wwPDB X-ray Structure Validation Summary Report (i)

Jan 20, 2024 – 03:34 pm GMT

PDB ID	:	7Q9S
Title	:	Crystal structure of PDE6D KRas peptide complex with Compound-1
Authors	:	Yelland, T.; Ismail, S.
Deposited on	:	2021-11-14
Resolution	:	1.85 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:

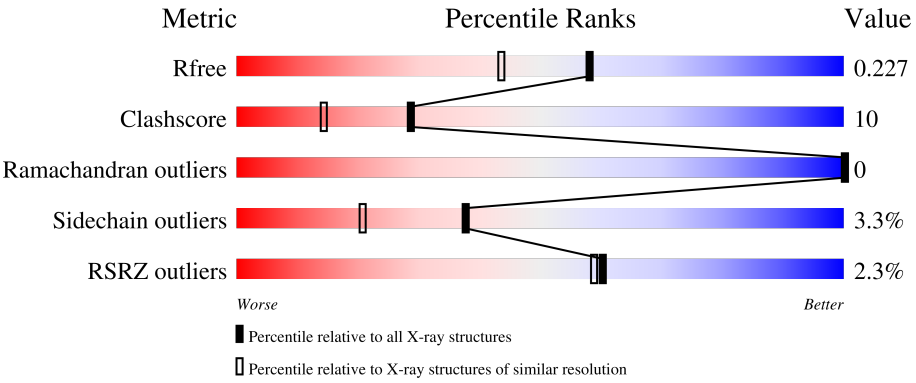
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	AAA	150	2% 89% 8%
1	BBB	150	% 80% 19%
2	CCC	13	38% 8% 54%
2	DDD	13	15% 23% 15% 62%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	9TI	BBB	201	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 2967 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.

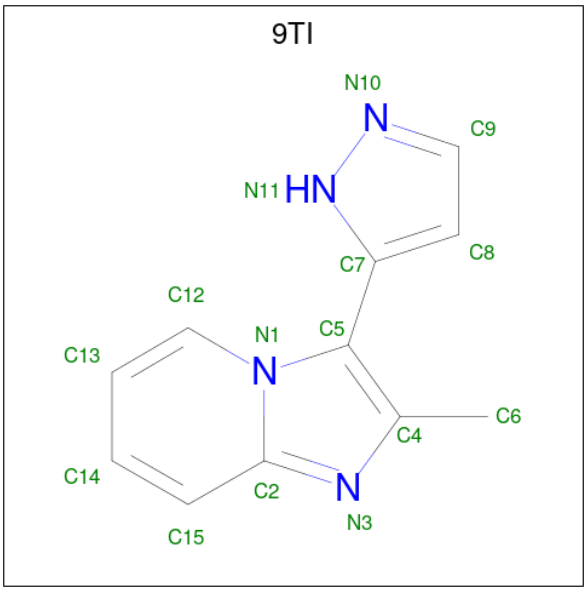
- Molecule 1 is a protein called Retinal rod rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BBB	149	Total	C	N	O	S	0	7	0
			1275	814	212	243	6			
1	AAA	150	Total	C	N	O	S	0	9	0
			1289	826	215	242	6			

- Molecule 2 is a protein called KRas.

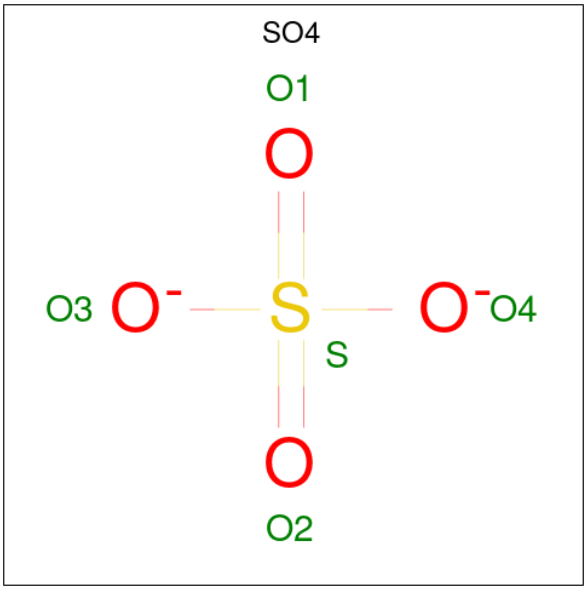
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	CCC	6	Total	C	N	O	S	0	0	0
			44	26	8	9	1			
2	DDD	5	Total	C	N	O	S	0	0	0
			39	23	7	8	1			

- Molecule 3 is 2-methyl-3-(1 {H}-pyrazol-5-yl)imidazo[1,2-a]pyridine (three-letter code: 9TI) (formula: $C_{11}H_{10}N_4$) (labeled as "Ligand of Interest" by depositor).



