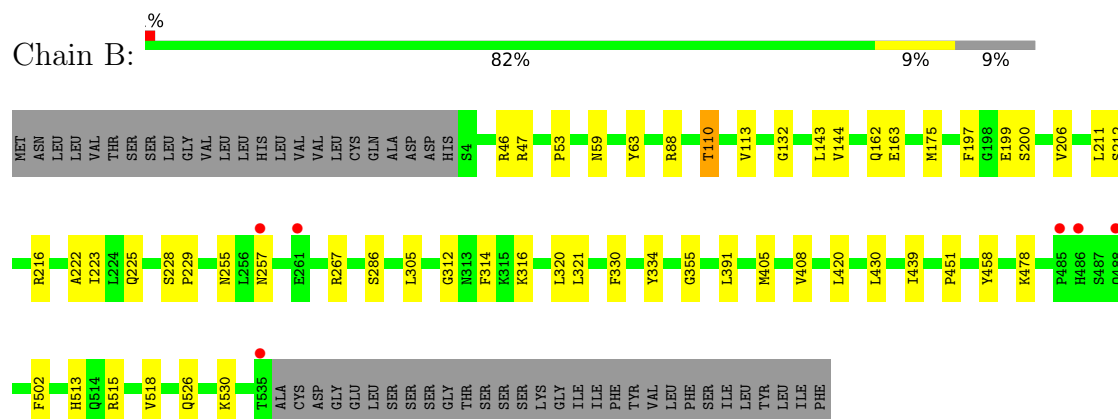
3 Residue-property plots [i](#)

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	91.90Å 105.67Å 150.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.80 – 2.00 45.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.80-2.00) 99.1 (45.80-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.201 , 0.246 0.202 , 0.246	Depositor DCC
R_{free} test set	2000 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.760	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9408	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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 42.85 % 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 1.9221e-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: CL, PEG, NAG, 8UQ

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	0.33	0/4439	0.51	0/6025
1	B	0.32	0/4416	0.51	0/5995
All	All	0.32	0/8855	0.51	0/12020

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	4292	0	4163	50	0
1	B	4275	0	4144	39	0
2	A	35	0	50	3	0
2	B	28	0	40	1	0
3	A	42	0	39	3	0
3	B	28	0	26	1	0
4	A	40	0	0	1	0
4	B	80	0	0	1	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
6	A	287	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	298	0	0	4	0
All	All	9408	0	8462	88	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 5.

