wwPDB X-ray Structure Validation Summary Report (i)

Dec 13, 2023 – 01:49 am GMT

PDB ID	:	2XYT
Title	:	Crystal structure of Aplysia californica AChBP in complex with d- tubocurarine
Authors	:	Brams, M.; Pandya, A.; Kuzmin, D.; van Elk, R.; Krijnen, L.; Yakel, J.L.; Tsetlin, V.; Smit, A.B.; Ulens, C.
Deposited on	:	2010-11-19
Resolution	:	2.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

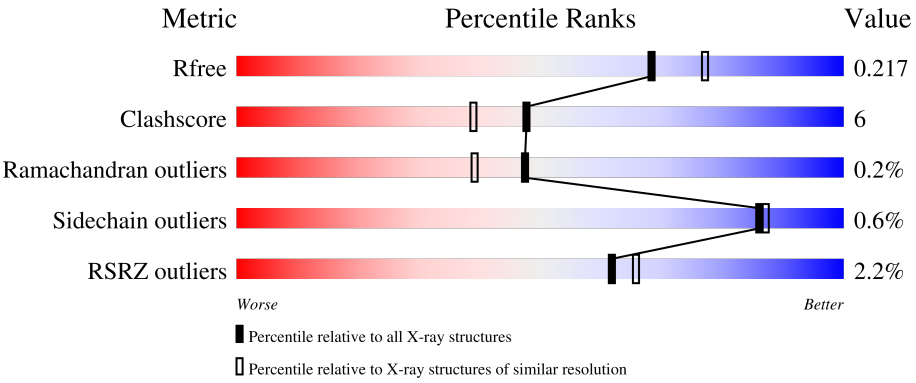
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	217	2% 83% 11% 6%
1	B	217	83% 11% 6%
1	C	217	6% 75% 19% 6%
1	D	217	3% 83% 11% 6%

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Mol	Chain	Length	Quality of chain
1	E	217	4% 77% 17% 6%
1	F	217	2% 86% 8% 6%
1	G	217	86% 8% 6%
1	H	217	84% 11% 6%
1	I	217	4% 83% 10% 6%
1	J	217	85% 9% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18839 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 SOLUBLE ACETYLCHOLINE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	8	0
			1699	1074	276	339	10			
1	B	205	Total	C	N	O	S	0	6	0
			1676	1059	272	335	10			
1	C	205	Total	C	N	O	S	0	10	0
			1718	1086	282	341	9			
1	D	205	Total	C	N	O	S	0	8	0
			1701	1074	280	338	9			
1	E	205	Total	C	N	O	S	0	15	0
			1764	1111	293	351	9			
1	F	205	Total	C	N	O	S	0	8	0
			1697	1074	277	337	9			
1	G	205	Total	C	N	O	S	0	12	0
			1734	1095	283	346	10			
1	H	205	Total	C	N	O	S	0	10	0
			1717	1086	282	340	9			
1	I	205	Total	C	N	O	S	0	9	0
			1713	1085	280	338	10			
1	J	205	Total	C	N	O	S	0	6	0
			1685	1066	274	335	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	VAL	ALA	conflict	UNP Q8WSF8
A	136	VAL	ALA	conflict	UNP Q8WSF8
B	41	VAL	ALA	conflict	UNP Q8WSF8
B	136	VAL	ALA	conflict	UNP Q8WSF8
C	41	VAL	ALA	conflict	UNP Q8WSF8
C	136	VAL	ALA	conflict	UNP Q8WSF8
D	41	VAL	ALA	conflict	UNP Q8WSF8
D	136	VAL	ALA	conflict	UNP Q8WSF8
E	41	VAL	ALA	conflict	UNP Q8WSF8

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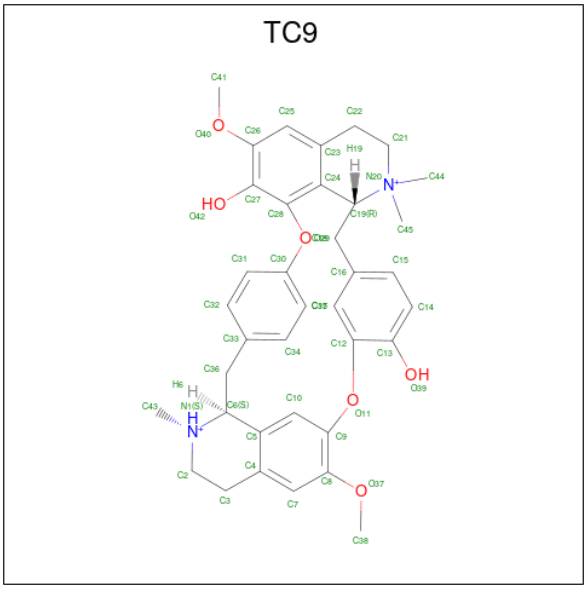
Chain	Residue	Modelled	Actual	Comment	Reference
E	136	VAL	ALA	conflict	UNP Q8WSF8

- Molecule 2 is D-TUBOCURARINE (three-letter code: TC9) (formula: $C_{37}H_{42}N_2O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O 45 37 2 6	0	0
2	D	1	Total C N O 45 37 2 6	0	0
2	F	1	Total C N O 45 37 2 6	0	0
2	G	1	Total C N O 45 37 2 6	0	0
2	H	1	Total C N O 45 37 2 6	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	142	Total O 142 142	0	0
3	B	170	Total O 170 170	0	0
3	C	141	Total O 141 141	0	0
3	D	120	Total O 120 120	0	0

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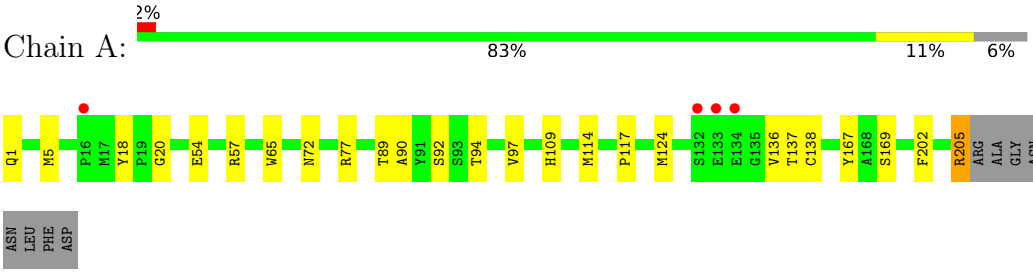
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	116	Total O 116 116	0	0
3	F	135	Total O 135 135	0	0
3	G	197	Total O 197 197	0	0
3	H	214	Total O 214 214	0	0
3	I	159	Total O 159 159	0	0
3	J	116	Total O 116 116	0	0

3 Residue-property plots (i)

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

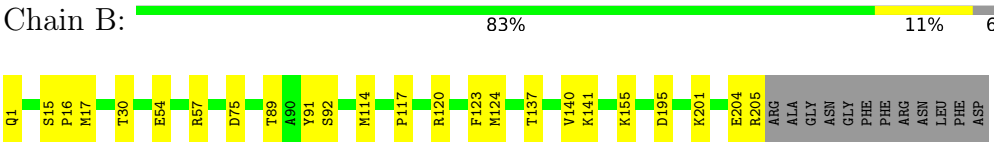
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain A:



