



# Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2022 – 03:37 pm BST

PDB ID : 7Q2N  
Title : Beta-lactoglobulin mutant FAF (I56F/L39A/M107F) in complex with desipramine (FAF-DSM)  
Authors : Loch, J.I.; Barciszewski, J.; Lewinski, K.  
Deposited on : 2021-10-25  
Resolution : 1.70 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.

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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 : 2.28.1  
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) : 2.28.1

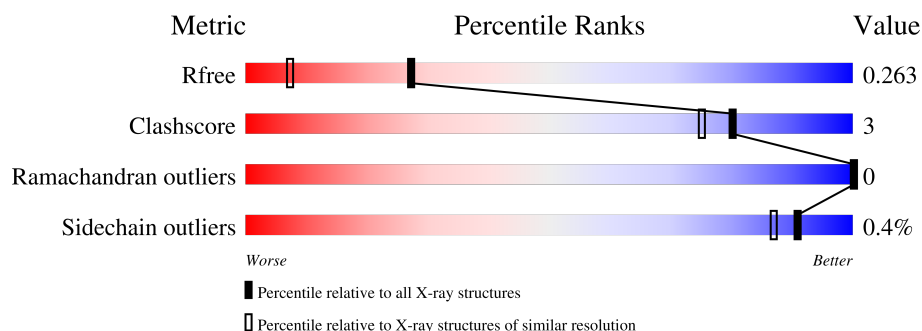
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	AAA	162	
1	BBB	162	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 2751 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.

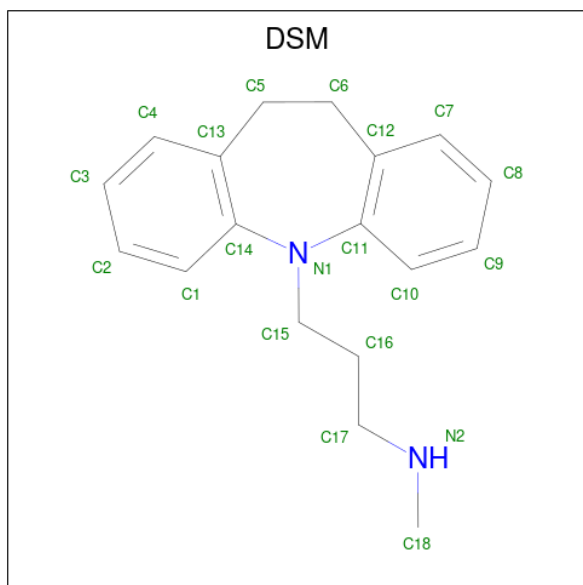
- Molecule 1 is a protein called Beta-lactoglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	158	Total	C	N	O	S	0	1	0
			1255	801	203	243	8			
1	BBB	157	Total	C	N	O	S	0	1	0
			1249	799	201	241	8			

There are 10 discrepancies between the modelled and reference sequences:

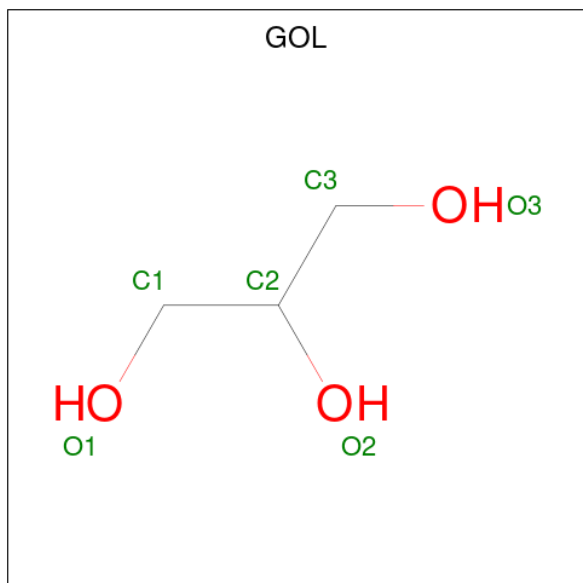
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	ALA	LEU	engineered mutation	UNP P02754
AAA	2	SER	ILE	engineered mutation	UNP P02754
AAA	39	ALA	LEU	engineered mutation	UNP P02754
AAA	56	PHE	ILE	engineered mutation	UNP P02754
AAA	107	PHE	MET	engineered mutation	UNP P02754
BBB	1	ALA	LEU	engineered mutation	UNP P02754
BBB	2	SER	ILE	engineered mutation	UNP P02754
BBB	39	ALA	LEU	engineered mutation	UNP P02754
BBB	56	PHE	ILE	engineered mutation	UNP P02754
BBB	107	PHE	MET	engineered mutation	UNP P02754