All (88) 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:58:TRP:HA	2:A:601:PEG:H11	1.70	0.73
1:A:62:THR:HG23	1:A:88[B]:ARG:HH22	1.56	0.71
1:A:6:LEU:C	1:A:16:MET:CE	2.66	0.69
1:B:163:GLU:HG3	1:B:267:ARG:HH22	1.59	0.68
1:A:132:GLY:HA3	1:A:143:LEU:HD23	1.77	0.67
1:A:6:LEU:HB3	1:A:16:MET:HE2	1.77	0.66
1:A:416:ASN:HD21	3:A:604:NAG:C1	2.10	0.65
1:A:6:LEU:CB	1:A:16:MET:HE2	2.26	0.65
1:A:6:LEU:O	1:A:16:MET:HE3	1.98	0.64
1:B:163:GLU:HG3	1:B:267:ARG:NH2	2.13	0.63
1:A:366:LEU:HD13	1:B:530:LYS:HG2	1.81	0.62
1:A:321:LEU:HD11	1:A:408:VAL:HG23	1.82	0.62
1:A:242:ARG:HH11	2:A:608:PEG:H31	1.65	0.61
1:A:425:HIS:ND1	6:A:705:HOH:O	2.32	0.59
1:A:16:MET:HE3	1:A:16:MET:HA	1.84	0.59
1:B:46:ARG:NE	1:B:163:GLU:OE1	2.36	0.58
1:A:62:THR:HG23	1:A:88[B]:ARG:NH2	2.20	0.57
1:B:47:ARG:NH2	1:B:162:GLN:OE1	2.38	0.56
1:A:110:THR:OG1	1:A:478:LYS:HG2	2.07	0.55
1:B:355:GLY:HA3	1:B:391:LEU:HD21	1.91	0.53
1:A:246:VAL:HG21	2:A:608:PEG:H42	1.91	0.53
1:A:468[B]:ARG:NH2	6:A:706:HOH:O	2.34	0.52
1:B:53:PRO:HB3	2:B:606:PEG:H41	1.92	0.52
1:A:451:PRO:HA	1:A:458:TYR:CD1	2.44	0.52
1:B:312:GLY:O	1:B:316:LYS:NZ	2.26	0.52
1:A:6:LEU:C	1:A:16:MET:HE3	2.34	0.52
1:A:455:GLU:O	3:A:605:NAG:H82	2.09	0.52
1:B:132:GLY:HA3	1:B:143:LEU:HD23	1.90	0.51
1:B:451:PRO:HA	1:B:458:TYR:CD1	2.45	0.51
1:B:228:SER:HB2	1:B:229:PRO:HD2	1.92	0.50
1:A:6:LEU:O	1:A:16:MET:CE	2.59	0.50
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ASN:O	1:A:485:PRO:HD3	2.11	0.50
1:A:6:LEU:CB	1:A:16:MET:CE	2.90	0.49
1:A:207:GLY:HA3	1:A:229:PRO:HD3	1.94	0.49
1:A:59:ASN:HD21	3:A:603:NAG:C7	2.25	0.48
1:B:405:MET:O	1:B:408:VAL:HG12	2.13	0.48
1:B:63:TYR:HB2	1:B:88[B]:ARG:HE	1.77	0.48
1:A:48:PRO:HB2	1:A:175:MET:HE2	1.96	0.48
1:A:211:LEU:HD23	1:A:314:PHE:HB3	1.96	0.47
1:A:223:ILE:HA	1:A:320:LEU:O	2.13	0.47
1:B:223:ILE:HA	1:B:320:LEU:O	2.15	0.47
1:B:255:ASN:OD1	1:B:257:ASN:HB2	2.14	0.47
1:B:200:SER:OG	6:B:701:HOH:O	2.21	0.46
1:B:405:MET:HA	1:B:408:VAL:HG12	1.97	0.46
1:A:6:LEU:HB2	1:A:16:MET:CE	2.46	0.46
1:A:474:ALA:O	1:A:478:LYS:HG3	2.15	0.46
1:A:240:GLU:O	1:A:244:ARG:HG3	2.16	0.45
1:A:199:GLU:HA	1:A:225:GLN:O	2.16	0.45
1:A:525:ASN:ND2	6:A:722:HOH:O	2.49	0.45
1:B:502:PHE:CZ	1:B:513:HIS:HB2	2.52	0.44
1:A:66:ASN:O	1:A:90:MET:HA	2.18	0.44
1:B:211:LEU:HD13	1:B:305:LEU:HD22	2.00	0.44
1:B:197:PHE:HB3	1:B:223:ILE:HB	2.01	0.43
1:B:312:GLY:HA2	1:B:314:PHE:CE2	2.53	0.43
1:A:325:LYS:HE2	6:A:813:HOH:O	2.19	0.43
1:B:88[B]:ARG:HG3	6:B:862:HOH:O	2.17	0.43
1:B:110:THR:HG21	1:B:478:LYS:HB2	2.01	0.43
1:A:413:LYS:HB3	1:A:413:LYS:HE3	1.63	0.43
1:A:350:GLU:O	6:A:701:HOH:O	2.21	0.42
1:B:515:ARG:HB3	1:B:518:VAL:HB	2.01	0.42
1:A:88[B]:ARG:HH11	1:A:88[B]:ARG:HG3	1.84	0.42
1:B:334:TYR:HB3	6:B:891:HOH:O	2.19	0.42
1:A:216:ARG:HG2	1:A:315:LYS:HB2	2.00	0.42
1:A:355:GLY:HA3	1:A:391:LEU:HD21	2.02	0.42
1:B:211:LEU:HD23	1:B:314:PHE:HB3	2.00	0.42
1:A:533:ASN:ND2	6:A:731:HOH:O	2.52	0.42
1:A:197:PHE:CB	1:A:223:ILE:HB	2.49	0.42
1:B:59:ASN:HD21	3:B:603:NAG:C1	2.33	0.42
1:B:420:LEU:HD23	1:B:502:PHE:HB3	2.02	0.42
1:B:430:LEU:HD21	1:B:439:ILE:HD12	2.02	0.42
1:A:48:PRO:HB2	1:A:175:MET:CE	2.50	0.41
1:B:321:LEU:O	1:B:420:LEU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:GLY:CA	1:B:143:LEU:HD23	2.51	0.41
1:B:502:PHE:CE1	1:B:513:HIS:HB2	2.56	0.41
1:B:175:MET:HE3	1:B:175:MET:HB2	1.97	0.41
1:B:113:VAL:HG22	1:B:144:VAL:HB	2.02	0.41
1:A:197:PHE:HB3	1:A:223:ILE:HB	2.01	0.41
1:B:199:GLU:HA	1:B:225:GLN:O	2.20	0.41
1:B:206:VAL:CG1	1:B:222:ALA:HB1	2.51	0.41
1:B:526:GLN:NE2	6:B:728:HOH:O	2.54	0.41
1:A:118:GLY:HA2	4:A:606:8UQ:CAQ	2.52	0.40
1:B:212:SER:O	1:B:216:ARG:HG3	2.21	0.40
