Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 09:11 am GMT

PDB ID	:	6EO6
Title	:	X-ray structure of the complex between human alpha-thrombin and modified 15-mer DNA aptamer containing 5-(3-(2-(1H-indol-3-yl)acetamide-N-yl)-1-propen-1-yl)-2'-deoxyuridine residue
Authors	:	Dolot, R.M.; Nawrot, B.; Yang, X.
Deposited on	:	2017-10-09
Resolution	:	1.69 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

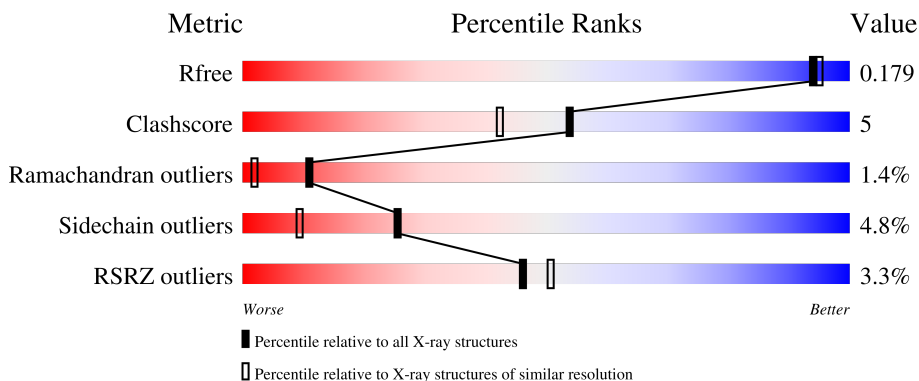|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.69 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	Percentile Ranks	Value
Rfree		0.179
Clashscore		5
Ramachandran outliers		1.4%
Sidechain outliers		4.8%
RSRZ outliers		3.3%

Worse *Better*

▌ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	D	15	53% 47%
2	L	36	3% / 67% 11% · 19%
3	H	259	3% / 82% 14% · ·

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 3230 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 DNA chain called GA63A - TBA MODIFIED APTAMER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	15	Total	C	N	O	P	0	0	0
			330	162	59	95	14			

- Molecule 2 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	29	Total	C	N	O	S	0	1	0
			248	155	40	52	1			

- Molecule 3 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	259	Total	C	N	O	S	0	13	0
			2194	1399	386	395	14			

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	K	0	0
			1	1		

- Molecule 5 is D-phenylalanyl-N-[(2S,3S)-6-{[amino(iminio)methyl]amino}-1-chloro-2-hydro xyhexan-3-yl]-L-prolinamide (three-letter code: 0G6) (formula: $C_{21}H_{34}ClN_6O_3$).
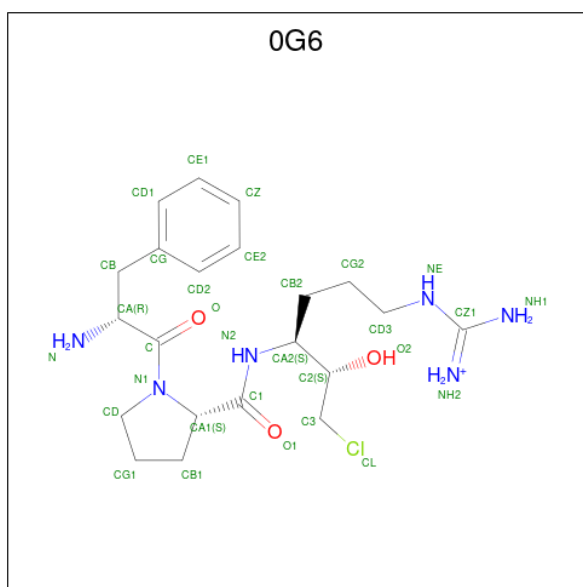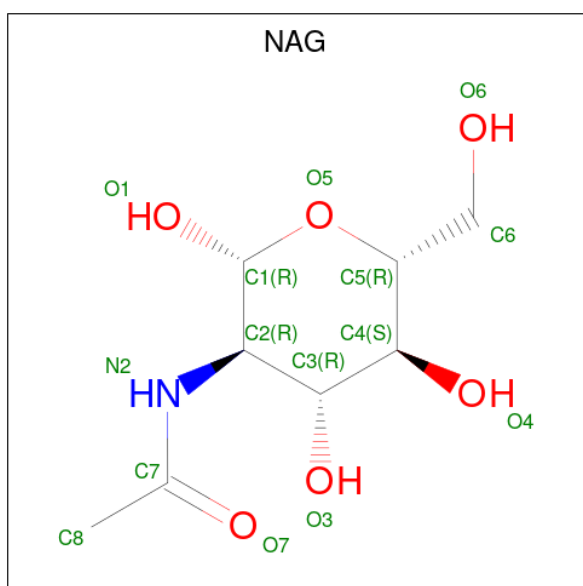
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	H	1	30	21	6	3	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
6	H	1	1	1	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	69	Total	O	0	0
			69	69		
8	L	41	Total	O	0	0
			41	41		
8	H	302	Total	O	0	0
			302	302		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
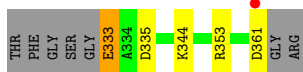
• Molecule 1: GA63A - TBA MODIFIED APTAMER

