



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2022 – 05:16 pm BST

PDB ID : 7PI1  
Title : Bacillus subtilis PabB  
Authors : Rooms, L.D.; Race, P.R.  
Deposited on : 2021-08-19  
Resolution : 1.73 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.30  
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) : 2.30

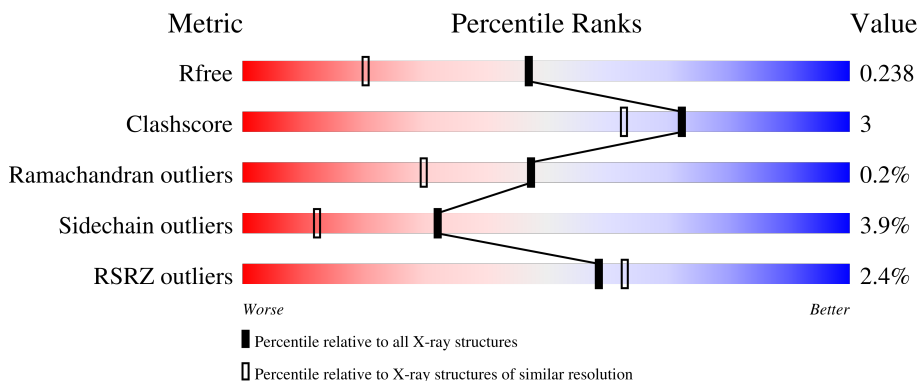
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.73 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	489	 83% 9% 7%
1	BBB	489	 84% 9% 7%
1	CCC	489	 84% 9% • 6%
1	DDD	489	 85% 7% • 6%

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 30347 atoms, of which 14479 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 Aminodeoxychorismate synthase component 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	456	7281	2333	3617	623	697	11	176	2	0
1	BBB	456	7215	2317	3571	616	700	11	171	1	0
1	CCC	458	7297	2339	3618	627	701	12	174	2	0
1	DDD	459	7318	2348	3625	627	706	12	176	3	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-18	MET	-	initiating methionine	UNP P28820
AAA	-17	ALA	-	expression tag	UNP P28820
AAA	-16	HIS	-	expression tag	UNP P28820
AAA	-15	HIS	-	expression tag	UNP P28820
AAA	-14	HIS	-	expression tag	UNP P28820
AAA	-13	HIS	-	expression tag	UNP P28820
AAA	-12	HIS	-	expression tag	UNP P28820
AAA	-11	HIS	-	expression tag	UNP P28820
AAA	-10	SER	-	expression tag	UNP P28820
AAA	-9	SER	-	expression tag	UNP P28820
AAA	-8	GLY	-	expression tag	UNP P28820
AAA	-7	LEU	-	expression tag	UNP P28820
AAA	-6	GLU	-	expression tag	UNP P28820
AAA	-5	VAL	-	expression tag	UNP P28820
AAA	-4	LEU	-	expression tag	UNP P28820
AAA	-3	PHE	-	expression tag	UNP P28820
AAA	-2	GLN	-	expression tag	UNP P28820
AAA	-1	GLY	-	expression tag	UNP P28820
AAA	0	PRO	-	expression tag	UNP P28820
BBB	-18	MET	-	initiating methionine	UNP P28820
BBB	-17	ALA	-	expression tag	UNP P28820

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-16	HIS	-	expression tag	UNP P28820
BBB	-15	HIS	-	expression tag	UNP P28820
BBB	-14	HIS	-	expression tag	UNP P28820
BBB	-13	HIS	-	expression tag	UNP P28820
BBB	-12	HIS	-	expression tag	UNP P28820
BBB	-11	HIS	-	expression tag	UNP P28820
BBB	-10	SER	-	expression tag	UNP P28820
BBB	-9	SER	-	expression tag	UNP P28820
BBB	-8	GLY	-	expression tag	UNP P28820
BBB	-7	LEU	-	expression tag	UNP P28820
BBB	-6	GLU	-	expression tag	UNP P28820
BBB	-5	VAL	-	expression tag	UNP P28820
BBB	-4	LEU	-	expression tag	UNP P28820
BBB	-3	PHE	-	expression tag	UNP P28820
BBB	-2	GLN	-	expression tag	UNP P28820
BBB	-1	GLY	-	expression tag	UNP P28820
BBB	0	PRO	-	expression tag	UNP P28820
CCC	-18	MET	-	initiating methionine	UNP P28820
CCC	-17	ALA	-	expression tag	UNP P28820
CCC	-16	HIS	-	expression tag	UNP P28820
CCC	-15	HIS	-	expression tag	UNP P28820
CCC	-14	HIS	-	expression tag	UNP P28820
CCC	-13	HIS	-	expression tag	UNP P28820
CCC	-12	HIS	-	expression tag	UNP P28820
CCC	-11	HIS	-	expression tag	UNP P28820
CCC	-10	SER	-	expression tag	UNP P28820
CCC	-9	SER	-	expression tag	UNP P28820
CCC	-8	GLY	-	expression tag	UNP P28820
CCC	-7	LEU	-	expression tag	UNP P28820
CCC	-6	GLU	-	expression tag	UNP P28820
CCC	-5	VAL	-	expression tag	UNP P28820
CCC	-4	LEU	-	expression tag	UNP P28820
CCC	-3	PHE	-	expression tag	UNP P28820
CCC	-2	GLN	-	expression tag	UNP P28820
CCC	-1	GLY	-	expression tag	UNP P28820
CCC	0	PRO	-	expression tag	UNP P28820
DDD	-18	MET	-	initiating methionine	UNP P28820
DDD	-17	ALA	-	expression tag	UNP P28820
DDD	-16	HIS	-	expression tag	UNP P28820
DDD	-15	HIS	-	expression tag	UNP P28820
DDD	-14	HIS	-	expression tag	UNP P28820
DDD	-13	HIS	-	expression tag	UNP P28820

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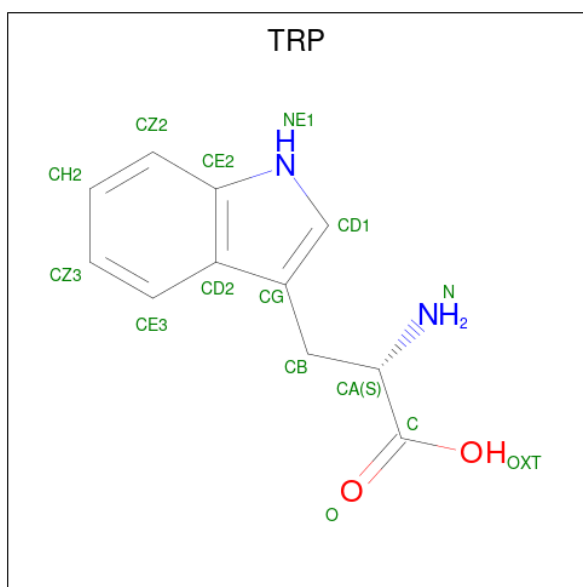
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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	-12	HIS	-	expression tag	UNP P28820
DDD	-11	HIS	-	expression tag	UNP P28820
DDD	-10	SER	-	expression tag	UNP P28820
DDD	-9	SER	-	expression tag	UNP P28820
DDD	-8	GLY	-	expression tag	UNP P28820
DDD	-7	LEU	-	expression tag	UNP P28820
DDD	-6	GLU	-	expression tag	UNP P28820
DDD	-5	VAL	-	expression tag	UNP P28820
DDD	-4	LEU	-	expression tag	UNP P28820
DDD	-3	PHE	-	expression tag	UNP P28820
DDD	-2	GLN	-	expression tag	UNP P28820
DDD	-1	GLY	-	expression tag	UNP P28820
DDD	0	PRO	-	expression tag	UNP P28820

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total Mg 1 1	0	0
2	BBB	1	Total Mg 1 1	0	0
2	CCC	1	Total Mg 1 1	0	0
2	DDD	1	Total Mg 1 1	0	0

- Molecule 3 is TRYPTOPHAN (three-letter code: TRP) (formula: C<sub>11</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
3	AAA	1	Total	C	H	N	O	0	0
			27	11	12	2	2		
3	BBB	1	Total	C	H	N	O	0	0
			27	11	12	2	2		
3	CCC	1	Total	C	H	N	O	0	0
			27	11	12	2	2		
3	DDD	1	Total	C	H	N	O	0	0
			27	11	12	2	2		