1:B:286:SER:O	4:B:605[A]:8UQ:CBE	2.69	0.40
1:A:15[A]:VAL:HG22	1:A:58:TRP:HB3	2.03	0.40
1:A:49:GLU:C	1:A:175:MET:HE1	2.46	0.40
1:A:321:LEU:O	1:A:420:LEU:HA	2.22	0.40
1:A:206:VAL:CG1	1:A:222:ALA:HB1	2.51	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	538/586 (92%)	516 (96%)	22 (4%)	0	100	100
1	B	536/586 (92%)	518 (97%)	18 (3%)	0	100	100
All	All	1074/1172 (92%)	1034 (96%)	40 (4%)	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	471/513 (92%)	470 (100%)	1 (0%)	87	92
1	B	470/513 (92%)	468 (100%)	2 (0%)	84	89
All	All	941/1026 (92%)	938 (100%)	3 (0%)	86	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	408	VAL
1	B	110	THR
1	B	330	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	66	ASN
1	A	525	ASN
1	B	59	ASN
1	B	65	ASN
1	B	66	ASN
1	B	409	ASN
1	B	500	GLN
1	B	514	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 3 are monoatomic - leaving 17 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
2	PEG	A	602	-	6,6,6	0.47	0	5,5,5	0.37	0
2	PEG	A	601	-	6,6,6	0.49	0	5,5,5	0.83	0
3	NAG	A	603	-	14,14,15	0.19	0	17,19,21	0.69	1 (5%)
3	NAG	A	604	-	14,14,15	0.66	1 (7%)	17,19,21	0.50	0
2	PEG	A	609	-	6,6,6	0.49	0	5,5,5	0.42	0
3	NAG	A	605	-	14,14,15	0.33	0	17,19,21	0.96	1 (5%)
2	PEG	A	608	-	6,6,6	0.47	0	5,5,5	0.72	0
3	NAG	B	604	1	14,14,15	0.46	0	17,19,21	0.57	0
2	PEG	B	607	-	6,6,6	0.49	0	5,5,5	0.45	0
4	8UQ	B	605[A]	-	44,44,44	2.94	9 (20%)	53,61,61	3.14	17 (32%)
2	PEG	B	606	-	6,6,6	0.48	0	5,5,5	0.40	0
2	PEG	B	602	-	6,6,6	0.51	0	5,5,5	0.69	0
4	8UQ	A	606	-	44,44,44	2.74	9 (20%)	53,61,61	3.20	17 (32%)
4	8UQ	B	605[B]	-	44,44,44	2.92	9 (20%)	53,61,61	3.07	15 (28%)
3	NAG	B	603	-	14,14,15	0.33	0	17,19,21	0.49	0
2	PEG	B	601	-	6,6,6	0.49	0	5,5,5	0.41	0
2	PEG	A	607	-	6,6,6	0.51	0	5,5,5	0.22	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
2	PEG	A	602	-	-	2/4/4/4	-
2	PEG	A	601	-	-	3/4/4/4	-
3	NAG	A	603	-	-	4/6/23/26	0/1/1/1
3	NAG	A	604	-	-	0/6/23/26	0/1/1/1
2	PEG	A	609	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	605	-	-	0/6/23/26	0/1/1/1
2	PEG	A	608	-	-	3/4/4/4	-
3	NAG	B	604	1	-	0/6/23/26	0/1/1/1
2	PEG	B	607	-	-	2/4/4/4	-
4	8UQ	B	605[A]	-	2/2/4/6	6/18/38/38	0/6/5/5
2	PEG	B	606	-	-	1/4/4/4	-
2	PEG	B	602	-	-	2/4/4/4	-
4	8UQ	A	606	-	2/2/4/6	10/18/38/38	0/6/5/5
4	8UQ	B	605[B]	-	2/2/4/6	7/18/38/38	0/6/5/5
3	NAG	B	603	-	-	1/6/23/26	0/1/1/1
2	PEG	B	601	-	-	1/4/4/4	-
2	PEG	A	607	-	-	2/4/4/4	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	605[A]	8UQ	CAK-CAJ	-9.38	1.41	1.53
4	B	605[B]	8UQ	CAK-CAJ	-9.37	1.41	1.53
4	A	606	8UQ	CAH-CAJ	-9.30	1.37	1.51
4	B	605[B]	8UQ	CAH-CAJ	-9.26	1.37	1.51
4	B	605[A]	8UQ	CAH-CAJ	-9.24	1.37	1.51
4	A	606	8UQ	CAK-CAJ	-7.59	1.44	1.53
4	B	605[A]	8UQ	CAM-CAG	-7.44	1.43	1.51
4	B	605[B]	8UQ	CAM-CAG	-7.31	1.43	1.51
4	A	606	8UQ	CBN-CAL	-6.46	1.35	1.52
4	A	606	8UQ	CAM-CAG	-6.35	1.44	1.51
4	B	605[B]	8UQ	CBN-CAL	-5.81	1.36	1.52
4	B	605[A]	8UQ	CBN-CAL	-5.76	1.37	1.52
4	B	605[A]	8UQ	CAZ-CBA	-5.63	1.39	1.51
4	A	606	8UQ	CAZ-CBA	-5.36	1.39	1.51
4	A	606	8UQ	CBN-CAQ	-5.25	1.41	1.53
4	B	605[B]	8UQ	CAZ-CBA	-5.21	1.39	1.51
4	B	605[B]	8UQ	CBN-CAQ	-5.17	1.41	1.53
4	B	605[A]	8UQ	CBN-CAQ	-5.17	1.41	1.53
4	B	605[A]	8UQ	CAR-CAQ	-4.02	1.40	1.52
4	B	605[B]	8UQ	CAR-CAQ	-3.96	1.40	1.52
4	A	606	8UQ	CAR-CAQ	-3.50	1.41	1.52
4	B	605[A]	8UQ	CAP-CAQ	-3.30	1.45	1.53
4	B	605[B]	8UQ	CAP-CAQ	-3.08	1.46	1.53
4	A	606	8UQ	CAP-CAQ	-2.79	1.46	1.53
4	A	606	8UQ	CAF-NAN	-2.52	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	605[B]	8UQ	CAF-NAN	-2.49	1.33	1.37
4	B	605[A]	8UQ	CAF-NAN	-2.45	1.33	1.37
3	A	604	NAG	O5-C1	-2.17	1.40	1.43