Chain D:

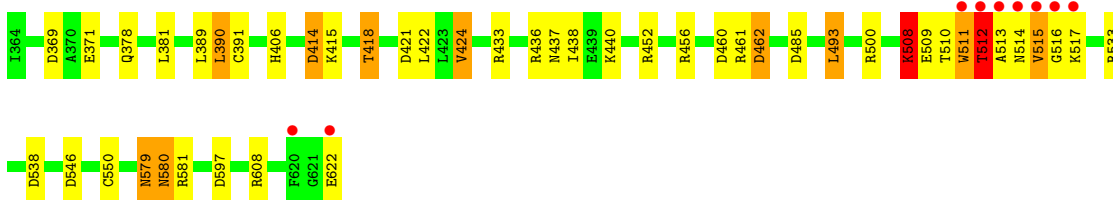• Molecule 2: Prothrombin

Chain L:

• Molecule 3: Prothrombin

Chain H:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	94.09Å 94.09Å 124.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	81.49 – 1.69 68.22 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.5 (81.49-1.69) 99.5 (68.22-1.69)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.145 , 0.168 0.159 , 0.179	Depositor DCC
R_{free} test set	3441 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3230	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 77Y, NA, 0G6, K, NAG

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	D	1.30	2/330 (0.6%)	1.32	4/509 (0.8%)
2	L	1.49	2/250 (0.8%)	1.44	3/332 (0.9%)
3	H	1.37	6/2249 (0.3%)	1.43	38/3041 (1.2%)
All	All	1.37	10/2829 (0.4%)	1.42	45/3882 (1.2%)

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
3	H	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	437	ASN	N-CA	23.28	1.93	1.46
2	L	333	GLU	CD-OE2	8.12	1.34	1.25
3	H	509	GLU	CB-CG	-8.04	1.36	1.52
3	H	414	ASP	CB-CG	-7.67	1.35	1.51
3	H	378	GLN	CD-NE2	-6.46	1.16	1.32
1	D	409	DT	O3'-P	-6.37	1.53	1.61
3	H	371	GLU	CD-OE2	-6.00	1.19	1.25
3	H	436	ARG	C-N	-5.93	1.20	1.34
2	L	335	ASP	CA-CB	5.75	1.66	1.53
1	D	401	DG	O3'-P	-5.30	1.54	1.61