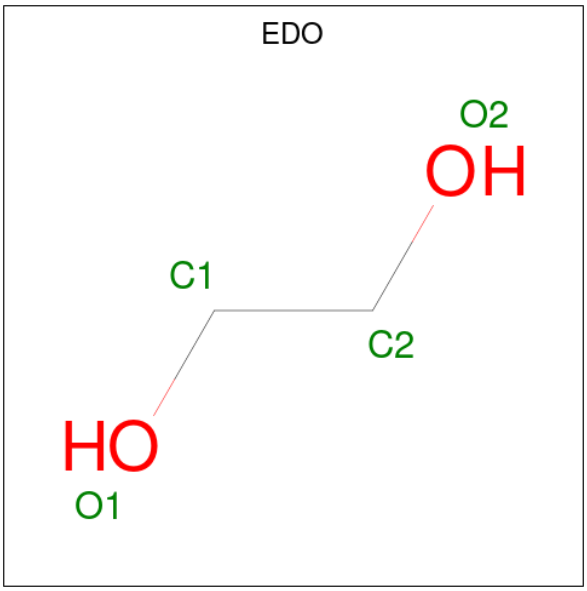
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	BBB	1	Total C N 15 11 4	0	0
3	AAA	1	Total C N 15 11 4	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



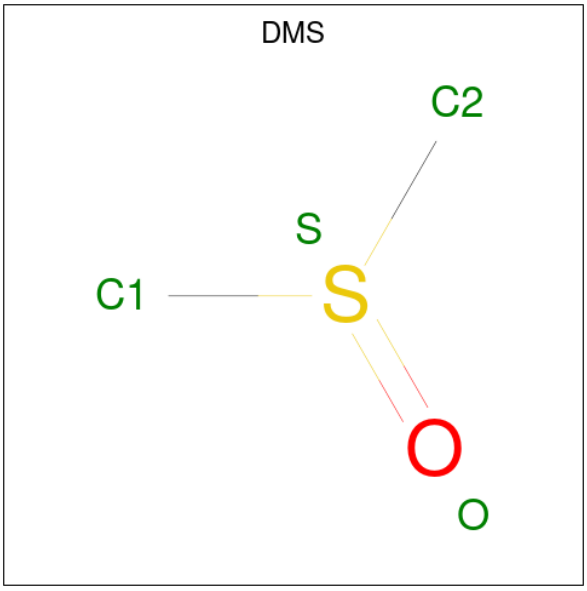
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	BBB	1	Total O S 5 4 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



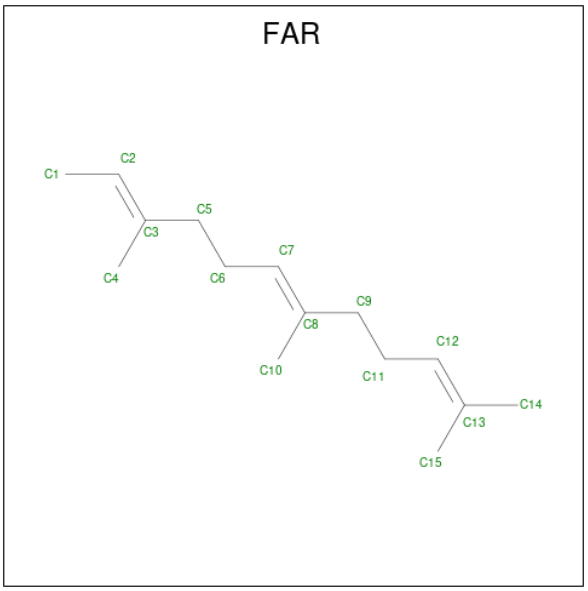
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	BBB	1	Total C O 4 2 2	0	0
5	BBB	1	Total C O 4 2 2	0	0
5	BBB	1	Total C O 4 2 2	0	0
5	BBB	1	Total C O 4 2 2	0	0
5	AAA	1	Total C O 4 2 2	0	0
5	AAA	1	Total C O 4 2 2	0	0
5	AAA	1	Total C O 4 2 2	0	0

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	1	Total C O S 4 2 1 1	0	0

- Molecule 7 is FARNESYL (three-letter code: FAR) (formula: $C_{15}H_{26}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	1	Total C 15 15	0	0
7	DDD	1	Total C 15 15	0	0

- Molecule 8 is water.