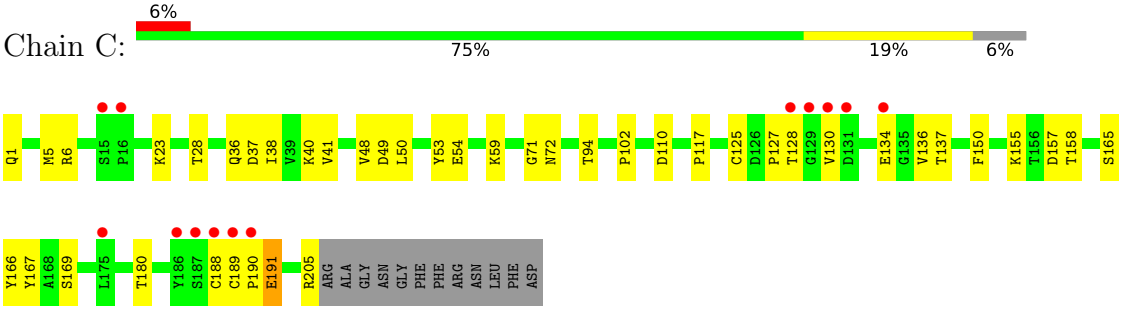
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain B:



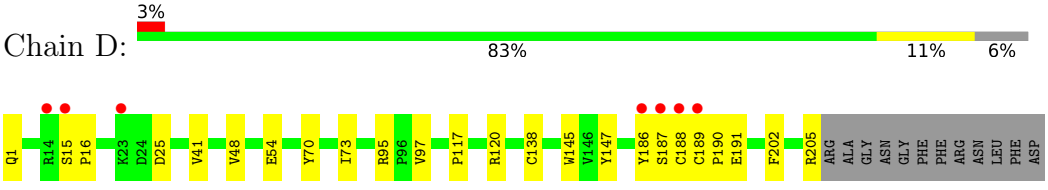
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain C:



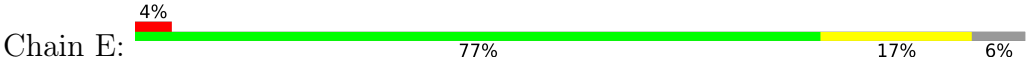
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

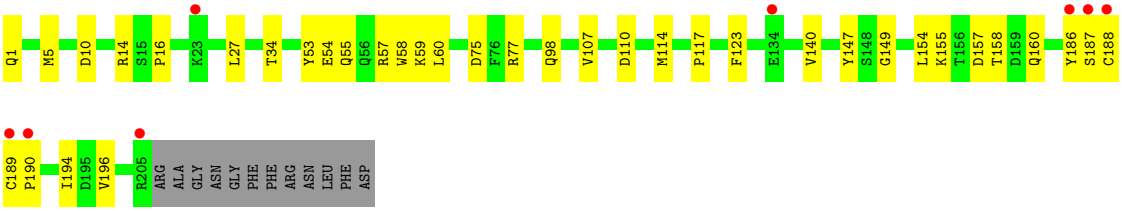
Chain D:



• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

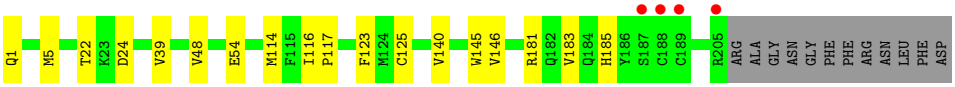
Chain E:





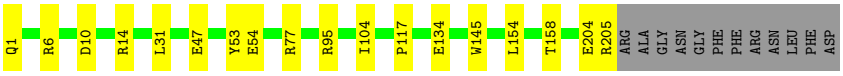
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain F:



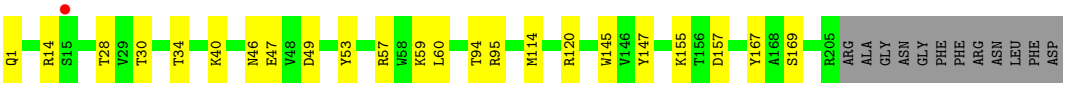
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain G:



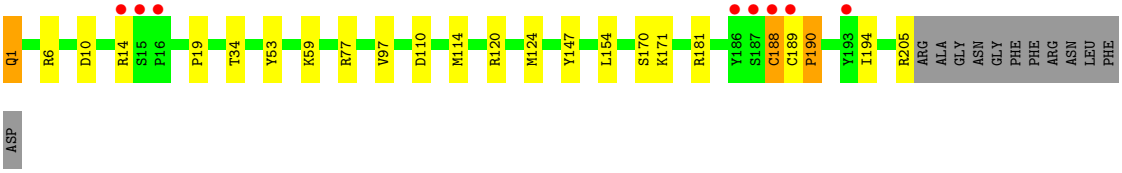
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain H:



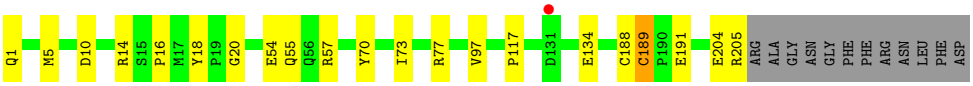
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain I:



• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.42Å 137.59Å 236.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.54 – 2.05 45.54 – 2.05	Depositor EDS
% Data completeness (in resolution range)	96.9 (45.54-2.05) 99.8 (45.54-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.36 (at 2.05Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.176 , 0.220 0.178 , 0.217	Depositor DCC
R_{free} test set	8557 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18839	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: TC9

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	0.37	0/1739	0.54	0/2372
1	B	0.41	0/1716	0.58	0/2341
1	C	0.36	0/1758	0.53	0/2397
1	D	0.32	0/1741	0.53	0/2375
1	E	0.33	0/1804	0.51	0/2459
1	F	0.35	0/1737	0.53	0/2372
1	G	0.38	0/1774	0.56	0/2420
1	H	0.40	0/1757	0.59	0/2395
1	I	0.36	0/1753	0.53	0/2388
1	J	0.32	0/1725	0.50	0/2351
All	All	0.36	0/17504	0.54	0/23870

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1699	0	1629	17	0
1	B	1676	0	1606	19	0
1	C	1718	0	1652	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1701	0	1635	19	0
1	E	1764	0	1692	35	0
1	F	1697	0	1630	18	0
1	G	1734	0	1664	17	0
1	H	1717	0	1655	24	0
1	I	1713	0	1652	21	0
1	J	1685	0	1618	14	0
2	B	45	0	41	8	0
2	D	45	0	41	15	0
2	F	45	0	41	5	0
2	G	45	0	41	3	0
2	H	45	0	41	3	0
3	A	142	0	0	3	0
3	B	170	0	0	1	0
3	C	141	0	0	2	0
3	D	120	0	0	1	0
3	E	116	0	0	1	0
3	F	135	0	0	1	0
3	G	197	0	0	2	0
3	H	214	0	0	0	0
3	I	159	0	0	3	0
3	J	116	0	0	1	0
All	All	18839	0	16638	207	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 6.