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	436	ARG	C-N-CA	-16.05	81.59	121.70
3	H	460	ASP	CB-CG-OD1	11.38	128.55	118.30
3	H	608	ARG	NE-CZ-NH1	10.36	125.48	120.30
3	H	452	ARG	NE-CZ-NH1	10.16	125.38	120.30
3	H	436	ARG	NE-CZ-NH2	-9.55	115.53	120.30
3	H	436	ARG	NE-CZ-NH1	9.38	124.99	120.30
3	H	485	ASP	CB-CG-OD1	8.91	126.32	118.30
3	H	369	ASP	CB-CG-OD1	8.62	126.06	118.30
1	D	410	DG	O5'-P-OP2	8.05	120.36	110.70
3	H	436	ARG	O-C-N	-7.81	110.21	122.70
3	H	456	ARG	NE-CZ-NH1	7.78	124.19	120.30
3	H	538	ASP	CB-CG-OD2	-7.55	111.50	118.30
2	L	333	GLU	CG-CD-OE2	7.30	132.91	118.30
3	H	597	ASP	CB-CG-OD1	7.13	124.72	118.30
3	H	461	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	D	409	DT	O5'-P-OP2	-6.83	99.55	105.70
3	H	424	VAL	CA-CB-CG1	6.63	120.85	110.90
3	H	461	ARG	NE-CZ-NH2	-6.44	117.08	120.30
3	H	452	ARG	NE-CZ-NH2	-6.43	117.08	120.30
3	H	414	ASP	CB-CG-OD1	-6.34	112.59	118.30
2	L	333	GLU	CG-CD-OE1	-6.16	105.99	118.30
3	H	369	ASP	CB-CG-OD2	-6.09	112.82	118.30
3	H	414	ASP	CB-CG-OD2	-6.01	112.89	118.30
3	H	546	ASP	CB-CG-OD1	6.00	123.70	118.30
3	H	462	ASP	CB-CG-OD1	5.97	123.67	118.30
3	H	509	GLU	CG-CD-OE2	-5.89	106.51	118.30
3	H	378	GLN	CB-CG-CD	5.78	126.63	111.60
3	H	440	LYS	CD-CE-NZ	-5.77	98.43	111.70
3	H	436	ARG	CA-C-N	5.74	129.83	117.20
3	H	508	LYS	CD-CE-NZ	5.70	124.80	111.70
2	L	335	ASP	N-CA-CB	5.69	120.84	110.60
3	H	485	ASP	CB-CG-OD2	-5.66	113.21	118.30
3	H	414	ASP	OD1-CG-OD2	5.54	133.82	123.30
3	H	511	TRP	C-N-CA	5.49	135.42	121.70
3	H	533	ARG	NE-CZ-NH2	-5.44	117.58	120.30
3	H	422	LEU	CB-CA-C	-5.35	100.03	110.20
3	H	500	ARG	NE-CZ-NH1	-5.26	117.67	120.30
3	H	533	ARG	NE-CZ-NH1	5.22	122.91	120.30
3	H	493	LEU	CB-CG-CD2	5.20	119.83	111.00
3	H	433	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	D	405	DG	O5'-P-OP2	5.16	116.89	110.70
3	H	622	GLU	CA-C-O	5.10	130.81	120.10
3	H	512	THR	N-CA-C	-5.10	97.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	460	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	D	403	DT	O5'-P-OP2	-5.06	101.15	105.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	511	TRP	Peptide
3	H	512	THR	Peptide

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	D	330	0	161	2	0
2	L	248	0	244	5	0
3	H	2194	0	2166	24	0
4	D	1	0	0	0	0
5	H	30	0	31	0	0
6	H	1	0	0	0	0
7	H	14	0	13	0	0
8	D	69	0	0	0	0
8	H	302	0	0	5	0
8	L	41	0	0	5	0
All	All	3230	0	2615	29	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 (29) 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:H:390[A]:LEU:C	3:H:390[A]:LEU:HD12	1.72	1.10
3:H:390[A]:LEU:HD12	3:H:390[A]:LEU:O	1.69	0.92
3:H:390[A]:LEU:HD13	8:H:859:HOH:O	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:390[A]:LEU:C	3:H:390[A]:LEU:CD1	2.48	0.82
3:H:381[A]:LEU:HD23	3:H:390[A]:LEU:HG	1.68	0.73
3:H:390[A]:LEU:CD1	8:H:859:HOH:O	2.33	0.73
3:H:390[A]:LEU:O	3:H:390[A]:LEU:CD1	2.38	0.70
2:L:344[B]:LYS:NZ	8:L:402:HOH:O	2.25	0.69
2:L:361:ASP:O	8:L:401:HOH:O	2.13	0.67
3:H:406:HIS:HD2	3:H:462:ASP:OD2	1.79	0.66
1:D:413:DT:H5'	3:H:438[A]:ILE:HD11	1.77	0.66
3:H:381[A]:LEU:CD2	3:H:390[A]:LEU:HG	2.26	0.65
3:H:510:THR:O	3:H:512:THR:HG23	1.97	0.64
3:H:389[B]:LEU:C	3:H:389[B]:LEU:HD23	2.21	0.62
2:L:333:GLU:CD	8:L:404:HOH:O	2.38	0.61
3:H:508:LYS:O	3:H:510:THR:HG23	2.00	0.61
2:L:333:GLU:HB2	8:L:404:HOH:O	2.02	0.58
3:H:513:ALA:HA	8:H:1051:HOH:O	2.06	0.55
3:H:579:ASN:C	3:H:579:ASN:HD22	2.12	0.53
3:H:415:LYS:HE3	8:H:1046:HOH:O	2.08	0.53
1:D:413:DT:C6	3:H:438[B]:ILE:HD11	2.43	0.52
2:L:333:GLU:CB	8:L:404:HOH:O	2.61	0.48
3:H:390[A]:LEU:O	3:H:391:CYS:SG	2.74	0.45
3:H:381[A]:LEU:HG	3:H:390[A]:LEU:HG	2.00	0.43
3:H:381[A]:LEU:CG	3:H:390[A]:LEU:HG	2.48	0.43
3:H:381[B]:LEU:CD2	3:H:424:VAL:HG22	2.49	0.42
3:H:579:ASN:ND2	3:H:581:ARG:H	2.18	0.41
3:H:580:ASN:ND2	8:H:805:HOH:O	2.47	0.41
3:H:418[B]:THR:HG22	3:H:421:ASP:OD2	2.20	0.41