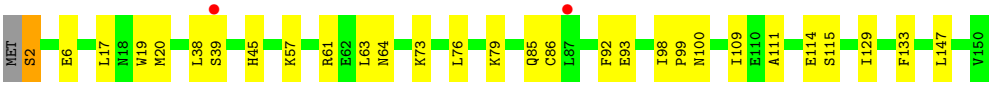
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	BBB	96	Total O 96 96	0	0
8	AAA	123	Total O 123 123	0	0
8	CCC	3	Total O 3 3	0	0
8	DDD	1	Total O 1 1	0	0

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.

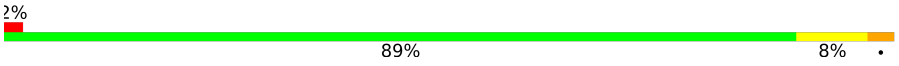
• Molecule 1: Retinal rod rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit delta

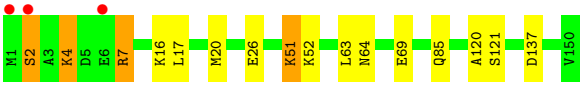
Chain BBB:



• Molecule 1: Retinal rod rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit delta

Chain AAA:



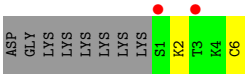


• Molecule 2: KRas

Chain CCC:

• Molecule 2: KRas

Chain DDD:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	77.10Å 81.12Å 118.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.66 – 1.85 40.66 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.66-1.85) 99.9 (40.66-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.199 , 0.227 0.203 , 0.227	Depositor DCC
R_{free} test set	1575 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	26.5	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.067 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2967	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% 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: EDO, DMS, FAR, 9TI, CMT, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	AAA	0.58	0/1315	0.75	0/1774
1	BBB	0.58	0/1301	0.73	0/1754
2	CCC	0.66	0/35	0.81	0/44
2	DDD	0.71	0/30	0.88	0/37
All	All	0.58	0/2681	0.74	0/3609

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	AAA	1289	0	1275	18	0
1	BBB	1275	0	1237	32	0
2	CCC	44	0	45	0	0
2	DDD	39	0	46	1	0
3	AAA	15	0	0	1	0
3	BBB	15	0	0	8	0
4	BBB	5	0	0	0	0
5	AAA	12	0	18	3	0
5	BBB	16	0	24	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AAA	4	0	6	0	0
7	AAA	15	0	24	0	0
7	DDD	15	0	24	2	0
8	AAA	123	0	0	3	0
8	BBB	96	0	0	1	0
8	CCC	3	0	0	0	0
8	DDD	1	0	0	0	0
All	All	2967	0	2699	53	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 10.

The worst 5 of 53 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:17:LEU:HD22	1:AAA:63[B]:LEU:HD11	1.39	1.03
1:BBB:61[A]:ARG:HB3	3:BBB:201:9TI:C12	2.09	0.83
1:BBB:61[A]:ARG:HG3	1:BBB:109:ILE:HD13	1.62	0.80
1:AAA:120:ALA:HB3	5:AAA:206:EDO:H11	1.71	0.71
1:BBB:85:GLN:NE2	8:BBB:301:HOH:O	2.23	0.70

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	AAA	157/150 (105%)	155 (99%)	2 (1%)	0	100	100
1	BBB	155/150 (103%)	153 (99%)	2 (1%)	0	100	100
2	CCC	4/13 (31%)	4 (100%)	0	0	100	100
2	DDD	3/13 (23%)	3 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	319/326 (98%)	315 (99%)	4 (1%)	0	100 100

There are no Ramachandran outliers to report.