The worst 5 of 207 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)
2:D:1206:TC9:H211	1:E:55[B]:GLN:HE22	1.04	1.11
2:B:1206:TC9:H452	1:C:165:SER:HA	1.39	1.03
1:B:89[B]:THR:HG21	1:C:102:PRO:HD3	1.45	0.98
1:I:154:LEU:H	1:I:194[B]:ILE:HD13	1.29	0.96
1:E:158:THR:HG22	1:E:160:GLN:H	1.34	0.93

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	211/217 (97%)	209 (99%)	2 (1%)	0	100 100
1	B	209/217 (96%)	208 (100%)	1 (0%)	0	100 100
1	C	213/217 (98%)	207 (97%)	6 (3%)	0	100 100
1	D	211/217 (97%)	205 (97%)	5 (2%)	1 (0%)	29 18
1	E	218/217 (100%)	214 (98%)	2 (1%)	2 (1%)	17 8
1	F	211/217 (97%)	207 (98%)	4 (2%)	0	100 100
1	G	215/217 (99%)	213 (99%)	2 (1%)	0	100 100
1	H	213/217 (98%)	211 (99%)	2 (1%)	0	100 100
1	I	212/217 (98%)	207 (98%)	4 (2%)	1 (0%)	29 18
1	J	209/217 (96%)	206 (99%)	3 (1%)	0	100 100
All	All	2122/2170 (98%)	2087 (98%)	31 (2%)	4 (0%)	47 39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	187	SER
1	D	187	SER
1	E	190	PRO
1	I	190	PRO

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	196/197 (100%)	194 (99%)	2 (1%)	76 75
1	B	194/197 (98%)	192 (99%)	2 (1%)	76 75
1	C	198/197 (100%)	197 (100%)	1 (0%)	88 89
1	D	196/197 (100%)	194 (99%)	2 (1%)	76 75
1	E	203/197 (103%)	202 (100%)	1 (0%)	88 89
1	F	195/197 (99%)	195 (100%)	0	100 100
1	G	200/197 (102%)	200 (100%)	0	100 100
1	H	198/197 (100%)	198 (100%)	0	100 100
1	I	197/197 (100%)	195 (99%)	2 (1%)	76 75
1	J	194/197 (98%)	193 (100%)	1 (0%)	88 89
All	All	1971/1970 (100%)	1960 (99%)	11 (1%)	86 87

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	189	CYS
1	I	1	GLN
1	J	189	CYS
1	I	188	CYS
1	C	191	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	68	ASN
1	J	55	GLN
1	J	185	HIS
1	E	3	ASN
1	E	184	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)

There are no monosaccharides 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	$\#\|Z\|>2$
2	TC9	G	1206	-	50,51,51	1.29	4 (8%)	73,77,77	2.04	9 (12%)
2	TC9	F	1206	-	50,51,51	1.44	8 (16%)	73,77,77	2.28	16 (21%)
2	TC9	D	1206	-	50,51,51	1.38	8 (16%)	73,77,77	2.07	11 (15%)
2	TC9	H	1206	-	50,51,51	1.36	7 (14%)	73,77,77	1.90	7 (9%)
2	TC9	B	1206	-	50,51,51	1.45	9 (18%)	73,77,77	2.34	14 (19%)

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	TC9	G	1206	-	-	2/20/49/49	-
2	TC9	F	1206	-	-	5/20/49/49	-
2	TC9	D	1206	-	-	5/20/49/49	-
2	TC9	H	1206	-	-	0/20/49/49	-
2	TC9	B	1206	-	-	4/20/49/49	-

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1206	TC9	C6-N1	3.15	1.53	1.48
2	B	1206	TC9	C26-C27	3.07	1.44	1.40
2	D	1206	TC9	C19-N20	-3.04	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1206	TC9	C26-C27	3.03	1.44	1.40
2	F	1206	TC9	C6-N1	3.02	1.52	1.48

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1206	TC9	C43-N1-C6	14.36	132.53	111.39
2	F	1206	TC9	C43-N1-C6	13.61	131.43	111.39
2	D	1206	TC9	C43-N1-C6	11.71	128.63	111.39
2	H	1206	TC9	C43-N1-C6	11.34	128.08	111.39
2	G	1206	TC9	C43-N1-C6	10.81	127.31	111.39

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1206	TC9	C27-C26-O40-C41
2	D	1206	TC9	C9-C8-O37-C38
2	G	1206	TC9	C27-C26-O40-C41
2	D	1206	TC9	C25-C26-O40-C41
2	D	1206	TC9	C7-C8-O37-C38

There are no ring outliers.

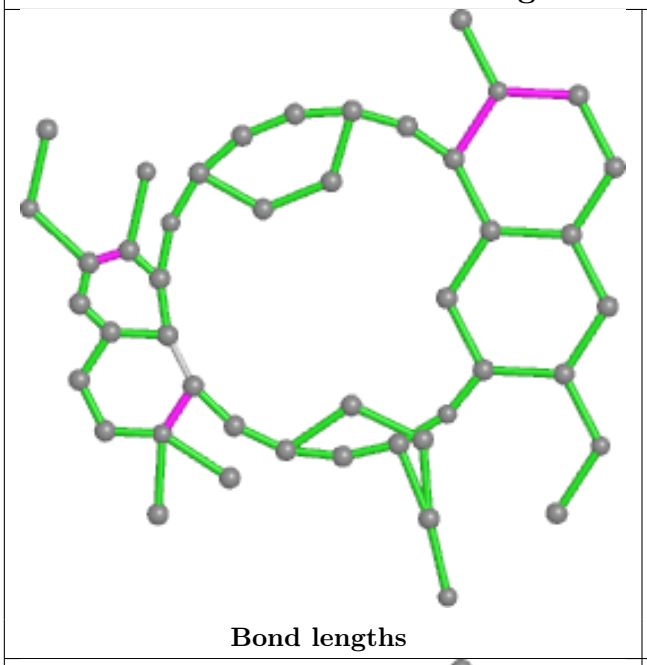
5 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1206	TC9	3	0
2	F	1206	TC9	5	0
2	D	1206	TC9	15	0
2	H	1206	TC9	3	0
2	B	1206	TC9	8	0

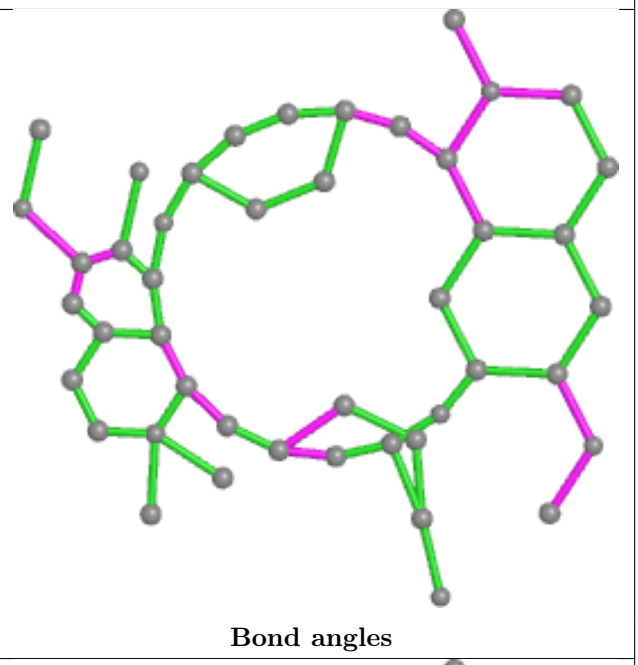
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