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	
2	L	28/36 (78%)	26 (93%)	2 (7%)	0	100	100
3	H	270/259 (104%)	256 (95%)	10 (4%)	4 (2%)	10	2
All	All	298/295 (101%)	282 (95%)	12 (4%)	4 (1%)	11	2

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	512	THR
3	H	514	ASN
3	H	515	VAL
3	H	516	GLY

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	
2	L	28/31 (90%)	27 (96%)	1 (4%)	35	16
3	H	238/225 (106%)	225 (94%)	13 (6%)	21	7
All	All	266/256 (104%)	252 (95%)	14 (5%)	25	7

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	353	ARG
3	H	390[A]	LEU
3	H	390[B]	LEU
3	H	414	ASP
3	H	418[A]	THR
3	H	418[B]	THR
3	H	493	LEU
3	H	508	LYS
3	H	512	THR
3	H	515	VAL
3	H	517	LYS
3	H	550	CYS

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Mol	Chain	Res	Type
3	H	579	ASN
3	H	580	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	H	378	GLN
3	H	406	HIS
3	H	579	ASN
3	H	580	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\#|Z| > 2$
1	77Y	D	404	1	34,38,39	1.59	7 (20%)	39,53,56	2.59	19 (48%)

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
1	77Y	D	404	1	-	0/18/32/33	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	404	77Y	C2'-C1'	3.64	1.62	1.52
1	D	404	77Y	C4-N3	-3.38	1.32	1.38
1	D	404	77Y	C30-C13	-2.90	1.36	1.42
1	D	404	77Y	O4-C4	2.87	1.29	1.23
1	D	404	77Y	C2-N3	-2.51	1.33	1.38
1	D	404	77Y	O3'-C3'	-2.42	1.38	1.43
1	D	404	77Y	C16-C12	2.04	1.42	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	404	77Y	O4-C4-C5	-5.85	116.84	124.61
1	D	404	77Y	C4-N3-C2	-5.39	120.38	127.35
1	D	404	77Y	C5-C4-N3	5.10	122.12	114.41
1	D	404	77Y	C28-C29-C30	-4.17	114.59	120.44
1	D	404	77Y	N3-C2-N1	3.59	119.66	114.89
1	D	404	77Y	O34-C32-N9	3.57	129.74	123.01
1	D	404	77Y	C27-C14-C13	-3.54	114.30	120.76
1	D	404	77Y	C2'-C3'-C4'	3.48	110.02	102.76
1	D	404	77Y	C3'-C2'-C1'	-3.47	93.85	102.54
1	D	404	77Y	C33-C32-N9	-3.23	111.82	116.19
1	D	404	77Y	C30-C13-C14	3.22	122.44	118.17
1	D	404	77Y	O2-C2-N1	-3.21	118.52	122.79
1	D	404	77Y	O4'-C4'-C3'	-2.91	98.88	105.67
1	D	404	77Y	O3'-C3'-C2'	-2.37	102.41	110.90
1	D	404	77Y	C6-N1-C2	2.28	123.61	121.30
1	D	404	77Y	C1'-N1-C6	-2.17	117.04	120.77
1	D	404	77Y	C4'-O4'-C1'	2.04	114.39	109.45
1	D	404	77Y	C27-C14-N15	2.02	136.40	130.80
1	D	404	77Y	O3'-C3'-C4'	2.02	117.81	110.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
5	0G6	H	701	3	30,31,32	1.06	2 (6%)	37,41,42	1.12	5 (13%)
7	NAG	H	703	3	14,14,15	1.83	3 (21%)	17,19,21	2.80	7 (41%)

