Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2022 – 01:15 pm BST

PDB ID	:	7NDP
Title	:	X-ray structure of acetylcholine-binding protein (AChBP) in complex with FL001856.
Authors	:	Cederfelt, D.; Boronat, P.; Dobritzsch, D.; Hennig, S.; Fitzgerald, E.A.; de Esch, I.J.P.; Danielson, U.H.
Deposited on	:	2021-02-02
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 following versions of software and data (see references ⓘ) were used in the production of this report:

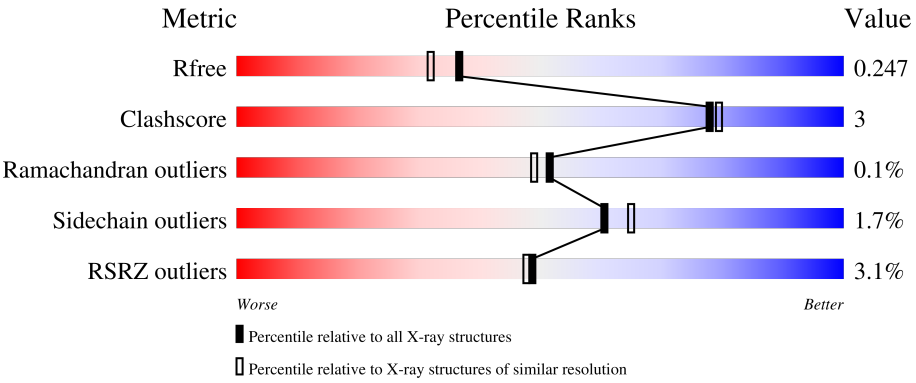
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	237	4% 78% 6% 15%
1	B	237	4% 79% 6% 15%
1	C	237	4% 76% 8% 16%
1	D	237	3% 76% 8% 15%
1	E	237	2% 78% 6% 15%

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Mol	Chain	Length	Quality of chain
1	F	237	4% 78% 7% 14%
1	G	237	79% 8% 13%
1	H	237	% 76% 10% 14%
1	I	237	2% 79% 6% 15%
1	J	237	% 76% 8% 16%
2	K	2	50% 50%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 16961 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 Acetylcholine-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1606	1007	275	319	5			
1	B	202	Total	C	N	O	S	0	0	0
			1613	1011	276	321	5			
1	C	200	Total	C	N	O	S	0	0	0
			1597	1003	274	315	5			
1	D	201	Total	C	N	O	S	0	0	0
			1606	1007	275	319	5			
1	E	201	Total	C	N	O	S	0	2	0
			1621	1018	278	320	5			
1	F	203	Total	C	N	O	S	0	0	0
			1620	1014	278	323	5			
1	G	206	Total	C	N	O	S	0	3	0
			1665	1042	287	331	5			
1	H	205	Total	C	N	O	S	0	1	0
			1644	1028	283	328	5			
1	I	202	Total	C	N	O	S	0	1	0
			1620	1015	279	321	5			
1	J	198	Total	C	N	O	S	0	1	0
			1594	1002	275	312	5			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	230	GLY	-	expression tag	UNP P58154
A	231	SER	-	expression tag	UNP P58154
A	232	HIS	-	expression tag	UNP P58154
A	233	HIS	-	expression tag	UNP P58154
A	234	HIS	-	expression tag	UNP P58154
A	235	HIS	-	expression tag	UNP P58154
A	236	HIS	-	expression tag	UNP P58154
A	237	HIS	-	expression tag	UNP P58154
B	230	GLY	-	expression tag	UNP P58154

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Chain	Residue	Modelled	Actual	Comment	Reference
B	231	SER	-	expression tag	UNP P58154
B	232	HIS	-	expression tag	UNP P58154
B	233	HIS	-	expression tag	UNP P58154
B	234	HIS	-	expression tag	UNP P58154
B	235	HIS	-	expression tag	UNP P58154
B	236	HIS	-	expression tag	UNP P58154
B	237	HIS	-	expression tag	UNP P58154
C	230	GLY	-	expression tag	UNP P58154
C	231	SER	-	expression tag	UNP P58154
C	232	HIS	-	expression tag	UNP P58154
C	233	HIS	-	expression tag	UNP P58154
C	234	HIS	-	expression tag	UNP P58154
C	235	HIS	-	expression tag	UNP P58154
C	236	HIS	-	expression tag	UNP P58154
C	237	HIS	-	expression tag	UNP P58154
D	230	GLY	-	expression tag	UNP P58154
D	231	SER	-	expression tag	UNP P58154
D	232	HIS	-	expression tag	UNP P58154
D	233	HIS	-	expression tag	UNP P58154
D	234	HIS	-	expression tag	UNP P58154
D	235	HIS	-	expression tag	UNP P58154
D	236	HIS	-	expression tag	UNP P58154
D	237	HIS	-	expression tag	UNP P58154
E	230	GLY	-	expression tag	UNP P58154
E	231	SER	-	expression tag	UNP P58154
E	232	HIS	-	expression tag	UNP P58154
E	233	HIS	-	expression tag	UNP P58154
E	234	HIS	-	expression tag	UNP P58154
E	235	HIS	-	expression tag	UNP P58154
E	236	HIS	-	expression tag	UNP P58154
E	237	HIS	-	expression tag	UNP P58154
F	230	GLY	-	expression tag	UNP P58154
F	231	SER	-	expression tag	UNP P58154
F	232	HIS	-	expression tag	UNP P58154
F	233	HIS	-	expression tag	UNP P58154
F	234	HIS	-	expression tag	UNP P58154
F	235	HIS	-	expression tag	UNP P58154
F	236	HIS	-	expression tag	UNP P58154
F	237	HIS	-	expression tag	UNP P58154
G	230	GLY	-	expression tag	UNP P58154
G	231	SER	-	expression tag	UNP P58154
G	232	HIS	-	expression tag	UNP P58154

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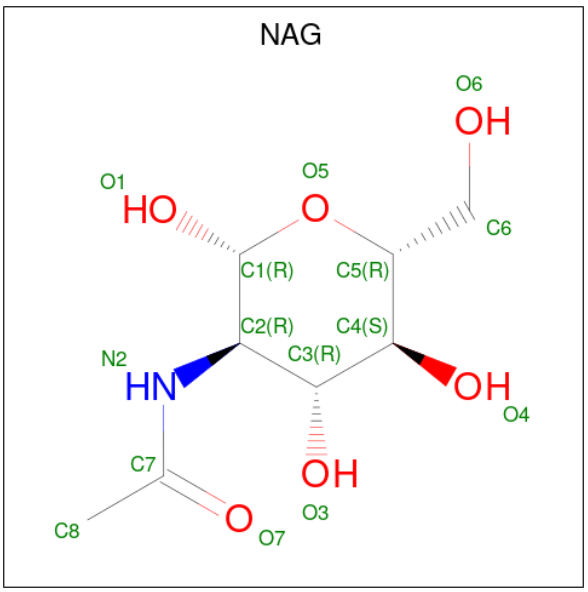
Chain	Residue	Modelled	Actual	Comment	Reference
G	233	HIS	-	expression tag	UNP P58154
G	234	HIS	-	expression tag	UNP P58154
G	235	HIS	-	expression tag	UNP P58154
G	236	HIS	-	expression tag	UNP P58154
G	237	HIS	-	expression tag	UNP P58154
H	230	GLY	-	expression tag	UNP P58154
H	231	SER	-	expression tag	UNP P58154
H	232	HIS	-	expression tag	UNP P58154
H	233	HIS	-	expression tag	UNP P58154
H	234	HIS	-	expression tag	UNP P58154
H	235	HIS	-	expression tag	UNP P58154
H	236	HIS	-	expression tag	UNP P58154
H	237	HIS	-	expression tag	UNP P58154
I	230	GLY	-	expression tag	UNP P58154
I	231	SER	-	expression tag	UNP P58154
I	232	HIS	-	expression tag	UNP P58154
I	233	HIS	-	expression tag	UNP P58154
I	234	HIS	-	expression tag	UNP P58154
I	235	HIS	-	expression tag	UNP P58154
I	236	HIS	-	expression tag	UNP P58154
I	237	HIS	-	expression tag	UNP P58154
J	230	GLY	-	expression tag	UNP P58154
J	231	SER	-	expression tag	UNP P58154
J	232	HIS	-	expression tag	UNP P58154
J	233	HIS	-	expression tag	UNP P58154
J	234	HIS	-	expression tag	UNP P58154
J	235	HIS	-	expression tag	UNP P58154
J	236	HIS	-	expression tag	UNP P58154
J	237	HIS	-	expression tag	UNP P58154

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

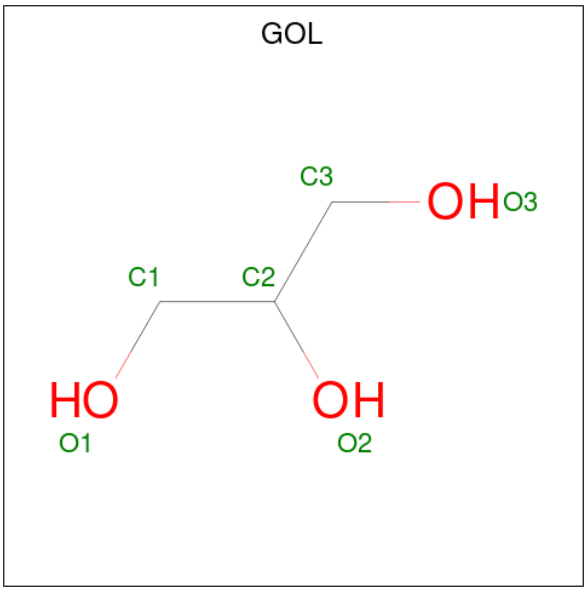
- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



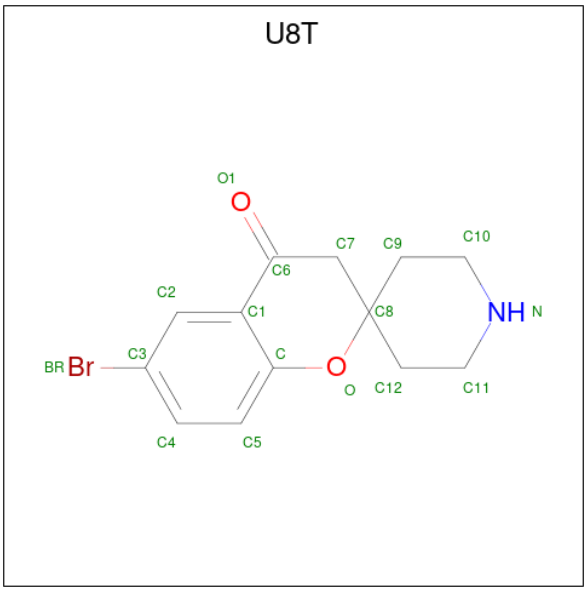
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	J	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



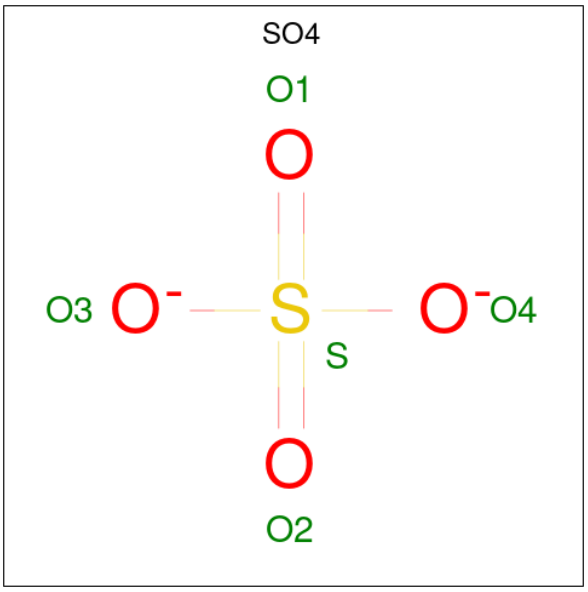
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0

- Molecule 5 is 6-bromanylspiro[3 {H}-chromene-2,4'-piperidine]-4-one (three-letter code: U8T) (formula: $C_{13}H_{14}BrNO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	Br	C	N	O	0	0
			17	1	13	1	2		
5	C	1	Total	Br	C	N	O	0	0
			17	1	13	1	2		
5	D	1	Total	Br	C	N	O	0	0
			17	1	13	1	2		
5	E	1	Total	Br	C	N	O	0	0
			17	1	13	1	2		
5	G	1	Total	Br	C	N	O	0	0
			17	1	13	1	2		
5	H	1	Total	Br	C	N	O	0	0
			17	1	13	1	2		
5	I	1	Total	Br	C	N	O	0	0
			17	1	13	1	2		
5	J	1	Total	Br	C	N	O	0	0
			17	1	13	1	2		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total O S 5 4 1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	1	Total Cl 1 1	0	0
7	J	1	Total Cl 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	35	Total O 35 35	0	0
8	B	23	Total O 23 23	0	0
8	C	27	Total O 27 27	0	0
8	D	52	Total O 54 54	0	2
8	E	46	Total O 46 46	0	0
8	F	40	Total O 41 41	0	1

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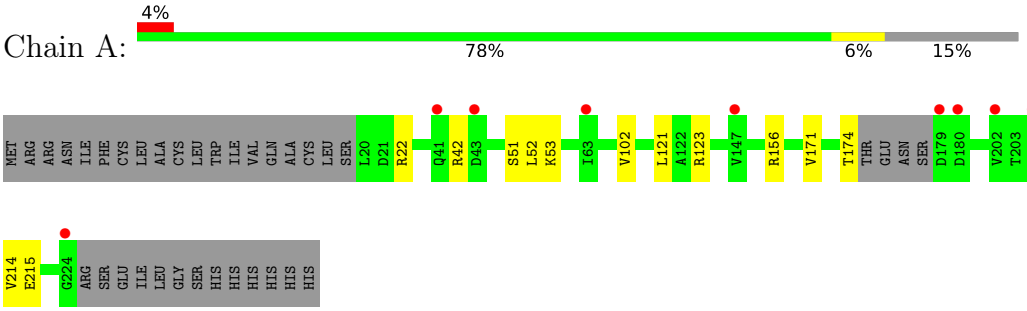
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	80	Total O 80 80	0	0
8	H	69	Total O 69 69	0	0
8	I	55	Total O 55 55	0	0
8	J	59	Total O 60 60	0	1

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.