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	606	8UQ	CAH-CAG-NAN	-9.85	119.33	123.65
4	B	605[A]	8UQ	CAH-CAG-NAN	-9.57	119.45	123.65
4	B	605[B]	8UQ	CAH-CAG-NAN	-9.30	119.57	123.65
4	A	606	8UQ	CAK-CAJ-CAH	8.05	121.94	111.52
4	B	605[A]	8UQ	CAJ-CAK-CAL	-8.01	82.52	110.60
4	B	605[B]	8UQ	CAJ-CAK-CAL	-7.81	83.23	110.60
4	A	606	8UQ	CAJ-CAK-CAL	-7.56	84.11	110.60
4	A	606	8UQ	CBN-CAQ-CAP	7.40	120.84	110.02
4	B	605[B]	8UQ	CAK-CAJ-CAH	7.35	121.03	111.52
4	B	605[B]	8UQ	CBN-CAL-CAK	7.19	123.36	109.69
4	B	605[A]	8UQ	CBN-CAQ-CAP	7.16	120.48	110.02
4	B	605[B]	8UQ	CBN-CAQ-CAP	7.05	120.33	110.02
4	A	606	8UQ	CBN-CAL-CAK	7.04	123.08	109.69
4	B	605[A]	8UQ	CBN-CAL-CAK	6.91	122.83	109.69
4	B	605[A]	8UQ	CAK-CAJ-CAH	6.85	120.39	111.52
4	A	606	8UQ	CAR-CAQ-CAP	6.67	122.25	111.17
4	B	605[B]	8UQ	CAR-CAQ-CAP	6.16	121.40	111.17
4	B	605[A]	8UQ	CAG-CAM-CAL	-6.04	100.19	111.77
4	B	605[A]	8UQ	CAR-CAQ-CAP	6.04	121.20	111.17
4	B	605[B]	8UQ	CAG-CAM-CAL	-5.95	100.36	111.77
4	A	606	8UQ	CAK-CAL-CAM	5.50	115.16	109.37
4	B	605[A]	8UQ	CBI-OBH-CBC	-5.19	109.89	117.51
4	A	606	8UQ	CAG-CAM-CAL	-5.03	102.12	111.77
4	A	606	8UQ	CAG-NAN-CAF	4.67	123.19	117.67
4	B	605[A]	8UQ	CAK-CAL-CAM	4.40	114.00	109.37
4	B	605[B]	8UQ	CAK-CAL-CAM	4.36	113.96	109.37
4	B	605[A]	8UQ	CAR-CAQ-CBN	4.26	118.24	111.17
4	B	605[B]	8UQ	CAG-NAN-CAF	4.22	122.66	117.67
4	B	605[B]	8UQ	CAR-CAQ-CBN	4.21	118.16	111.17
4	B	605[A]	8UQ	CAG-NAN-CAF	4.05	122.47	117.67
4	A	606	8UQ	CBA-CAZ-NAY	-3.87	104.91	113.07
4	B	605[B]	8UQ	CBI-OBH-CBC	-3.70	112.08	117.51
4	A	606	8UQ	CAP-CAJ-CAK	3.55	113.72	109.55
4	B	605[A]	8UQ	CAP-CAJ-CAK	3.47	113.62	109.55
4	A	606	8UQ	CAR-CAQ-CBN	3.31	116.67	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	605[B]	8UQ	CAP-CAJ-CAK	3.08	113.17	109.55
4	A	606	8UQ	CBI-OBH-CBC	-2.81	113.39	117.51
3	A	605	NAG	C1-O5-C5	2.73	115.85	112.19
4	B	605[A]	8UQ	CBA-CAZ-NAY	-2.43	107.95	113.07
4	A	606	8UQ	CAC-CAB-CAA	-2.22	119.57	122.00
4	B	605[B]	8UQ	CAA-CAF-CAE	2.20	122.04	119.58
4	A	606	8UQ	CAH-CAI-NAT	-2.18	115.92	119.47
4	B	605[B]	8UQ	CAH-CAI-CAE	-2.18	118.61	120.92
3	A	603	NAG	C1-O5-C5	2.16	115.08	112.19
4	B	605[A]	8UQ	CAC-CAB-CAA	-2.13	119.67	122.00
4	A	606	8UQ	CAM-CAG-NAN	2.10	119.76	116.39
4	B	605[A]	8UQ	CAH-CAI-CAE	-2.09	118.71	120.92
4	B	605[A]	8UQ	OBH-CBC-CBD	2.06	117.64	114.55
4	B	605[A]	8UQ	CAA-CAF-CAE	2.04	121.86	119.58
4	A	606	8UQ	CAA-CAF-CAE	2.03	121.85	119.58
4	B	605[B]	8UQ	CBA-CAZ-NAY	-2.00	108.85	113.07