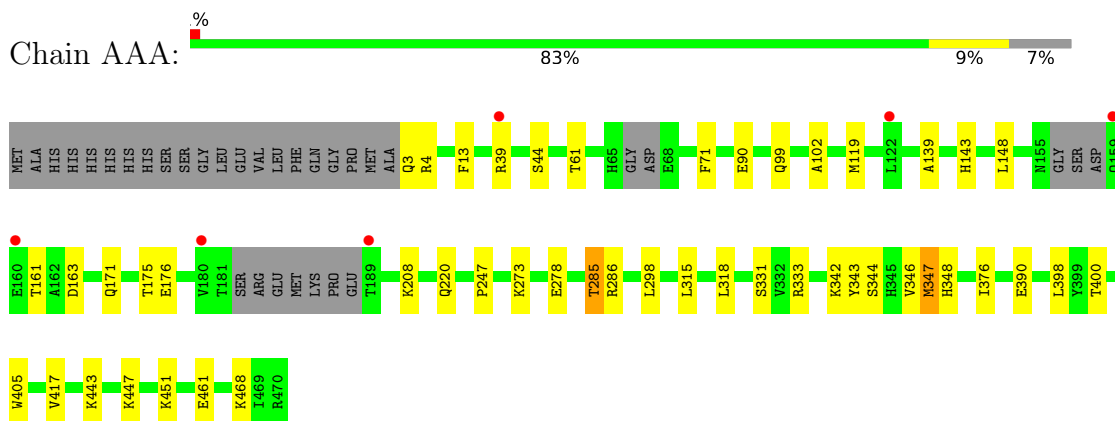
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	281	Total	O	0	0
			281	281		
4	BBB	352	Total	O	0	0
			352	352		
4	CCC	204	Total	O	0	0
			204	204		
4	DDD	287	Total	O	0	0
			287	287		

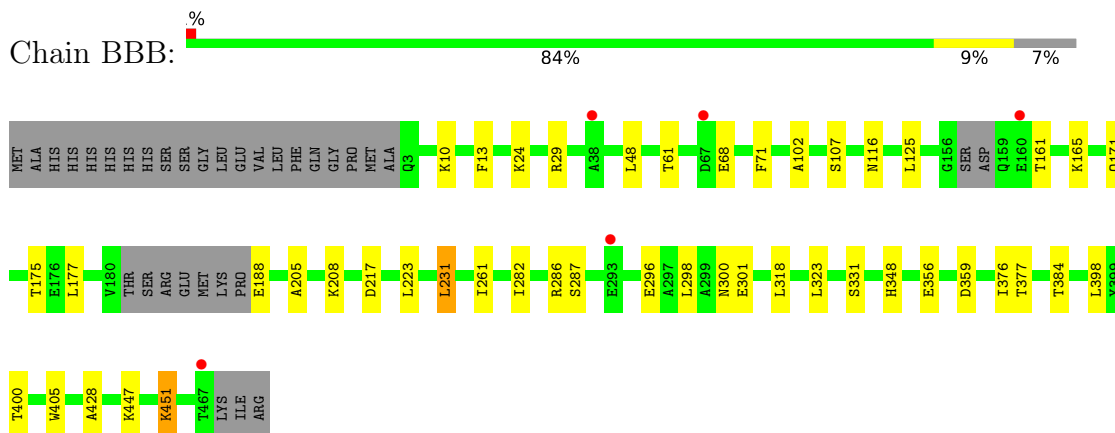
### 3 Residue-property plots [i](#)

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.

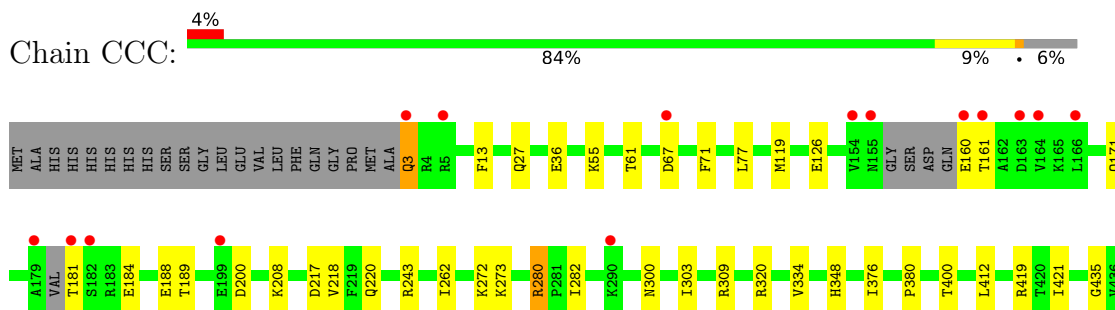
- Molecule 1: Aminodeoxychorismate synthase component 1

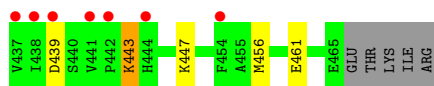


- Molecule 1: Aminodeoxychorismate synthase component 1

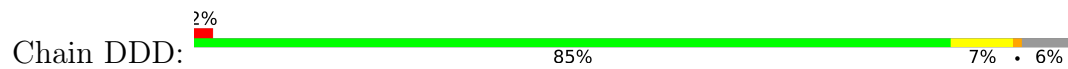


- Molecule 1: Aminodeoxychorismate synthase component 1





- Molecule 1: Aminodeoxychorismate synthase component 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.08Å 170.70Å 224.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.83 – 1.73 50.77 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.83-1.73) 99.9 (50.77-1.73)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.199 , 0.236 0.205 , 0.238	Depositor DCC
$R_{free}$ test set	10342 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.0	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	30347	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.64	0/3749	0.80	0/5061
1	BBB	0.66	0/3727	0.80	0/5035
1	CCC	0.64	0/3767	0.79	0/5087
1	DDD	0.66	0/3784	0.85	3/5110 (0.1%)
All	All	0.65	0/15027	0.81	3/20293 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	187	PRO	N-CA-CB	-14.10	86.38	103.30
1	DDD	187	PRO	N-CA-C	7.94	132.73	112.10
1	DDD	187	PRO	CB-CA-C	-6.78	95.05	112.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	3664	3617	3600	27	0
1	BBB	3644	3571	3552	22	0
1	CCC	3679	3618	3601	25	0
1	DDD	3693	3625	3609	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
2	CCC	1	0	0	0	0
2	DDD	1	0	0	0	0
3	AAA	15	12	9	0	0
3	BBB	15	12	9	0	0
3	CCC	15	12	9	0	0
3	DDD	15	12	9	0	0
4	AAA	281	0	0	4	0
4	BBB	352	0	0	2	1
4	CCC	204	0	0	2	0
4	DDD	287	0	0	6	0
All	All	15868	14479	14398	99	1