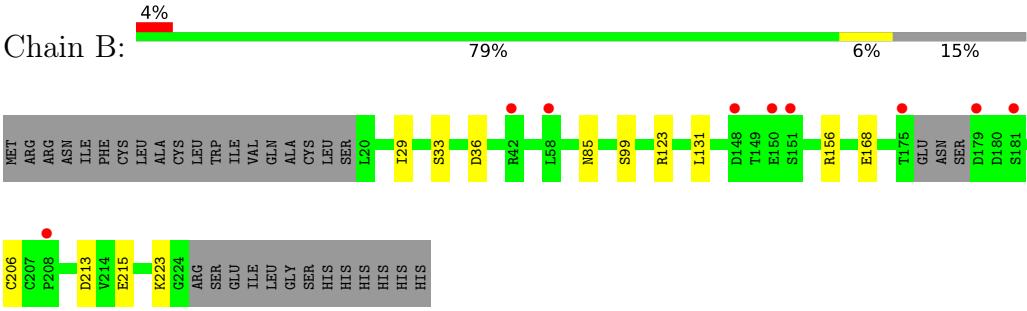
• Molecule 1: Acetylcholine-binding protein

Chain A:



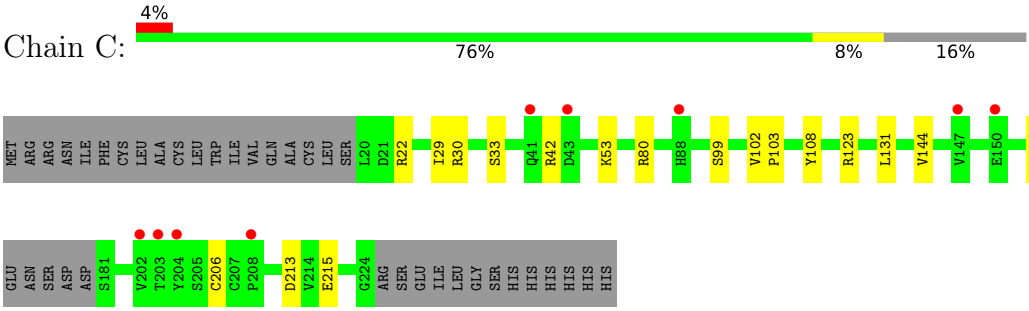
• Molecule 1: Acetylcholine-binding protein

Chain B:



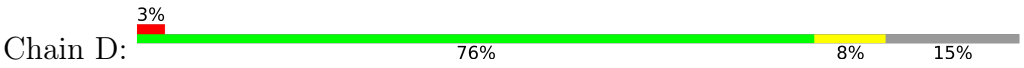
• Molecule 1: Acetylcholine-binding protein

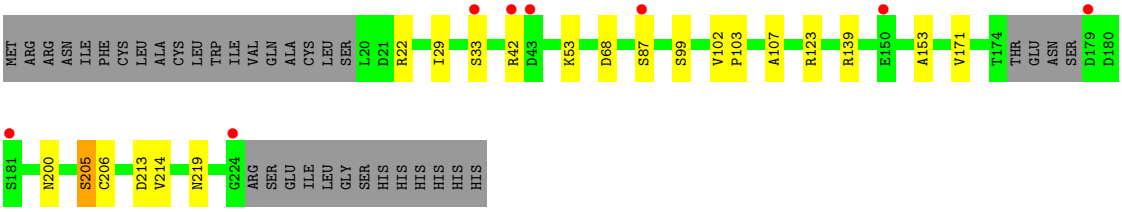
Chain C:



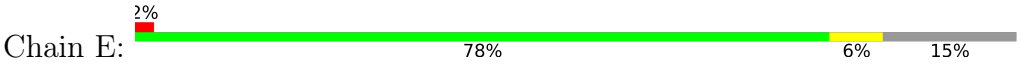
• Molecule 1: Acetylcholine-binding protein

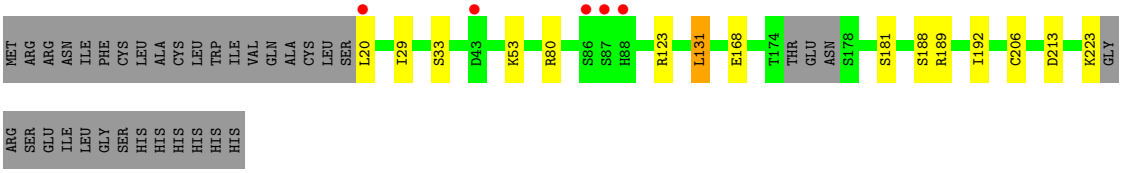
Chain D:



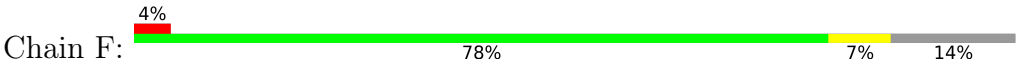


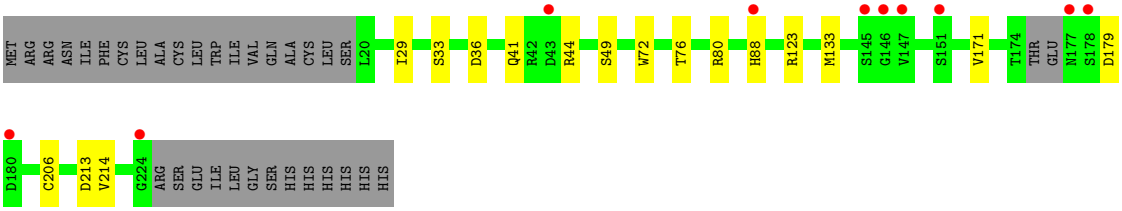
• Molecule 1: Acetylcholine-binding protein



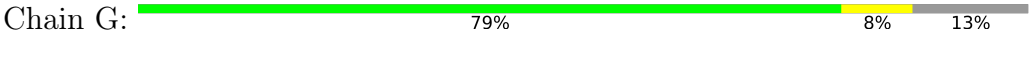


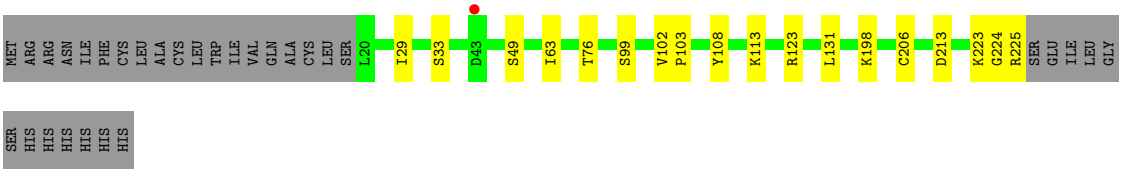
• Molecule 1: Acetylcholine-binding protein



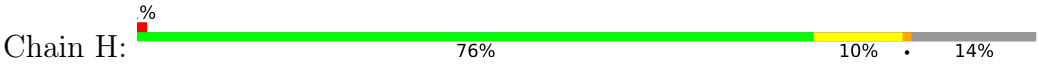


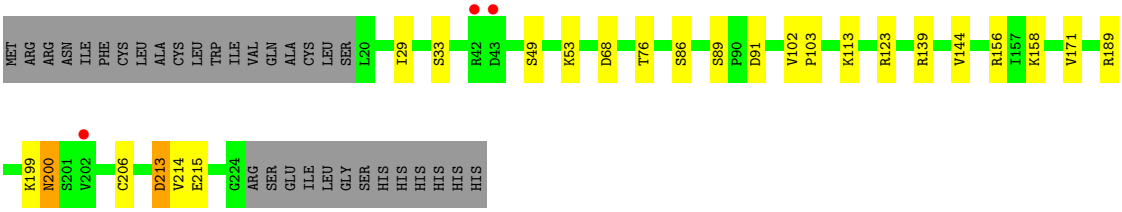
• Molecule 1: Acetylcholine-binding protein





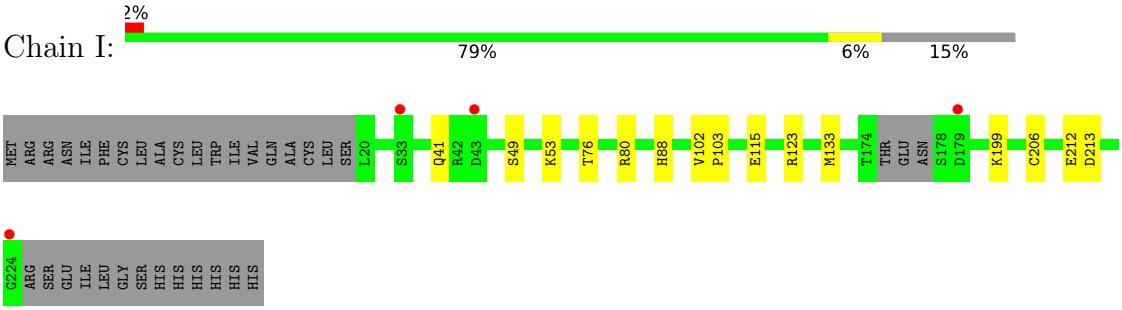
• Molecule 1: Acetylcholine-binding protein





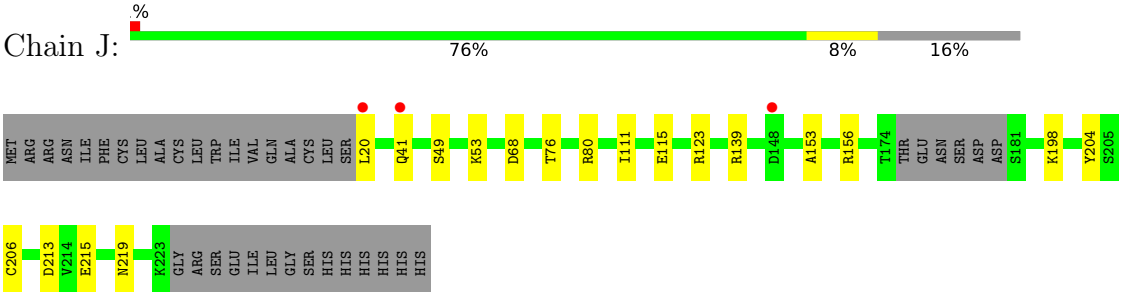
• Molecule 1: Acetylcholine-binding protein

Chain I:



• Molecule 1: Acetylcholine-binding protein

Chain J:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.70Å 121.10Å 241.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.53 – 2.00 47.53 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.53-2.00) 99.6 (47.53-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.212 , 0.243 0.220 , 0.247	Depositor DCC
R_{free} test set	7578 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16961	wwPDB-VP
Average B, all atoms (Å^2)	58.0	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 23.58 % 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 4.5329e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GOL, CL, NAG, SO4, U8T

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	0.69	0/1641	0.84	0/2238
1	B	0.66	0/1648	0.82	0/2248
1	C	0.67	0/1632	0.83	1/2226 (0.0%)
1	D	0.67	0/1641	0.86	1/2238 (0.0%)
1	E	0.68	0/1662	0.84	0/2266
1	F	0.67	0/1655	0.85	0/2257
1	G	0.69	0/1710	0.85	0/2332
1	H	0.72	0/1683	0.88	1/2296 (0.0%)
1	I	0.67	0/1658	0.87	1/2261 (0.0%)
1	J	0.67	0/1632	0.84	1/2226 (0.0%)
All	All	0.68	0/16562	0.85	5/22588 (0.0%)

