



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:45 PM UTC

PDB ID : 7NB1 / pdb_00007nb1
Title : Crystal structure of human choline alpha in complex with an inhibitor
Authors : Casale, E.; Fasolini, M.
Deposited on : 2021-01-25
Resolution : 2.30 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

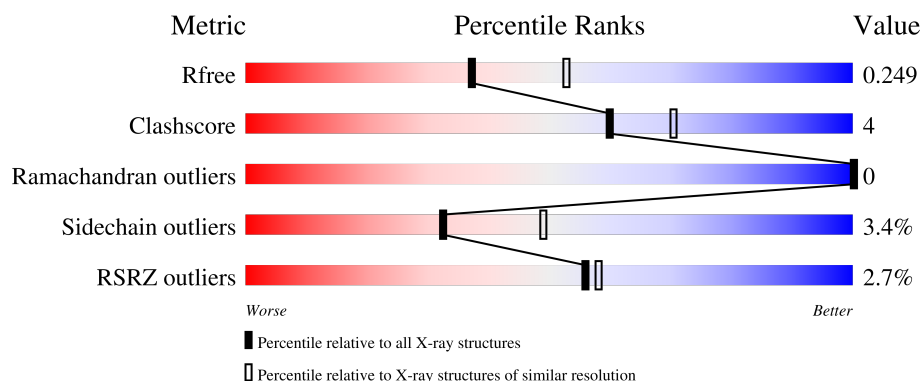
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

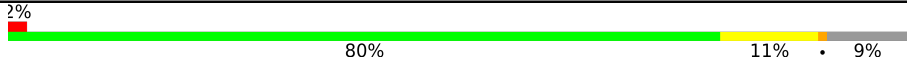
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	AAA	384	
1	BBB	384	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6039 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.

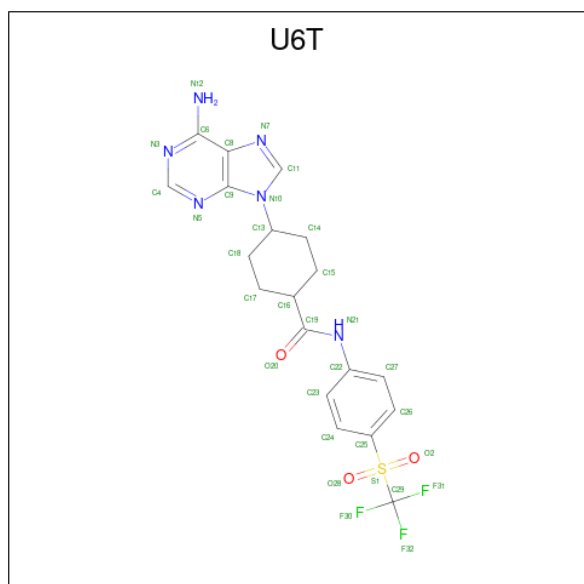
- Molecule 1 is a protein called Choline kinase alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	351	Total	C	N	O	S	0	0	0
			2909	1884	487	522	16			
1	BBB	353	Total	C	N	O	S	0	0	0
			2879	1868	478	517	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	74	GLY	-	expression tag	UNP P35790
BBB	74	GLY	-	expression tag	UNP P35790

- Molecule 2 is 4-(6-aminopurin-9-yl)- {N}-[4-(trifluoromethylsulfonyl)phenyl]cyclohexane-1-carboxamide (CCD ID: U6T) (formula: C₁₉H₁₉F₃N₆O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	F	N	O	S	0	0
			32	19	3	6	3	1		
2	BBB	1	Total	C	F	N	O	S	0	0
			32	19	3	6	3	1		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	AAA	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	BBB	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

