



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:49 AM UTC

PDB ID : 7AIS / pdb_00007ais
Title : Crystal structure of Torpedo Californica acetylcholinesterase in complex with 6-[(3-Chloro-6,7,10,11-tetrahydro-9-methyl-7,11-methanocycloocta[b]quinolin-12-yl)amino]-N-(4-hydroxy-3-methoxybenzyl)hexanamide
Authors : Coquelle, N.; Colletier, J.P.
Deposited on : 2020-09-28
Resolution : 1.75 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

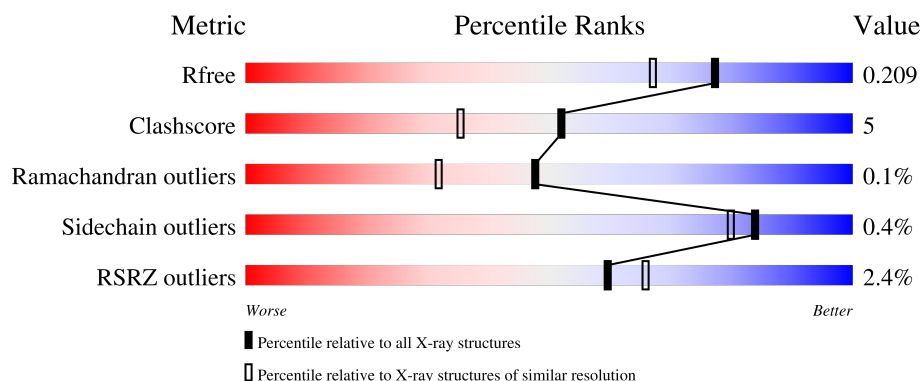
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

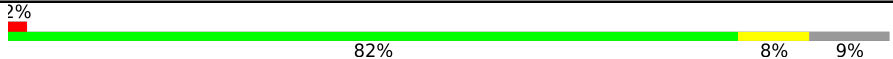
The reported resolution of this entry is 1.75 Å.

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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	

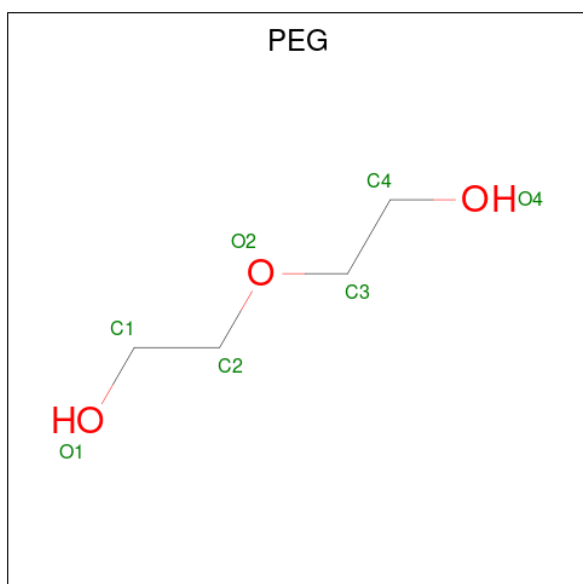
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	602	-	-	X	-



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



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

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

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

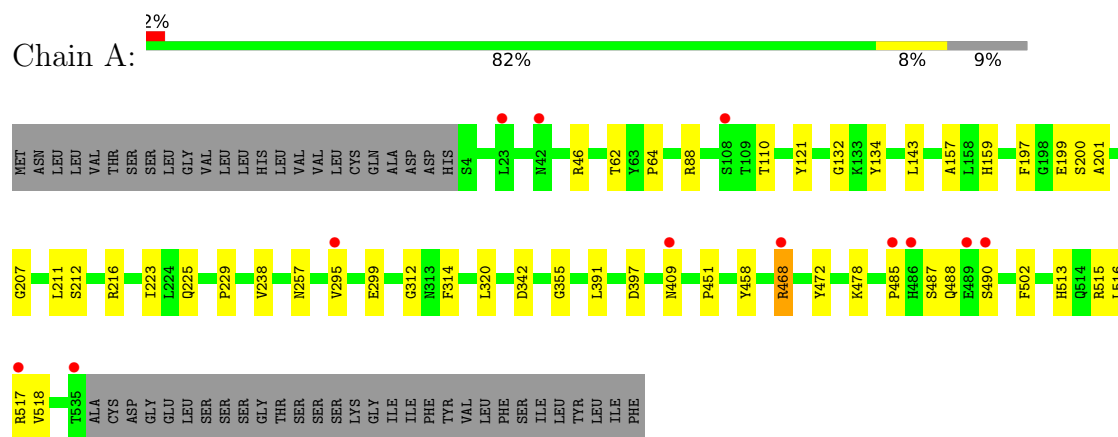
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	526	Total O 526 526	0	0
6	B	540	Total O 540 540	0	0