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
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
All	All	0	10

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	123	ARG	CG-CD-NE	-7.38	96.31	111.80
1	D	123	ARG	CG-CD-NE	-7.31	96.44	111.80
1	J	123	ARG	CG-CD-NE	-7.29	96.49	111.80
1	H	123	ARG	CG-CD-NE	-6.53	98.09	111.80
1	C	108	TYR	CB-CG-CD1	5.37	124.22	121.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	CYS	Peptide
1	B	206	CYS	Peptide
1	C	206	CYS	Peptide
1	D	206	CYS	Peptide
1	E	206	CYS	Peptide
1	F	206	CYS	Peptide
1	G	206	CYS	Peptide
1	H	206	CYS	Peptide
1	I	206	CYS	Peptide
1	J	206	CYS	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	1606	0	1552	10	0
1	B	1613	0	1559	7	0
1	C	1597	0	1552	10	0
1	D	1606	0	1552	16	0
1	E	1621	0	1579	9	0
1	F	1620	0	1563	11	0
1	G	1665	0	1618	8	0
1	H	1644	0	1590	14	0
1	I	1620	0	1571	8	0
1	J	1594	0	1554	10	0
2	K	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	14	0	13	0	0
3	B	14	0	13	1	0
3	F	14	0	13	0	0
3	G	14	0	13	1	0
3	H	14	0	13	0	0
3	J	14	0	13	0	0
4	A	12	0	16	1	0
4	D	12	0	16	3	0
4	E	6	0	8	1	0
5	B	17	0	0	1	0
5	C	17	0	0	1	0
5	D	17	0	0	1	0
5	E	17	0	0	0	0
5	G	17	0	0	2	0
5	H	17	0	0	2	0
5	I	17	0	0	1	0
5	J	17	0	0	3	0
6	G	5	0	0	0	0
7	I	1	0	0	0	0
7	J	1	0	0	0	0
8	A	35	0	0	0	0
8	B	23	0	0	0	0
8	C	27	0	0	0	0
8	D	54	0	0	1	0
8	E	46	0	0	0	0
8	F	41	0	0	1	0
8	G	80	0	0	1	0
8	H	69	0	0	1	0
8	I	55	0	0	0	0
8	J	60	0	0	1	0
All	All	16961	0	15833	95	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 3.

All (95) 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:H:91:ASP:OD2	8:H:401:HOH:O	1.83	0.94
1:D:171:VAL:HG12	1:D:214:VAL:HG23	1.54	0.88
1:F:171:VAL:HG12	1:F:214:VAL:HG23	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:VAL:HG12	1:A:214:VAL:HG23	1.55	0.86
1:D:42:ARG:HH21	1:F:88:HIS:HB2	1.42	0.85
1:H:171:VAL:HG12	1:H:214:VAL:HG23	1.61	0.80
5:I:301:U8T:BR	1:J:53:LYS:HE3	2.40	0.77
1:E:189[B]:ARG:HH11	1:E:189[B]:ARG:HG3	1.55	0.70
1:G:63:ILE:HG22	1:H:189:ARG:HD3	1.77	0.66
1:D:107:ALA:H	4:D:301:GOL:H11	1.63	0.64
1:F:36:ASP:OD1	8:F:401:HOH:O	2.16	0.62
1:A:102:VAL:HG22	4:A:302:GOL:H12	1.82	0.61
1:J:115:GLU:OE2	8:J:401:HOH:O	2.16	0.60
5:C:301:U8T:BR	1:D:53:LYS:HE3	2.57	0.59
1:H:86:SER:HA	1:H:89:SER:OG	2.02	0.59
1:G:33:SER:HB2	1:G:99:SER:O	2.02	0.59
1:B:29:ILE:O	1:B:33:SER:HB3	2.03	0.58
1:G:29:ILE:O	1:G:33:SER:HB3	2.03	0.58
1:J:41:GLN:HE21	1:J:80:ARG:HG3	1.67	0.58
1:B:85:ASN:HD22	3:B:301:NAG:H83	1.69	0.58
1:D:29:ILE:O	1:D:33:SER:HB3	2.04	0.58
1:E:181:SER:OG	1:E:192:ILE:HG21	2.04	0.57
1:B:33:SER:HB2	1:B:99:SER:O	2.05	0.57
1:J:156:ARG:HD2	1:J:215:GLU:OE2	2.04	0.57
1:C:156:ARG:HD2	1:C:215:GLU:OE2	2.05	0.57
1:D:107:ALA:N	4:D:301:GOL:H11	2.19	0.57
1:A:52:LEU:HD12	1:A:52:LEU:N	2.22	0.55
1:A:156:ARG:HD2	1:A:215:GLU:OE2	2.07	0.55
5:D:303:U8T:BR	1:E:53:LYS:HE3	2.62	0.55
1:D:33:SER:HB2	1:D:99:SER:O	2.07	0.54
1:E:189[B]:ARG:HG3	1:E:189[B]:ARG:NH1	2.24	0.53
1:B:156:ARG:HD2	1:B:215:GLU:OE2	2.07	0.53
1:C:29:ILE:O	1:C:33:SER:HB3	2.09	0.53
5:G:302:U8T:BR	1:H:53:LYS:HE3	2.63	0.53
5:H:302:U8T:BR	1:I:53:LYS:HE3	2.63	0.53
1:D:68:ASP:HB2	1:D:139:ARG:HH21	1.73	0.53
1:F:29:ILE:O	1:F:33:SER:HB3	2.10	0.51
1:H:156:ARG:HD2	1:H:215:GLU:OE2	2.08	0.51
1:A:22:ARG:NH2	1:E:168:GLU:OE2	2.44	0.51
1:H:29:ILE:O	1:H:33:SER:HB3	2.10	0.51
1:H:68:ASP:HB2	1:H:139[B]:ARG:HH21	1.76	0.50
1:C:33:SER:OG	1:C:99:SER:O	2.22	0.50
5:J:302:U8T:N	5:J:302:U8T:O	2.44	0.50
1:B:188:SER:O	1:B:223:LYS:CE	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:SER:O	1:E:223:LYS:CE	2.60	0.50
1:D:107:ALA:H	4:D:301:GOL:C1	2.24	0.49
5:B:302:U8T:BR	1:C:53:LYS:HE3	2.69	0.48
5:H:302:U8T:C2	1:I:133:MET:HE1	2.44	0.47
1:D:68:ASP:HB2	1:D:139:ARG:NH2	2.29	0.47
1:G:108:TYR:OH	5:G:302:U8T:N	2.47	0.47
1:H:158:LYS:HE2	1:H:213:ASP:OD2	2.15	0.46
1:H:113:LYS:HE3	1:I:115:GLU:HG3	1.98	0.46
1:J:204:TYR:OH	5:J:302:U8T:C4	2.63	0.46
1:F:72:TRP:HH2	5:J:302:U8T:BR	2.54	0.46
1:J:68:ASP:HB2	1:J:139:ARG:NH2	2.30	0.45
1:I:49:SER:HB2	1:I:76:THR:OG1	2.16	0.45
1:J:111:ILE:HD11	1:J:139:ARG:HG2	1.98	0.45
1:C:80:ARG:NH2	3:G:301:NAG:O5	2.50	0.45
1:D:87:SER:HB3	2:K:1:NAG:HN2	1.82	0.45
1:G:113:LYS:HE2	1:G:113:LYS:HB3	1.81	0.44
1:D:42:ARG:NH2	1:F:88:HIS:HB2	2.21	0.44
1:F:72:TRP:HB3	1:F:133:MET:CE	2.47	0.44
1:J:41:GLN:NE2	1:J:80:ARG:HG3	2.30	0.44
1:A:52:LEU:N	1:A:52:LEU:CD1	2.80	0.44
1:A:53:LYS:HB3	1:A:53:LYS:HE3	1.89	0.44
1:C:102:VAL:HG13	1:C:103:PRO:HD2	2.00	0.43
1:F:44:ARG:HD3	1:F:44:ARG:HA	1.77	0.43
1:I:102:VAL:HG13	1:I:103:PRO:HD2	2.01	0.43
1:H:102:VAL:HG13	1:H:103:PRO:HD2	2.01	0.43
1:D:205:SER:HB2	8:D:401:HOH:O	2.19	0.43
1:D:102:VAL:HG13	1:D:103:PRO:HD2	2.01	0.43
1:F:88:HIS:O	1:F:88:HIS:ND1	2.50	0.43
1:I:41:GLN:HE21	1:I:80:ARG:HG3	1.84	0.43
1:E:80:ARG:HD3	1:E:80:ARG:HA	1.60	0.42
1:I:199:LYS:HE2	1:I:212:GLU:OE1	2.18	0.42
1:B:36:ASP:OD2	1:C:30:ARG:NH1	2.53	0.42
1:H:49:SER:HB2	1:H:76:THR:OG1	2.19	0.42
1:H:200:ASN:HD22	1:H:200:ASN:HA	1.75	0.42
1:H:144:VAL:HG12	1:H:144:VAL:O	2.20	0.41
1:A:51:SER:HB2	1:A:174:THR:HG22	2.03	0.41
1:G:102:VAL:HG13	1:G:103:PRO:HD2	2.01	0.41
1:B:168:GLU:OE2	1:C:22:ARG:NH2	2.54	0.41
1:A:121:LEU:HD11	4:E:401:GOL:H31	2.02	0.41
1:F:41:GLN:NE2	1:F:80:ARG:HG3	2.35	0.41
1:D:153:ALA:O	1:D:219:ASN:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:LYS:HE3	8:G:434:HOH:O	2.21	0.41
1:A:42:ARG:NH2	1:I:88:HIS:HB2	2.36	0.41
1:G:49:SER:HB2	1:G:76:THR:OG1	2.21	0.41
1:C:144:VAL:HG12	1:C:144:VAL:O	2.21	0.40
1:F:49:SER:HB2	1:F:76:THR:OG1	2.21	0.40
1:J:49:SER:HB2	1:J:76:THR:OG1	2.21	0.40
1:C:168:GLU:OE2	1:D:22:ARG:NH2	2.54	0.40
1:J:153:ALA:O	1:J:219:ASN:HA	2.22	0.40
1:E:29:ILE:O	1:E:33:SER:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	197/237 (83%)	195 (99%)	2 (1%)	0	100	100
1	B	198/237 (84%)	197 (100%)	1 (0%)	0	100	100
1	C	196/237 (83%)	195 (100%)	1 (0%)	0	100	100
1	D	197/237 (83%)	196 (100%)	1 (0%)	0	100	100
1	E	199/237 (84%)	198 (100%)	1 (0%)	0	100	100
1	F	199/237 (84%)	198 (100%)	1 (0%)	0	100	100
1	G	207/237 (87%)	204 (99%)	2 (1%)	1 (0%)	29	23
1	H	204/237 (86%)	203 (100%)	1 (0%)	0	100	100
1	I	199/237 (84%)	197 (99%)	2 (1%)	0	100	100
1	J	195/237 (82%)	193 (99%)	2 (1%)	0	100	100
All	All	1991/2370 (84%)	1976 (99%)	14 (1%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	224	GLY

5.3.2 Protein sidechains (i)

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	187/220 (85%)	185 (99%)	2 (1%)	73	78
1	B	188/220 (86%)	184 (98%)	4 (2%)	53	57
1	C	186/220 (84%)	182 (98%)	4 (2%)	52	55
1	D	187/220 (85%)	184 (98%)	3 (2%)	62	67
1	E	190/220 (86%)	185 (97%)	5 (3%)	46	48
1	F	189/220 (86%)	186 (98%)	3 (2%)	62	67
1	G	195/220 (89%)	189 (97%)	6 (3%)	40	40
1	H	192/220 (87%)	189 (98%)	3 (2%)	62	67
1	I	189/220 (86%)	188 (100%)	1 (0%)	88	92
1	J	186/220 (84%)	183 (98%)	3 (2%)	62	67
All	All	1889/2200 (86%)	1855 (98%)	34 (2%)	60	63

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ARG
1	A	213	ASP
1	B	123	ARG
1	B	131	LEU
1	B	198	LYS
1	B	213	ASP
1	C	42	ARG
1	C	123	ARG
1	C	131	LEU
1	C	213	ASP
1	D	200	ASN
1	D	205	SER
1	D	213	ASP

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Mol	Chain	Res	Type
1	E	20	LEU
1	E	123	ARG
1	E	131[A]	LEU
1	E	131[B]	LEU
1	E	213	ASP
1	F	123	ARG
1	F	179	ASP
1	F	213	ASP
1	G	123	ARG
1	G	131[A]	LEU
1	G	131[B]	LEU
1	G	198	LYS
1	G	213	ASP
1	G	225	ARG
1	H	199	LYS
1	H	200	ASN
1	H	213	ASP
1	I	213	ASP
1	J	20	LEU
1	J	198	LYS
1	J	213	ASP

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	200	ASN
1	D	200	ASN
1	F	41	GLN
1	G	41	GLN
1	I	41	GLN
1	I	74	GLN