- Molecule 2 is 3-(10,11-DIHYDRO-5H-DIBENZO[B,F]AZEPIN-5-YL)-N-METHYLPROPA N-1-AMINE (three-letter code: DSM) (formula: C<sub>18</sub>H<sub>22</sub>N<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	N	0	0
			20	18	2		
2	AAA	1	Total	C	N	0	0
			20	18	2		
2	AAA	1	Total	C	N	0	0
			20	18	2		
2	BBB	1	Total	C	N	0	0
			20	18	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

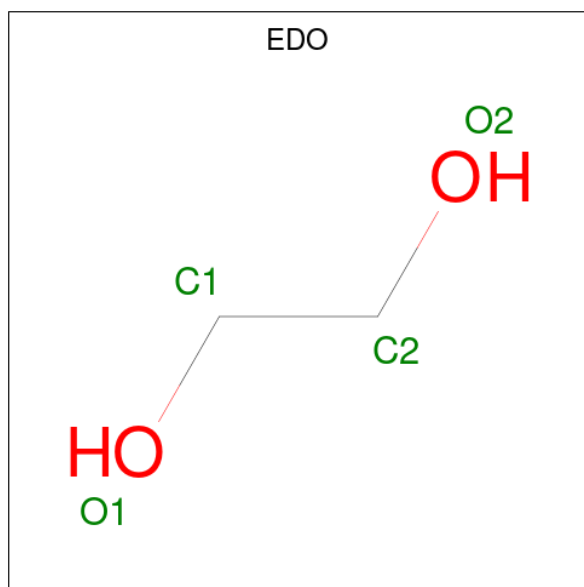


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

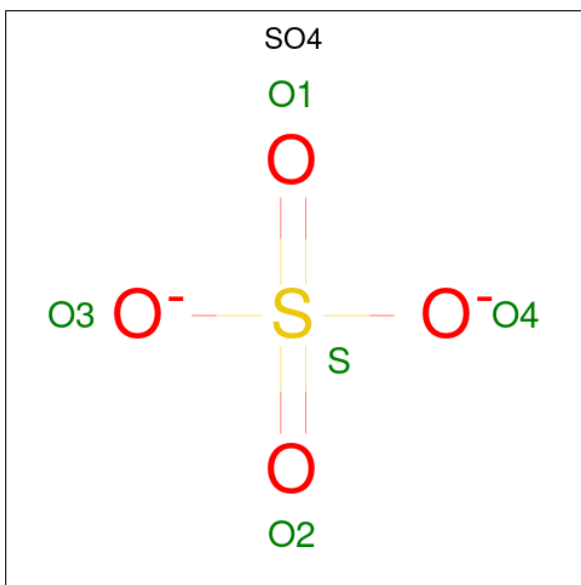
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Cl	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	71	Total	O	0	0
			71	71		
7	BBB	75	Total	O	0	0
			75	75		

### 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. 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. 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: Beta-lactoglobulin

Chain AAA:  93% 5% .



- Molecule 1: Beta-lactoglobulin

Chain BBB:  93% . .