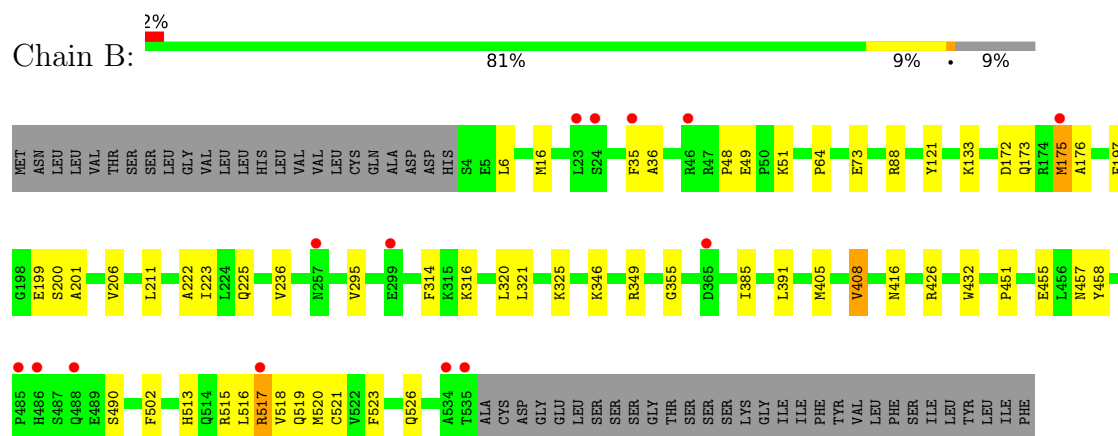
3 Residue-property plots [i](#)

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	91.90Å 106.75Å 150.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.16 – 1.75 46.16 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.16-1.75) 99.9 (46.16-1.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.67 (at 1.42Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.187 , 0.208 0.189 , 0.209	Depositor DCC
R_{free} test set	11173 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.1	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	0.97	EDS
Total number of atoms	9823	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 40.48 % 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 2.7170e-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, PEG, 8UH, CL

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	0.38	4/4446 (0.1%)	0.62	6/6035 (0.1%)
1	B	0.42	3/4439 (0.1%)	0.57	3/6025 (0.0%)
All	All	0.40	7/8885 (0.1%)	0.60	9/12060 (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	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	468[A]	ARG	C-N	7.37	1.41	1.33
1	A	468[B]	ARG	C-N	7.37	1.41	1.33
1	A	409[A]	ASN	CA-C	6.75	1.61	1.52
1	A	409[B]	ASN	CA-C	6.75	1.61	1.52
1	B	175	MET	C-O	-5.30	1.17	1.24
1	B	48	PRO	CG-CD	-5.27	1.32	1.50
1	B	173	GLN	C-O	-5.14	1.18	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	468[A]	ARG	CA-C-O	13.00	135.95	119.05
1	A	468[B]	ARG	CA-C-O	13.00	135.95	119.05
1	A	468[A]	ARG	N-CA-C	10.91	125.72	111.75
1	A	468[B]	ARG	N-CA-C	10.91	125.72	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409[A]	ASN	CA-C-O	7.61	128.81	120.82
1	A	409[B]	ASN	CA-C-O	7.61	128.81	120.82
1	B	175	MET	CA-C-N	7.39	130.49	120.44
1	B	175	MET	C-N-CA	7.39	130.49	120.44
1	B	48	PRO	CA-CB-CG	-5.13	94.75	104.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	488	GLN	Peptide

5.2 Too-close contacts [i](#)

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	4296	0	4169	33	0
1	B	4292	0	4163	50	4
2	A	38	0	0	2	1
2	B	38	0	0	5	0
3	A	42	0	39	1	0
3	B	28	0	23	13	4
4	A	21	0	30	0	0
5	A	2	0	0	0	0
6	A	526	0	0	10	0
6	B	540	0	0	10	1
All	All	9823	0	8424	88	5