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 (99) 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:DDD:186:LYS:HD3	1:DDD:186:LYS:H	1.38	0.88
1:DDD:186:LYS:HD3	1:DDD:186:LYS:N	1.94	0.78
1:CCC:27:GLN:HE22	1:CCC:181:THR:HA	1.56	0.70
1:CCC:320:ARG:HD3	1:CCC:334:VAL:HG23	1.76	0.66
1:BBB:286:ARG:NH1	1:BBB:301:GLU:OE2	2.33	0.62
1:AAA:171:GLN:HG2	4:AAA:863:HOH:O	2.01	0.60
1:AAA:39:ARG:HG2	1:AAA:344:SER:HB3	1.82	0.60
1:BBB:331:SER:HB2	1:BBB:356:GLU:HG2	1.83	0.59
1:BBB:376:ILE:HD13	1:BBB:400:THR:HB	1.85	0.58
1:AAA:39:ARG:HB2	1:AAA:247:PRO:HB2	1.85	0.58
1:AAA:220:GLN:HE22	1:AAA:315:LEU:HD11	1.69	0.58
1:DDD:376:ILE:HD13	1:DDD:400:THR:HB	1.86	0.58
1:AAA:171:GLN:O	1:AAA:175:THR:HG23	2.05	0.57
1:AAA:285:THR:HB	1:AAA:348:HIS:CD2	2.40	0.57
1:BBB:116:ASN:OD1	4:BBB:601:HOH:O	2.18	0.56
1:DDD:243:ARG:HD2	4:DDD:707:HOH:O	2.05	0.56
1:CCC:188:GLU:O	1:CCC:189:THR:HG22	2.06	0.56
1:DDD:4:ARG:HA	1:DDD:154:VAL:O	2.06	0.55
1:CCC:303:ILE:O	1:CCC:309:ARG:NH1	2.38	0.55
1:CCC:439:ASP:OD1	1:CCC:439:ASP:N	2.23	0.54
1:DDD:154:VAL:HG11	1:DDD:162:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:231:LEU:CD1	1:BBB:428:ALA:HB2	2.38	0.53
1:DDD:292:ASN:O	1:DDD:296:GLU:HG2	2.08	0.53
1:AAA:398:LEU:HG	1:AAA:417:VAL:HG11	1.91	0.53
1:CCC:3:GLN:HA	1:CCC:3:GLN:HE21	1.73	0.53
1:BBB:231:LEU:HD13	1:BBB:428:ALA:HB2	1.92	0.51
1:AAA:376:ILE:HD13	1:AAA:400:THR:HB	1.92	0.51
1:AAA:44:SER:OG	1:AAA:143:HIS:HE1	1.93	0.51
1:AAA:331:SER:O	1:AAA:333:ARG:NH1	2.43	0.51
1:BBB:282:ILE:HG23	1:BBB:348:HIS:HB3	1.93	0.49
1:AAA:344:SER:HB2	4:AAA:845:HOH:O	2.13	0.49
1:AAA:343:TYR:OH	1:AAA:348:HIS:CE1	2.66	0.49
1:BBB:287:SER:OG	1:BBB:451:LYS:HE3	2.12	0.49
1:CCC:218:VAL:HA	1:CCC:380:PRO:HD2	1.94	0.49
1:DDD:29:ARG:HG2	1:DDD:48:LEU:O	2.13	0.49
1:CCC:3:GLN:HE21	1:CCC:3:GLN:CA	2.26	0.49
1:BBB:125:LEU:HD12	4:BBB:686:HOH:O	2.14	0.48
1:AAA:443:LYS:HD2	4:AAA:779:HOH:O	2.12	0.48
1:BBB:171:GLN:O	1:BBB:175:THR:HG23	2.12	0.48
1:CCC:320:ARG:HD3	1:CCC:334:VAL:CG2	2.43	0.47
1:BBB:61:THR:O	1:BBB:71:PHE:HA	2.15	0.47
1:CCC:272:LYS:HB3	1:CCC:412:LEU:HG	1.96	0.47
1:DDD:284:GLY:O	1:DDD:348:HIS:HA	2.15	0.47
1:CCC:443:LYS:O	1:CCC:447:LYS:HG2	2.15	0.46
1:AAA:39:ARG:HG3	1:AAA:343:TYR:HB2	1.96	0.46
1:DDD:186:LYS:N	1:DDD:186:LYS:CD	2.72	0.46
1:AAA:342:LYS:HG2	1:AAA:347:MET:HG3	1.97	0.46
1:DDD:240:LYS:HG2	1:DDD:243:ARG:NH2	2.30	0.46
1:AAA:102:ALA:O	1:AAA:405:TRP:HA	2.16	0.46
1:CCC:282:ILE:HG23	1:CCC:348:HIS:HB3	1.98	0.45
1:CCC:36:GLU:OE2	1:CCC:243:ARG:HD2	2.16	0.45
1:AAA:461:GLU:OE2	1:DDD:64:LYS:NZ	2.49	0.45
1:AAA:318:LEU:C	1:AAA:318:LEU:HD23	2.36	0.45
1:BBB:323:LEU:HD12	1:BBB:323:LEU:HA	1.87	0.45
1:CCC:412:LEU:HD12	1:CCC:412:LEU:C	2.36	0.45
1:DDD:158:ASP:O	1:DDD:161:THR:HG22	2.16	0.45
1:DDD:280:ARG:NH2	4:DDD:614:HOH:O	2.50	0.44
1:CCC:3:GLN:HA	1:CCC:3:GLN:NE2	2.32	0.44
1:DDD:188:GLU:HB2	1:DDD:189:THR:H	1.61	0.44
1:CCC:61:THR:O	1:CCC:71:PHE:HA	2.16	0.44
1:AAA:286:ARG:HD3	1:AAA:298:LEU:HB3	1.99	0.44
1:DDD:39:ARG:C	1:DDD:40:GLY:O	2.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:318:LEU:HD23	1:AAA:318:LEU:O	2.18	0.44
1:CCC:262:ILE:HB	1:CCC:421:ILE:HB	1.99	0.44
1:CCC:280[A]:ARG:HB3	4:CCC:712:HOH:O	2.17	0.43
1:CCC:376:ILE:HD13	1:CCC:400:THR:HB	1.99	0.43
1:BBB:376:ILE:CD1	1:BBB:400:THR:HB	2.49	0.43
1:DDD:273:LYS:HE3	4:DDD:712:HOH:O	2.17	0.43
1:AAA:3:GLN:HA	1:AAA:3:GLN:OE1	2.19	0.43
1:DDD:302:LEU:HD22	1:DDD:349:ILE:HD11	2.00	0.43
1:AAA:343:TYR:OH	1:AAA:348:HIS:HE1	2.02	0.43
1:BBB:24:LYS:HB3	1:BBB:177:LEU:HD12	2.01	0.43
1:DDD:36:GLU:OE2	1:DDD:243:ARG:HD2	2.18	0.43
1:DDD:282:ILE:HG23	1:DDD:348:HIS:HB3	2.00	0.42
1:CCC:55:LYS:NZ	4:CCC:623:HOH:O	2.52	0.42
1:BBB:286:ARG:HH11	1:BBB:301:GLU:HG3	1.85	0.42
1:DDD:264:GLY:HA3	4:DDD:611:HOH:O	2.19	0.42
1:AAA:139:ALA:HB1	1:AAA:148:LEU:HD11	2.01	0.42
1:DDD:282:ILE:HG12	1:DDD:350:VAL:HG22	2.01	0.42
1:AAA:447:LYS:O	1:AAA:451:LYS:HG2	2.19	0.42
1:AAA:61:THR:O	1:AAA:71:PHE:HA	2.20	0.42
1:BBB:231:LEU:HD12	1:BBB:231:LEU:HA	1.86	0.42
1:CCC:27:GLN:NE2	1:CCC:181:THR:HA	2.29	0.42
1:CCC:220:GLN:HE21	1:CCC:435:GLY:HA3	1.85	0.42
1:BBB:261:ILE:HG12	1:BBB:398:LEU:CD2	2.50	0.41
1:BBB:318:LEU:O	1:BBB:318:LEU:HD23	2.20	0.41
1:DDD:3:GLN:O	1:DDD:3:GLN:HG3	2.20	0.41
1:DDD:102:ALA:O	1:DDD:405:TRP:HA	2.20	0.41
1:AAA:220:GLN:NE2	1:AAA:315:LEU:HD11	2.34	0.41
1:BBB:205:ALA:HB3	1:BBB:223:LEU:HD21	2.03	0.41
1:CCC:419:ARG:HA	1:CCC:456:MET:SD	2.60	0.41
1:BBB:377:THR:C	1:BBB:384:THR:HG21	2.41	0.40
1:DDD:244:GLU:HG2	4:DDD:856:HOH:O	2.22	0.40
1:BBB:29:ARG:HG2	1:BBB:48:LEU:O	2.21	0.40
1:BBB:102:ALA:O	1:BBB:405:TRP:HA	2.22	0.40
1:CCC:443:LYS:N	1:CCC:443:LYS:HD2	2.37	0.40
1:AAA:344:SER:CB	4:AAA:845:HOH:O	2.68	0.40
1:CCC:77:LEU:HD12	1:CCC:77:LEU:HA	1.96	0.40
1:DDD:244:GLU:CG	4:DDD:859:HOH:O	2.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BBB:601:HOH:O	4:BBB:739:HOH:O[1_655]	2.03	0.17