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.82Å 73.34Å 179.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.38 – 1.70 44.93 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.38-1.70) 99.9 (44.93-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.203 , 0.233 0.243 , 0.263	Depositor DCC
$R_{free}$ test set	1042 reflections (2.54%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.0	Xtriage
Anisotropy	0.825	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>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2751	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.31% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, EDO, CL, DSM

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	0.66	0/1279	0.84	0/1727
1	BBB	0.67	0/1275	0.82	0/1726
All	All	0.67	0/2554	0.83	0/3453

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	1255	0	1258	5	0
1	BBB	1249	0	1255	6	0
2	AAA	60	0	66	1	0
2	BBB	20	0	22	1	0
3	AAA	6	0	8	0	0
4	AAA	1	0	0	1	0
5	AAA	4	0	6	0	0
6	AAA	5	0	0	0	0
6	BBB	5	0	0	0	0
7	AAA	71	0	0	1	0
7	BBB	75	0	0	2	0
All	All	2751	0	2615	14	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (14) 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:BBB:59:GLN:HE22	1:BBB:159:GLN:HB3	1.48	0.79
4:AAA:205:CL:CL	7:BBB:308:HOH:O	2.47	0.70
1:AAA:21:SER:O	1:AAA:161:HIS:HE1	1.81	0.65
1:BBB:59:GLN:NE2	1:BBB:159:GLN:HB3	2.17	0.57
1:BBB:73:ALA:HB1	1:BBB:82:PHE:HB3	1.87	0.56
1:AAA:73:ALA:HB1	1:AAA:82:PHE:HB3	1.91	0.52
1:AAA:161:HIS:HD2	7:AAA:320:HOH:O	1.94	0.50
1:BBB:56:PHE:HB2	1:BBB:71:ILE:HG13	1.94	0.48
1:BBB:73:ALA:HB1	1:BBB:82:PHE:CB	2.46	0.45
1:AAA:155:GLN:O	1:AAA:161:HIS:HA	2.18	0.43
1:BBB:63:ASN:HB2	7:BBB:359:HOH:O	2.19	0.43
2:AAA:202:DSM:H162	2:AAA:202:DSM:H183	1.73	0.42
2:BBB:201:DSM:H152	2:BBB:201:DSM:H1	1.81	0.42
1:AAA:102:TYR:OH	1:AAA:135:LYS:HD3	2.21	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	155/162 (96%)	153 (99%)	2 (1%)	0	100	100
1	BBB	156/162 (96%)	153 (98%)	3 (2%)	0	100	100
All	All	311/324 (96%)	306 (98%)	5 (2%)	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	138/141 (98%)	137 (99%)	1 (1%)	84	77
1	BBB	138/141 (98%)	138 (100%)	0	100	100
All	All	276/282 (98%)	275 (100%)	1 (0%)	91	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	60	LYS

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 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\# Z  > 2$
6	SO4	AAA	207	-	4,4,4	0.37	0	6,6,6	0.08	0
2	DSM	AAA	201	-	22,22,22	0.16	0	29,29,29	0.56	0
5	EDO	AAA	206	-	3,3,3	0.19	0	2,2,2	0.16	0
2	DSM	AAA	202	-	22,22,22	0.24	0	29,29,29	0.63	0
3	GOL	AAA	203	-	5,5,5	0.17	0	5,5,5	0.42	0
2	DSM	BBB	201	-	22,22,22	0.29	0	29,29,29	0.57	0
6	SO4	BBB	202	-	4,4,4	0.40	0	6,6,6	0.07	0
2	DSM	AAA	204	-	22,22,22	0.15	0	29,29,29	0.67	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
2	DSM	AAA	201	-	-	4/5/18/18	0/2/3/3
5	EDO	AAA	206	-	-	1/1/1/1	-
2	DSM	AAA	202	-	-	2/5/18/18	0/3/3/3
3	GOL	AAA	203	-	-	2/4/4/4	-
2	DSM	BBB	201	-	-	4/5/18/18	0/3/3/3
2	DSM	AAA	204	-	-	0/5/18/18	0/2/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	201	DSM	C16-C15-N1-C11
2	BBB	201	DSM	C16-C15-N1-C14
2	AAA	201	DSM	N1-C15-C16-C17
2	AAA	202	DSM	C15-C16-C17-N2
2	AAA	201	DSM	C16-C17-N2-C18
5	AAA	206	EDO	O1-C1-C2-O2
2	AAA	201	DSM	C15-C16-C17-N2
2	AAA	202	DSM	C16-C17-N2-C18