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:B:520:MET:N	3:B:602:NAG:O5	1.91	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:TYR:OH	2:B:601:8UH:CBJ	2.13	0.95
1:B:517:ARG:O	3:B:602:NAG:N2	2.02	0.92
1:A:299:GLU:OE1	6:A:702:HOH:O	1.90	0.89
3:A:604:NAG:O4	6:A:701:HOH:O	1.86	0.82
1:B:416:ASN:ND2	6:B:701:HOH:O	2.11	0.82
1:B:521:CYS:H	3:B:602:NAG:C1	1.96	0.79
1:B:405:MET:HG3	3:B:602:NAG:C8	2.12	0.79
1:A:342:ASP:OD2	6:A:703:HOH:O	2.01	0.79
1:A:478:LYS:NZ	6:A:705:HOH:O	2.23	0.72
1:B:36:ALA:HB1	1:B:49:GLU:O	1.89	0.71
1:B:321:LEU:HD11	1:B:408:VAL:HG23	1.72	0.69
1:B:455:GLU:OE1	1:B:455:GLU:N	2.23	0.68
1:B:519:GLN:HB3	3:B:602:NAG:H62	1.76	0.67
1:A:134:TYR:OH	6:A:704:HOH:O	2.12	0.67
1:B:35:PHE:CE1	1:B:176:ALA:HB2	2.31	0.65
1:B:517:ARG:NE	3:B:602:NAG:O3	2.26	0.63
1:B:520:MET:N	3:B:602:NAG:C1	2.65	0.59
1:B:405:MET:HG3	3:B:602:NAG:H83	1.84	0.59
1:B:516:LEU:O	1:B:517:ARG:O	2.20	0.59
1:B:517:ARG:C	3:B:602:NAG:HN2	2.05	0.58
1:A:355:GLY:HA3	1:A:391:LEU:HD21	1.87	0.56
1:A:211:LEU:HD23	1:A:314:PHE:HB3	1.86	0.56
1:B:520:MET:HB2	3:B:602:NAG:H2	1.89	0.55
2:B:601:8UH:CAS	2:B:601:8UH:CAD	2.85	0.55
1:A:159:HIS:HD2	6:A:723:HOH:O	1.89	0.54
1:B:526:GLN:NE2	6:B:702:HOH:O	2.15	0.54
1:B:349:ARG:NH1	6:B:705:HOH:O	2.20	0.54
1:B:516:LEU:O	1:B:517:ARG:C	2.51	0.53
1:A:62:THR:HG23	1:A:88[B]:ARG:NH2	2.23	0.53
1:B:355:GLY:HA3	1:B:391:LEU:HD21	1.90	0.53
1:B:416:ASN:ND2	6:B:708:HOH:O	2.25	0.53
1:A:132:GLY:CA	1:A:143:LEU:HD23	2.40	0.52
1:A:451:PRO:HA	1:A:458:TYR:CD1	2.45	0.52
1:A:516:LEU:O	1:A:517:ARG:C	2.53	0.52
2:B:601:8UH:CBF	2:B:601:8UH:CAW	2.86	0.52
1:B:6:LEU:HB2	1:B:16:MET:HE3	1.91	0.51
1:B:325:LYS:HE2	6:B:976:HOH:O	2.11	0.51
2:B:601:8UH:OAX	6:B:704:HOH:O	2.19	0.51
1:A:46[B]:ARG:NH1	6:A:712:HOH:O	2.37	0.49
1:B:236:VAL:HG23	1:B:295:VAL:HG12	1.93	0.49
1:B:211:LEU:HD23	1:B:314:PHE:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:LYS:NZ	6:B:717:HOH:O	2.46	0.49
1:B:200:SER:OG	1:B:201:ALA:N	2.46	0.48
1:A:110:THR:OG1	1:A:478:LYS:HG2	2.13	0.48
1:B:121:TYR:HH	2:B:601:8UH:CBJ	2.21	0.48
1:B:6:LEU:CB	1:B:16:MET:HE3	2.44	0.47
1:B:457:ASN:ND2	6:B:719:HOH:O	2.46	0.47
1:B:517:ARG:C	3:B:602:NAG:C1	2.87	0.47
1:B:451:PRO:HA	1:B:458:TYR:CD1	2.50	0.47
1:B:515:ARG:HB3	1:B:518:VAL:HB	1.96	0.47
1:A:121:TYR:OH	2:A:601:8UH:CBJ	2.63	0.47
1:A:468[B]:ARG:NH1	6:A:710:HOH:O	2.33	0.46
1:B:521:CYS:N	3:B:602:NAG:C1	2.73	0.46
1:B:223:ILE:HA	1:B:320:LEU:O	2.16	0.45
1:A:257:ASN:ND2	6:A:706:HOH:O	2.25	0.45
1:A:397:ASP:OD1	1:A:517:ARG:HD3	2.16	0.45
1:B:502:PHE:CZ	1:B:513:HIS:HB2	2.51	0.45
1:A:397:ASP:CG	1:A:517:ARG:HD3	2.42	0.45
1:A:62:THR:HG23	1:A:88[B]:ARG:HH22	1.82	0.44
1:B:314:PHE:O	1:B:316:LYS:HD2	2.18	0.44
1:B:426:ARG:NH2	1:B:432:TRP:O	2.48	0.44
1:B:206:VAL:CG1	1:B:222:ALA:HB1	2.48	0.44
1:A:238:VAL:HG12	1:A:295[B]:VAL:HG11	2.00	0.43
1:A:485:PRO:C	1:A:487:SER:H	2.26	0.43
1:B:73[B]:GLU:OE1	6:B:706:HOH:O	2.21	0.43
1:A:199:GLU:HA	1:A:225:GLN:O	2.18	0.43
1:A:515:ARG:HB3	1:A:518:VAL:HB	2.01	0.43
1:B:36:ALA:HA	1:B:51:LYS:N	2.34	0.43
1:A:157:ALA:CB	1:A:295[B]:VAL:HG21	2.49	0.42
1:A:312:GLY:HA2	1:A:314:PHE:CE2	2.53	0.42
1:A:212:SER:O	1:A:216:ARG:HG3	2.19	0.42
1:B:64:PRO:O	1:B:88[B]:ARG:HG2	2.20	0.42
1:A:207:GLY:HA3	1:A:229:PRO:HD3	2.00	0.42
1:A:478:LYS:NZ	6:A:707:HOH:O	2.25	0.41
1:B:197:PHE:CB	1:B:223:ILE:HB	2.50	0.41
1:A:200:SER:OG	1:A:201:ALA:N	2.50	0.41
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.54	0.41
1:B:520:MET:O	1:B:523:PHE:HB3	2.20	0.41
1:B:199:GLU:HA	1:B:225:GLN:O	2.20	0.41
1:B:517:ARG:CZ	3:B:602:NAG:O4	2.69	0.41
1:A:64:PRO:O	1:A:88[B]:ARG:HG2	2.21	0.41
1:B:199:GLU:OE1	1:B:200:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:LYS:NZ	6:B:703:HOH:O	2.19	0.41
1:A:223:ILE:HA	1:A:320:LEU:O	2.20	0.41
2:A:601:8UH:OAX	2:A:601:8UH:CAV	2.68	0.41
1:B:346:LYS:HE2	1:B:385:ILE:HD11	2.03	0.40