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	AAA	142/135 (105%)	136 (96%)	6 (4%)	30 13
1	BBB	139/135 (103%)	135 (97%)	4 (3%)	42 26
2	CCC	4/11 (36%)	4 (100%)	0	100 100
2	DDD	4/11 (36%)	4 (100%)	0	100 100
All	All	289/292 (99%)	279 (96%)	10 (4%)	38 18

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	7[B]	ARG
1	AAA	16	LYS
1	AAA	51	LYS
1	BBB	100	ASN
1	AAA	2	SER

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	CMT	DDD	6	2,7	7,7,7	2.03	1 (14%)	6,8,8	2.09	2 (33%)
2	CMT	CCC	101	2,7	7,7,7	1.93	1 (14%)	6,8,8	1.71	2 (33%)

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	CMT	DDD	6	2,7	-	4/8/8/8	-
2	CMT	CCC	101	2,7	-	2/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	6	CMT	OXT-C	5.10	1.45	1.33
2	CCC	101	CMT	OXT-C	4.92	1.45	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	DDD	6	CMT	OXT-C-CA	3.53	120.56	111.52
2	CCC	101	CMT	OXT-C-O	-2.83	118.31	123.84
2	DDD	6	CMT	OXT-C-O	-2.72	118.52	123.84
2	CCC	101	CMT	OXT-C-CA	2.43	117.73	111.52

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	DDD	6	CMT	CA-C-OXT-C1
2	DDD	6	CMT	O-C-OXT-C1
2	DDD	6	CMT	N-CA-CB-SG

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Mol	Chain	Res	Type	Atoms
2	CCC	101	CMT	OXT-C-CA-N
2	CCC	101	CMT	OXT-C-CA-CB

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 (i)

13 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	$\#\|Z\| > 2$
5	EDO	BBB	204	-	3,3,3	0.07	0	2,2,2	0.17	0
5	EDO	BBB	203	-	3,3,3	0.05	0	2,2,2	0.25	0
5	EDO	AAA	204	-	3,3,3	0.07	0	2,2,2	0.26	0
3	9TI	AAA	203	-	14,17,17	3.13	5 (35%)	9,24,24	1.25	1 (11%)
3	9TI	BBB	201	1	14,17,17	3.58	6 (42%)	9,24,24	1.34	2 (22%)
4	SO4	BBB	202	-	4,4,4	0.39	0	6,6,6	0.06	0
5	EDO	BBB	205	-	3,3,3	0.07	0	2,2,2	0.21	0
5	EDO	AAA	205	-	3,3,3	0.05	0	2,2,2	0.16	0
6	DMS	AAA	201	-	3,3,3	0.23	0	3,3,3	0.15	0
5	EDO	AAA	206	-	3,3,3	0.04	0	2,2,2	0.12	0
5	EDO	BBB	206	-	3,3,3	0.05	0	2,2,2	0.09	0
7	FAR	DDD	101	2	14,14,14	0.23	0	16,16,16	0.66	0
7	FAR	AAA	202	2	14,14,14	0.27	0	16,16,16	0.74	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	EDO	BBB	204	-	-	0/1/1/1	-
5	EDO	BBB	203	-	-	1/1/1/1	-
5	EDO	AAA	204	-	-	0/1/1/1	-
3	9TI	AAA	203	-	-	0/0/4/4	0/3/3/3
3	9TI	BBB	201	1	-	0/0/4/4	0/3/3/3
5	EDO	AAA	205	-	-	1/1/1/1	-
5	EDO	BBB	205	-	-	1/1/1/1	-
5	EDO	AAA	206	-	-	0/1/1/1	-
5	EDO	BBB	206	-	-	0/1/1/1	-
7	FAR	DDD	101	2	-	4/14/14/14	-
7	FAR	AAA	202	2	-	1/14/14/14	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BBB	201	9TI	C5-C7	-9.50	1.33	1.49
3	AAA	203	9TI	C5-C7	-8.24	1.35	1.49
3	BBB	201	9TI	C8-C7	-5.25	1.33	1.40
3	AAA	203	9TI	C8-C7	-4.89	1.34	1.40
3	BBB	201	9TI	C15-C2	-4.60	1.34	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	BBB	201	9TI	C8-C7-C5	-2.50	125.76	128.77
3	AAA	203	9TI	C8-C7-N11	-2.32	107.48	110.42
3	BBB	201	9TI	C13-C12-N1	-2.16	118.01	120.78

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	DDD	101	FAR	C12-C11-C9-C8
5	BBB	203	EDO	O1-C1-C2-O2
5	BBB	205	EDO	O1-C1-C2-O2
5	AAA	205	EDO	O1-C1-C2-O2
7	DDD	101	FAR	C1-C2-C3-C5