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
5	0G6	H	701	3	-	1/31/41/43	0/2/2/2
7	NAG	H	703	3	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	703	NAG	C1-C2	5.28	1.60	1.52
7	H	703	NAG	O5-C1	-2.87	1.39	1.43
7	H	703	NAG	C2-N2	2.44	1.50	1.46
5	H	701	0G6	CA1-N1	2.12	1.51	1.47
5	H	701	0G6	O-C	2.08	1.26	1.22

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	703	NAG	O5-C1-C2	-6.21	101.48	111.29
7	H	703	NAG	C1-C2-N2	5.50	119.89	110.49
7	H	703	NAG	C8-C7-N2	4.07	122.99	116.10
7	H	703	NAG	C4-C3-C2	-3.63	105.70	111.02
7	H	703	NAG	C2-N2-C7	-3.42	118.04	122.90
7	H	703	NAG	O7-C7-N2	-3.09	116.27	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	701	0G6	O2-C2-C3	-2.89	101.19	109.74
5	H	701	0G6	CA2-N2-C1	-2.28	119.04	123.07
5	H	701	0G6	CB1-CA1-N1	2.25	106.37	103.03
5	H	701	0G6	CB2-CA2-C2	-2.21	108.68	112.51
7	H	703	NAG	C6-C5-C4	2.17	118.08	113.00
5	H	701	0G6	CZ-CE1-CD1	-2.03	117.09	120.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	701	0G6	O2-C2-CA2-CB2
7	H	703	NAG	C4-C5-C6-O6
7	H	703	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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 0G6 H 701

Bond lengths

Bond angles

Torsions

Rings
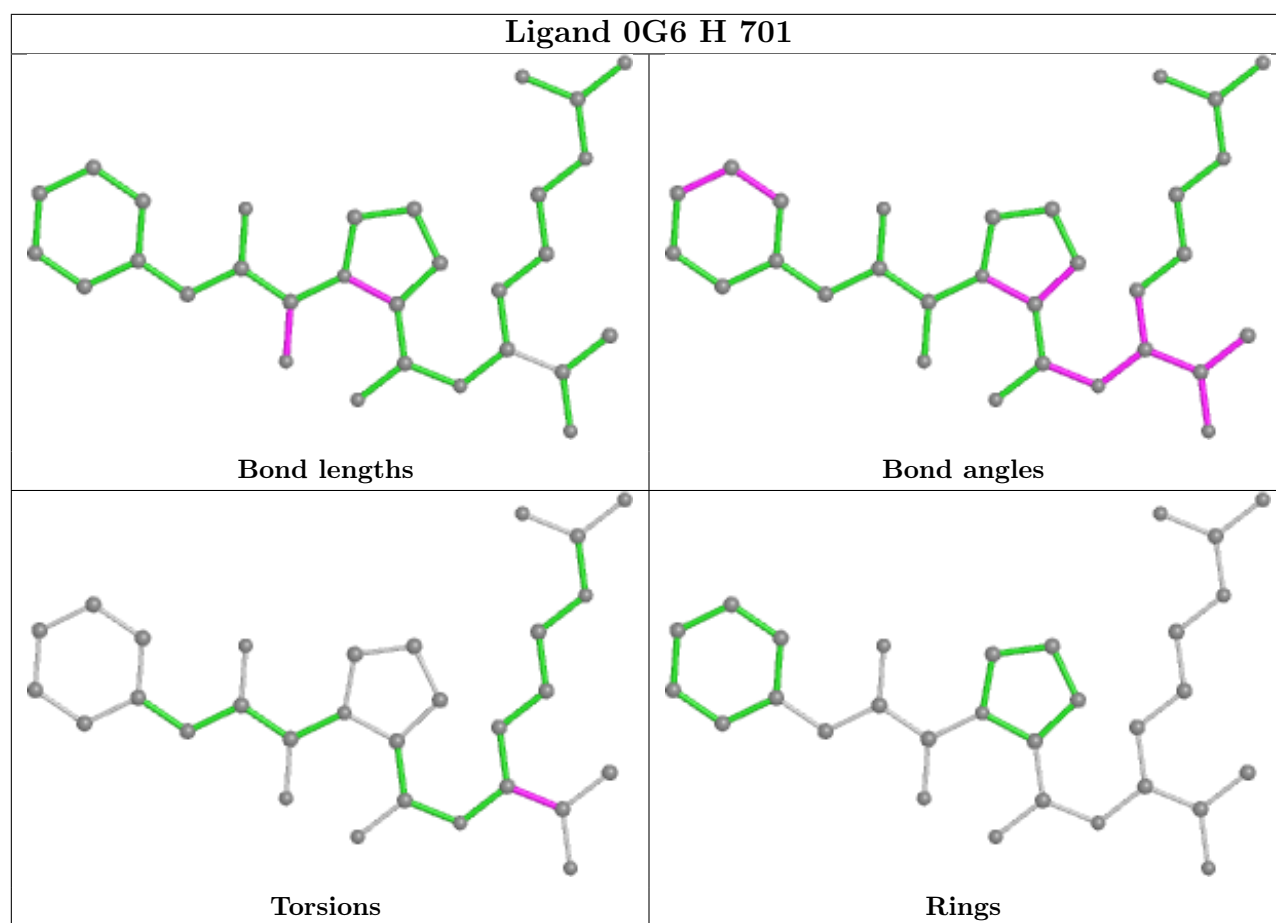
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	436:ARG	C	437:ASN	N	1.20