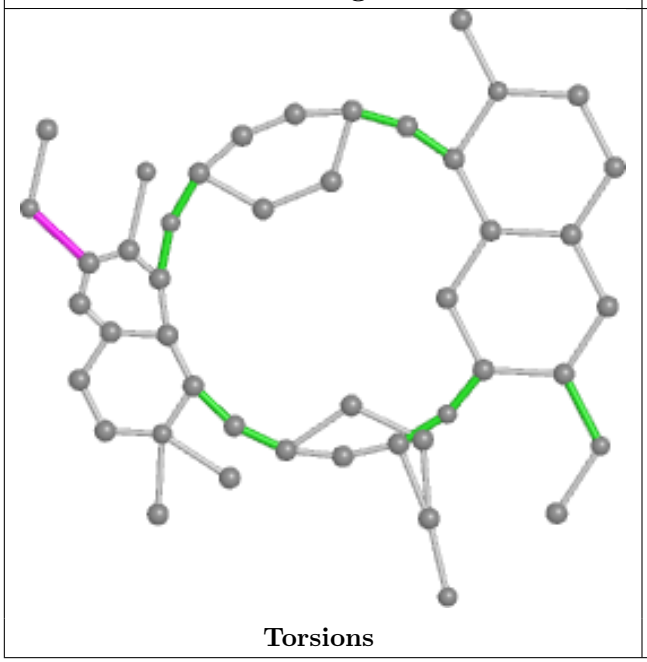
Ligand TC9 G 1206



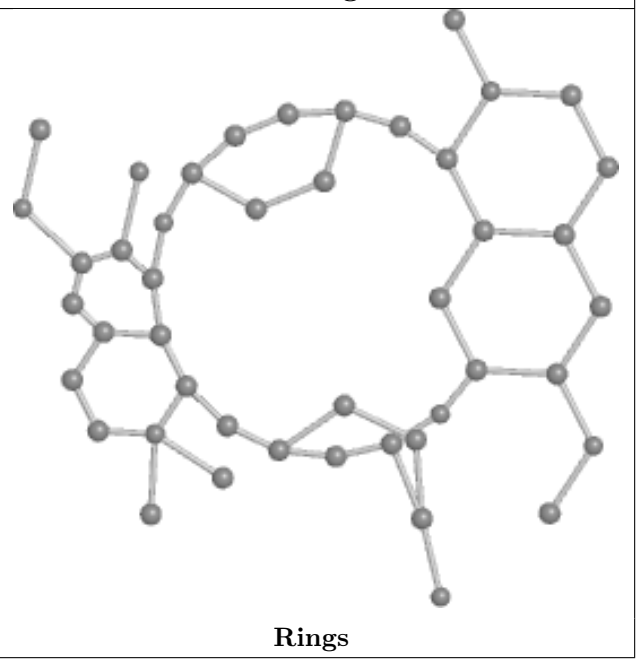
Bond lengths



Bond angles

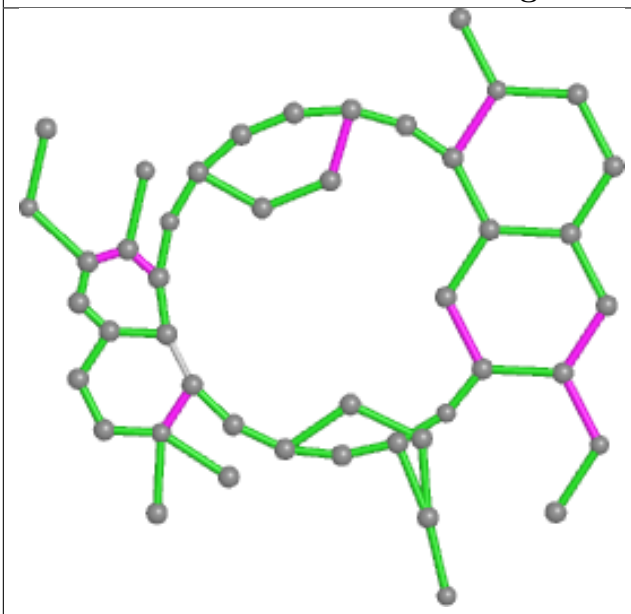


Torsions

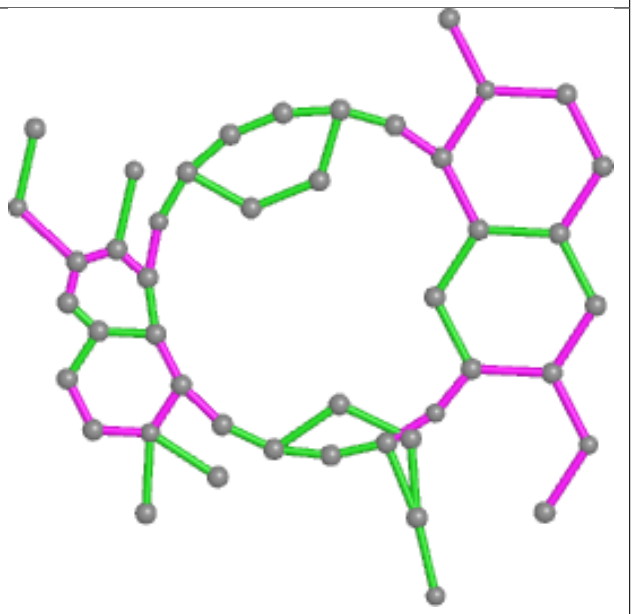


Rings

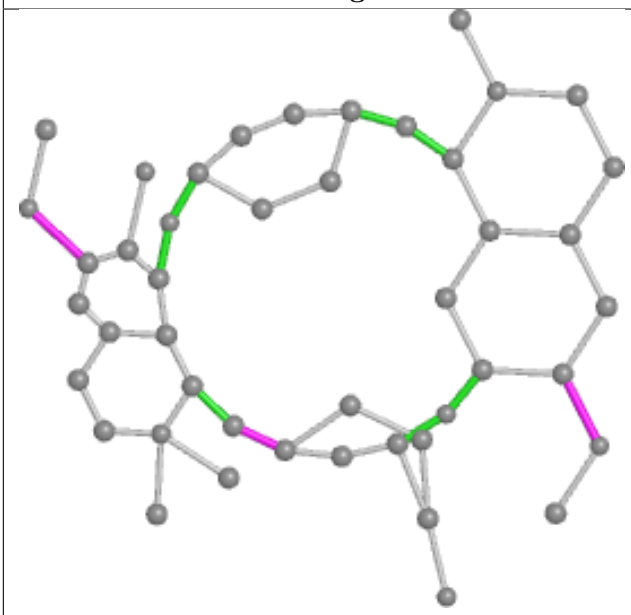
Ligand TC9 F 1206



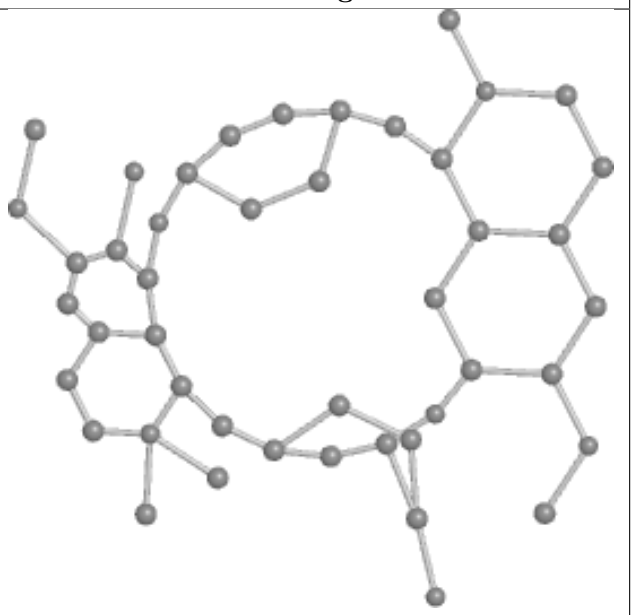
Bond lengths



Bond angles

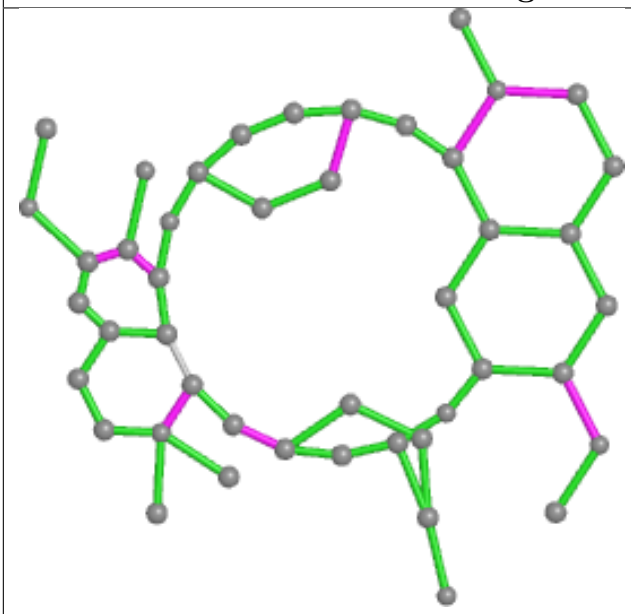


Torsions

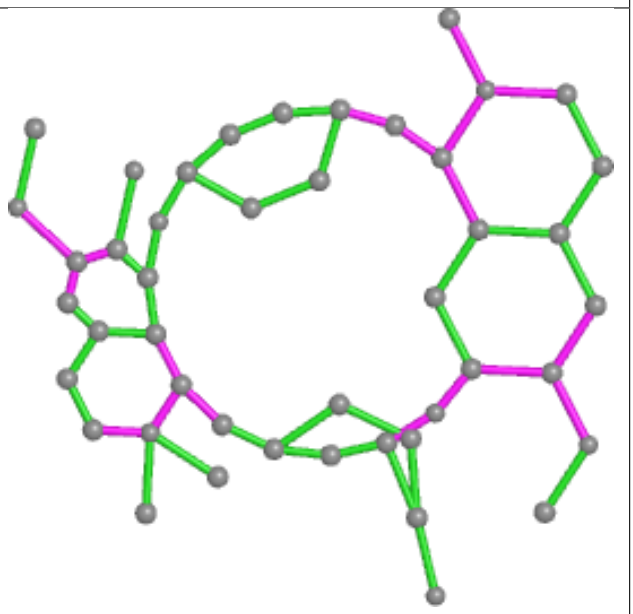


Rings

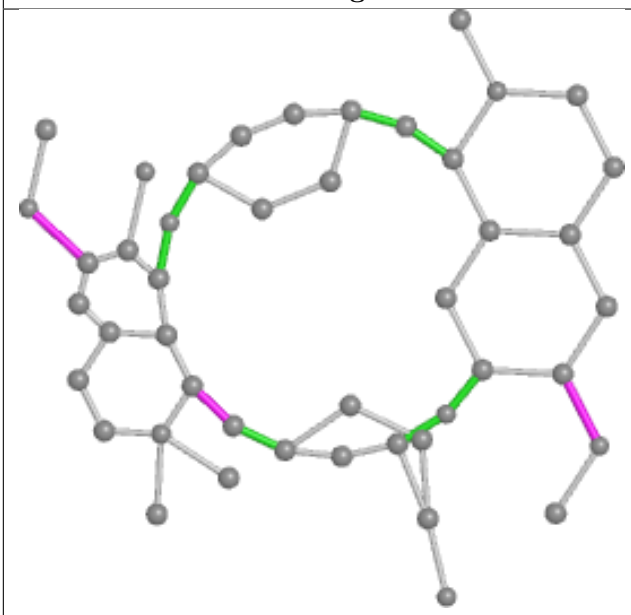
Ligand TC9 D 1206



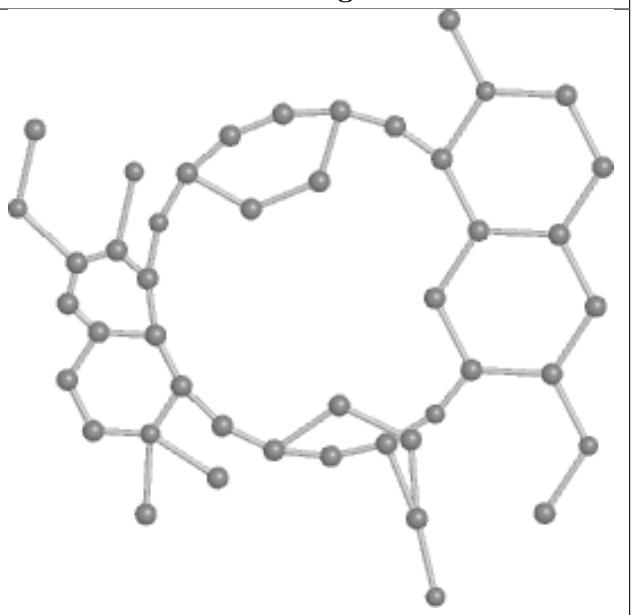
Bond lengths



Bond angles