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	606	8UQ	CAQ
4	A	606	8UQ	CAL
4	B	605[A]	8UQ	CAQ
4	B	605[A]	8UQ	CAL
4	B	605[B]	8UQ	CAQ
4	B	605[B]	8UQ	CAL

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	606	8UQ	CBB-CBC-OBH-CBI
3	A	603	NAG	O5-C5-C6-O6
3	A	603	NAG	C4-C5-C6-O6
3	A	603	NAG	C8-C7-N2-C2
3	A	603	NAG	O7-C7-N2-C2
4	A	606	8UQ	CBD-CBC-OBH-CBI
2	A	601	PEG	O2-C3-C4-O4
2	A	608	PEG	O1-C1-C2-O2
2	B	601	PEG	O1-C1-C2-O2
4	B	605[B]	8UQ	CBB-CBC-OBH-CBI
4	B	605[A]	8UQ	CBB-CBC-OBH-CBI
2	B	602	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	606	8UQ	NAT-CAS-CAU-CAV
4	A	606	8UQ	CBJ-CBK-CBL-CBM
4	A	606	8UQ	CBK-CBL-CBM-CAV
4	B	605[B]	8UQ	CBD-CBC-OBH-CBI
4	B	605[A]	8UQ	CBD-CBC-OBH-CBI
2	A	607	PEG	O2-C3-C4-O4
2	A	609	PEG	O2-C3-C4-O4
4	A	606	8UQ	CAU-CAV-CBM-CBL
4	A	606	8UQ	CAU-CAS-NAT-CAI
4	B	605[A]	8UQ	CAU-CAS-NAT-CAI
2	A	607	PEG	O1-C1-C2-O2
4	B	605[B]	8UQ	OAX-CAW-CBJ-CBK
4	B	605[B]	8UQ	NAY-CAW-CBJ-CBK
4	A	606	8UQ	OAX-CAW-CBJ-CBK
4	B	605[B]	8UQ	CAU-CAS-NAT-CAI
2	A	602	PEG	C1-C2-O2-C3
4	A	606	8UQ	NAY-CAW-CBJ-CBK
2	B	607	PEG	O2-C3-C4-O4
2	B	607	PEG	O1-C1-C2-O2
2	A	601	PEG	C4-C3-O2-C2
2	A	602	PEG	O2-C3-C4-O4
2	A	609	PEG	O1-C1-C2-O2
2	A	609	PEG	C1-C2-O2-C3
2	A	608	PEG	C1-C2-O2-C3
2	B	602	PEG	C1-C2-O2-C3
2	B	606	PEG	C1-C2-O2-C3
4	B	605[B]	8UQ	CAH-CAI-NAT-CAS
2	A	608	PEG	C4-C3-O2-C2
4	A	606	8UQ	CAH-CAI-NAT-CAS
4	B	605[A]	8UQ	CAH-CAI-NAT-CAS
4	B	605[A]	8UQ	CAW-CBJ-CBK-CBL
2	A	601	PEG	O1-C1-C2-O2
3	B	603	NAG	C4-C5-C6-O6
4	B	605[A]	8UQ	OAX-CAW-CBJ-CBK
4	B	605[B]	8UQ	CAW-CBJ-CBK-CBL

There are no ring outliers.

9 monomers are involved in 10 short contacts:

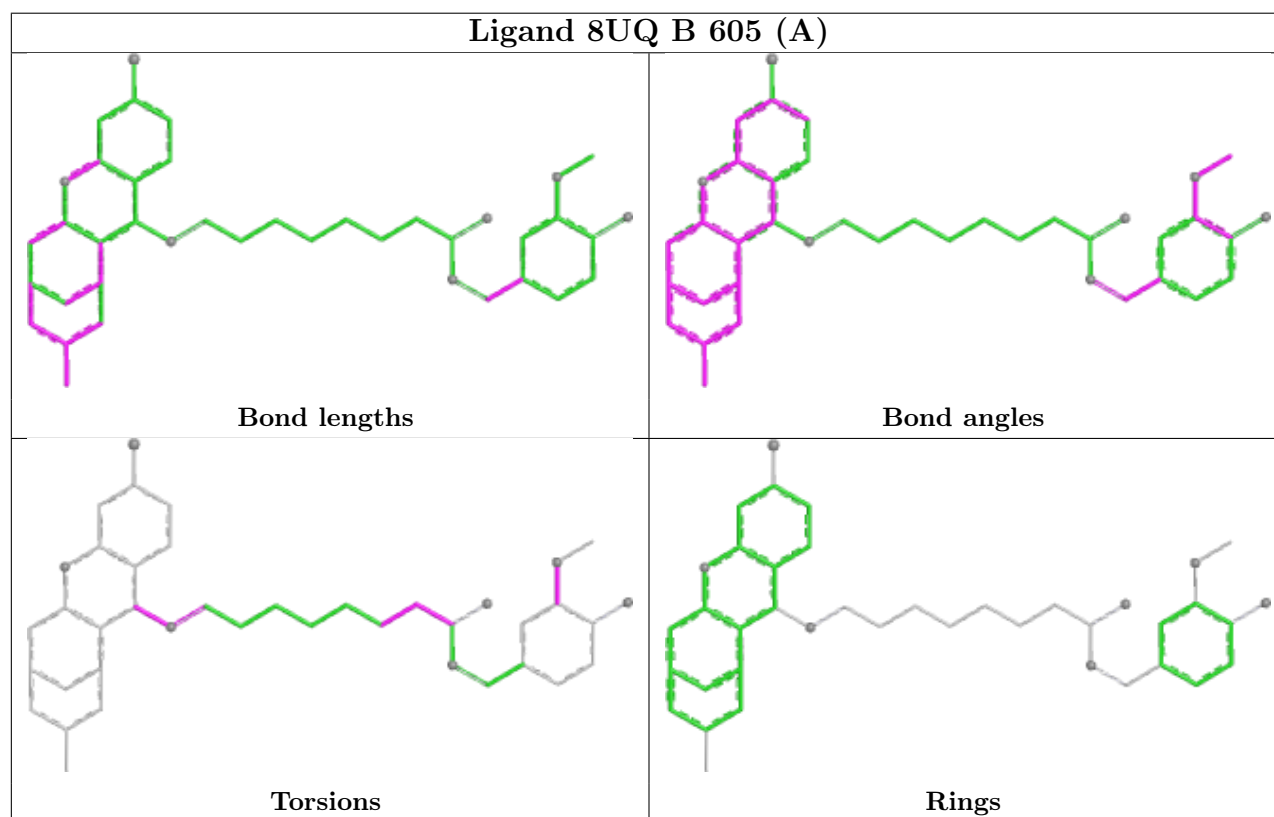
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	PEG	1	0
3	A	603	NAG	1	0