All (5) 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)
1:B:175:MET:CB	3:B:603:NAG:N2[2_735]	1.39	0.81
1:B:175:MET:CB	3:B:603:NAG:C2[2_735]	1.56	0.64
1:B:175:MET:CB	3:B:603:NAG:C1[2_735]	1.56	0.64
2:A:601:8UH:CBI	6:B:1062:HOH:O[4_436]	1.88	0.32
1:B:172:ASP:OD1	3:B:603:NAG:O4[2_735]	1.99	0.21

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	539/586 (92%)	518 (96%)	21 (4%)	0	100	100
1	B	538/586 (92%)	520 (97%)	17 (3%)	1 (0%)	43	27
All	All	1077/1172 (92%)	1038 (96%)	38 (4%)	1 (0%)	48	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	517	ARG

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	472/513 (92%)	470 (100%)	2 (0%)	84	80
1	B	471/513 (92%)	469 (100%)	2 (0%)	84	80
All	All	943/1026 (92%)	939 (100%)	4 (0%)	84	80

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	PHE
1	A	490	SER
1	B	408	VAL
1	B	490	SER

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	178	GLN
1	B	178	GLN
1	B	257	ASN
1	B	374	GLN
1	B	514	GLN
1	B	526	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 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	602	-	14,14,15	1.59	2 (14%)	17,19,21	2.40	5 (29%)
3	NAG	B	603	-	14,14,15	1.50	3 (21%)	17,19,21	1.50	5 (29%)
4	PEG	A	605	-	6,6,6	0.49	0	5,5,5	0.31	0
3	NAG	A	603	1	14,14,15	0.55	0	17,19,21	0.39	0
2	8UH	B	601	-	42,42,42	2.89	12 (28%)	51,59,59	2.36	13 (25%)
4	PEG	A	606	-	6,6,6	0.68	0	5,5,5	0.45	0
3	NAG	A	602	1	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	A	604	1	14,14,15	0.40	0	17,19,21	0.43	0
4	PEG	A	607	-	6,6,6	0.55	0	5,5,5	0.50	0
2	8UH	A	601	-	42,42,42	3.21	22 (52%)	51,59,59	3.29	24 (47%)

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	602	-	-	0/6/23/26	0/1/1/1
3	NAG	B	603	-	-	2/6/23/26	0/1/1/1
4	PEG	A	605	-	-	4/4/4/4	-
3	NAG	A	603	1	-	2/6/23/26	0/1/1/1
2	8UH	B	601	-	-	3/16/36/36	0/6/5/5
4	PEG	A	606	-	-	3/4/4/4	-
3	NAG	A	602	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	604	1	-	2/6/23/26	0/1/1/1
4	PEG	A	607	-	-	3/4/4/4	-
2	8UH	A	601	-	-	6/16/36/36	0/6/5/5