### 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	450/489 (92%)	437 (97%)	13 (3%)	0	100	100
1	BBB	451/489 (92%)	440 (98%)	10 (2%)	1 (0%)	47	30
1	CCC	454/489 (93%)	435 (96%)	19 (4%)	0	100	100
1	DDD	456/489 (93%)	436 (96%)	17 (4%)	3 (1%)	22	8
All	All	1811/1956 (93%)	1748 (96%)	59 (3%)	4 (0%)	47	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	187	PRO
1	BBB	68	GLU
1	DDD	40	GLY
1	DDD	39	ARG

#### 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	395/420 (94%)	378 (96%)	17 (4%)	29	10
1	BBB	391/420 (93%)	376 (96%)	15 (4%)	33	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	CCC	396/420 (94%)	378 (96%)	18 (4%)	27 9
1	DDD	398/420 (95%)	384 (96%)	14 (4%)	36 16
All	All	1580/1680 (94%)	1516 (96%)	64 (4%)	32 11

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	4	ARG
1	AAA	13	PHE
1	AAA	90	GLU
1	AAA	99	GLN
1	AAA	119	MET
1	AAA	161	THR
1	AAA	163	ASP
1	AAA	176	GLU
1	AAA	208[A]	LYS
1	AAA	208[B]	LYS
1	AAA	273	LYS
1	AAA	278	GLU
1	AAA	285	THR
1	AAA	346	VAL
1	AAA	347	MET
1	AAA	390	GLU
1	AAA	468	LYS
1	BBB	10	LYS
1	BBB	13	PHE
1	BBB	107	SER
1	BBB	161	THR
1	BBB	165	LYS
1	BBB	188	GLU
1	BBB	208	LYS
1	BBB	217	ASP
1	BBB	231	LEU
1	BBB	296	GLU
1	BBB	298	LEU
1	BBB	300	ASN
1	BBB	359	ASP
1	BBB	447	LYS
1	BBB	451	LYS
1	CCC	3	GLN
1	CCC	13	PHE

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Mol	Chain	Res	Type
1	CCC	67	ASP
1	CCC	119	MET
1	CCC	126	GLU
1	CCC	160	GLU
1	CCC	161	THR
1	CCC	171	GLN
1	CCC	184	GLU
1	CCC	200	ASP
1	CCC	208	LYS
1	CCC	217	ASP
1	CCC	273	LYS
1	CCC	280[A]	ARG
1	CCC	280[B]	ARG
1	CCC	300	ASN
1	CCC	443	LYS
1	CCC	461	GLU
1	DDD	4	ARG
1	DDD	5	ARG
1	DDD	13	PHE
1	DDD	30	LYS
1	DDD	158	ASP
1	DDD	161	THR
1	DDD	185	MET
1	DDD	186	LYS
1	DDD	187	PRO
1	DDD	207	GLU
1	DDD	217	ASP
1	DDD	302	LEU
1	DDD	318	LEU
1	DDD	461	GLU

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
3	TRP	DDD	501	-	14,16,16	0.83	1 (7%)	16,22,22	1.11	2 (12%)
3	TRP	BBB	501	-	14,16,16	0.83	1 (7%)	16,22,22	0.86	0
3	TRP	CCC	501	-	14,16,16	0.80	1 (7%)	16,22,22	1.08	2 (12%)
3	TRP	AAA	502	-	14,16,16	0.88	1 (7%)	16,22,22	0.94	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
3	TRP	DDD	501	-	-	0/7/8/8	0/2/2/2
3	TRP	BBB	501	-	-	0/7/8/8	0/2/2/2
3	TRP	CCC	501	-	-	0/7/8/8	0/2/2/2
3	TRP	AAA	502	-	-	0/7/8/8	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	502	TRP	OXT-C	-2.23	1.23	1.30
3	DDD	501	TRP	OXT-C	-2.11	1.23	1.30
3	CCC	501	TRP	OXT-C	-2.04	1.23	1.30
3	BBB	501	TRP	OXT-C	-2.03	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	DDD	501	TRP	OXT-C-O	-2.45	118.53	124.09
3	CCC	501	TRP	OXT-C-O	-2.32	118.83	124.09
3	DDD	501	TRP	OXT-C-CA	2.24	121.03	113.38
3	CCC	501	TRP	OXT-C-CA	2.17	120.77	113.38

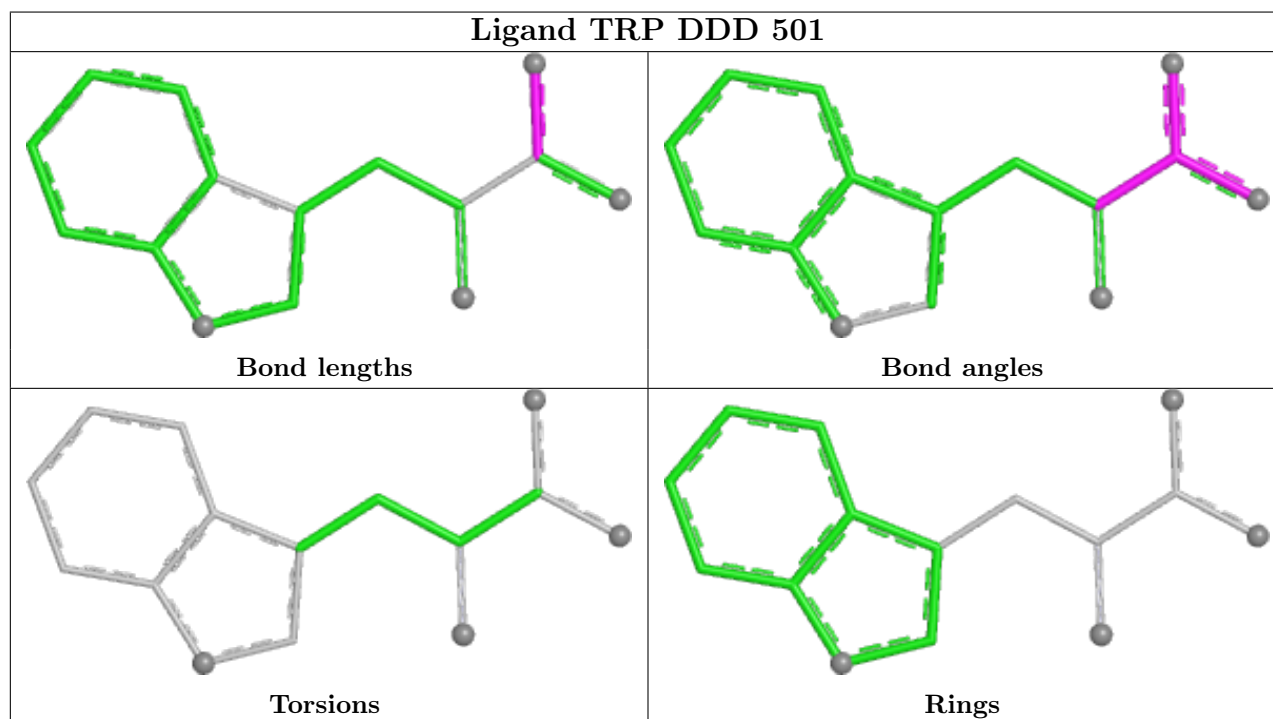
There are no chirality outliers.