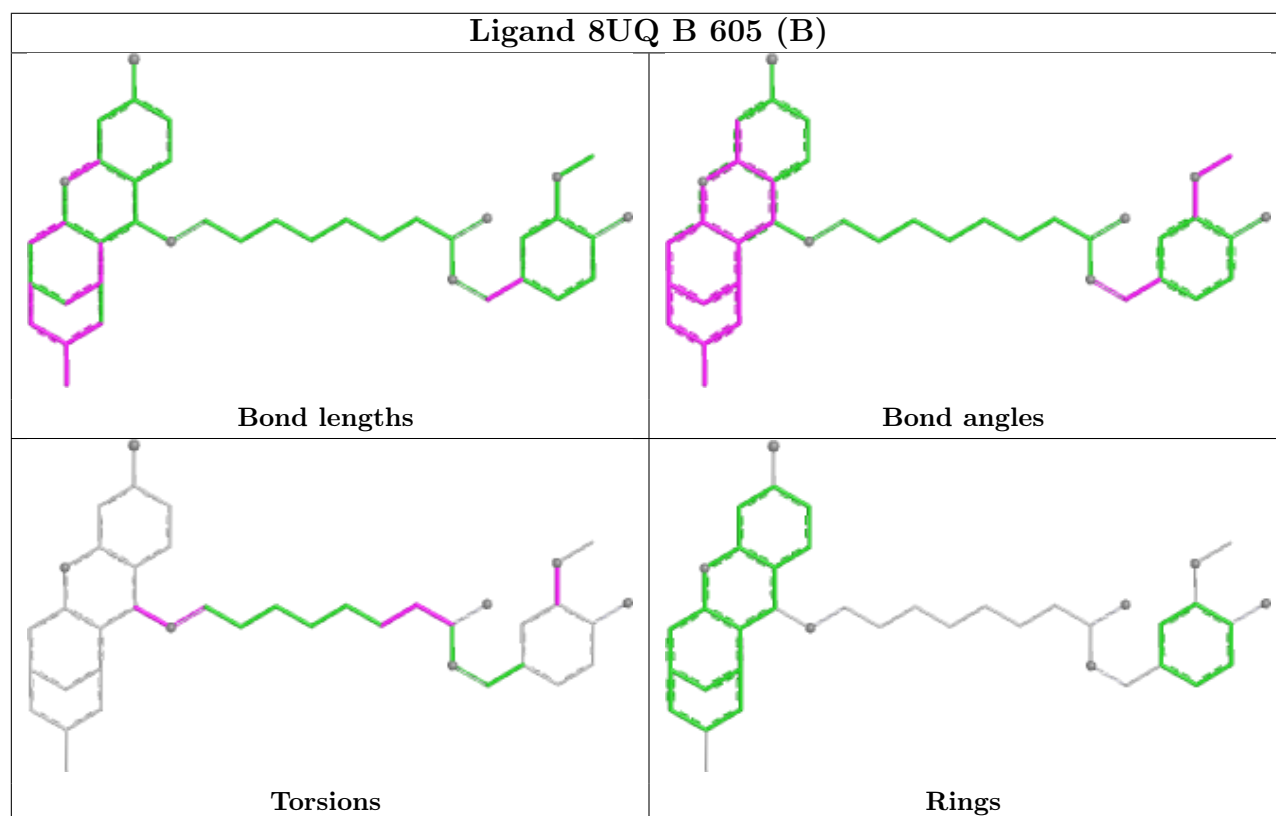
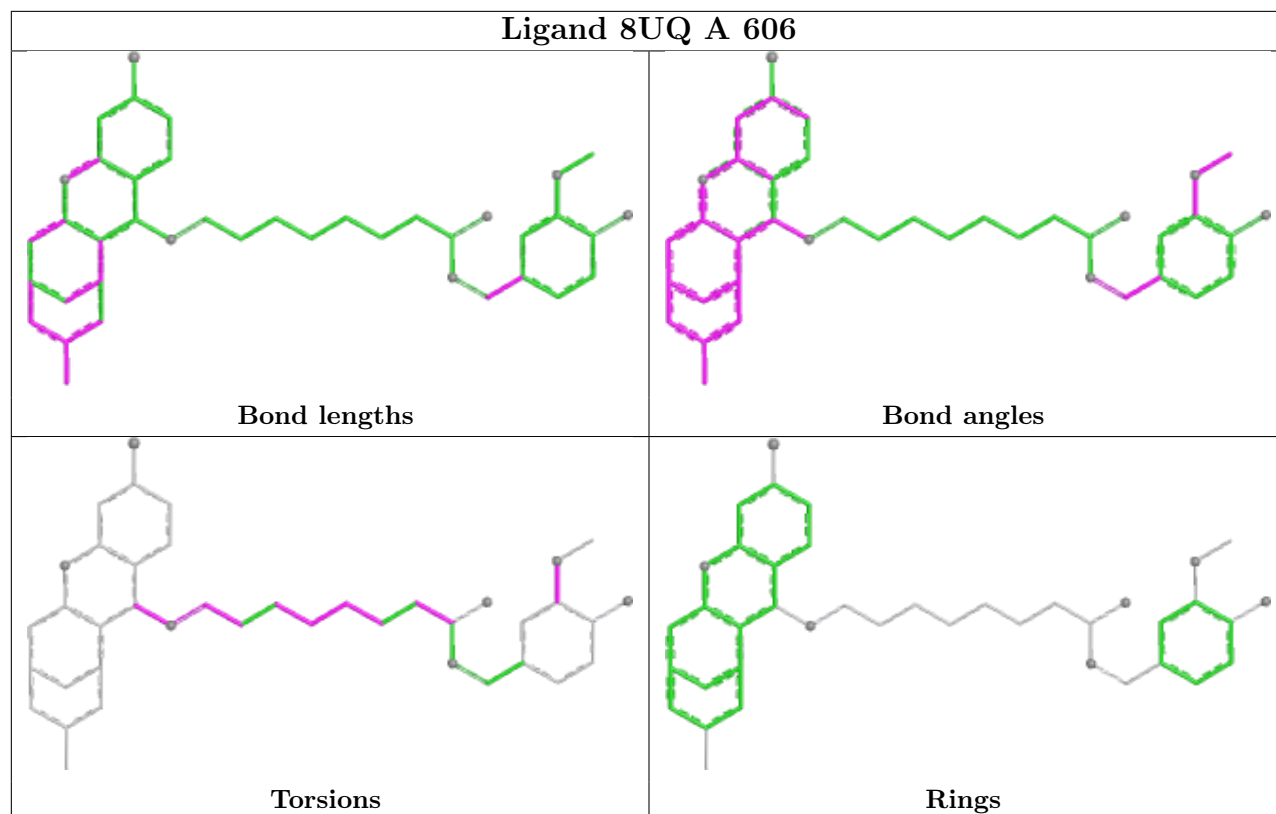
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	NAG	1	0
3	A	605	NAG	1	0
2	A	608	PEG	2	0
4	B	605[A]	8UQ	1	0
2	B	606	PEG	1	0
4	A	606	8UQ	1	0
3	B	603	NAG	1	0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	532/586 (90%)	0.41	7 (1%) 75 74	20, 34, 51, 109	9 (1%)
1	B	532/586 (90%)	0.38	6 (1%) 78 77	15, 34, 51, 85	8 (1%)
All	All	1064/1172 (90%)	0.39	13 (1%) 76 76	15, 34, 51, 109	17 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	535	THR	4.9
1	B	486	HIS	3.9
1	A	485	PRO	3.8
1	A	486	HIS	3.1
1	B	261	GLU	2.9
1	B	485	PRO	2.9
1	B	257	ASN	2.8
1	A	535	THR	2.6
1	A	253	ASN	2.5
1	A	490	SER	2.3
1	A	452	LEU	2.3
1	B	488	GLN	2.2
1	A	468[A]	ARG	2.1