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	8UH	CAZ-CBA	-8.06	1.33	1.51
2	B	601	8UH	CAL-CBL	-6.89	1.32	1.51
2	A	601	8UH	CAL-CBL	-6.83	1.32	1.51
2	A	601	8UH	CAK-CAJ	6.38	1.61	1.53
2	A	601	8UH	CAS-NAT	-6.07	1.33	1.45
2	A	601	8UH	CAK-CAL	-6.06	1.44	1.53
2	B	601	8UH	CBL-CAQ	5.77	1.42	1.32
2	A	601	8UH	CAZ-CBA	-5.76	1.38	1.51
2	B	601	8UH	CAK-CAJ	5.58	1.60	1.53
2	A	601	8UH	CAM-CAG	-5.48	1.45	1.51
2	A	601	8UH	CAR-CAQ	-5.41	1.37	1.50
2	B	601	8UH	CAR-CAQ	-5.35	1.37	1.50
2	B	601	8UH	CAM-CAG	-5.34	1.45	1.51
2	B	601	8UH	CAK-CAL	-5.27	1.46	1.53
2	A	601	8UH	CBL-CAQ	5.24	1.41	1.32
3	B	602	NAG	C1-C2	-5.07	1.45	1.52
2	A	601	8UH	CAM-CAL	-4.53	1.47	1.53
2	B	601	8UH	CAM-CAL	-4.04	1.48	1.53
2	A	601	8UH	CAF-NAN	-3.99	1.31	1.37
2	A	601	8UH	CBE-CBD	-3.67	1.33	1.39
2	B	601	8UH	CAH-CAJ	-3.67	1.45	1.51
2	A	601	8UH	CAI-NAT	-3.48	1.26	1.37
2	A	601	8UH	CAH-CAJ	-3.31	1.46	1.51
2	B	601	8UH	CAF-NAN	-3.25	1.32	1.37
3	B	603	NAG	C3-C2	-3.20	1.45	1.52
2	A	601	8UH	CAE-CAF	-3.13	1.37	1.42
3	B	602	NAG	O5-C1	2.89	1.48	1.43
2	A	601	8UH	CAI-CAH	-2.78	1.34	1.40
2	A	601	8UH	CBJ-CAW	-2.77	1.45	1.51
3	B	603	NAG	O5-C1	2.77	1.48	1.43
3	B	603	NAG	C1-C2	2.77	1.56	1.52
2	B	601	8UH	CBJ-CAW	-2.69	1.46	1.51
2	A	601	8UH	CAW-NAY	-2.58	1.27	1.33
2	A	601	8UH	CBE-CBF	-2.48	1.34	1.38
2	A	601	8UH	CAA-CAF	-2.40	1.38	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	8UH	CAI-CAE	-2.39	1.39	1.43
2	A	601	8UH	CAD-CAE	-2.19	1.37	1.42
2	B	601	8UH	CAD-CAE	-2.17	1.37	1.42
2	A	601	8UH	OBH-CBC	-2.02	1.33	1.37

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	8UH	CAH-CAG-NAN	-11.75	118.49	123.65
2	B	601	8UH	CAH-CAG-NAN	-11.06	118.80	123.65
2	A	601	8UH	CBI-OBH-CBC	-10.41	102.25	117.51
3	B	602	NAG	C1-O5-C5	6.36	120.70	112.19
2	A	601	8UH	CAZ-NAY-CAW	6.07	132.28	122.42
2	A	601	8UH	CAG-NAN-CAF	5.84	124.58	117.67
2	B	601	8UH	CBK-CBJ-CAW	-5.51	97.89	113.19
2	A	601	8UH	CBA-CAZ-NAY	-5.09	102.33	113.07
2	A	601	8UH	CBF-CBE-CBD	-4.89	115.61	120.50
2	B	601	8UH	CAG-NAN-CAF	4.71	123.24	117.67
2	B	601	8UH	CAP-CAJ-CAH	-4.50	106.62	111.33
3	B	602	NAG	C2-N2-C7	4.41	128.81	122.90
2	A	601	8UH	CAP-CAJ-CAH	-4.06	107.07	111.33
2	A	601	8UH	CBC-CBB-CBA	-3.99	114.14	120.04
2	A	601	8UH	CAV-CAU-CAS	-3.65	96.71	113.56
3	B	602	NAG	C1-C2-N2	-3.58	104.80	110.43
2	A	601	8UH	CBK-CBJ-CAW	-3.49	103.51	113.19
2	A	601	8UH	CAR-CAQ-CBL	-3.48	118.09	122.46
2	A	601	8UH	CAB-CAA-CAF	3.34	122.22	119.47
2	A	601	8UH	CBE-CBF-CBA	3.25	125.27	121.00
2	A	601	8UH	CAZ-CBA-CBF	-3.00	114.82	120.94
2	B	601	8UH	CAC-CAB-CAA	-2.99	118.73	122.00
2	B	601	8UH	CBF-CBA-CBB	2.98	122.66	118.55
2	A	601	8UH	CAC-CAB-CAA	-2.93	118.79	122.00
3	B	603	NAG	C2-N2-C7	2.92	126.82	122.90
2	A	601	8UH	CAE-CAF-NAN	-2.91	119.72	122.80
2	B	601	8UH	CAR-CAQ-CBL	-2.78	118.96	122.46
3	B	602	NAG	O4-C4-C5	-2.74	102.58	109.32
3	B	603	NAG	C1-C2-N2	2.73	114.74	110.43
3	B	602	NAG	O3-C3-C4	2.64	116.60	110.38
2	A	601	8UH	CBE-CBD-CBC	2.54	122.43	119.55
2	B	601	8UH	CAZ-CBA-CBB	-2.51	115.28	120.63
2	B	601	8UH	CAK-CAJ-CAH	2.49	114.74	111.52
2	B	601	8UH	CAH-CAI-NAT	-2.43	115.52	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	8UH	CAG-CAM-CAL	-2.41	110.27	113.84
2	A	601	8UH	CAR-CAQ-CAP	2.37	119.93	116.14
2	B	601	8UH	OBH-CBC-CBD	2.35	118.07	114.55
2	A	601	8UH	CAH-CAI-NAT	-2.28	115.76	119.47
3	B	603	NAG	C1-O5-C5	2.25	115.20	112.19
2	A	601	8UH	CBB-CBC-CBD	2.24	122.30	120.04
2	A	601	8UH	CAH-CAI-CAE	2.22	123.27	120.92
2	A	601	8UH	CAM-CAG-NAN	2.20	119.93	116.39
2	A	601	8UH	CAU-CAS-NAT	-2.16	105.62	111.46
3	B	603	NAG	O4-C4-C3	2.14	115.42	110.38
3	B	603	NAG	O3-C3-C2	-2.03	105.18	109.40
2	B	601	8UH	CAB-CAA-CAF	2.02	121.14	119.47
2	A	601	8UH	CAZ-CBA-CBB	2.01	124.92	120.63