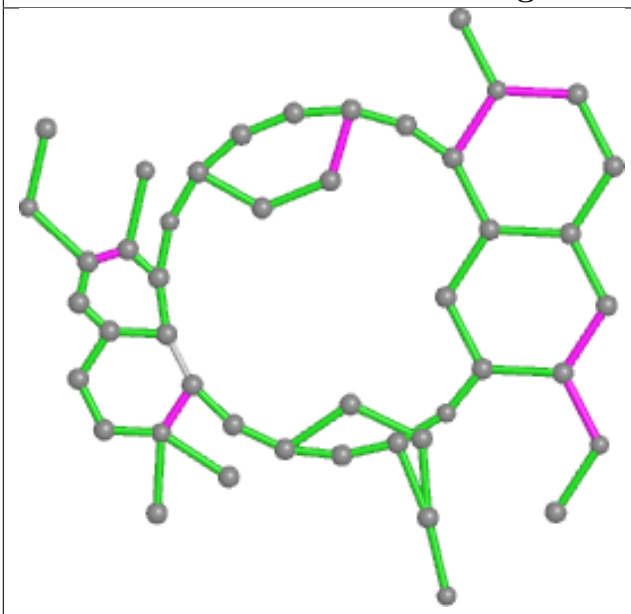


Torsions

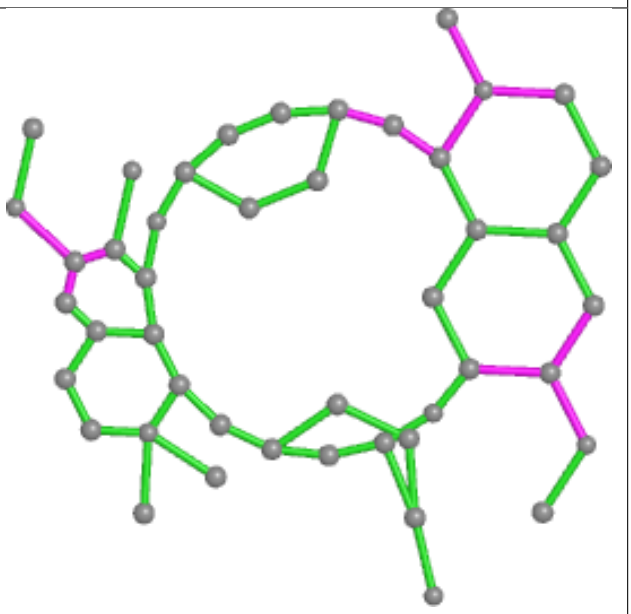


Rings

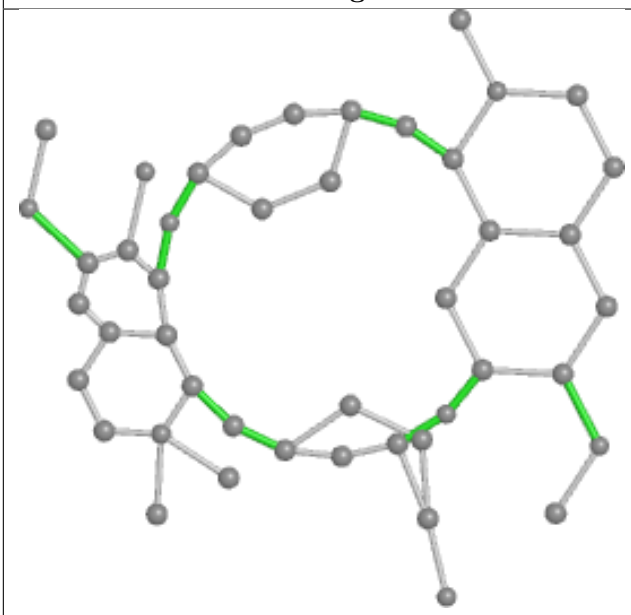
Ligand TC9 H 1206



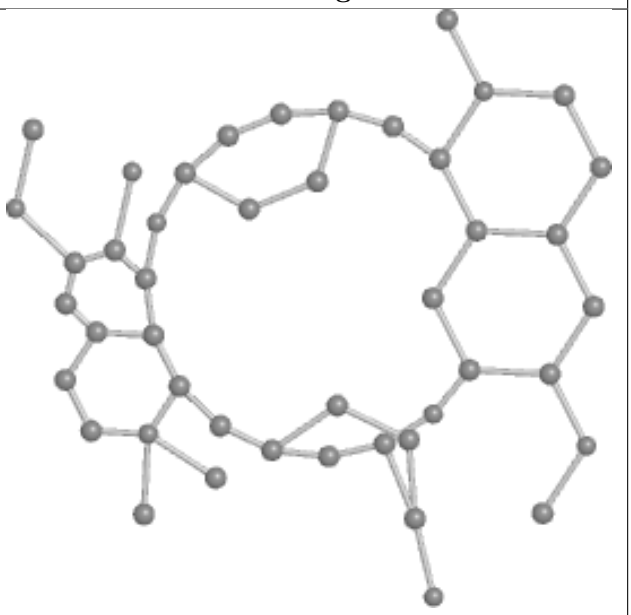
Bond lengths



Bond angles

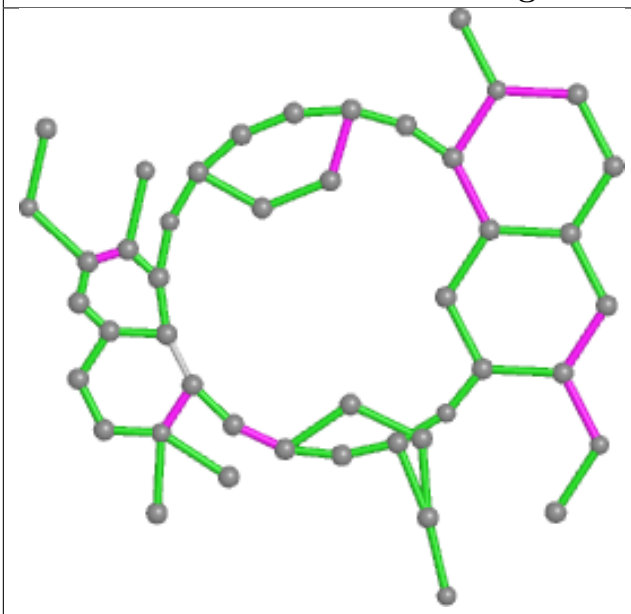


Torsions

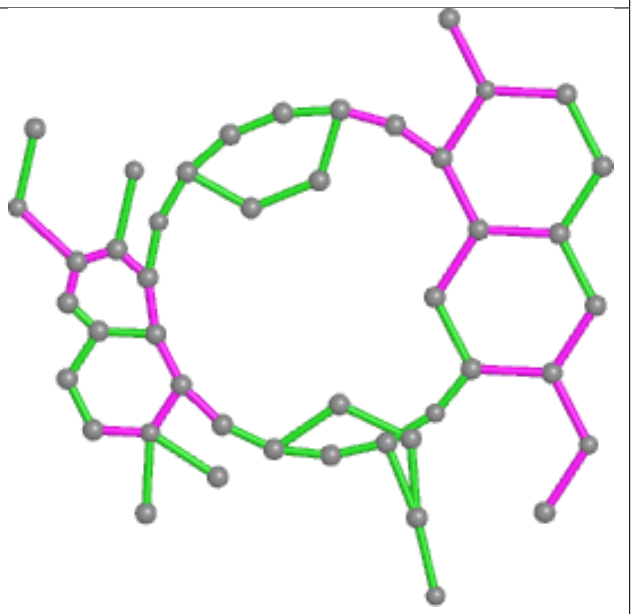


Rings

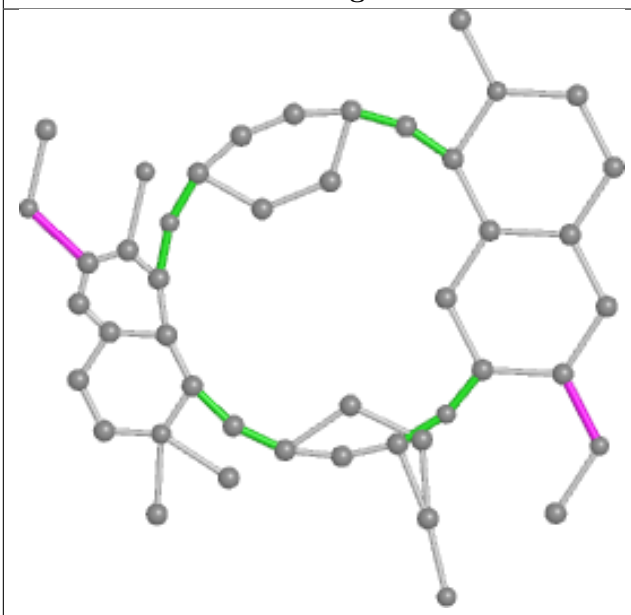
Ligand TC9 B 1206



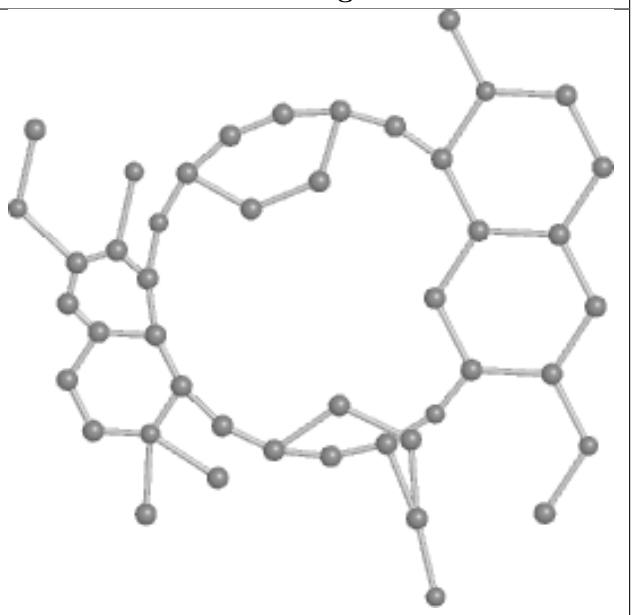
Bond lengths



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	205/217 (94%)	-0.26	4 (1%) 65 69	18, 31, 54, 85	0
1	B	205/217 (94%)	-0.21	0 100 100	13, 26, 50, 77	0
1	C	205/217 (94%)	0.02	13 (6%) 20 21	18, 32, 68, 120	0
1	D	205/217 (94%)	-0.15	7 (3%) 45 49	24, 36, 65, 105	0
1	E	205/217 (94%)	0.02	8 (3%) 39 42	24, 38, 71, 131	0
1	F	205/217 (94%)	-0.22	4 (1%) 65 69	22, 34, 61, 92	0
1	G	205/217 (94%)	-0.23	0 100 100	16, 27, 51, 79	0
1	H	205/217 (94%)	-0.11	1 (0%) 91 92	15, 24, 46, 70	0
1	I	205/217 (94%)	-0.19	8 (3%) 39 42	18, 30, 63, 117	0
1	J	205/217 (94%)	-0.21	1 (0%) 91 92	23, 37, 66, 87	0
All	All	2050/2170 (94%)	-0.16	46 (2%) 62 66	13, 32, 62, 131	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	186	TYR	8.0
1	I	189	CYS	6.3
1	E	187	SER	6.2
1	I	187	SER	6.1
1	C	188	CYS	5.4