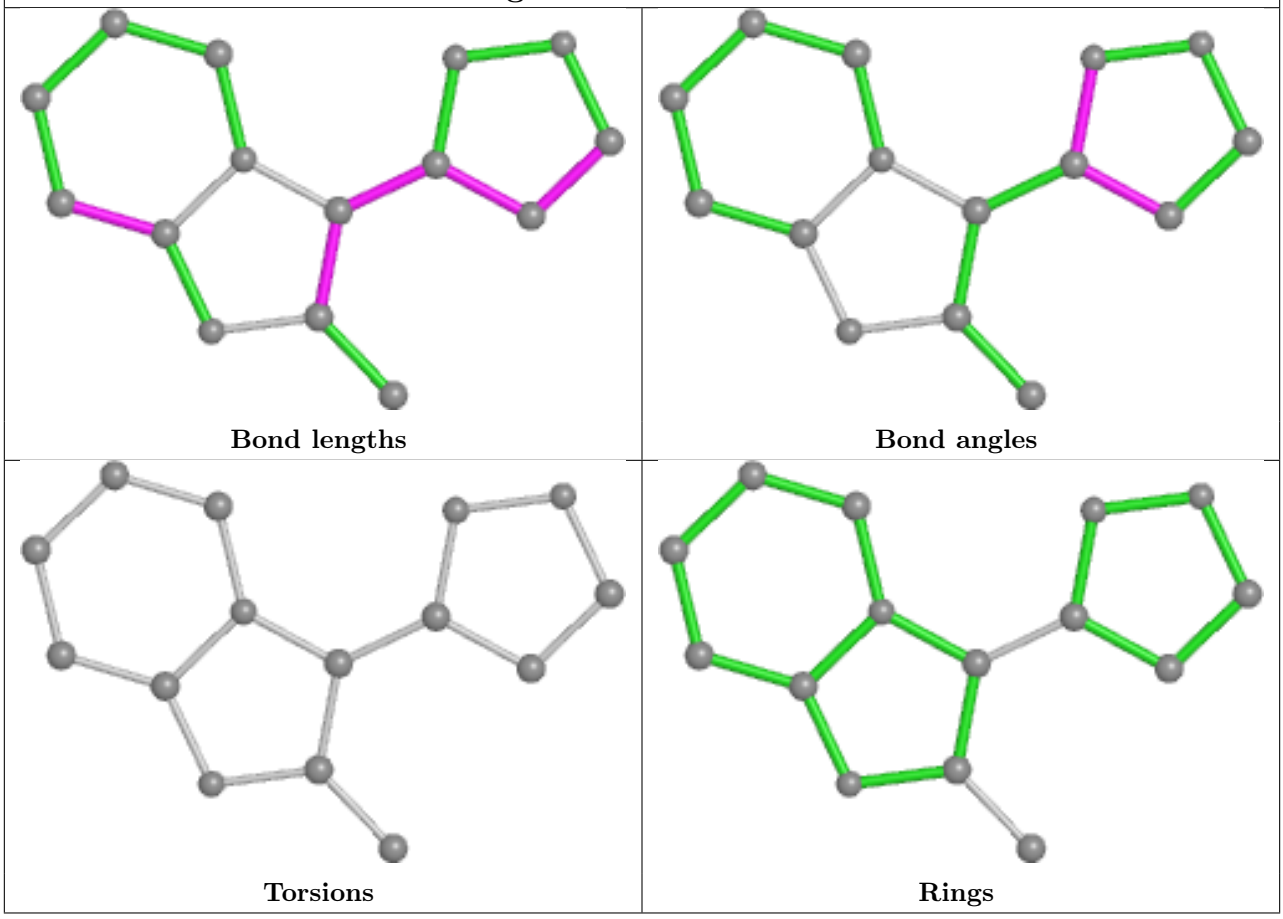
There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	BBB	203	EDO	3	0
3	AAA	203	9TI	1	0
3	BBB	201	9TI	8	0
5	AAA	205	EDO	1	0
5	AAA	206	EDO	2	0
7	DDD	101	FAR	2	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.