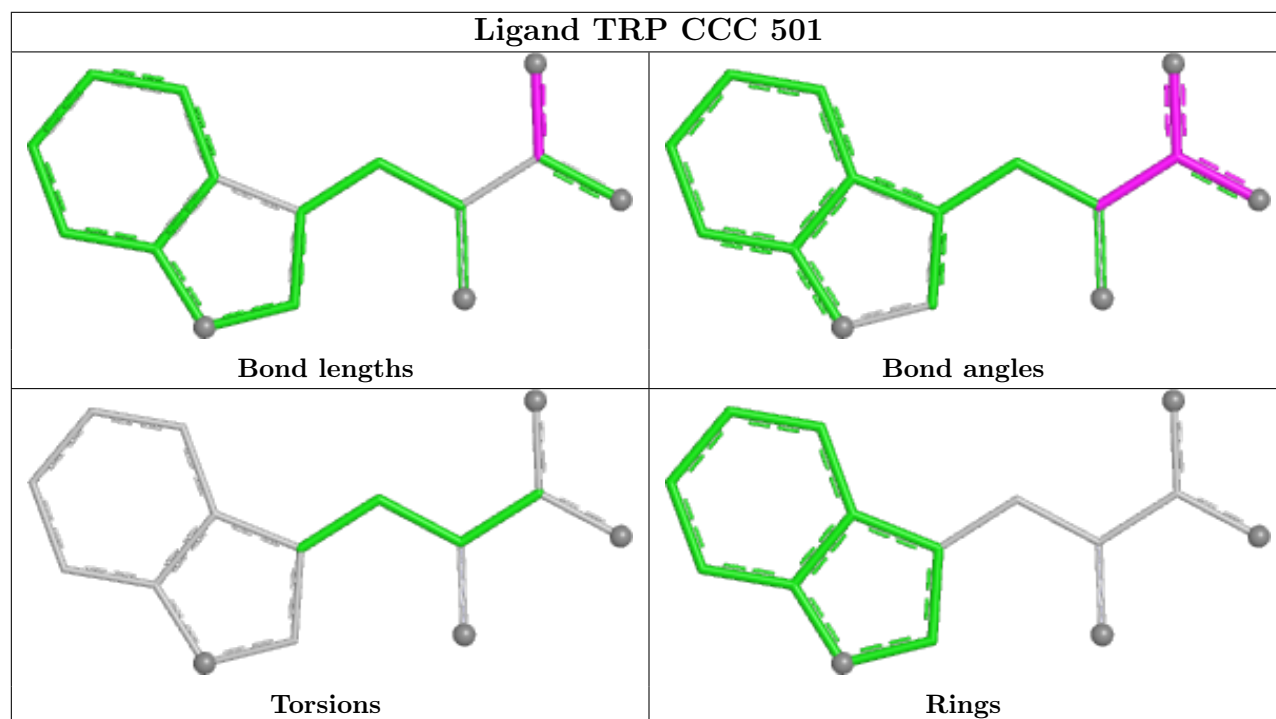
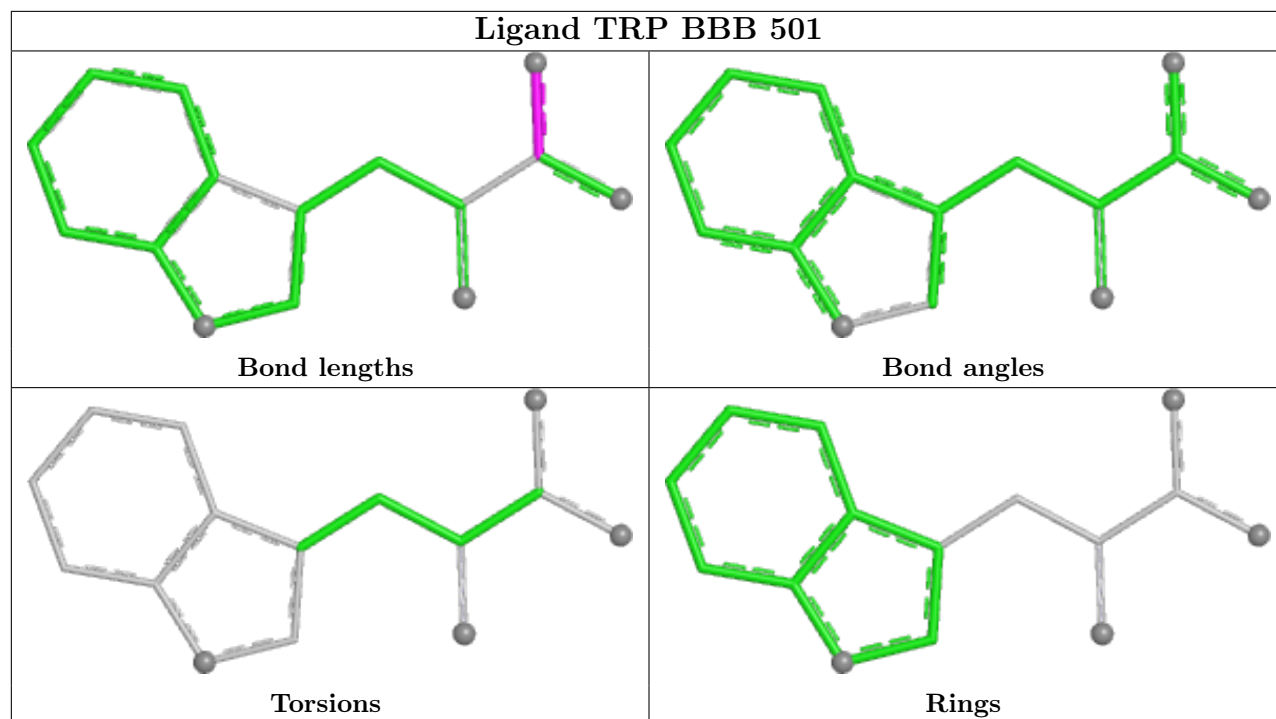
There are no torsion outliers.

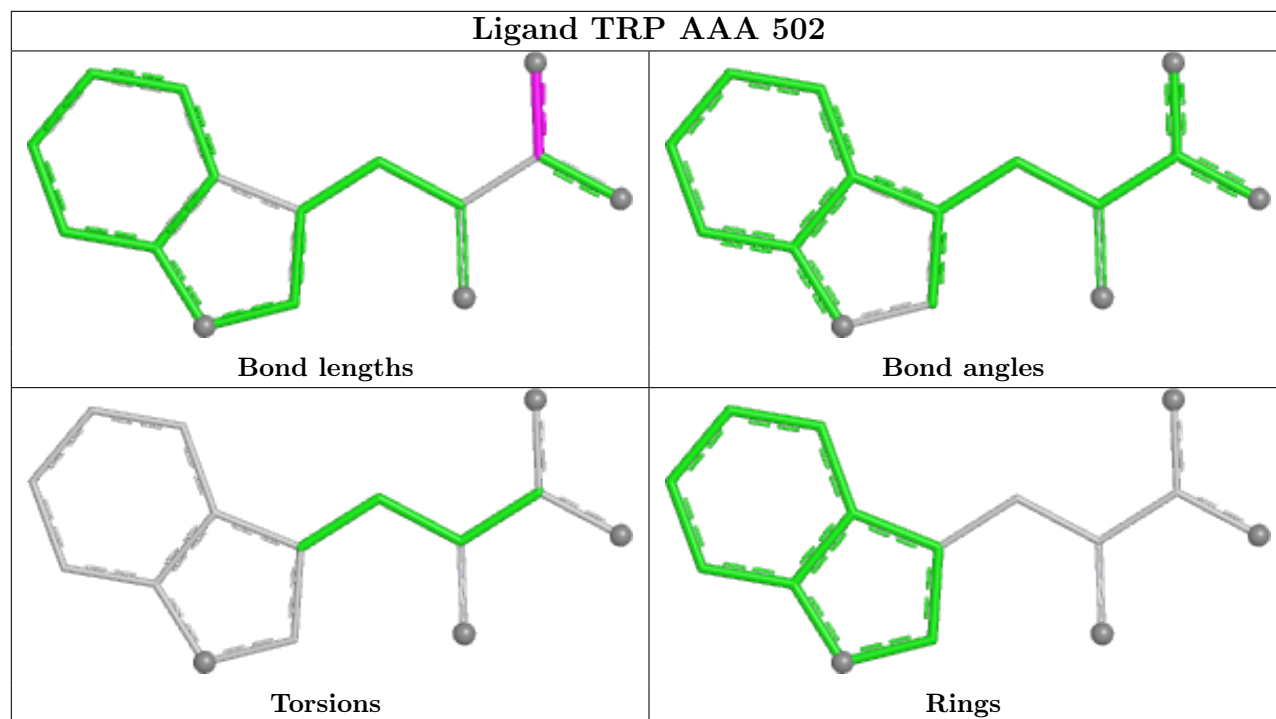
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AAA	456/489 (93%)	-0.05	6 (1%) 77 81	21, 33, 61, 114	0
1	BBB	456/489 (93%)	-0.13	5 (1%) 80 84	20, 31, 55, 80	0
1	CCC	458/489 (93%)	0.28	22 (4%) 30 34	24, 40, 73, 95	0
1	DDD	459/489 (93%)	0.07	10 (2%) 62 66	22, 34, 63, 115	0
All	All	1829/1956 (93%)	0.04	43 (2%) 59 63	20, 34, 64, 115	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	438	ILE	4.8
1	DDD	160	GLU	4.5
1	AAA	39	ARG	4.4
1	DDD	159	GLN	4.4
1	CCC	441	VAL	4.4
1	CCC	163	ASP	4.2
1	CCC	181	THR	3.9
1	DDD	154	VAL	3.8
1	CCC	160	GLU	3.7
1	CCC	454	PHE	3.7
1	CCC	161	THR	3.7
1	CCC	154	VAL	3.6
1	CCC	444	HIS	3.5
1	AAA	159	GLN	3.5
1	CCC	179	ALA	3.3
1	CCC	67	ASP	3.2
1	CCC	290	LYS	3.1
1	DDD	3	GLN	3.1
1	DDD	67	ASP	3.0
1	CCC	155	ASN	3.0
1	CCC	439	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	DDD	329	TYR	2.9
1	BBB	67	ASP	2.8
1	CCC	437	VAL	2.7
1	BBB	38	ALA	2.7
1	CCC	3	GLN	2.7
1	AAA	180	VAL	2.7
1	AAA	189	THR	2.7
1	DDD	185	MET	2.6
1	BBB	467	THR	2.6
1	AAA	122	LEU	2.5
1	AAA	160	GLU	2.5
1	DDD	333	ARG	2.5
1	BBB	160	GLU	2.5
1	CCC	182	SER	2.3
1	CCC	5	ARG	2.2
1	BBB	293	GLU	2.2
1	DDD	5	ARG	2.2
1	CCC	164	VAL	2.1
1	DDD	94	GLU	2.0
1	CCC	199	GLU	2.0
1	CCC	166	LEU	2.0
1	CCC	442	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 [\(i\)](#)