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)

2 monosaccharides 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	$\#\|Z\| > 2$
2	NAG	K	1	2,1	14,14,15	0.67	0	17,19,21	1.41	4 (23%)
2	NAG	K	2	2	14,14,15	0.79	0	17,19,21	1.55	3 (17%)

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	NAG	K	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	2	NAG	O5-C5-C6	3.62	112.87	107.20
2	K	1	NAG	C4-C3-C2	2.81	115.14	111.02
2	K	2	NAG	C3-C4-C5	-2.80	105.24	110.24
2	K	1	NAG	O5-C1-C2	-2.50	107.34	111.29
2	K	1	NAG	O5-C5-C6	2.27	110.77	107.20
2	K	2	NAG	O5-C5-C4	-2.24	105.38	110.83
2	K	1	NAG	C2-N2-C7	2.02	125.78	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	1	NAG	O5-C5-C6-O6

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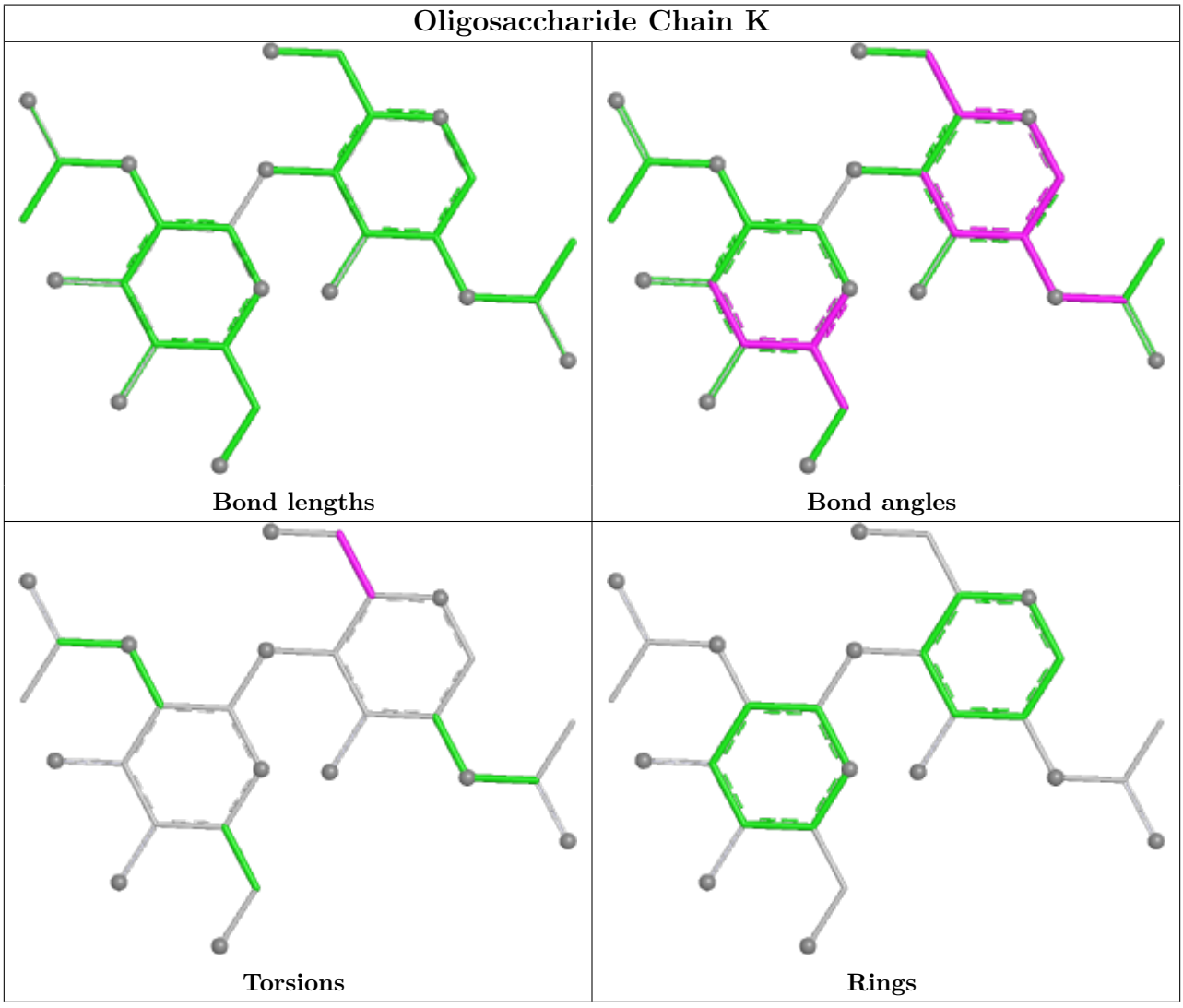
Mol	Chain	Res	Type	Atoms
2	K	1	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1	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 oligosaccharide.



5.6 Ligand geometry

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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	U8T	J	302	-	19,19,19	1.64	3 (15%)	21,28,28	2.05	6 (28%)
6	SO4	G	303	-	4,4,4	0.33	0	6,6,6	0.09	0
5	U8T	B	302	-	19,19,19	1.23	1 (5%)	21,28,28	1.81	5 (23%)
5	U8T	E	402	-	19,19,19	1.63	3 (15%)	21,28,28	1.92	6 (28%)
5	U8T	H	302	-	19,19,19	1.35	1 (5%)	21,28,28	1.96	8 (38%)
5	U8T	I	301	-	19,19,19	1.14	1 (5%)	21,28,28	1.81	8 (38%)
5	U8T	G	302	-	19,19,19	1.69	3 (15%)	21,28,28	2.94	9 (42%)
5	U8T	C	301	-	19,19,19	1.34	2 (10%)	21,28,28	1.79	6 (28%)
4	GOL	A	303	-	5,5,5	0.11	0	5,5,5	0.28	0
3	NAG	J	301	1	14,14,15	0.82	0	17,19,21	1.97	5 (29%)
3	NAG	A	301	1	14,14,15	0.61	0	17,19,21	1.83	3 (17%)
3	NAG	H	301	1	14,14,15	0.84	1 (7%)	17,19,21	1.39	3 (17%)
3	NAG	G	301	1	14,14,15	0.73	0	17,19,21	1.67	4 (23%)
3	NAG	F	301	1	14,14,15	0.45	0	17,19,21	1.33	2 (11%)
3	NAG	B	301	1	14,14,15	0.71	0	17,19,21	1.87	4 (23%)
4	GOL	D	301	-	5,5,5	0.28	0	5,5,5	0.74	0
4	GOL	A	302	-	5,5,5	0.14	0	5,5,5	0.39	0
5	U8T	D	303	-	19,19,19	1.51	3 (15%)	21,28,28	2.73	7 (33%)
4	GOL	D	302	-	5,5,5	0.13	0	5,5,5	0.31	0
4	GOL	E	401	-	5,5,5	0.14	0	5,5,5	0.38	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
5	U8T	J	302	-	-	-	1/3/3/3
5	U8T	B	302	-	-	-	0/3/3/3
5	U8T	E	402	-	-	-	0/3/3/3
5	U8T	H	302	-	-	-	0/3/3/3
5	U8T	I	301	-	-	-	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	U8T	G	302	-	-	-	0/3/3/3
5	U8T	C	301	-	-	-	1/3/3/3
4	GOL	A	303	-	-	0/4/4/4	-
3	NAG	J	301	1	-	1/6/23/26	0/1/1/1
3	NAG	A	301	1	-	3/6/23/26	0/1/1/1
3	NAG	H	301	1	-	2/6/23/26	0/1/1/1
3	NAG	G	301	1	-	2/6/23/26	0/1/1/1
3	NAG	F	301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	301	1	-	2/6/23/26	0/1/1/1
4	GOL	D	301	-	-	1/4/4/4	-
4	GOL	A	302	-	-	4/4/4/4	-
5	U8T	D	303	-	-	-	0/3/3/3
4	GOL	D	302	-	-	4/4/4/4	-
4	GOL	E	401	-	-	4/4/4/4	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	402	U8T	C1-C	5.05	1.50	1.40
5	J	302	U8T	C1-C	4.83	1.49	1.40
5	G	302	U8T	C1-C	4.79	1.49	1.40
5	H	302	U8T	C1-C	4.69	1.49	1.40
5	B	302	U8T	C1-C	4.60	1.49	1.40
5	D	303	U8T	C1-C	4.29	1.48	1.40
5	C	301	U8T	C1-C	4.16	1.48	1.40
5	I	301	U8T	C1-C	3.57	1.47	1.40
5	G	302	U8T	C7-C8	2.73	1.55	1.53
5	J	302	U8T	C1-C6	2.64	1.52	1.48
5	E	402	U8T	C1-C6	2.57	1.52	1.48
5	G	302	U8T	C2-C1	-2.44	1.36	1.39
5	J	302	U8T	C2-C3	2.34	1.42	1.38
5	C	301	U8T	C1-C6	2.19	1.51	1.48
5	D	303	U8T	C1-C6	2.16	1.51	1.48
5	E	402	U8T	C2-C3	2.14	1.42	1.38
5	D	303	U8T	O-C	-2.12	1.34	1.37
3	H	301	NAG	C1-C2	2.07	1.55	1.52

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	303	U8T	C-C1-C6	-6.73	115.98	119.85
5	G	302	U8T	BR-C3-C2	-6.45	110.31	119.27
3	J	301	NAG	C2-N2-C7	5.76	131.11	122.90
5	G	302	U8T	C-C1-C6	5.46	123.00	119.85
5	D	303	U8T	BR-C3-C4	-5.34	111.54	119.30
5	B	302	U8T	O-C8-C7	5.21	116.07	109.64
5	G	302	U8T	O-C8-C7	5.10	115.94	109.64
5	J	302	U8T	C-C1-C6	-4.88	117.04	119.85
5	H	302	U8T	O-C8-C7	4.84	115.61	109.64
5	G	302	U8T	BR-C3-C4	4.82	126.31	119.30
5	D	303	U8T	BR-C3-C2	4.61	125.67	119.27
5	D	303	U8T	C2-C1-C6	4.26	126.47	119.42
5	J	302	U8T	O-C-C5	4.18	123.00	116.61
3	F	301	NAG	O5-C5-C6	4.14	113.70	107.20
5	G	302	U8T	C10-N-C11	4.07	122.03	110.34
3	H	301	NAG	C1-O5-C5	3.94	117.53	112.19
5	E	402	U8T	O-C8-C7	3.89	114.45	109.64
5	C	301	U8T	C-C1-C6	-3.89	117.62	119.85
3	B	301	NAG	C4-C3-C2	-3.85	105.38	111.02
5	E	402	U8T	O-C-C5	3.69	122.25	116.61
3	A	301	NAG	O5-C5-C6	3.63	112.89	107.20
5	I	301	U8T	O-C8-C7	3.61	114.10	109.64
3	A	301	NAG	O5-C1-C2	-3.53	105.71	111.29
5	I	301	U8T	C8-O-C	3.52	123.35	116.76
5	C	301	U8T	C2-C1-C6	3.41	125.06	119.42
3	A	301	NAG	C3-C4-C5	3.33	116.18	110.24
3	G	301	NAG	C1-O5-C5	3.30	116.67	112.19
5	G	302	U8T	O-C-C5	3.26	121.60	116.61
5	H	302	U8T	C-C1-C6	-3.22	118.00	119.85
3	G	301	NAG	O5-C5-C6	3.19	112.20	107.20
3	G	301	NAG	O5-C1-C2	3.11	116.20	111.29
5	E	402	U8T	C12-C11-N	-3.08	104.39	110.89
3	J	301	NAG	C1-C2-N2	-3.05	105.28	110.49
5	J	302	U8T	C2-C1-C6	3.03	124.43	119.42
3	B	301	NAG	O5-C1-C2	-3.03	106.51	111.29
3	B	301	NAG	C1-O5-C5	3.00	116.26	112.19
5	J	302	U8T	O-C-C1	-2.99	117.86	121.94
5	E	402	U8T	O-C-C1	-2.94	117.93	121.94
5	I	301	U8T	O-C-C5	2.92	121.08	116.61
5	H	302	U8T	C2-C1-C6	2.91	124.22	119.42
5	D	303	U8T	C10-N-C11	2.87	118.59	110.34
3	B	301	NAG	C8-C7-N2	2.81	120.86	116.10
5	H	302	U8T	C8-O-C	2.80	122.00	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	302	U8T	C-C1-C6	-2.76	118.27	119.85
5	D	303	U8T	C9-C8-C12	2.74	113.11	109.56
5	I	301	U8T	O-C-C1	-2.70	118.26	121.94
5	B	302	U8T	O-C-C5	2.63	120.64	116.61
5	G	302	U8T	C9-C10-N	2.61	116.39	110.89
3	F	301	NAG	O5-C1-C2	-2.57	107.23	111.29
5	E	402	U8T	C5-C4-C3	2.40	122.31	119.19
5	G	302	U8T	C9-C8-C12	-2.40	106.46	109.56
5	G	302	U8T	O-C-C1	-2.37	118.72	121.94
5	C	301	U8T	O-C8-C7	2.36	112.56	109.64
5	C	301	U8T	C8-O-C	2.35	121.16	116.76
5	H	302	U8T	C7-C6-C1	2.35	119.74	116.49
5	I	301	U8T	C10-N-C11	2.32	117.01	110.34
3	H	301	NAG	C2-N2-C7	2.29	126.16	122.90
3	J	301	NAG	O5-C5-C6	2.29	110.79	107.20
5	D	303	U8T	C12-C11-N	2.27	115.69	110.89
5	B	302	U8T	C8-O-C	2.26	121.00	116.76
5	H	302	U8T	O1-C6-C7	-2.26	118.04	121.16
5	H	302	U8T	BR-C3-C4	-2.24	116.05	119.30
5	B	302	U8T	C7-C6-C1	2.21	119.55	116.49
5	J	302	U8T	C7-C6-C1	2.19	119.52	116.49
3	H	301	NAG	O5-C1-C2	2.17	114.72	111.29
5	I	301	U8T	C7-C6-C1	2.15	119.47	116.49
5	J	302	U8T	C5-C4-C3	2.15	121.98	119.19
3	G	301	NAG	C3-C4-C5	-2.13	106.43	110.24
5	I	301	U8T	C-C1-C6	-2.13	118.63	119.85
5	C	301	U8T	BR-C3-C4	-2.10	116.25	119.30
5	H	302	U8T	O-C-C1	-2.08	119.10	121.94
5	I	301	U8T	C2-C1-C6	2.06	122.83	119.42
3	J	301	NAG	O3-C3-C4	-2.06	105.59	110.35
5	E	402	U8T	C2-C1-C6	2.04	122.79	119.42
5	C	301	U8T	O-C-C1	-2.03	119.17	121.94
3	J	301	NAG	C4-C3-C2	2.03	113.99	111.02