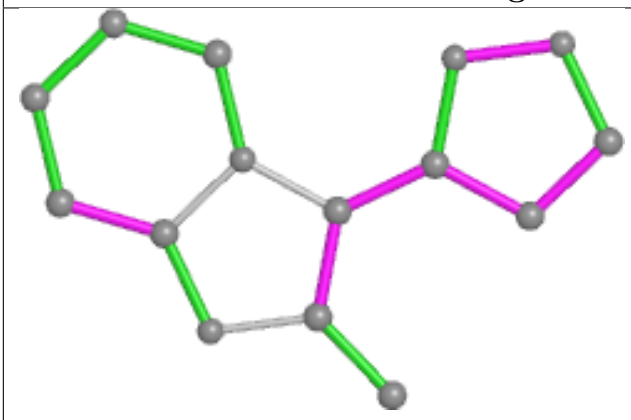
Ligand 9TI AAA 203



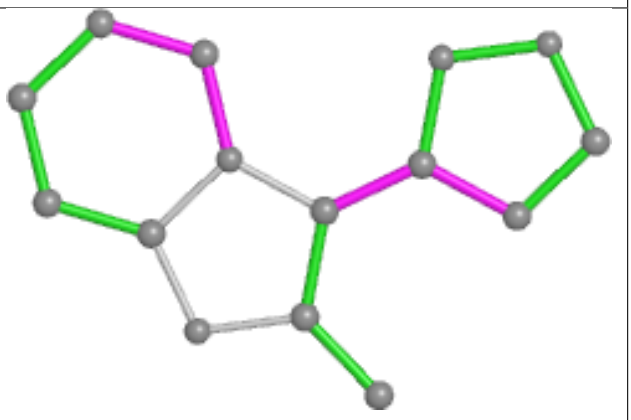
Bond lengths | **Bond angles**

Torsions | **Rings**

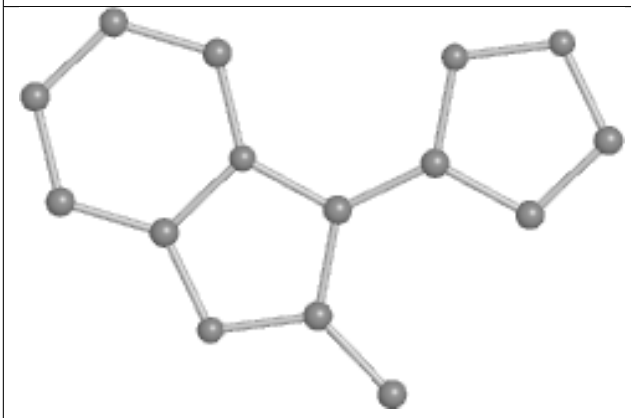
Ligand 9TI BBB 201



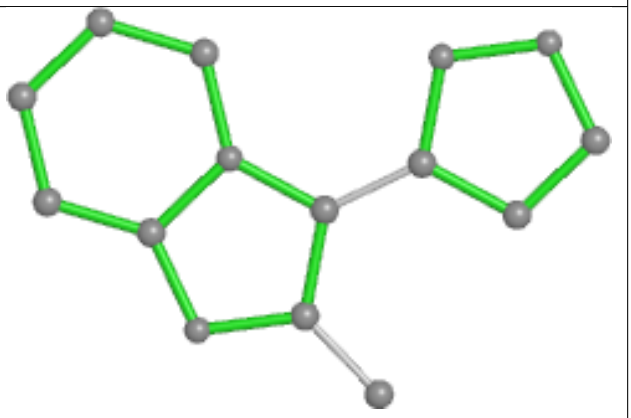
Bond lengths



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	AAA	150/150 (100%)	0.01	3 (2%) 65 64	15, 28, 51, 88	0
1	BBB	149/150 (99%)	0.09	2 (1%) 77 78	20, 31, 52, 77	0
2	CCC	5/13 (38%)	0.08	0 100 100	23, 34, 45, 62	0
2	DDD	4/13 (30%)	1.82	2 (50%) 0 0	54, 54, 72, 81	0
All	All	308/326 (94%)	0.08	7 (2%) 60 59	15, 30, 54, 88	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	1	MET	4.3
1	AAA	2	SER	3.1
1	BBB	39	SER	2.3
2	DDD	1	SER	2.3
2	DDD	3	THR	2.3

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, 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	CMT	DDD	6	8/8	0.80	0.19	39,58,65,82	0
2	CMT	CCC	101	8/8	0.98	0.08	23,24,27,27	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