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<sup>th</sup> 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.

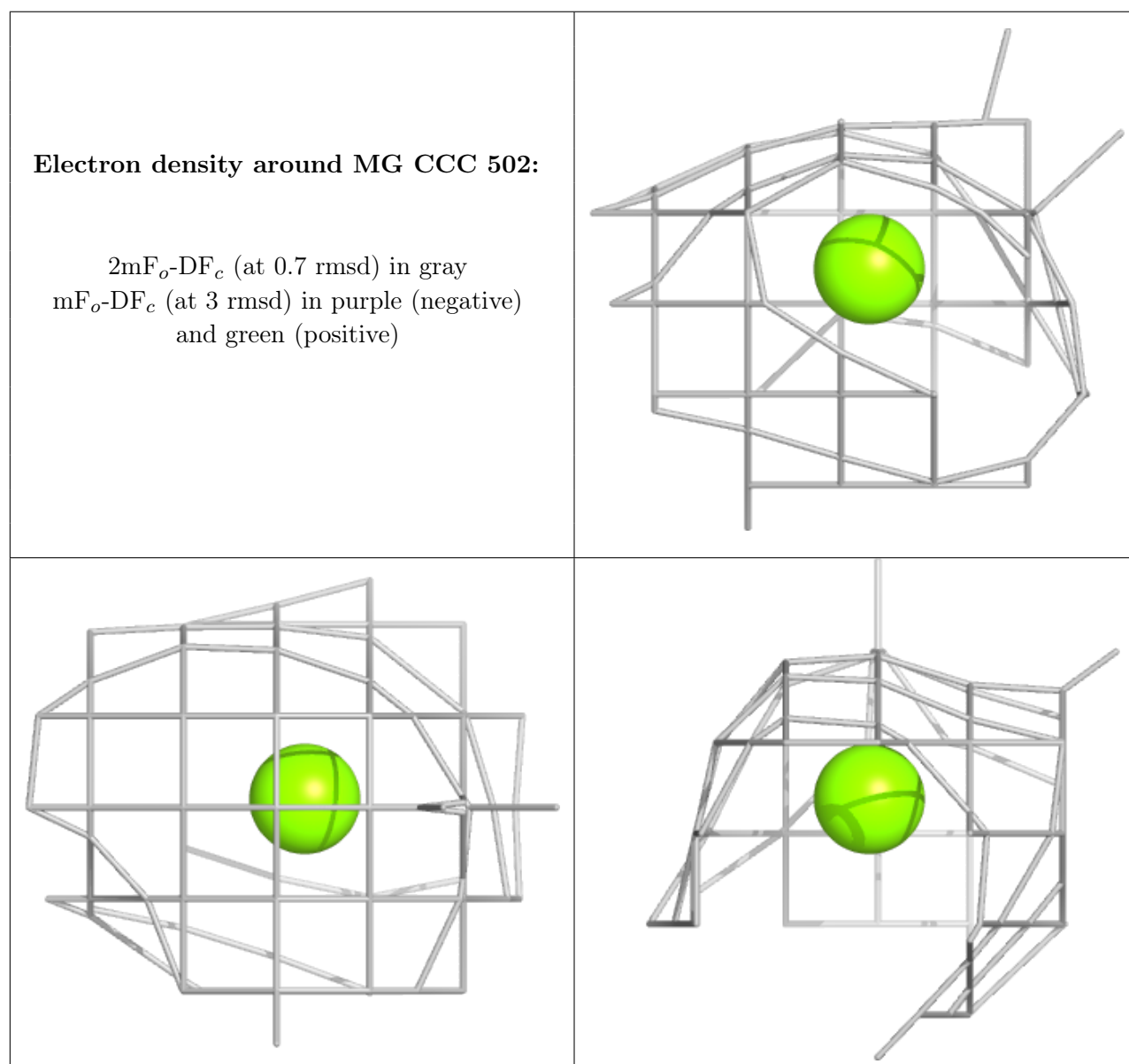
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	CCC	502	1/1	0.95	0.10	42,42,42,42	1

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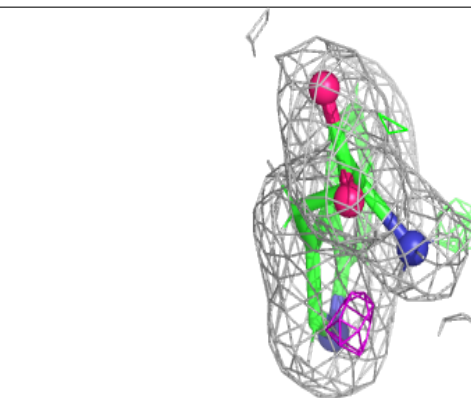
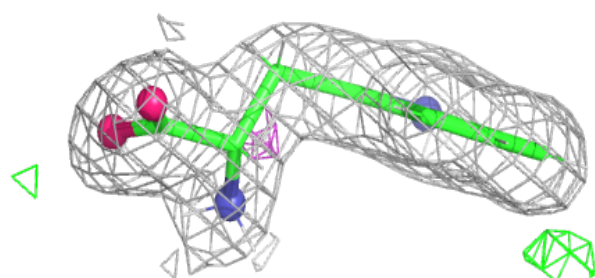
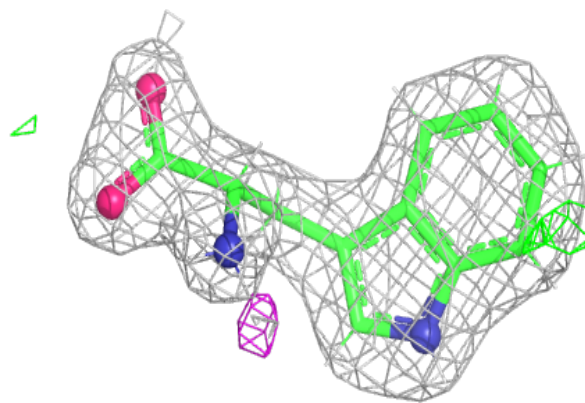
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	TRP	CCC	501	15/15	0.96	0.08	24,27,36,38	0
3	TRP	DDD	501	15/15	0.96	0.09	25,27,37,42	0
3	TRP	BBB	501	15/15	0.97	0.07	20,22,26,28	0
3	TRP	AAA	502	15/15	0.98	0.07	22,24,27,29	0
2	MG	AAA	501	1/1	0.98	0.06	54,54,54,54	0
2	MG	DDD	502	1/1	0.99	0.04	33,33,33,33	0
2	MG	BBB	502	1/1	1.00	0.03	37,37,37,37	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.