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(Å²)	Q<0.9
1	D	14/15 (93%)	-0.59	0	100	100	24, 29, 38, 84	0
2	L	29/36 (80%)	-0.31	1 (3%)	45	50	19, 26, 54, 84	0
3	H	259/259 (100%)	-0.38	9 (3%)	44	49	16, 23, 51, 133	0
All	All	302/310 (97%)	-0.38	10 (3%)	46	51	16, 24, 51, 133	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	513	ALA	7.0
3	H	515	VAL	6.5
3	H	622	GLU	4.7
3	H	517	LYS	4.6
3	H	511	TRP	4.0
3	H	512	THR	3.8
3	H	516	GLY	3.4
3	H	514	ASN	3.3
2	L	361	ASP	2.9
3	H	620	PHE	2.0

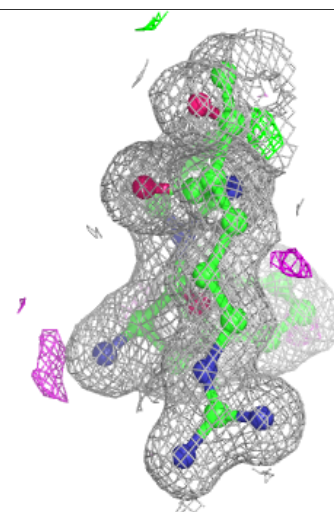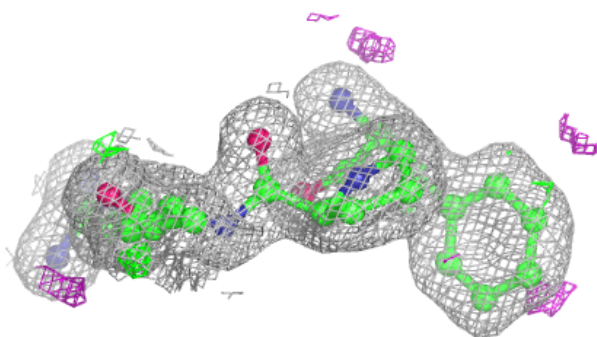## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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(Å²)	Q<0.9
1	77Y	D	404	35/36	0.98	0.06	19,24,27,29	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.
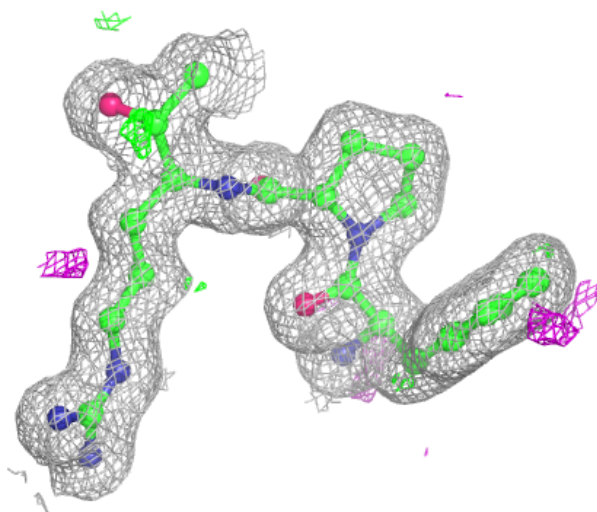
6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	H	703	14/15	0.68	0.27	57,85,93,104	0
5	0G6	H	701	30/31	0.98	0.07	16,19,23,26	0
4	K	D	501	1/1	0.99	0.08	23,23,23,23	0
6	NA	H	702	1/1	1.00	0.07	19,19,19,19	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 0G6 H 701:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.