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

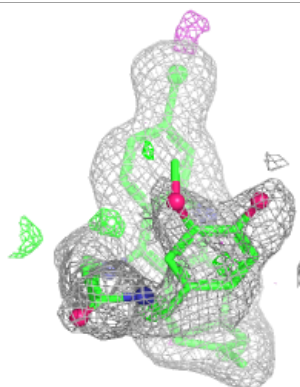
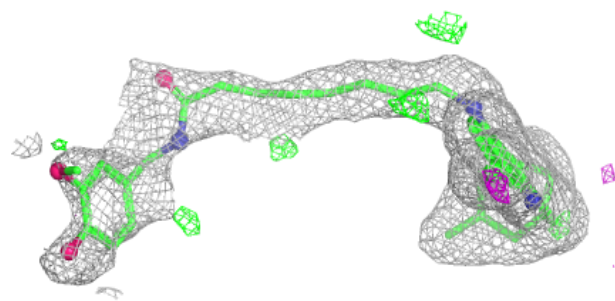
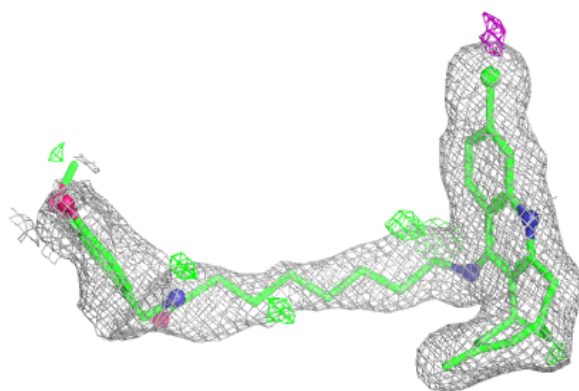
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	605	14/15	0.65	0.16	75,91,99,102	0
3	NAG	B	603	14/15	0.71	0.16	53,61,68,70	0
2	PEG	B	601	7/7	0.72	0.21	52,55,69,71	0
3	NAG	A	604	14/15	0.75	0.15	43,58,66,72	0
2	PEG	A	602	7/7	0.75	0.20	41,46,53,56	0
3	NAG	A	603	14/15	0.75	0.15	61,79,85,88	0
2	PEG	B	607	7/7	0.76	0.15	62,64,69,72	0
2	PEG	B	602	7/7	0.80	0.18	42,60,68,71	0
2	PEG	A	601	7/7	0.82	0.18	44,47,60,65	0
3	NAG	B	604	14/15	0.83	0.12	36,43,54,60	0
2	PEG	A	609	7/7	0.88	0.12	49,52,56,59	0
2	PEG	A	608	7/7	0.89	0.13	43,48,53,54	0
4	8UQ	B	605[A]	40/40	0.89	0.17	28,34,86,87	40
4	8UQ	B	605[B]	40/40	0.89	0.17	27,34,81,85	40
5	CL	B	608	1/1	0.89	0.14	61,61,61,61	0
4	8UQ	A	606	40/40	0.92	0.16	21,32,115,120	0
2	PEG	A	607	7/7	0.92	0.10	35,44,48,49	0
5	CL	A	610	1/1	0.93	0.13	69,69,69,69	0
2	PEG	B	606	7/7	0.93	0.10	43,47,55,56	0
5	CL	A	611	1/1	0.95	0.09	49,49,49,49	0