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	603	NAG	C4-C5-C6-O6
2	A	601	8UH	CBJ-CAW-NAY-CAZ
3	B	603	NAG	O5-C5-C6-O6
2	A	601	8UH	OAX-CAW-NAY-CAZ
4	A	605	PEG	O2-C3-C4-O4
3	A	603	NAG	O5-C5-C6-O6
3	A	604	NAG	O5-C5-C6-O6
2	B	601	8UH	CBA-CAZ-NAY-CAW
2	A	601	8UH	CBB-CBC-OBH-CBI
3	A	602	NAG	C8-C7-N2-C2
3	A	602	NAG	O7-C7-N2-C2
3	A	603	NAG	C4-C5-C6-O6
4	A	606	PEG	O1-C1-C2-O2
3	A	604	NAG	C4-C5-C6-O6
4	A	605	PEG	O1-C1-C2-O2
4	A	606	PEG	O2-C3-C4-O4
4	A	607	PEG	O2-C3-C4-O4
2	A	601	8UH	CBD-CBC-OBH-CBI
2	B	601	8UH	CBD-CBC-OBH-CBI
2	B	601	8UH	CBB-CBC-OBH-CBI
2	A	601	8UH	CAU-CAS-NAT-CAI
4	A	607	PEG	C1-C2-O2-C3
4	A	605	PEG	C1-C2-O2-C3
2	A	601	8UH	CAU-CAV-CBK-CBJ

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Mol	Chain	Res	Type	Atoms
4	A	605	PEG	C4-C3-O2-C2
4	A	607	PEG	O1-C1-C2-O2
4	A	606	PEG	C4-C3-O2-C2

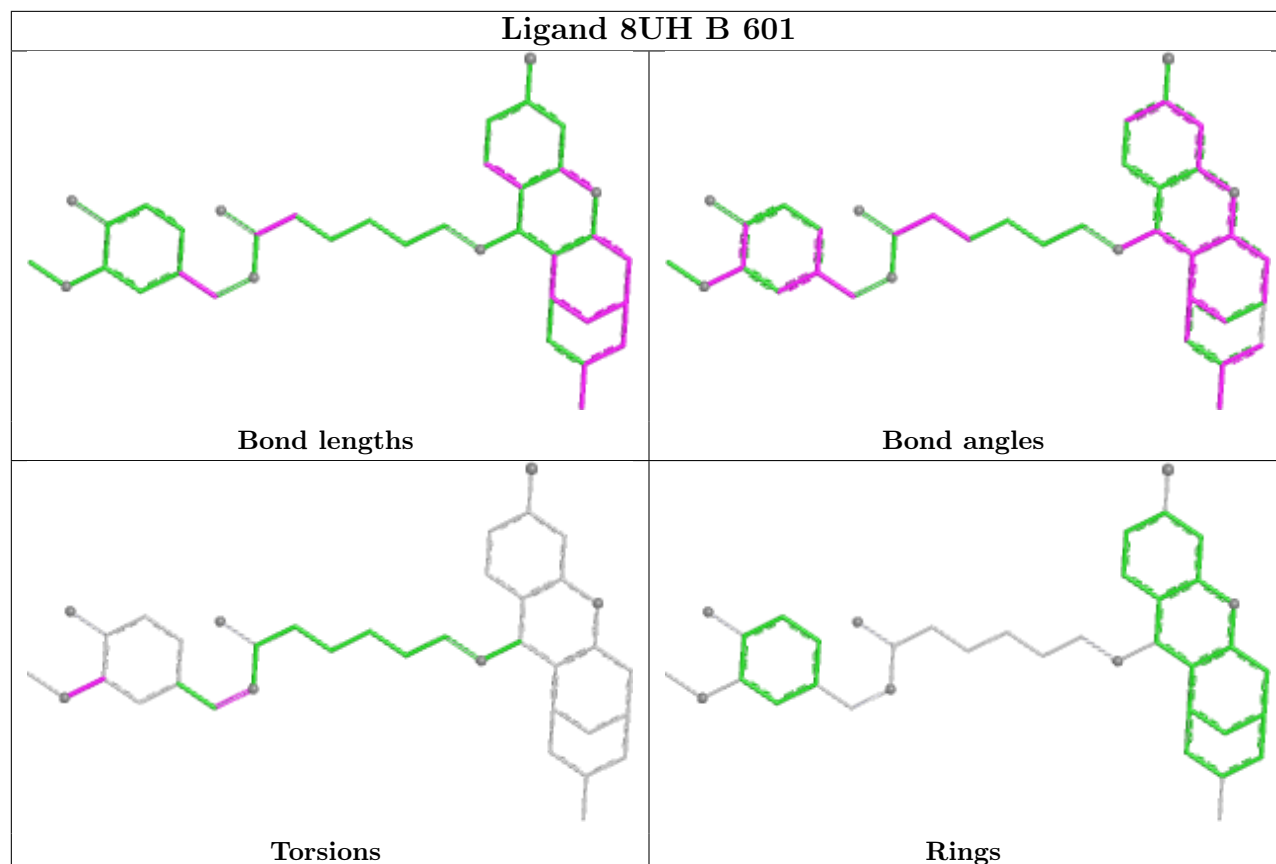
There are no ring outliers.