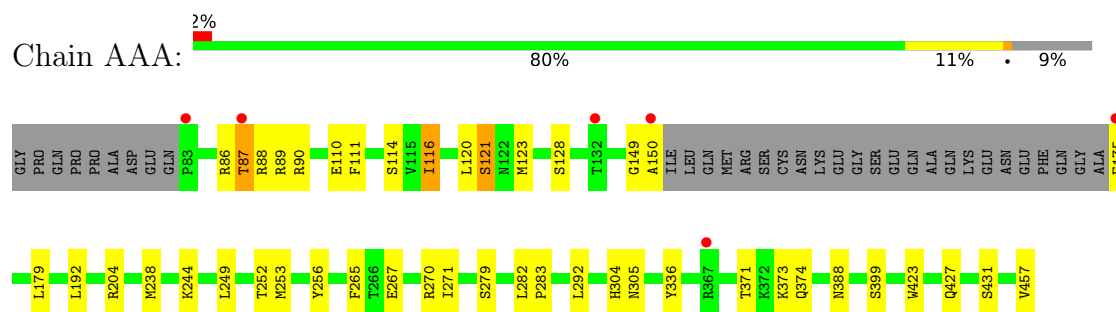
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	78	Total	O	0	0
			78	78		
4	BBB	64	Total	O	0	0
			64	64		

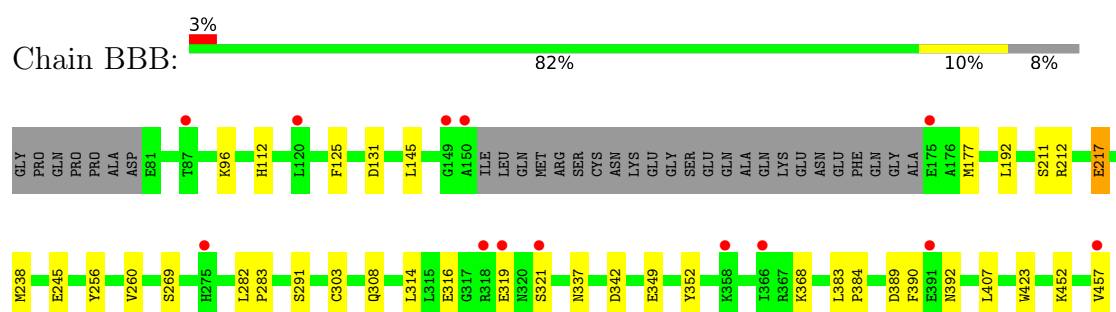
3 Residue-property plots [i](#)

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: Choline kinase alpha



• Molecule 1: Choline kinase alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.85Å 122.00Å 132.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.86 – 2.30 44.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.86-2.30) 99.9 (44.86-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.195 , 0.249 0.195 , 0.249	Depositor DCC
R_{free} test set	2094 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6039	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, U6T

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	AAA	0.55	0/2985	1.07	1/4020 (0.0%)
1	BBB	0.56	1/2955 (0.0%)	1.06	1/3989 (0.0%)
All	All	0.55	1/5940 (0.0%)	1.06	2/8009 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	319	GLU	C-O	5.58	1.31	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	116	ILE	N-CA-C	-5.82	106.55	111.56
1	BBB	245	GLU	CB-CG-CD	5.05	121.19	112.60

There are no chirality outliers.

There are no planarity outliers.

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	AAA	2909	0	2880	30	0
1	BBB	2879	0	2811	19	0
2	AAA	32	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BBB	32	0	0	0	0
3	AAA	30	0	35	1	0
3	BBB	15	0	17	1	0
4	AAA	78	0	0	1	0
4	BBB	64	0	0	1	0
All	All	6039	0	5743	50	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 4.