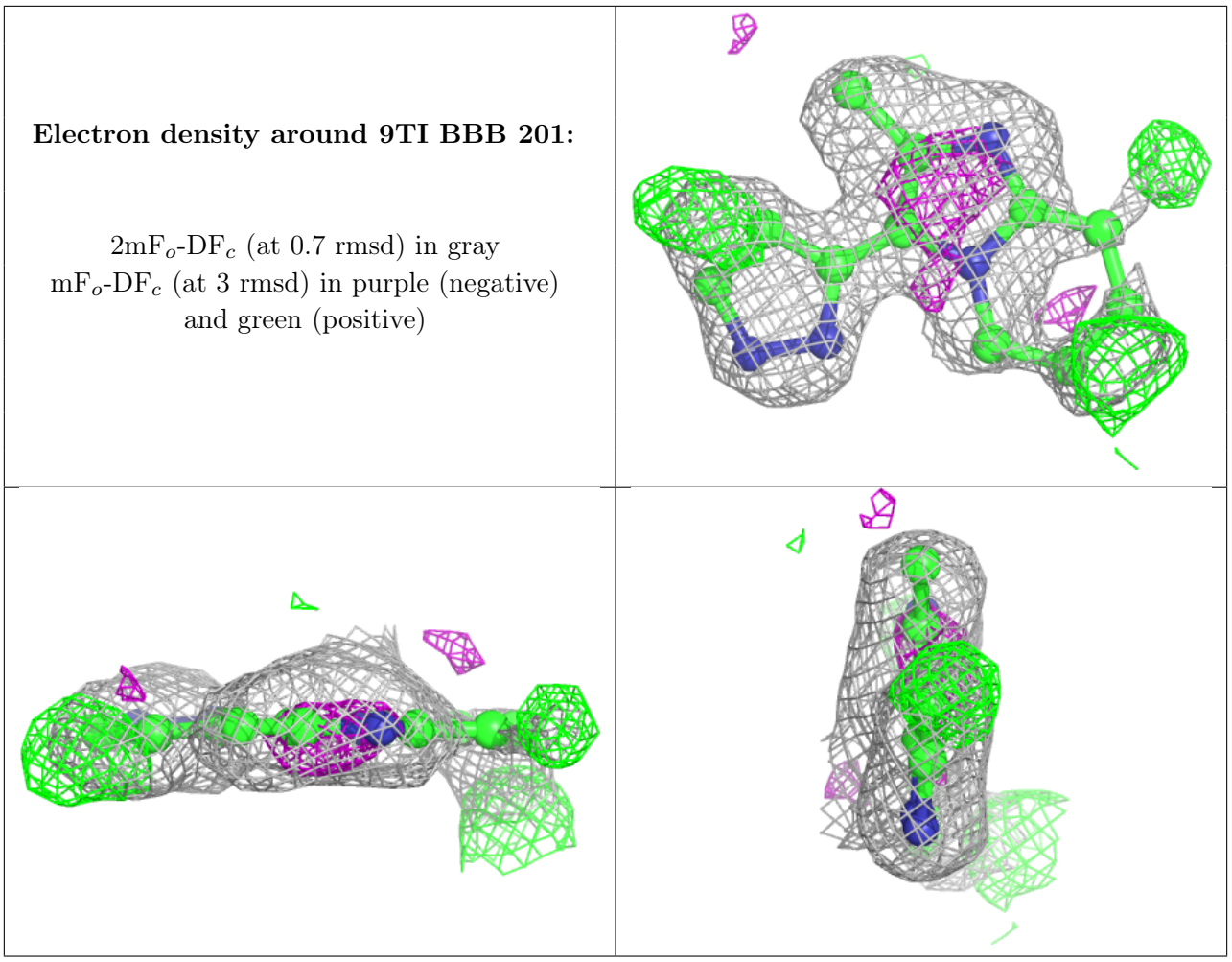
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	EDO	AAA	204	4/4	0.65	0.22	47,48,53,53	0
5	EDO	BBB	205	4/4	0.76	0.13	64,65,66,67	0
5	EDO	BBB	203	4/4	0.77	0.17	43,45,45,48	0
5	EDO	AAA	205	4/4	0.77	0.26	70,70,74,81	0
3	9TI	BBB	201	15/15	0.82	0.22	19,23,28,28	15
5	EDO	BBB	206	4/4	0.82	0.18	53,53,59,62	0
7	FAR	DDD	101	15/15	0.83	0.15	36,42,47,48	0
3	9TI	AAA	203	15/15	0.86	0.14	21,24,28,28	0
4	SO4	BBB	202	5/5	0.87	0.12	43,50,56,61	5
5	EDO	AAA	206	4/4	0.89	0.20	50,51,55,58	0
7	FAR	AAA	202	15/15	0.90	0.12	25,28,32,32	0
5	EDO	BBB	204	4/4	0.90	0.10	50,58,61,61	0
6	DMS	AAA	201	4/4	0.91	0.18	53,58,58,61	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.