5 monomers are involved in 26 short contacts:

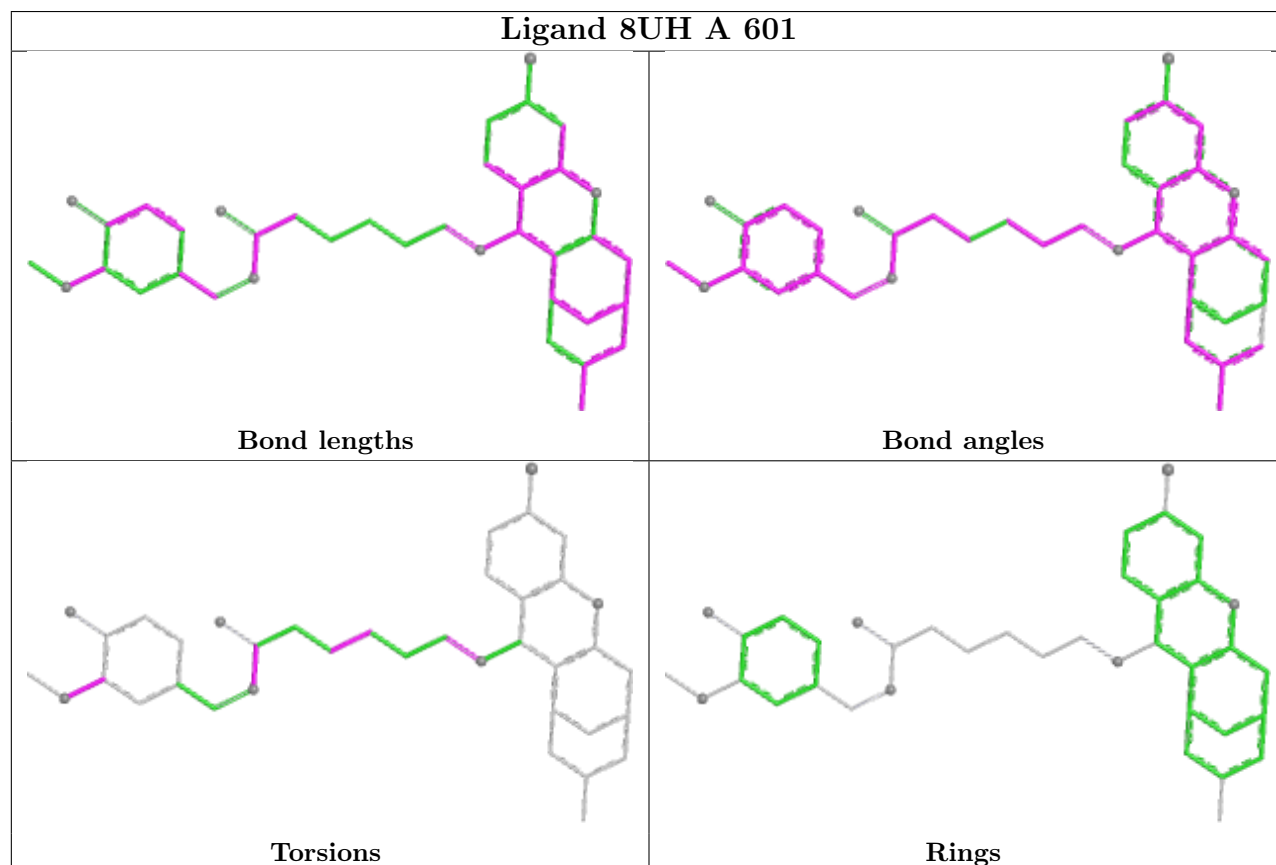
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	NAG	13	0
3	B	603	NAG	0	4
2	B	601	8UH	5	0
3	A	604	NAG	1	0
2	A	601	8UH	2	1

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.