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	301	NAG	C3-C2-N2-C7
4	A	302	GOL	O1-C1-C2-C3
4	D	302	GOL	O1-C1-C2-O2
4	D	302	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	E	401	GOL	O1-C1-C2-C3
4	E	401	GOL	C1-C2-C3-O3
3	A	301	NAG	O5-C5-C6-O6
3	G	301	NAG	O5-C5-C6-O6
3	F	301	NAG	O5-C5-C6-O6
3	F	301	NAG	C4-C5-C6-O6
3	G	301	NAG	C4-C5-C6-O6
3	A	301	NAG	C4-C5-C6-O6
3	B	301	NAG	C8-C7-N2-C2
3	B	301	NAG	O7-C7-N2-C2
4	D	302	GOL	O2-C2-C3-O3
4	E	401	GOL	O2-C2-C3-O3
4	A	302	GOL	C1-C2-C3-O3
4	D	302	GOL	O1-C1-C2-C3
4	A	302	GOL	O1-C1-C2-O2
4	A	302	GOL	O2-C2-C3-O3
4	E	401	GOL	O1-C1-C2-O2
3	H	301	NAG	C4-C5-C6-O6
4	D	301	GOL	O2-C2-C3-O3
3	H	301	NAG	O5-C5-C6-O6
3	A	301	NAG	C3-C2-N2-C7

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	301	U8T	C10-C11-C12-C8-C9-N
5	J	302	U8T	C10-C11-C12-C8-C9-N

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	302	U8T	3	0
5	B	302	U8T	1	0
5	H	302	U8T	2	0
5	I	301	U8T	1	0
5	G	302	U8T	2	0
5	C	301	U8T	1	0
3	G	301	NAG	1	0
3	B	301	NAG	1	0
4	D	301	GOL	3	0
4	A	302	GOL	1	0
5	D	303	U8T	1	0

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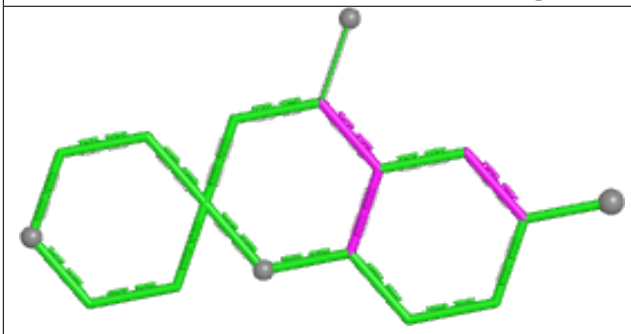
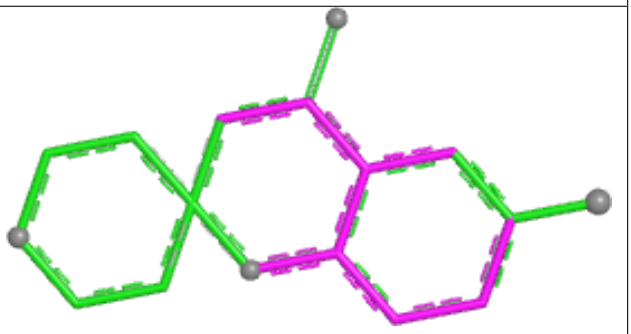
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	401	GOL	1	0

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 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.

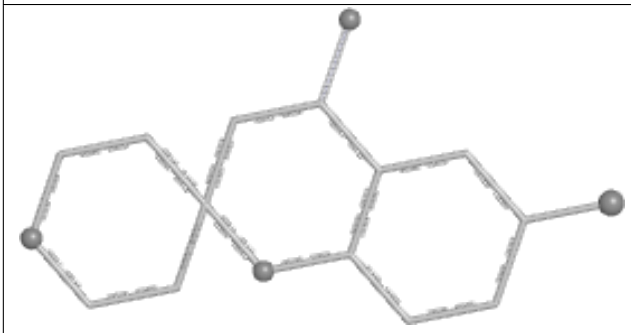
Ligand U8T J 302



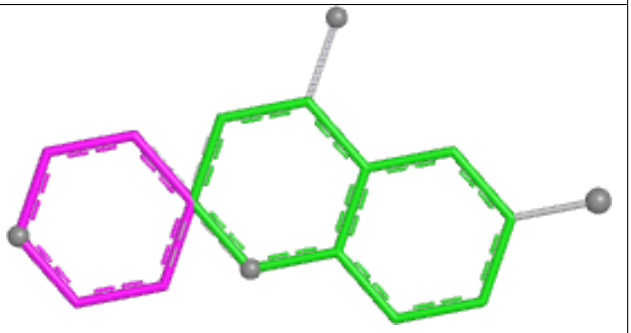
Bond lengths



Bond angles

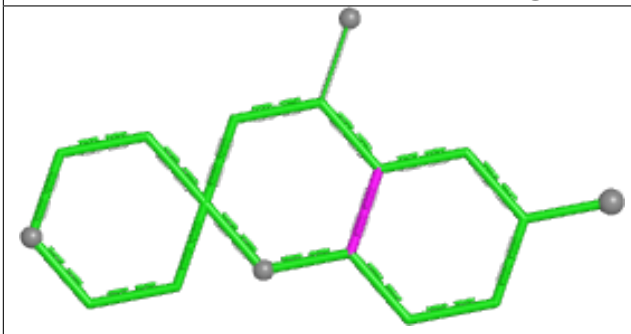


Torsions



Rings

Ligand U8T B 302



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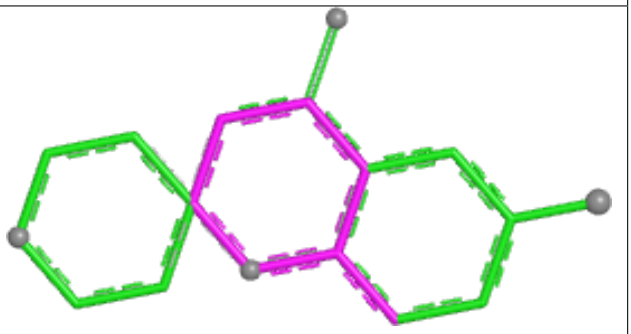
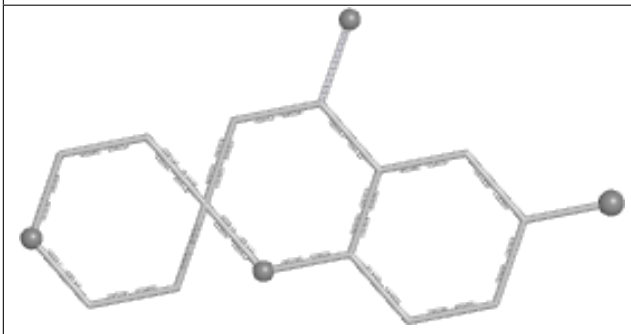


Bond angles



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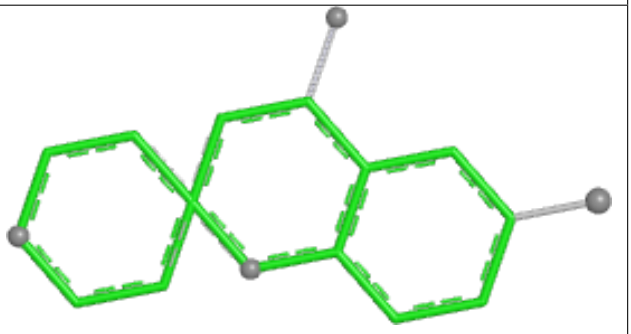
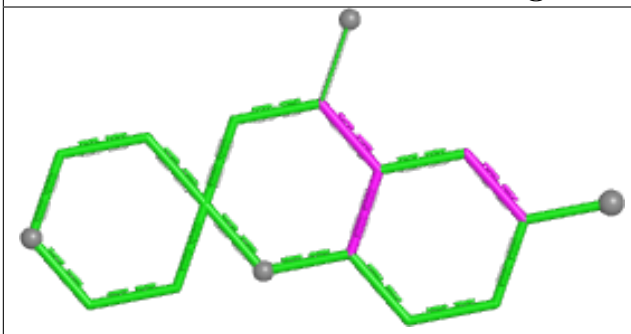
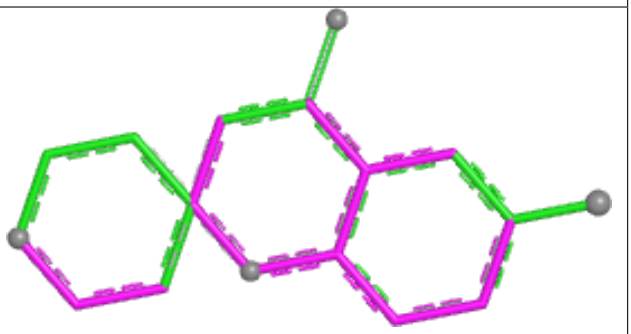