All (50) 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:AAA:371:THR:H	1:AAA:374:GLN:HE21	1.31	0.76
1:AAA:192:LEU:CD1	1:AAA:238:MET:SD	2.84	0.66
1:AAA:267:GLU:CG	1:AAA:270:ARG:HG3	2.29	0.63
1:AAA:292:LEU:HD22	1:AAA:457:VAL:HG11	1.84	0.60
1:AAA:238:MET:HE2	1:AAA:238:MET:HA	1.83	0.59
1:AAA:121:SER:N	1:AAA:123:MET:HE2	2.18	0.59
1:BBB:238:MET:HA	1:BBB:238:MET:HE2	1.84	0.58
1:AAA:123:MET:HE1	1:AAA:149:GLY:HA3	1.86	0.58
1:BBB:217:GLU:H	1:BBB:217:GLU:CD	2.11	0.57
1:AAA:267:GLU:HG3	1:AAA:270:ARG:HG3	1.86	0.57
1:AAA:371:THR:H	1:AAA:374:GLN:NE2	2.01	0.56
1:BBB:390:PHE:C	1:BBB:392:ASN:H	2.16	0.53
1:BBB:192:LEU:CD1	1:BBB:238:MET:SD	2.96	0.53
1:AAA:267:GLU:HG2	1:AAA:270:ARG:HG3	1.90	0.52
1:BBB:352:TYR:O	4:BBB:601:HOH:O	2.19	0.52
1:AAA:120:LEU:C	1:AAA:123:MET:HE2	2.36	0.51
1:AAA:86:ARG:O	1:AAA:89:ARG:HB3	2.12	0.50
1:AAA:149:GLY:O	1:AAA:150:ALA:C	2.54	0.50
1:AAA:88:ARG:NH2	1:AAA:111:PHE:O	2.44	0.50
1:BBB:212:ARG:NH2	1:BBB:314:LEU:HD22	2.26	0.50
1:AAA:457:VAL:O	1:AAA:457:VAL:HG12	2.13	0.49
1:AAA:423:TRP:O	1:AAA:427:GLN:HG2	2.13	0.49
2:AAA:501:U6T:O20	2:AAA:501:U6T:C23	2.61	0.49
1:AAA:252:THR:HG22	1:AAA:256:TYR:CE2	2.49	0.48
1:BBB:282:LEU:N	1:BBB:283:PRO:CD	2.77	0.47
1:BBB:423:TRP:CH2	3:BBB:502:EPE:H91	2.50	0.47
1:AAA:304:HIS:O	1:AAA:305:ASN:HB2	2.15	0.46
1:AAA:267:GLU:H	1:AAA:267:GLU:CD	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:303:CYS:SG	1:BBB:337:ASN:HB3	2.56	0.45
1:BBB:452:LYS:HG2	1:BBB:457:VAL:HG23	1.98	0.45
1:AAA:116:ILE:HG23	2:AAA:501:U6T:C27	2.47	0.45
1:AAA:282:LEU:N	1:AAA:283:PRO:CD	2.80	0.44
1:BBB:308:GLN:HB3	1:BBB:349:GLU:HG3	2.00	0.44
1:BBB:125:PHE:HB2	1:BBB:145:LEU:HB3	2.00	0.43
1:AAA:121:SER:CA	1:AAA:123:MET:HE2	2.48	0.43
1:AAA:192:LEU:HD12	1:AAA:238:MET:SD	2.59	0.43
1:AAA:249:LEU:HG	1:AAA:253:MET:HE2	2.01	0.43
1:BBB:192:LEU:HD12	1:BBB:238:MET:SD	2.59	0.42
1:AAA:373:LYS:HE2	4:AAA:674:HOH:O	2.19	0.42
1:BBB:383:LEU:N	1:BBB:384:PRO:HD2	2.35	0.42
1:AAA:87:THR:HA	1:AAA:90:ARG:HG3	2.01	0.42
1:AAA:265:PHE:O	1:AAA:271:ILE:HD11	2.20	0.41
1:BBB:177:MET:HE3	1:BBB:177:MET:HB3	1.94	0.41
1:AAA:244:LYS:HD3	1:AAA:336:TYR:CZ	2.54	0.41
1:AAA:431:SER:O	3:AAA:503:EPE:H51	2.20	0.41
1:BBB:390:PHE:C	1:BBB:392:ASN:N	2.79	0.41
1:AAA:116:ILE:HG23	2:AAA:501:U6T:C22	2.51	0.41
1:BBB:256:TYR:O	1:BBB:260:VAL:HG23	2.21	0.41
1:BBB:211:SER:HA	1:BBB:316:GLU:HG3	2.02	0.40
1:BBB:368:LYS:HD3	1:BBB:368:LYS:HA	1.92	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	AAA	347/384 (90%)	336 (97%)	11 (3%)	0	100	100
1	BBB	349/384 (91%)	338 (97%)	11 (3%)	0	100	100
All	All	696/768 (91%)	674 (97%)	22 (3%)	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	AAA	314/342 (92%)	303 (96%)	11 (4%)	32	48
1	BBB	305/342 (89%)	295 (97%)	10 (3%)	33	50
All	All	619/684 (90%)	598 (97%)	21 (3%)	32	49