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

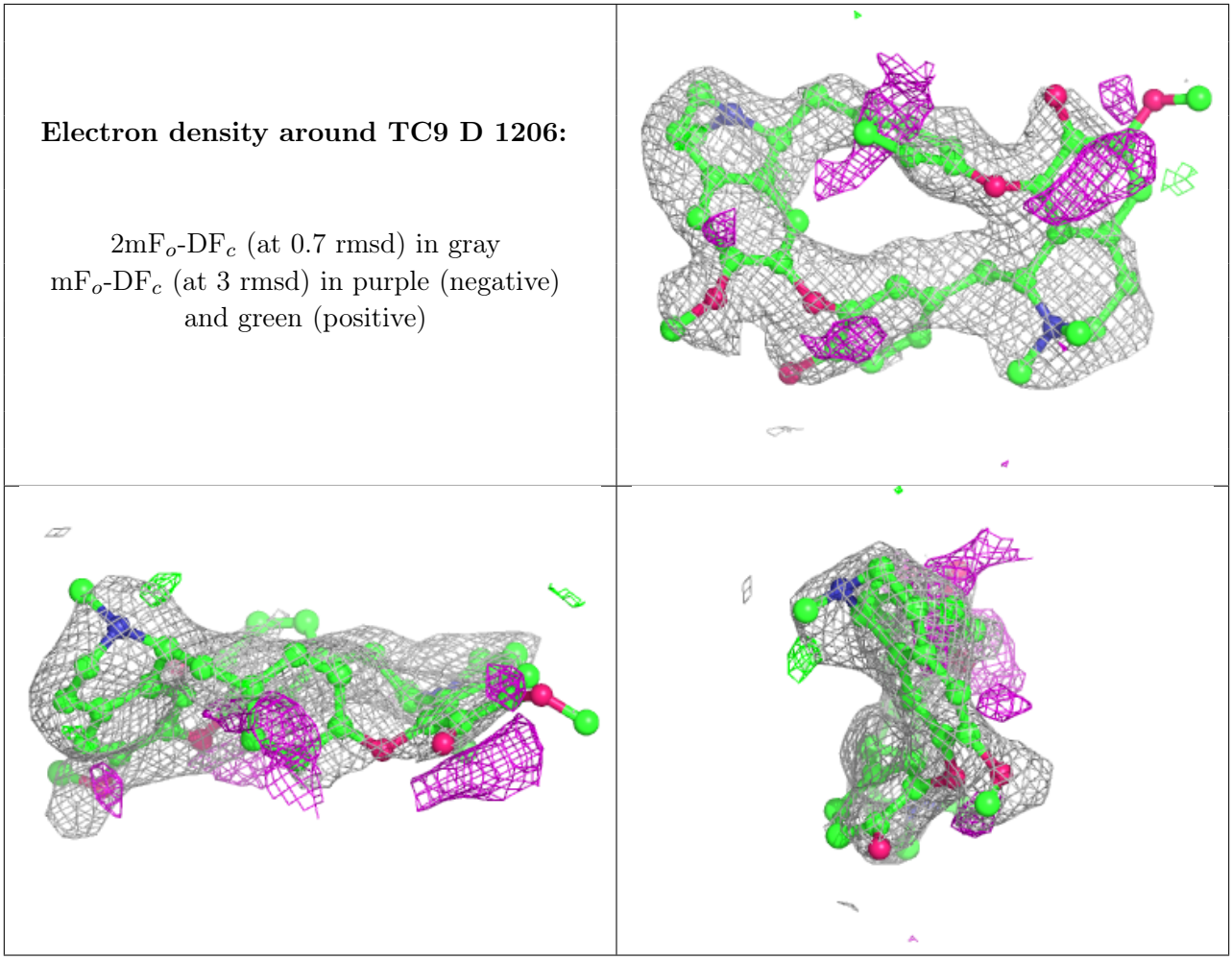
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	TC9	D	1206	45/45	0.72	0.28	38,75,91,96	0
2	TC9	F	1206	45/45	0.79	0.20	35,66,72,74	0
2	TC9	B	1206	45/45	0.81	0.20	25,46,60,66	0
2	TC9	H	1206	45/45	0.91	0.12	21,31,45,50	0
2	TC9	G	1206	45/45	0.95	0.11	13,23,45,58	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.

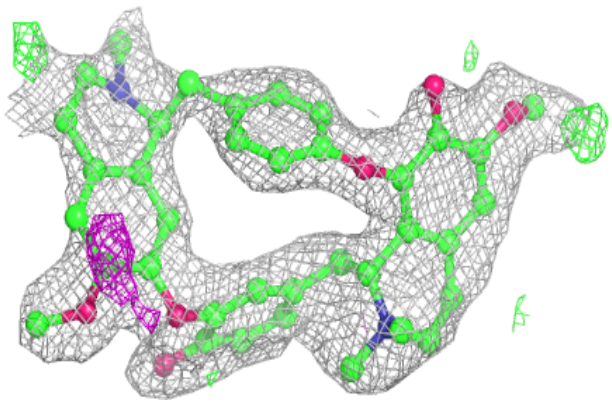
Electron density around TC9 D 1206:

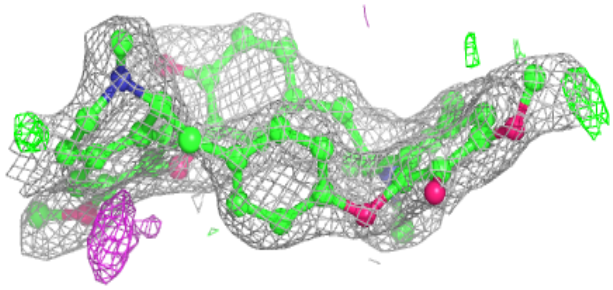
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

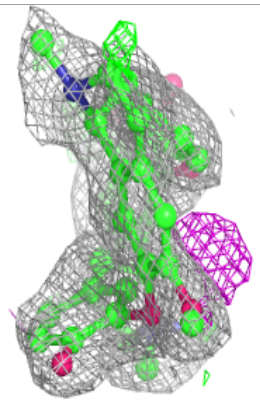


Electron density around TC9 F 1206:

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

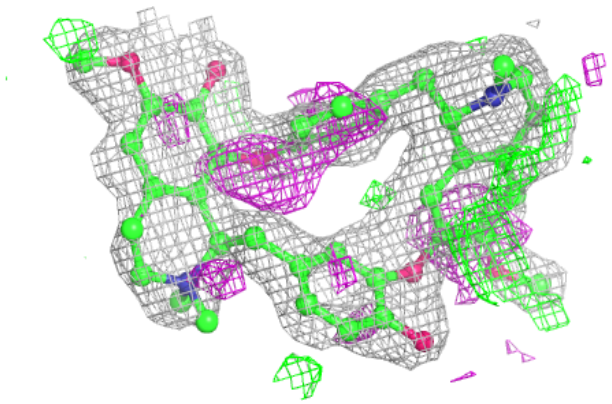


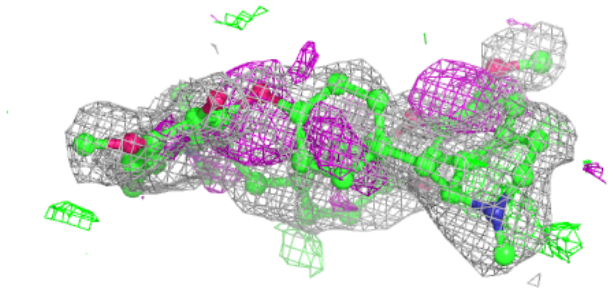


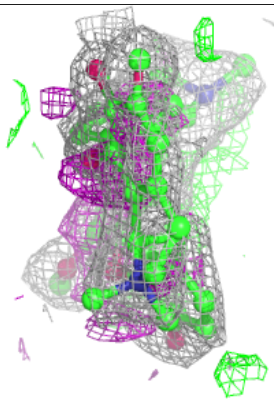


Electron density around TC9 B 1206:

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

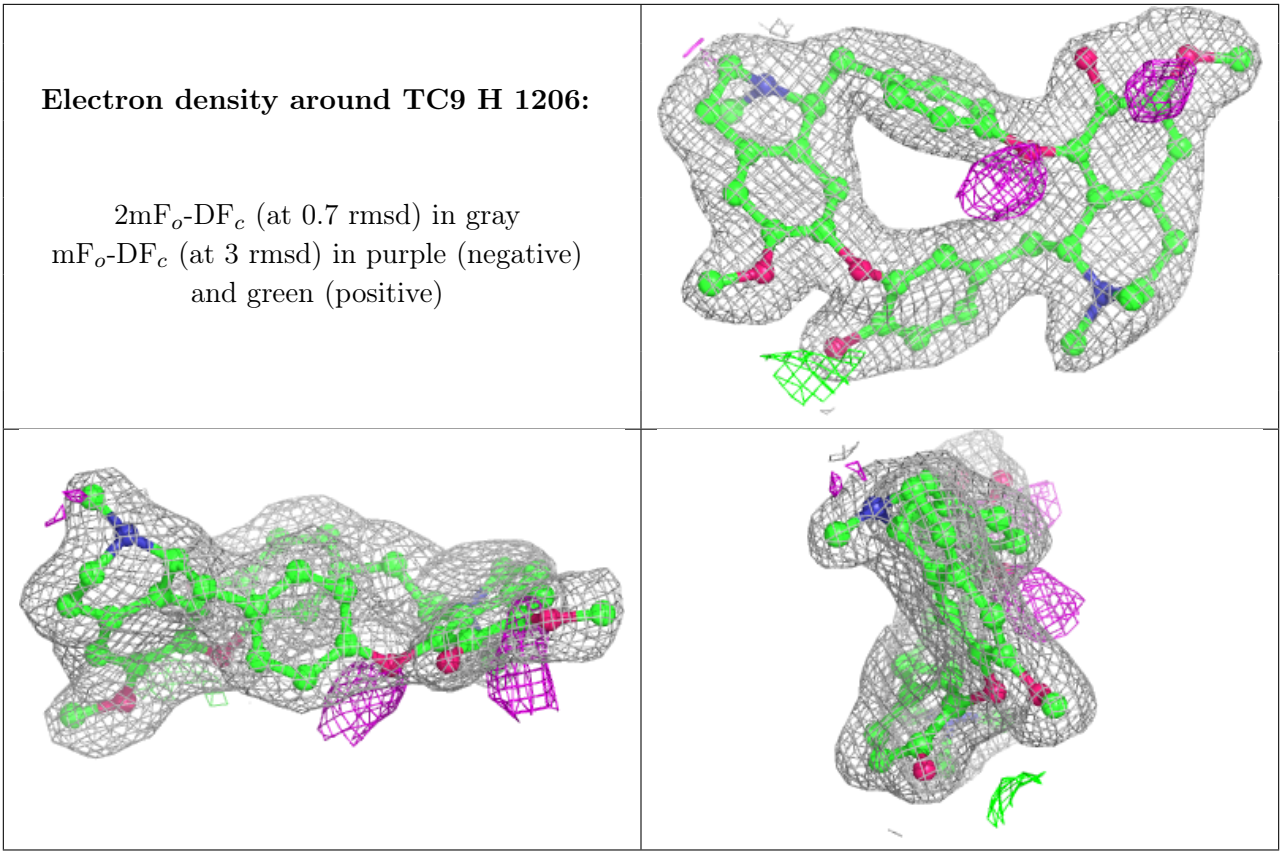






Electron density around TC9 H 1206:

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



Electron density around TC9 G 1206:

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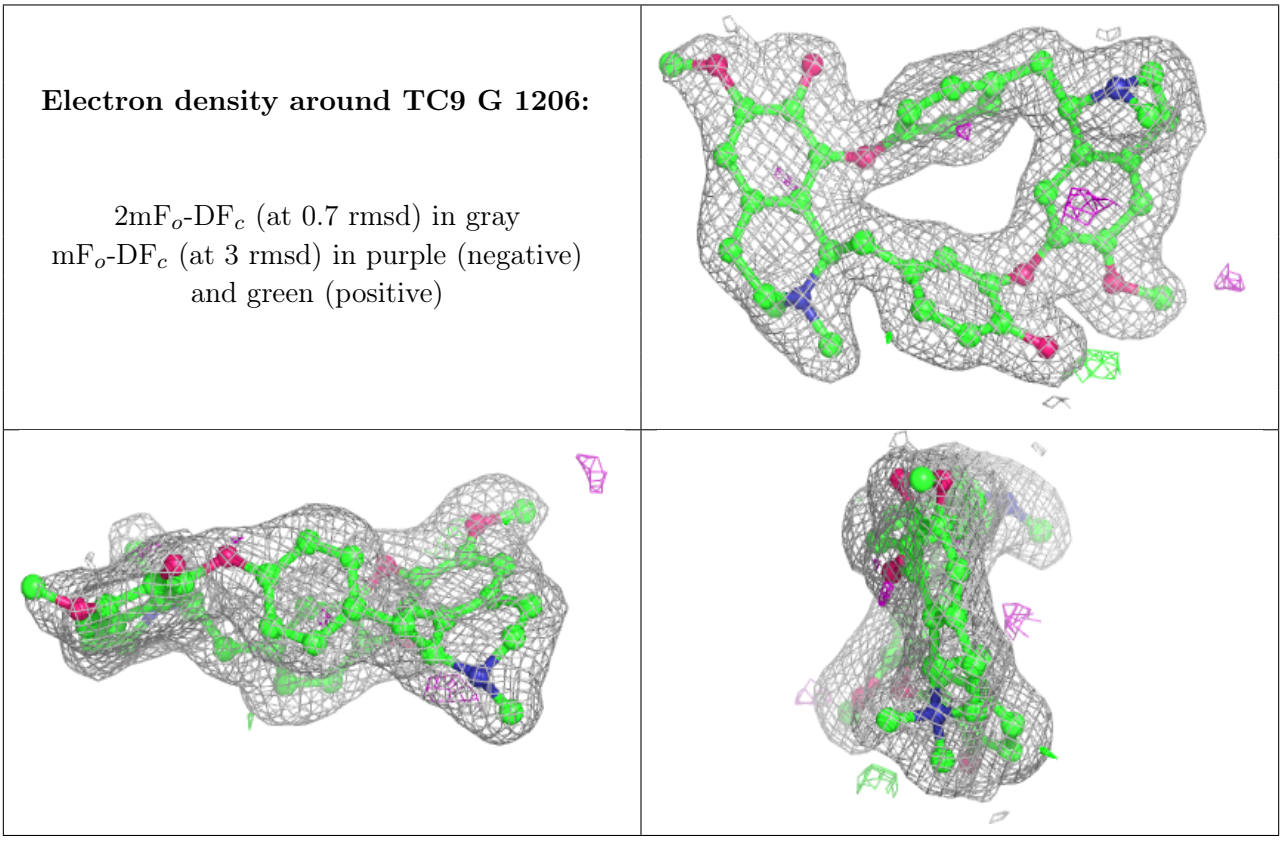
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.