Rings

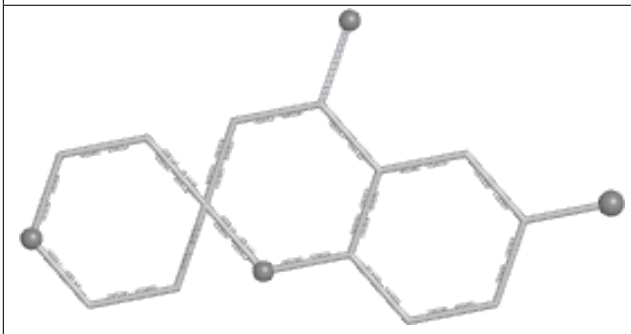
Ligand U8T E 402



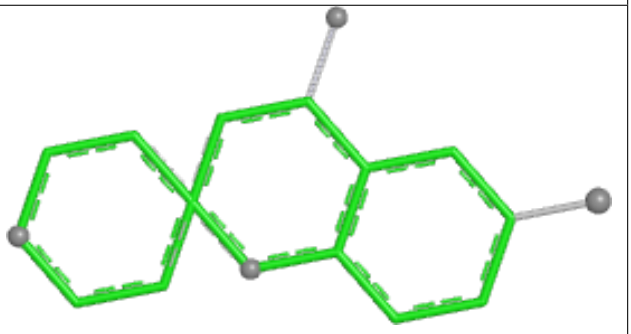
Bond lengths



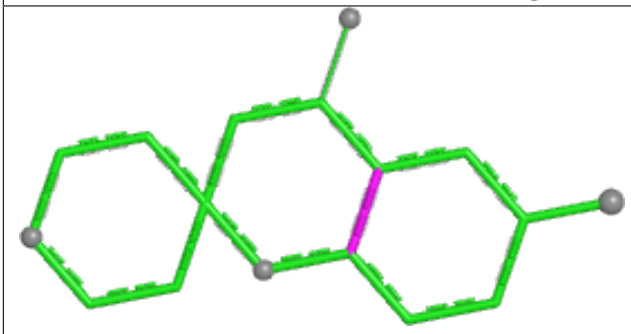
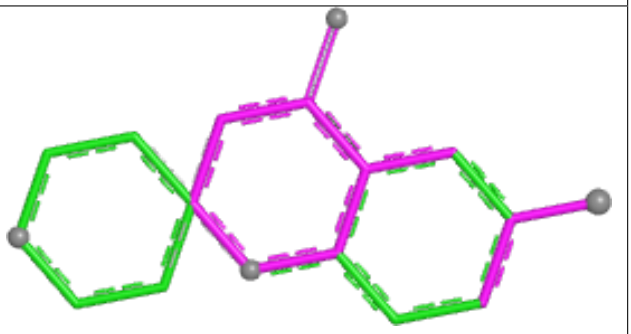
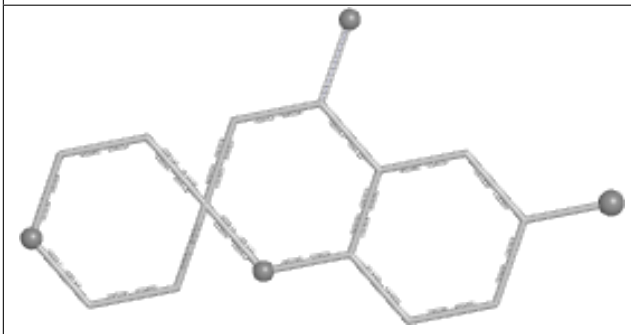
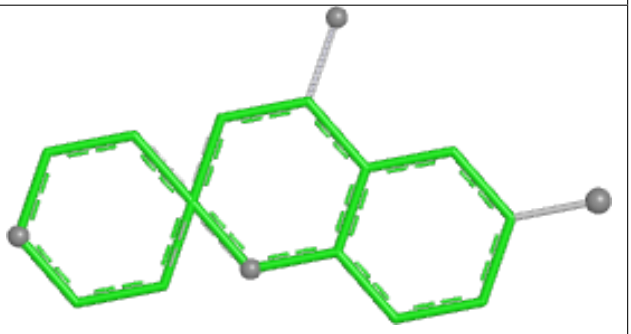
Bond angles



Torsions



Rings

Ligand U8T H 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

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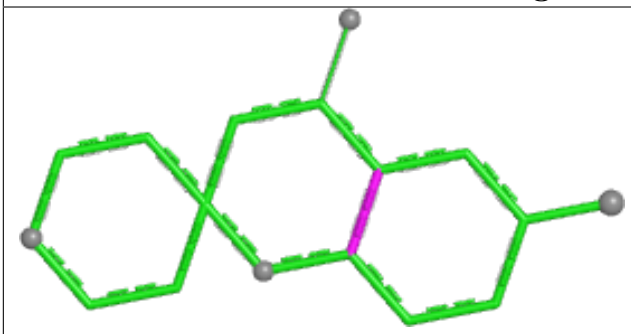
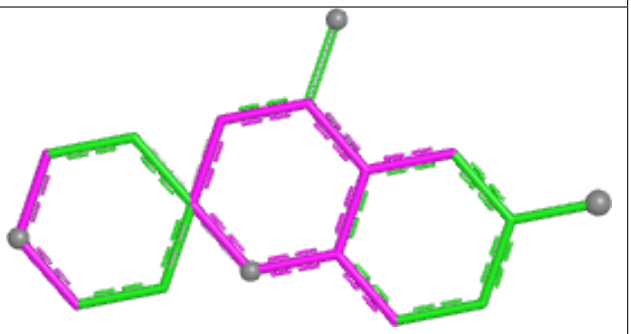
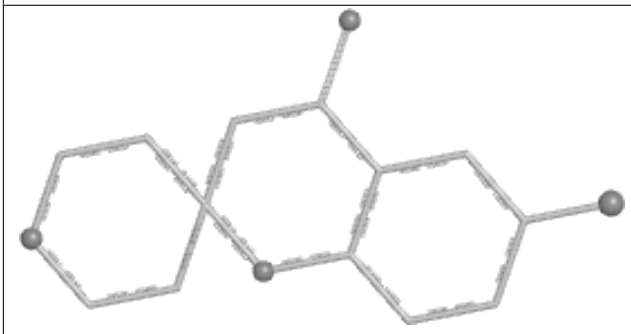
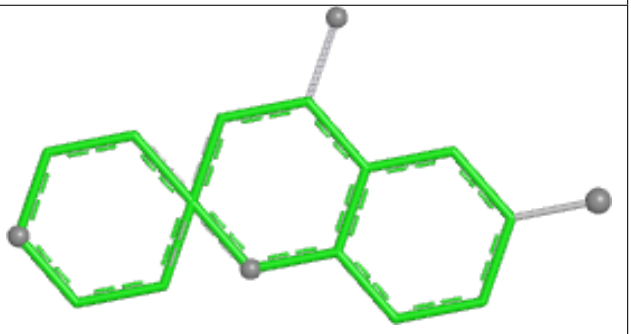
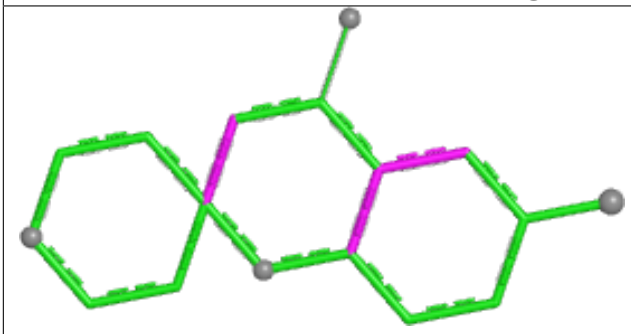
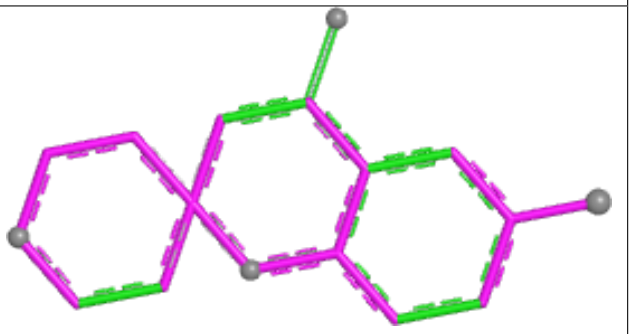
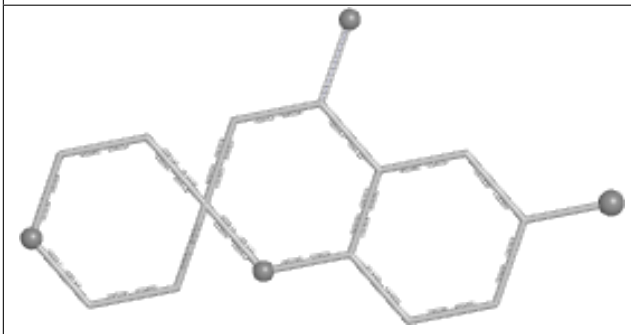
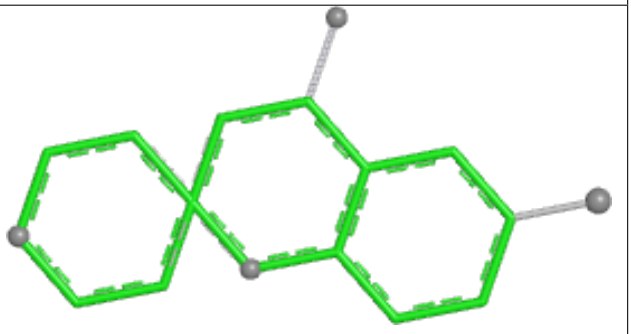
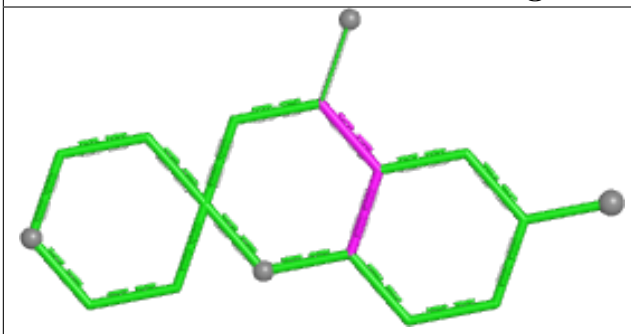
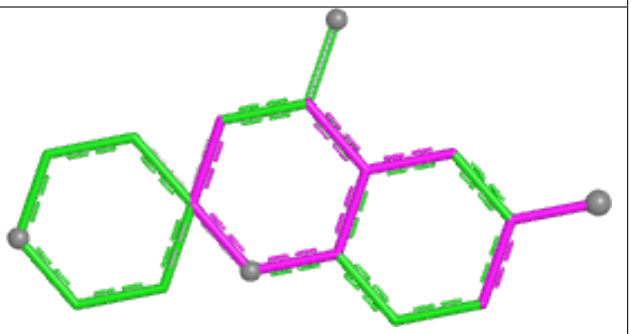
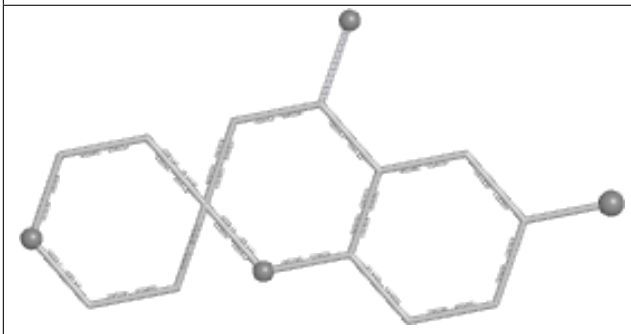
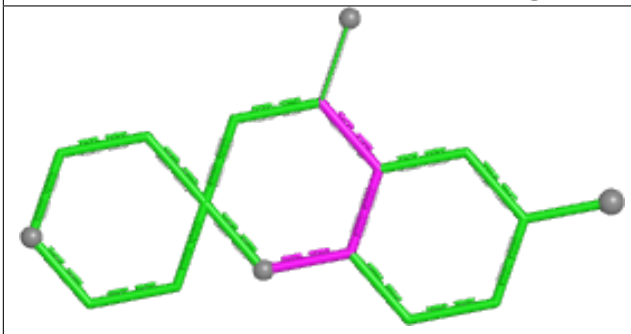
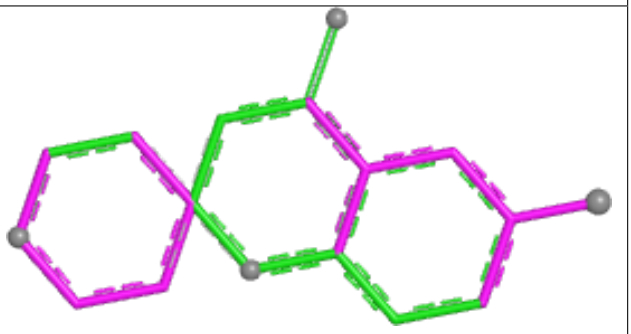
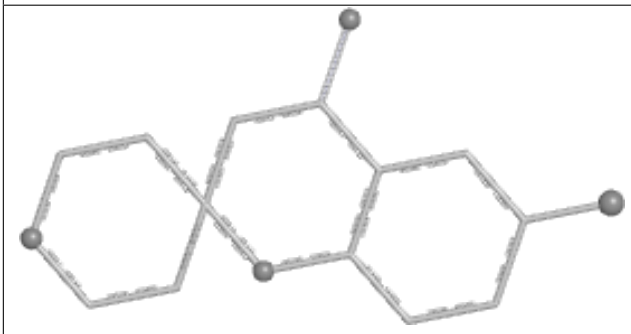
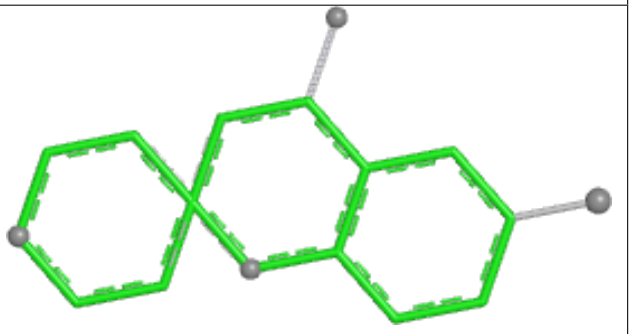
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand U8T G 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand U8T C 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand U8T D 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