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	87	THR
1	AAA	110	GLU
1	AAA	114	SER
1	AAA	121	SER
1	AAA	128	SER
1	AAA	175	GLU
1	AAA	179	LEU
1	AAA	204	ARG
1	AAA	279	SER
1	AAA	388	ASN
1	AAA	399	SER
1	BBB	96	LYS
1	BBB	112	HIS
1	BBB	131	ASP
1	BBB	217	GLU
1	BBB	269	SER
1	BBB	291	SER
1	BBB	321	SER
1	BBB	342	ASP
1	BBB	389	ASP
1	BBB	407	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

5 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	EPE	BBB	502	-	15,15,15	1.10	1 (6%)	19,20,20	1.20	2 (10%)
2	U6T	BBB	501	-	35,35,35	2.35	7 (20%)	53,53,53	2.03	11 (20%)
2	U6T	AAA	501	-	35,35,35	2.25	4 (11%)	53,53,53	2.41	14 (26%)
3	EPE	AAA	502	-	15,15,15	0.69	1 (6%)	19,20,20	0.98	1 (5%)
3	EPE	AAA	503	-	15,15,15	1.14	1 (6%)	19,20,20	1.40	3 (15%)

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	EPE	BBB	502	-	-	5/9/19/19	0/1/1/1
2	U6T	BBB	501	-	-	0/27/37/37	0/4/4/4
2	U6T	AAA	501	-	-	6/27/37/37	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPE	AAA	502	-	-	5/9/19/19	0/1/1/1
3	EPE	AAA	503	-	-	5/9/19/19	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	501	U6T	C25-S1	-11.46	1.62	1.76
2	AAA	501	U6T	C25-S1	-11.29	1.63	1.76
3	BBB	502	EPE	O2S-S	4.06	1.56	1.45
3	AAA	503	EPE	O2S-S	3.61	1.55	1.45
2	BBB	501	U6T	C29-S1	-2.99	1.70	1.85
2	AAA	501	U6T	C22-N21	-2.89	1.35	1.41
2	BBB	501	U6T	C8-N7	-2.84	1.33	1.39
2	AAA	501	U6T	C8-C6	2.74	1.48	1.41
2	AAA	501	U6T	C29-S1	-2.69	1.72	1.85
2	BBB	501	U6T	C9-N10	-2.67	1.32	1.37
2	BBB	501	U6T	C22-N21	-2.66	1.36	1.41
3	AAA	502	EPE	O3S-S	2.32	1.55	1.47
2	BBB	501	U6T	C8-C6	2.31	1.47	1.41
2	BBB	501	U6T	C11-N7	2.23	1.36	1.31