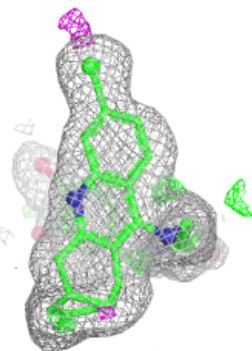
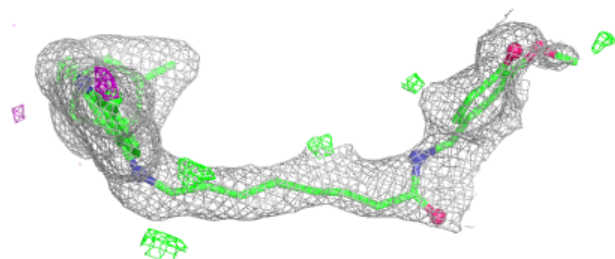
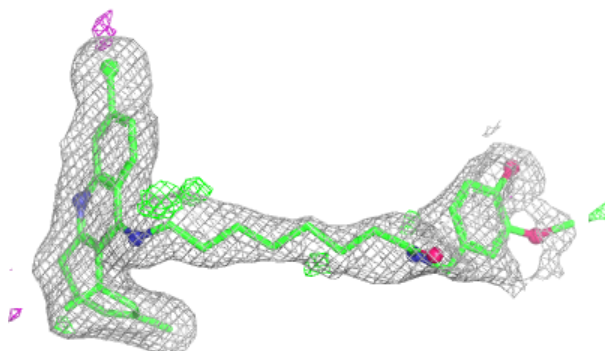
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

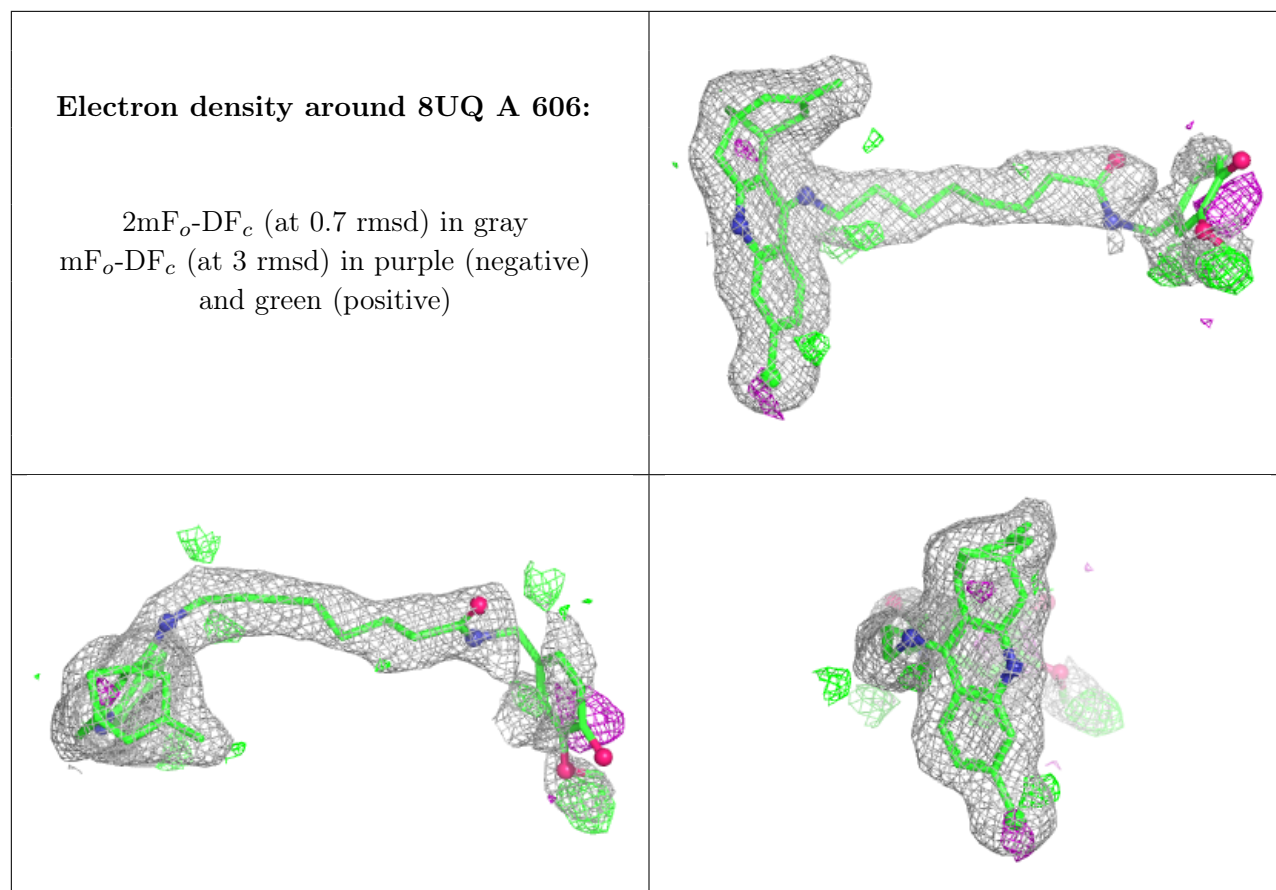
Electron density around 8UQ B 605 (A):

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

**Electron density around 8UQ B 605 (B):**

$2mF_o-DF_c$ (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.