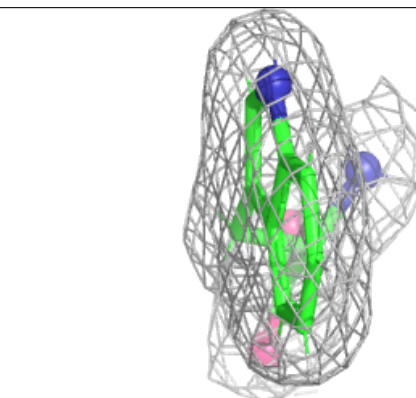
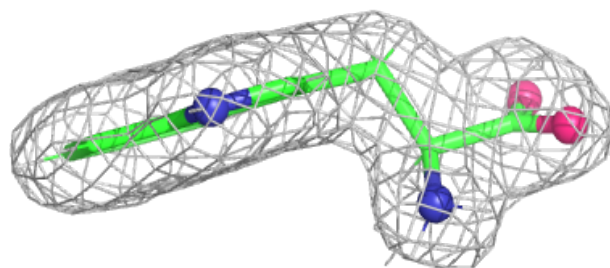
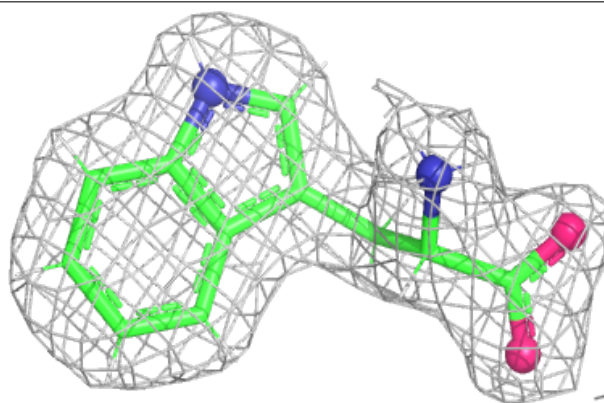


**Electron density around TRP CCC 501:**

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

**Electron density around TRP DDD 501:**

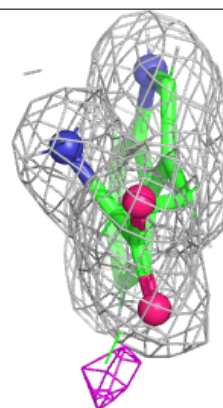
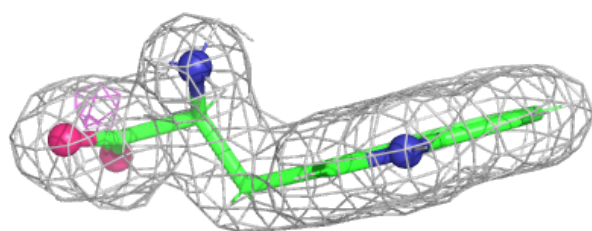
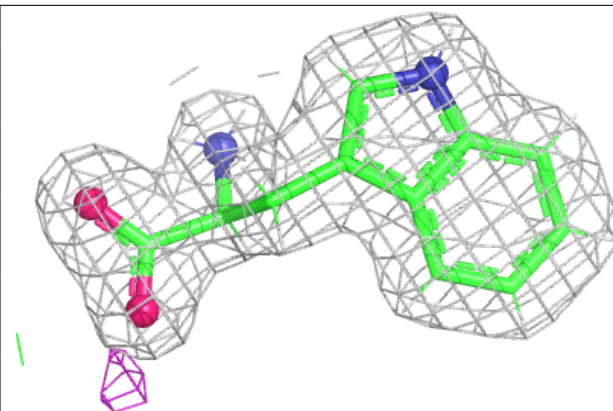
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



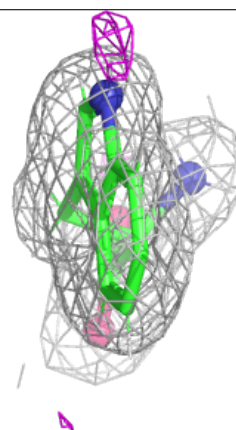
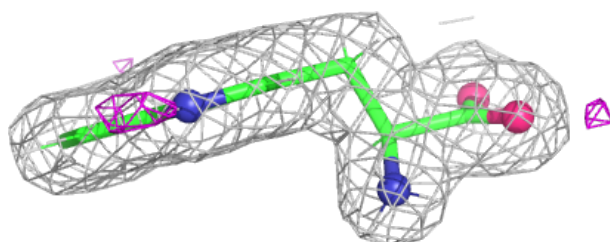
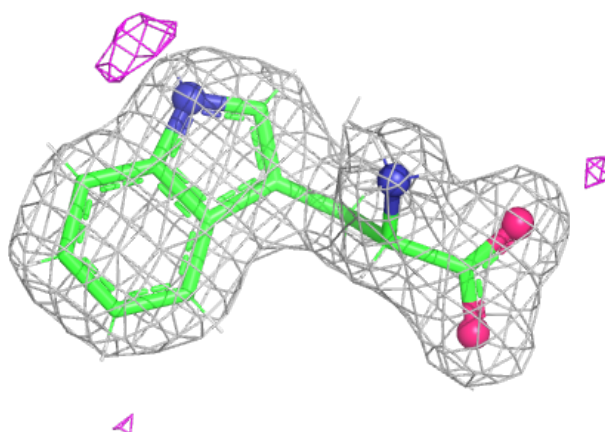


**Electron density around TRP BBB 501:**

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

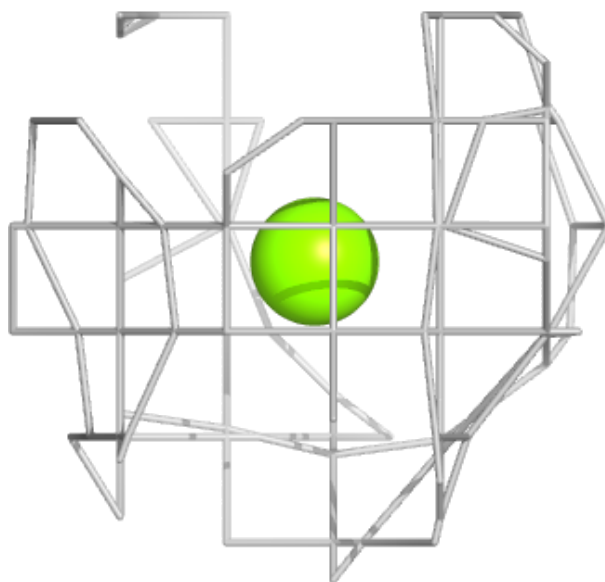
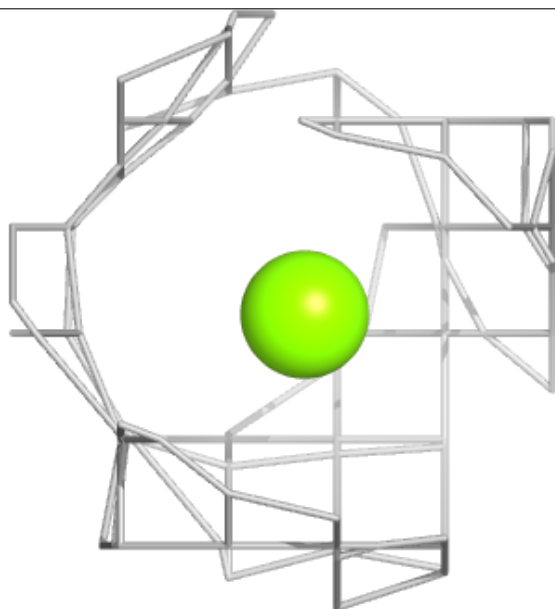
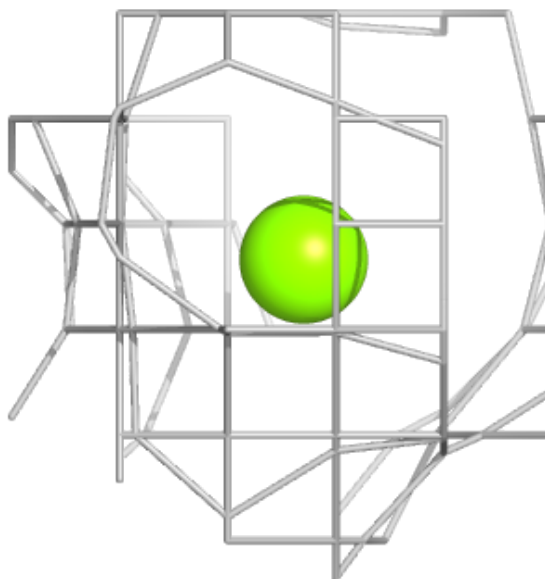
**Electron density around TRP AAA 502:**