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	501	U6T	O28-S1-O2	-10.32	106.10	119.06
2	BBB	501	U6T	O28-S1-O2	-9.26	107.44	119.06
2	AAA	501	U6T	C8-C9-N5	-5.73	118.83	126.72
2	AAA	501	U6T	N3-C4-N5	-4.91	121.16	128.58
2	AAA	501	U6T	C4-N5-C9	4.79	123.52	111.83
2	BBB	501	U6T	N3-C4-N5	-4.64	121.56	128.58
2	BBB	501	U6T	C8-C9-N5	-4.42	120.63	126.72
2	AAA	501	U6T	N5-C9-N10	3.93	133.85	127.17
2	BBB	501	U6T	C4-N5-C9	3.89	121.33	111.83
3	AAA	503	EPE	O3S-S-O1S	3.89	121.12	111.40
2	AAA	501	U6T	C26-C25-S1	3.68	122.49	119.36
2	AAA	501	U6T	N10-C11-N7	-3.42	109.09	113.94
3	BBB	502	EPE	O2S-S-C10	-3.35	101.66	106.73
2	AAA	501	U6T	C29-S1-C25	3.13	108.22	102.52
2	BBB	501	U6T	C18-C13-N10	-3.04	108.03	111.40
3	BBB	502	EPE	O3S-S-O1S	2.95	118.78	111.40
2	AAA	501	U6T	C14-C15-C16	2.76	116.04	111.18
2	BBB	501	U6T	N5-C9-N10	2.74	131.82	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	501	U6T	O2-S1-C29	2.64	112.87	104.70
2	BBB	501	U6T	O28-S1-C29	2.64	112.87	104.70
2	AAA	501	U6T	C9-N10-C11	2.52	108.38	105.74
2	AAA	501	U6T	C8-N7-C11	2.24	106.97	103.45
2	BBB	501	U6T	N10-C11-N7	-2.20	110.81	113.94
3	AAA	502	EPE	O3S-S-C10	-2.18	101.74	106.00
3	AAA	503	EPE	O2S-S-O1S	-2.17	106.77	113.82
2	BBB	501	U6T	C29-S1-C25	2.14	106.42	102.52
3	AAA	503	EPE	O3S-S-O2S	-2.09	106.17	111.40
2	AAA	501	U6T	C9-C8-N7	-2.04	108.24	110.58
2	AAA	501	U6T	C18-C13-N10	-2.03	109.16	111.40
2	BBB	501	U6T	N12-C6-N3	2.03	122.89	118.38
2	BBB	501	U6T	O2-S1-C25	2.02	110.88	108.35

There are no chirality outliers.

All (21) torsion outliers are listed below:

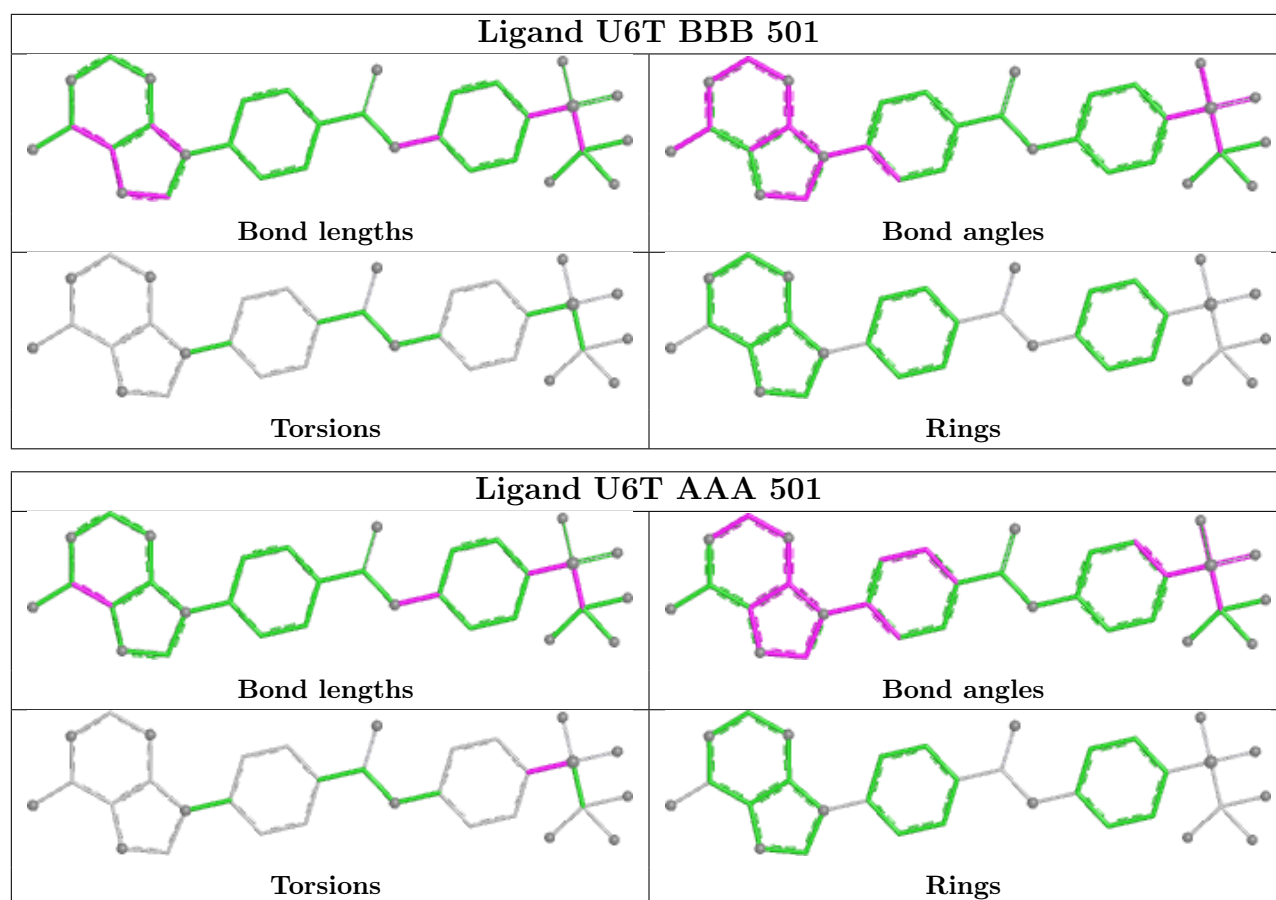
Mol	Chain	Res	Type	Atoms
2	AAA	501	U6T	C24-C25-S1-C29
2	AAA	501	U6T	C26-C25-S1-C29
3	AAA	502	EPE	C9-C10-S-O2S
3	AAA	503	EPE	C10-C9-N1-C2
3	AAA	503	EPE	N4-C7-C8-O8
2	AAA	501	U6T	C24-C25-S1-O2
2	AAA	501	U6T	C26-C25-S1-O2
3	AAA	502	EPE	C10-C9-N1-C6
3	AAA	503	EPE	C10-C9-N1-C6
3	BBB	502	EPE	C10-C9-N1-C2
3	AAA	502	EPE	C8-C7-N4-C3
3	AAA	502	EPE	C8-C7-N4-C5
3	AAA	503	EPE	C8-C7-N4-C3
3	BBB	502	EPE	S-C10-C9-N1
3	AAA	503	EPE	C8-C7-N4-C5
3	AAA	502	EPE	C10-C9-N1-C2
3	BBB	502	EPE	C10-C9-N1-C6
2	AAA	501	U6T	C24-C25-S1-O28
3	BBB	502	EPE	C8-C7-N4-C3
3	BBB	502	EPE	C8-C7-N4-C5
2	AAA	501	U6T	C26-C25-S1-O28

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	502	EPE	1	0
2	AAA	501	U6T	3	0
3	AAA	503	EPE	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	AAA	351/384 (91%)	-0.08	6 (1%) 69 70	31, 48, 89, 113	1 (0%)
1	BBB	353/384 (91%)	0.01	13 (3%) 45 48	32, 53, 98, 158	0
All	All	704/768 (91%)	-0.03	19 (2%) 56 58	31, 51, 91, 158	1 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	150	ALA	4.4
1	BBB	150	ALA	4.2
1	AAA	83	PRO	3.9
1	BBB	87	THR	3.3
1	BBB	366	ILE	3.1
1	BBB	120	LEU	3.0
1	BBB	318	ARG	2.8
1	AAA	175	GLU	2.7
1	BBB	319	GLU	2.5
1	AAA	132	THR	2.4
1	BBB	175	GLU	2.4
1	AAA	367	ARG	2.4
1	BBB	391	GLU	2.4
1	AAA	87	THR	2.4
1	BBB	358	LYS	2.3
1	BBB	457	VAL	2.3
1	BBB	149	GLY	2.2
1	BBB	321	SER	2.1
1	BBB	275	HIS	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 [i](#)