Ligand 8UH B 601



Ligand 8UH A 601



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	532/586 (90%)	0.14	12 (2%) 61 67	18, 29, 46, 91	11 (2%)
1	B	532/586 (90%)	0.17	14 (2%) 57 63	18, 30, 45, 87	10 (1%)
All	All	1064/1172 (90%)	0.16	26 (2%) 59 66	18, 29, 46, 91	21 (1%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	535	THR	5.8
1	B	485	PRO	4.8
1	B	175	MET	4.4
1	B	35	PHE	4.1
1	A	468[A]	ARG	4.0
1	A	485	PRO	3.4
1	A	486	HIS	3.3
1	A	23	LEU	3.1
1	B	486	HIS	2.9
1	B	534	ALA	2.9
1	B	517	ARG	2.8
1	A	489	GLU	2.6
1	B	365	ASP	2.6
1	A	490	SER	2.6
1	B	488	GLN	2.4
1	A	517	ARG	2.4
1	B	299	GLU	2.3
1	B	23	LEU	2.2
1	A	42	ASN	2.2
1	A	535	THR	2.2
1	B	257	ASN	2.1
1	B	24	SER	2.1
1	A	295[A]	VAL	2.1
1	B	46[A]	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	409[A]	ASN	2.0
1	A	108	SER	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](#)

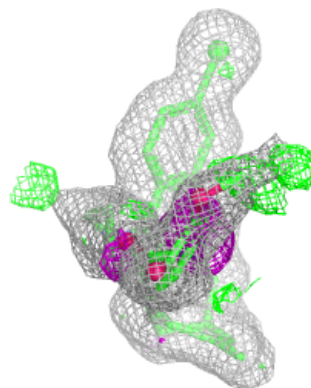
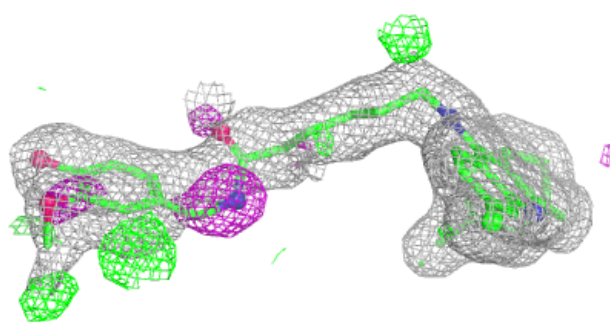
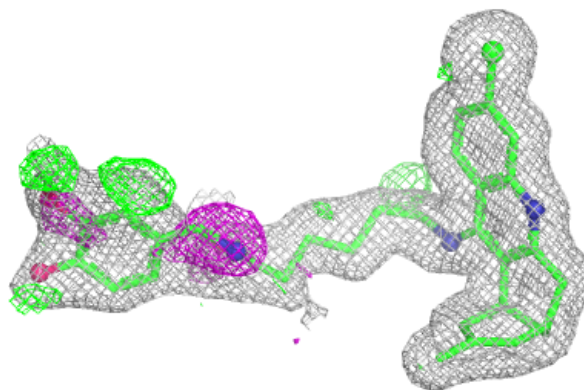
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	NAG	B	603	14/15	0.16	0.33	44,48,51,56	0
3	NAG	B	602	14/15	0.37	0.28	42,50,59,63	0
3	NAG	A	602	14/15	0.71	0.14	49,56,61,61	0
5	CL	A	609	1/1	0.75	0.29	30,30,30,30	0
3	NAG	A	604	14/15	0.76	0.12	62,68,72,72	0
4	PEG	A	607	7/7	0.82	0.23	20,20,20,20	0
4	PEG	A	605	7/7	0.85	0.13	48,54,63,67	0
3	NAG	A	603	14/15	0.86	0.11	39,45,54,57	0
4	PEG	A	606	7/7	0.89	0.13	36,42,59,62	0
2	8UH	B	601	38/38	0.93	0.12	21,26,51,56	0
2	8UH	A	601	38/38	0.93	0.12	22,27,53,54	0
5	CL	A	608	1/1	0.97	0.23	30,30,30,30	0

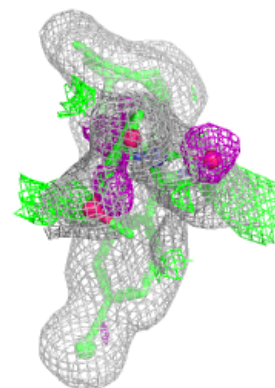
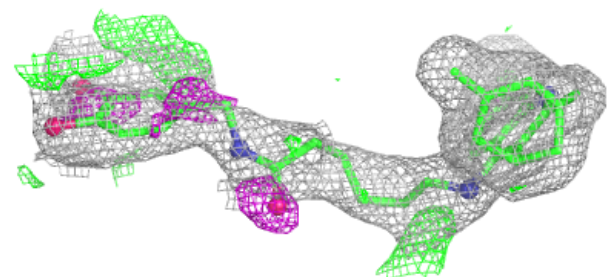
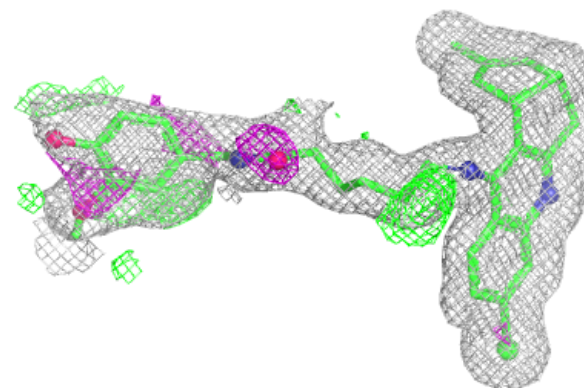
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8UH 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 8UH 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 [i](#)

There are no such residues in this entry.