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



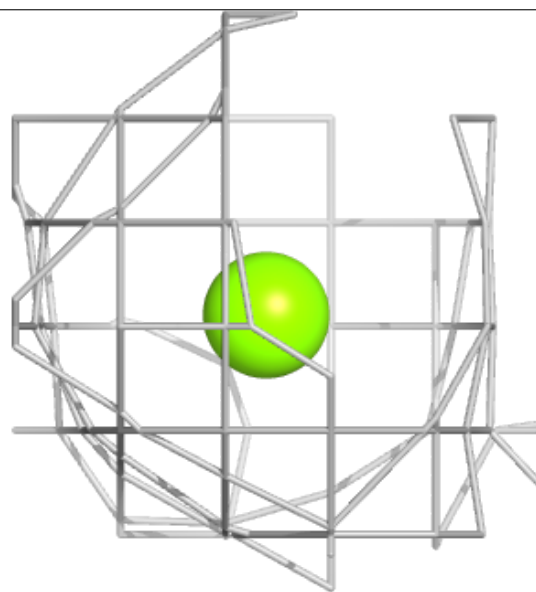
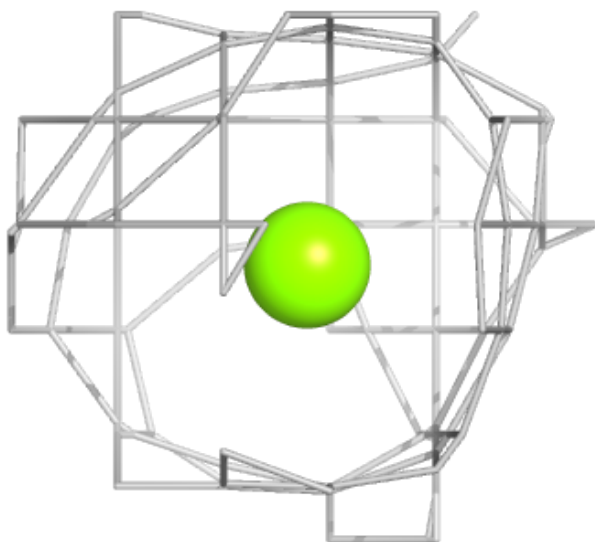
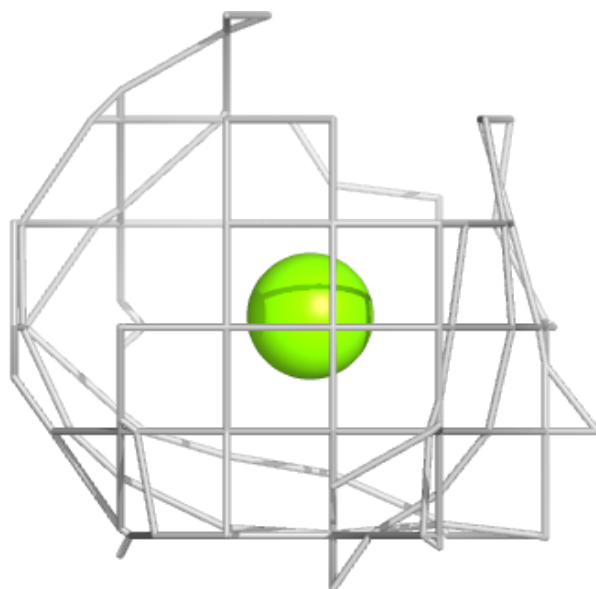
**Electron density around MG AAA 501:**

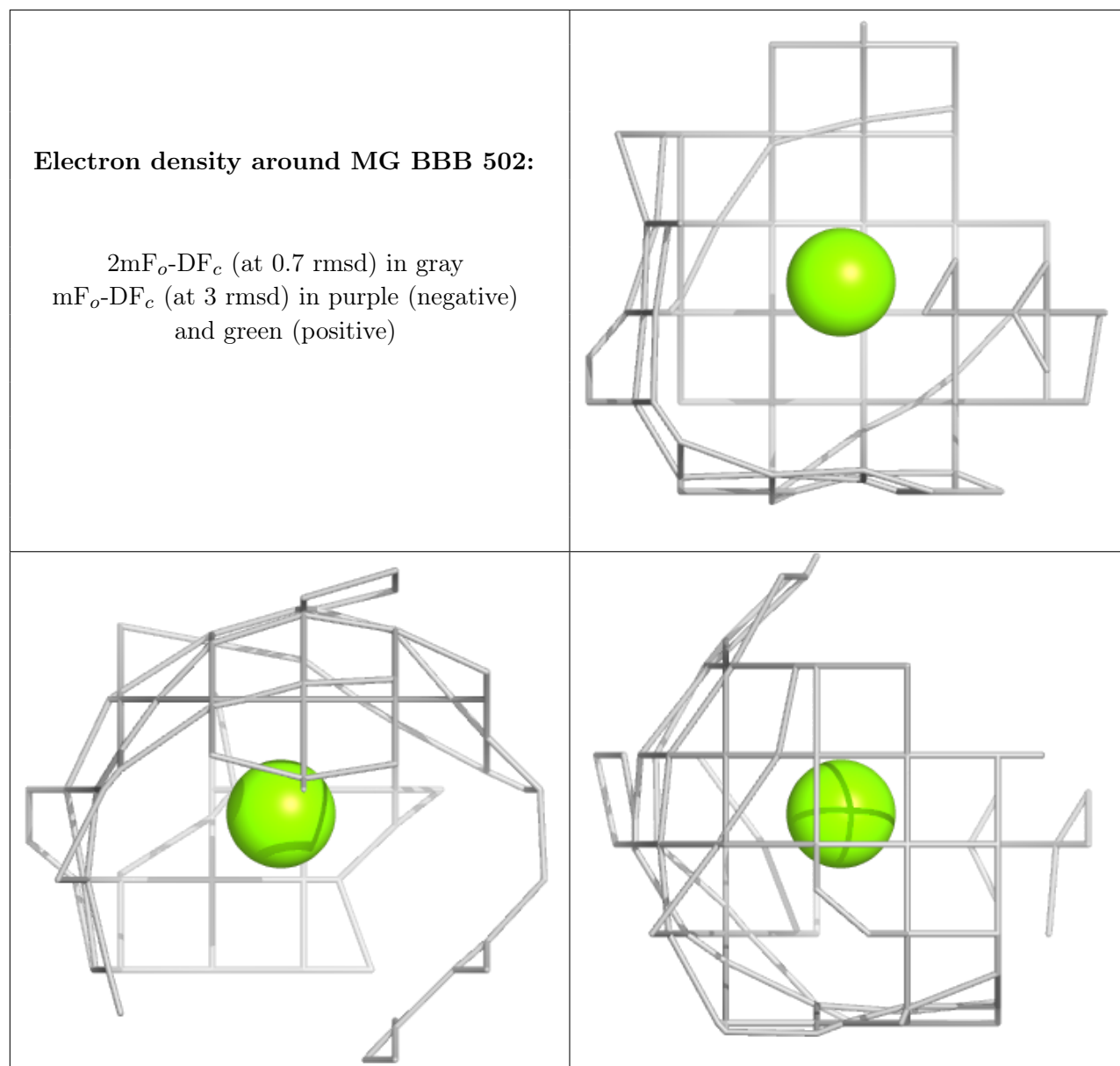
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MG DDD 502:**

$2mF_o-DF_c$  (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.