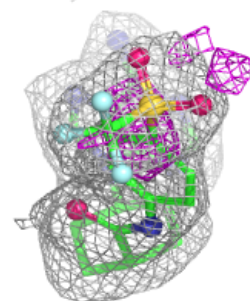
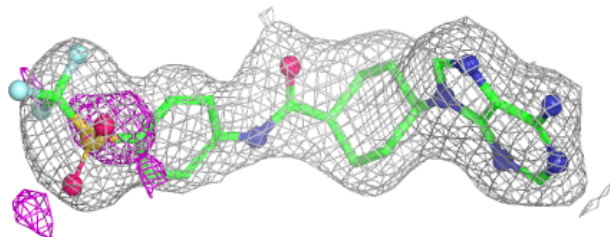
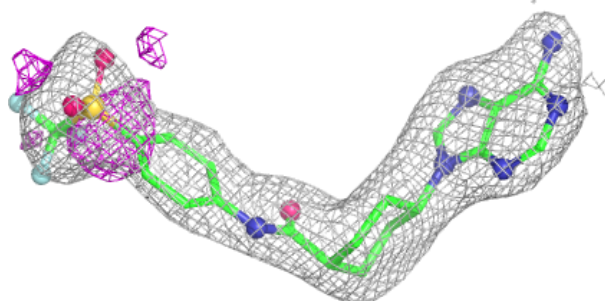
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	EPE	AAA	503	15/15	0.81	0.21	63,103,129,132	0
3	EPE	BBB	502	15/15	0.81	0.25	96,111,127,131	0
3	EPE	AAA	502	15/15	0.84	0.21	86,97,108,122	0
2	U6T	BBB	501	32/32	0.92	0.10	36,45,110,119	0
2	U6T	AAA	501	32/32	0.92	0.10	39,49,121,129	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.

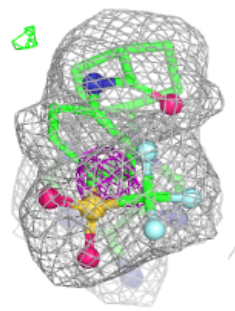
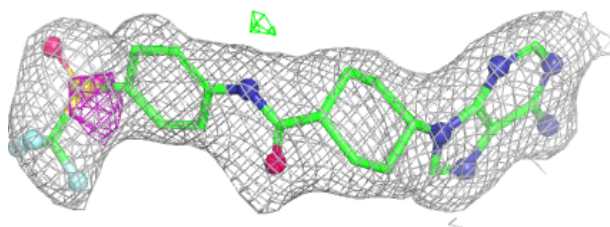
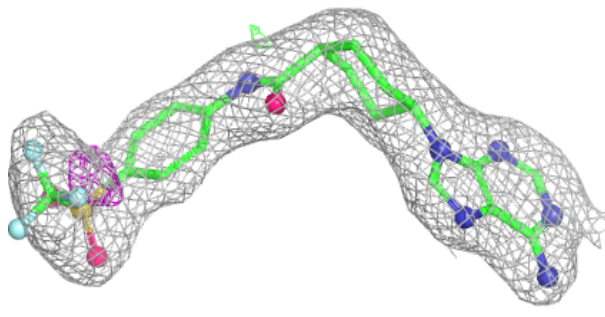
Electron density around U6T BBB 501:

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 U6T AAA 501:

$2mF_o-DF_c$ (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.