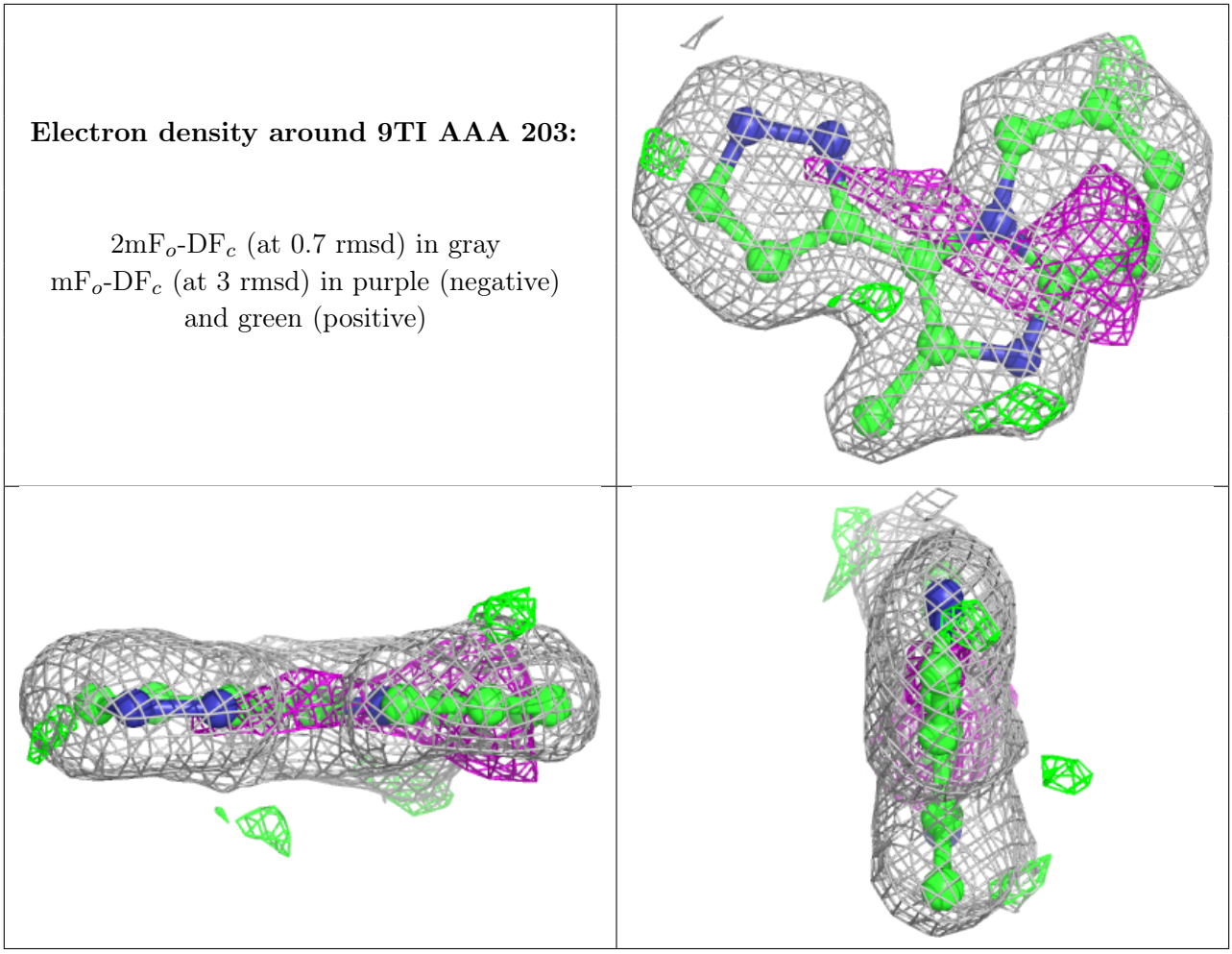
Electron density around 9TI BBB 201:

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



Electron density around 9TI AAA 203:

$2mF_o$-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.