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, 95^{th} 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	201/237 (84%)	0.25	9 (4%)	33	32	42, 59, 92, 124	0
1	B	202/237 (85%)	0.28	9 (4%)	33	32	44, 62, 97, 125	0
1	C	200/237 (84%)	0.25	10 (5%)	28	28	43, 60, 98, 128	0
1	D	201/237 (84%)	0.09	8 (3%)	38	37	39, 53, 86, 131	0
1	E	201/237 (84%)	0.15	5 (2%)	57	56	37, 51, 78, 113	0
1	F	203/237 (85%)	0.21	10 (4%)	29	28	38, 54, 91, 124	0
1	G	206/237 (86%)	-0.04	1 (0%)	91	90	38, 47, 70, 103	0
1	H	205/237 (86%)	0.02	3 (1%)	73	72	37, 47, 88, 111	0
1	I	202/237 (85%)	0.03	4 (1%)	65	63	36, 50, 84, 118	0
1	J	198/237 (83%)	0.09	3 (1%)	73	72	37, 50, 73, 107	0
All	All	2019/2370 (85%)	0.13	62 (3%)	49	48	36, 53, 89, 131	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	224	GLY	5.5
1	A	180	ASP	5.2
1	F	224	GLY	4.9
1	B	181	SER	4.7
1	B	175	THR	4.5
1	B	42	ARG	4.5
1	D	43	ASP	4.5
1	A	147	VAL	4.3
1	C	204	TYR	4.3
1	A	202	VAL	4.2
1	D	179	ASP	4.1
1	A	43	ASP	4.1
1	D	224	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	179	ASP	3.9
1	F	177	ASN	3.9
1	A	204	TYR	3.8
1	A	224	GLY	3.7
1	C	88	HIS	3.6
1	F	43	ASP	3.5
1	B	179	ASP	3.4
1	F	88	HIS	3.4
1	A	63	ILE	3.3
1	J	148	ASP	3.2
1	F	145	SER	3.2
1	H	42	ARG	3.2
1	G	43	ASP	3.1
1	D	87	SER	3.0
1	C	41	GLN	2.9
1	E	87	SER	2.9
1	I	179	ASP	2.8
1	C	175	THR	2.8
1	C	203	THR	2.8
1	J	20	LEU	2.8
1	B	150	GLU	2.8
1	C	43	ASP	2.7
1	B	148	ASP	2.6
1	C	202	VAL	2.6
1	C	150	GLU	2.5
1	C	147	VAL	2.5
1	I	43	ASP	2.5
1	F	151	SER	2.5
1	I	33	SER	2.4
1	C	208	PRO	2.3
1	D	33	SER	2.3
1	F	146	GLY	2.3
1	E	86	SER	2.3
1	J	41	GLN	2.3
1	D	181	SER	2.2
1	E	88	HIS	2.2
1	F	147	VAL	2.2
1	E	20	LEU	2.2
1	D	42	ARG	2.2
1	H	202	VAL	2.2
1	B	151	SER	2.1
1	B	58	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	180	ASP	2.1
1	H	43	ASP	2.1
1	F	178	SER	2.1
1	E	43	ASP	2.1
1	A	41	GLN	2.1
1	D	150	GLU	2.1
1	B	208	PRO	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)

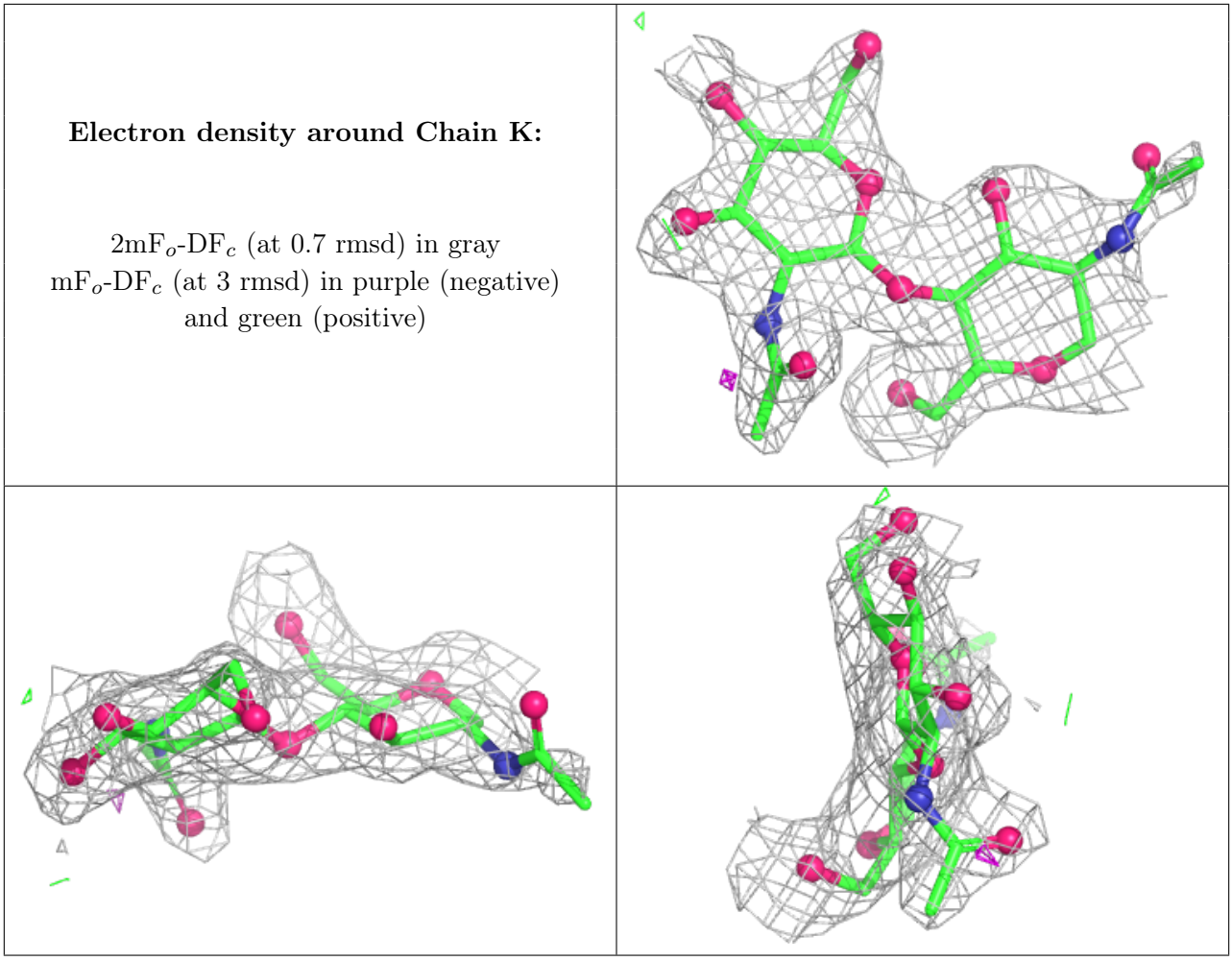
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	NAG	K	1	14/15	0.81	0.24	72,84,99,111	0
2	NAG	K	2	14/15	0.85	0.24	64,78,83,84	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain K:

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



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, 95^{th} 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	J	301	14/15	0.47	0.32	92,104,114,117	0
3	NAG	G	301	14/15	0.64	0.28	95,103,114,117	0
3	NAG	H	301	14/15	0.67	0.22	94,102,114,114	0
3	NAG	A	301	14/15	0.71	0.28	82,101,106,110	0
5	U8T	E	402	17/17	0.72	0.26	69,82,119,125	0
5	U8T	J	302	17/17	0.73	0.21	76,84,98,107	0
3	NAG	F	301	14/15	0.75	0.25	84,104,113,118	0
3	NAG	B	301	14/15	0.76	0.18	95,107,116,117	0
4	GOL	D	301	6/6	0.79	0.18	52,75,76,81	0
5	U8T	H	302	17/17	0.81	0.14	59,79,101,139	0

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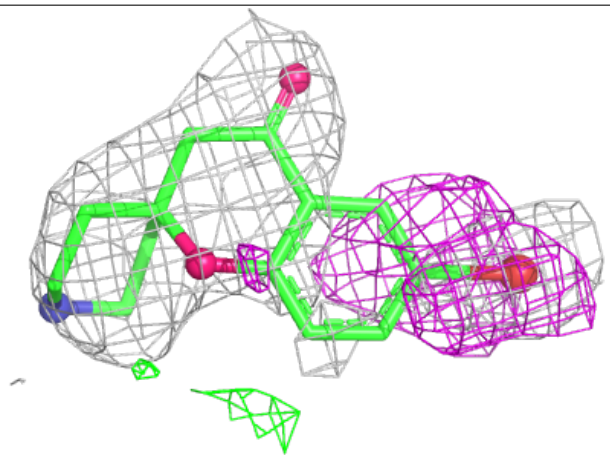
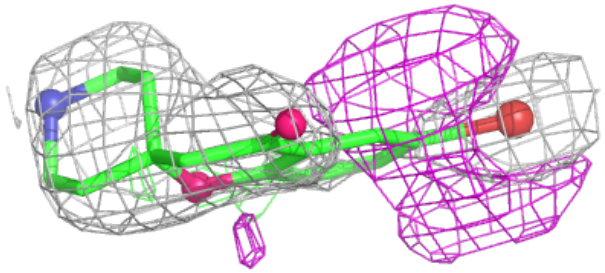
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	E	401	6/6	0.83	0.13	44,67,73,85	0
4	GOL	A	303	6/6	0.86	0.14	67,83,83,84	0
4	GOL	D	302	6/6	0.86	0.21	53,70,72,86	0
5	U8T	D	303	17/17	0.88	0.10	54,64,90,110	0
5	U8T	B	302	17/17	0.88	0.16	82,100,116,160	0
5	U8T	G	302	17/17	0.89	0.14	57,84,98,118	0
6	SO4	G	303	5/5	0.89	0.13	113,117,124,125	0
4	GOL	A	302	6/6	0.91	0.16	54,75,81,94	0
5	U8T	C	301	17/17	0.93	0.16	81,93,116,146	0
5	U8T	I	301	17/17	0.93	0.12	54,67,99,153	0
7	CL	I	302	1/1	0.98	0.06	44,44,44,44	0
7	CL	J	303	1/1	1.00	0.07	44,44,44,44	0

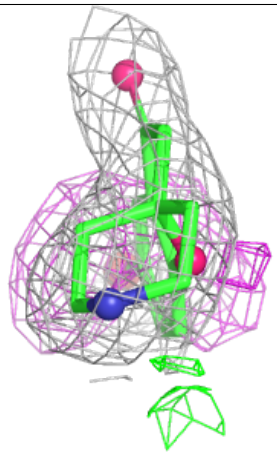
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around U8T E 402:

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

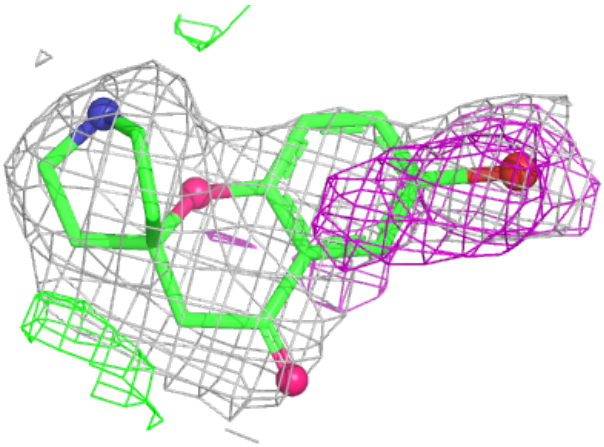


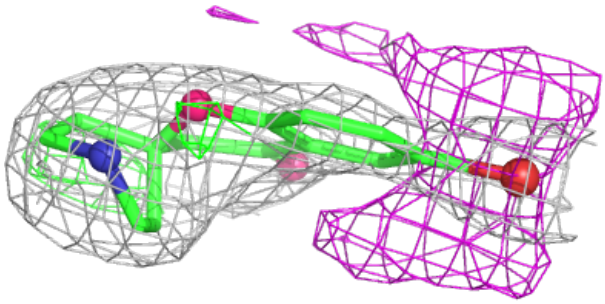


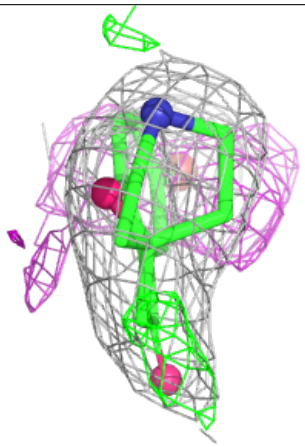


Electron density around U8T J 302:

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

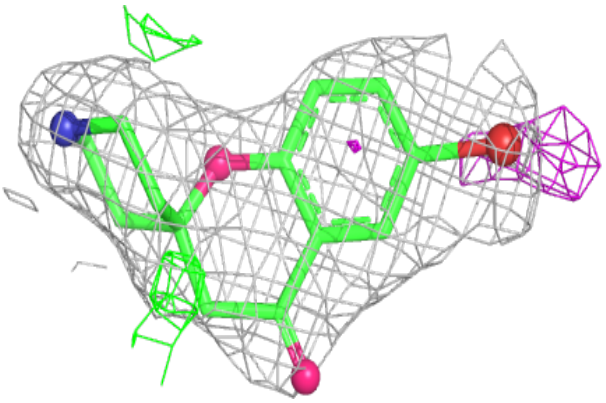


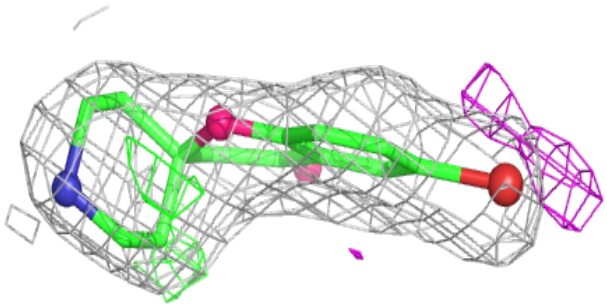


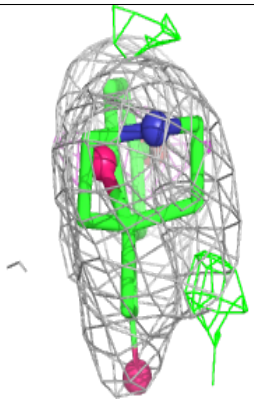


Electron density around U8T H 302:

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

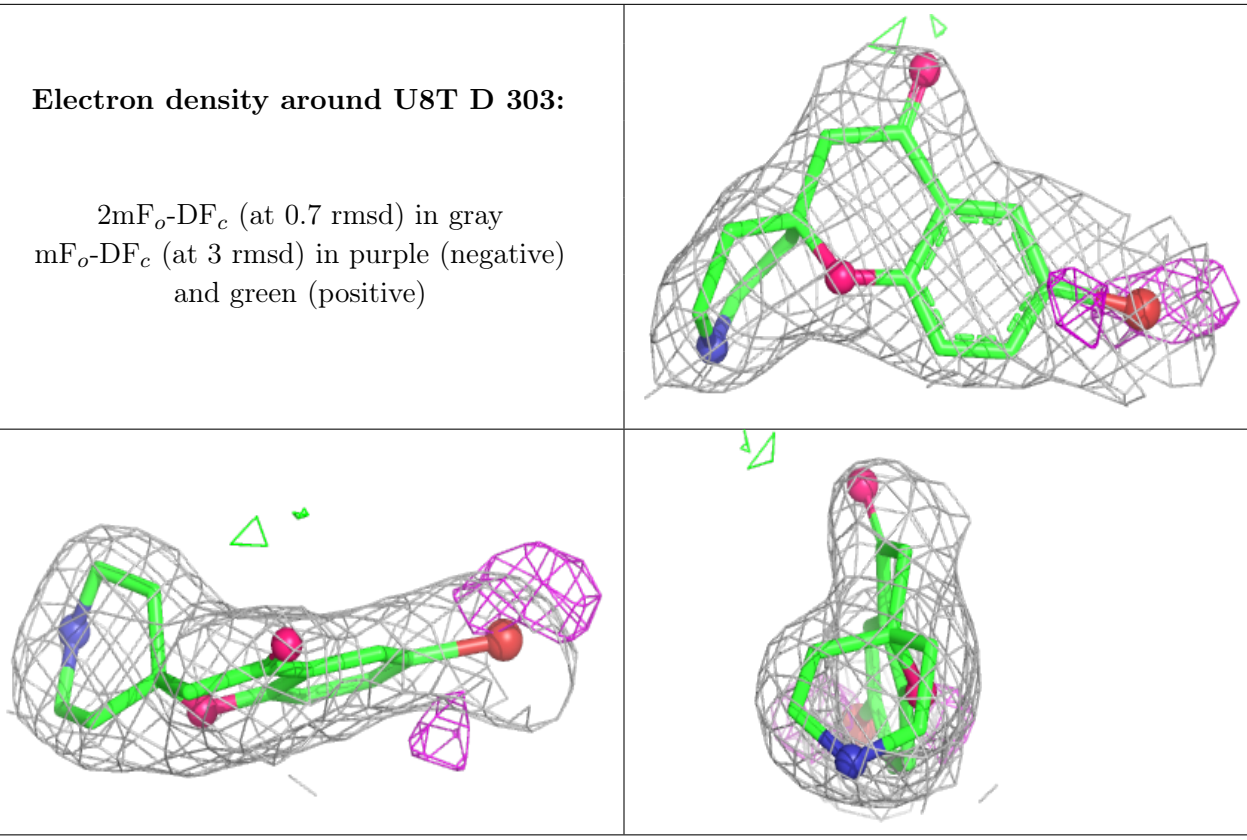






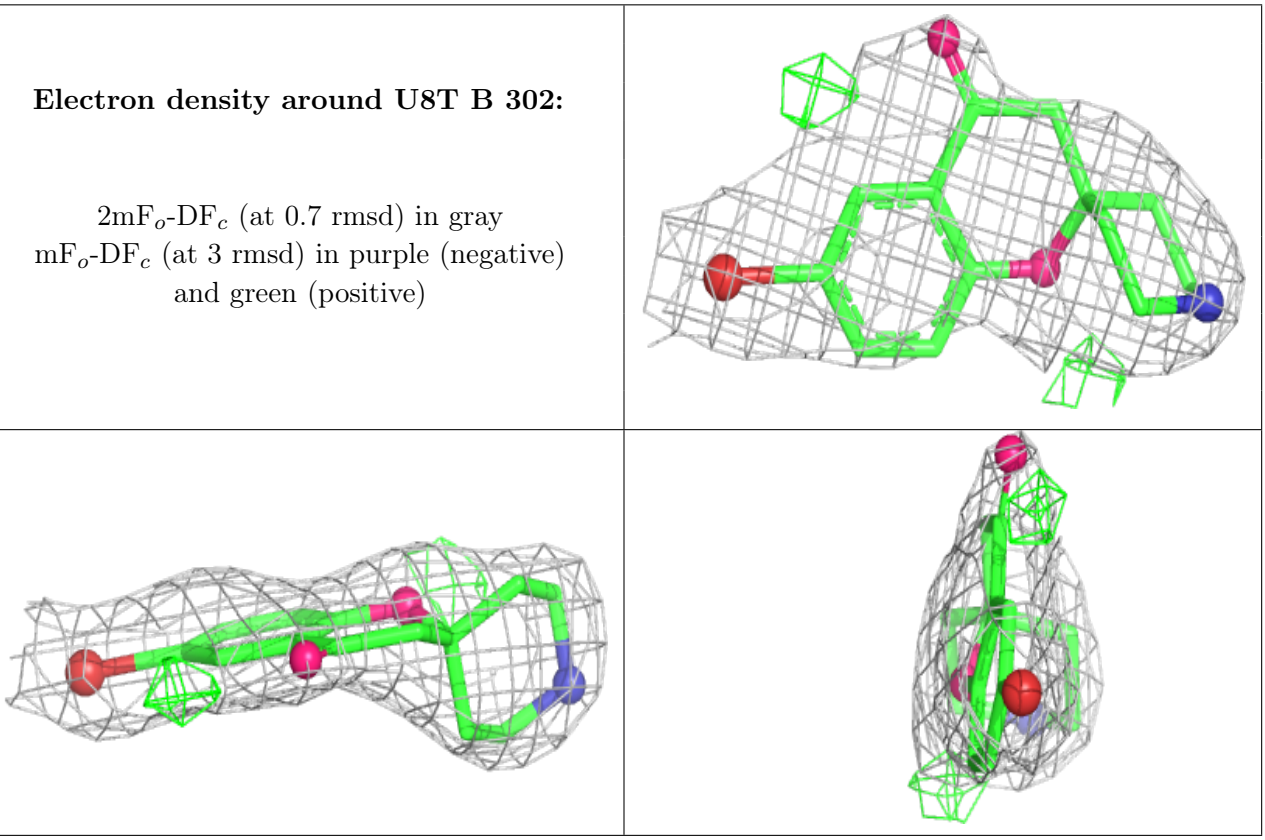
Electron density around U8T D 303:

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



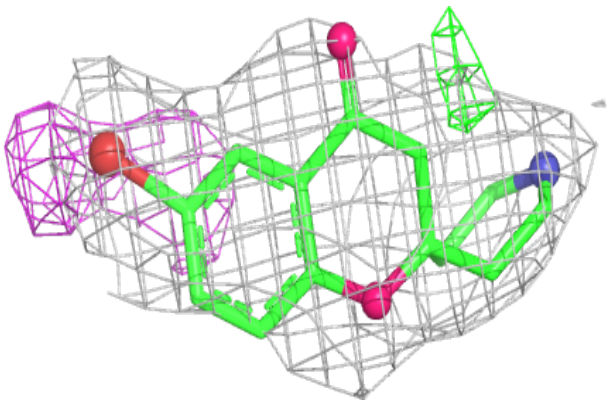
Electron density around U8T B 302:

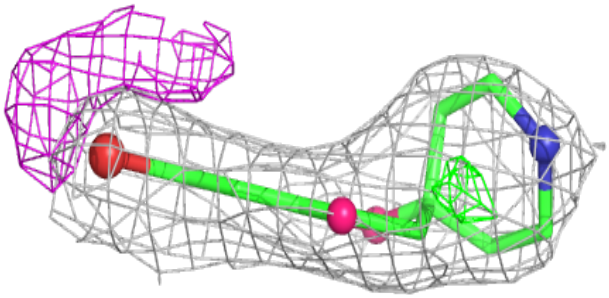
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

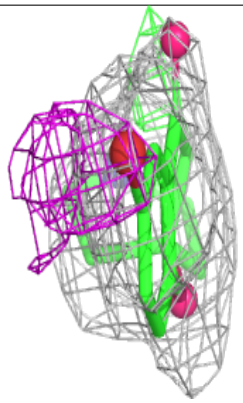


Electron density around U8T G 302:

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

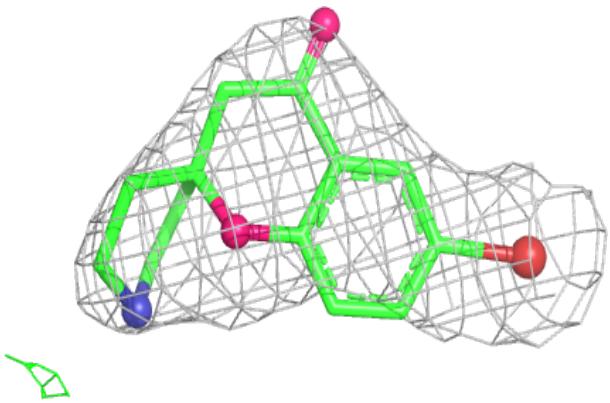


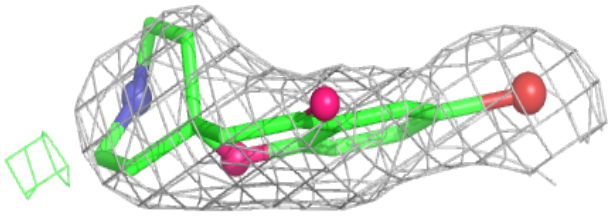


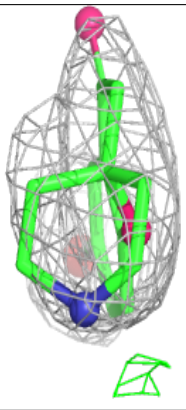


Electron density around U8T C 301:

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

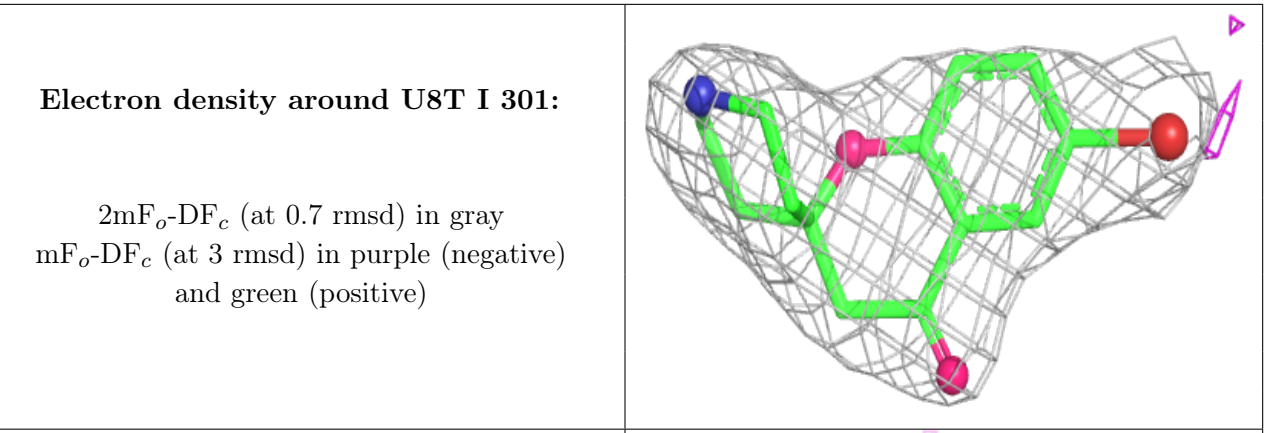






Electron density around U8T I 301:

$2mF_o$-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.