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Mol	Chain	Res	Type	Atoms
2	BBB	201	DSM	C16-C15-N1-C11
3	AAA	203	GOL	O1-C1-C2-O2
2	BBB	201	DSM	C15-C16-C17-N2
3	AAA	203	GOL	O1-C1-C2-C3
2	BBB	201	DSM	C16-C17-N2-C18

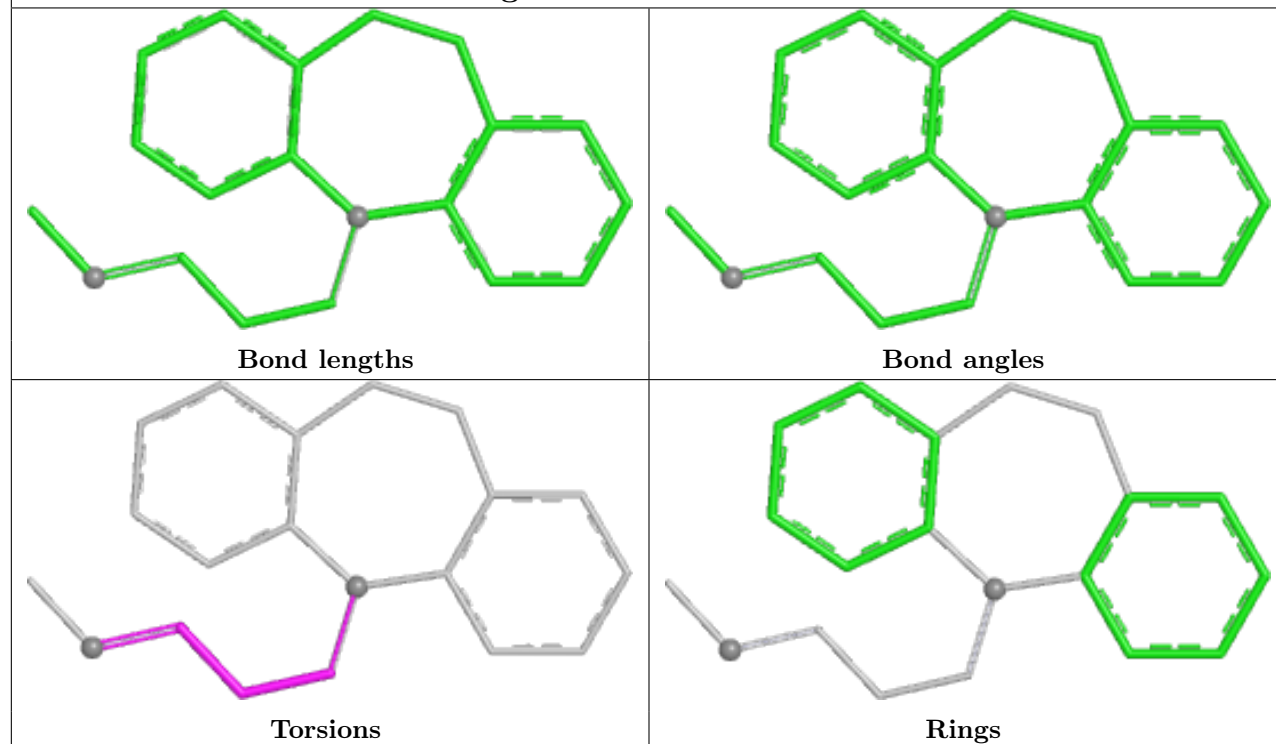
There are no ring outliers.

2 monomers are involved in 2 short contacts:

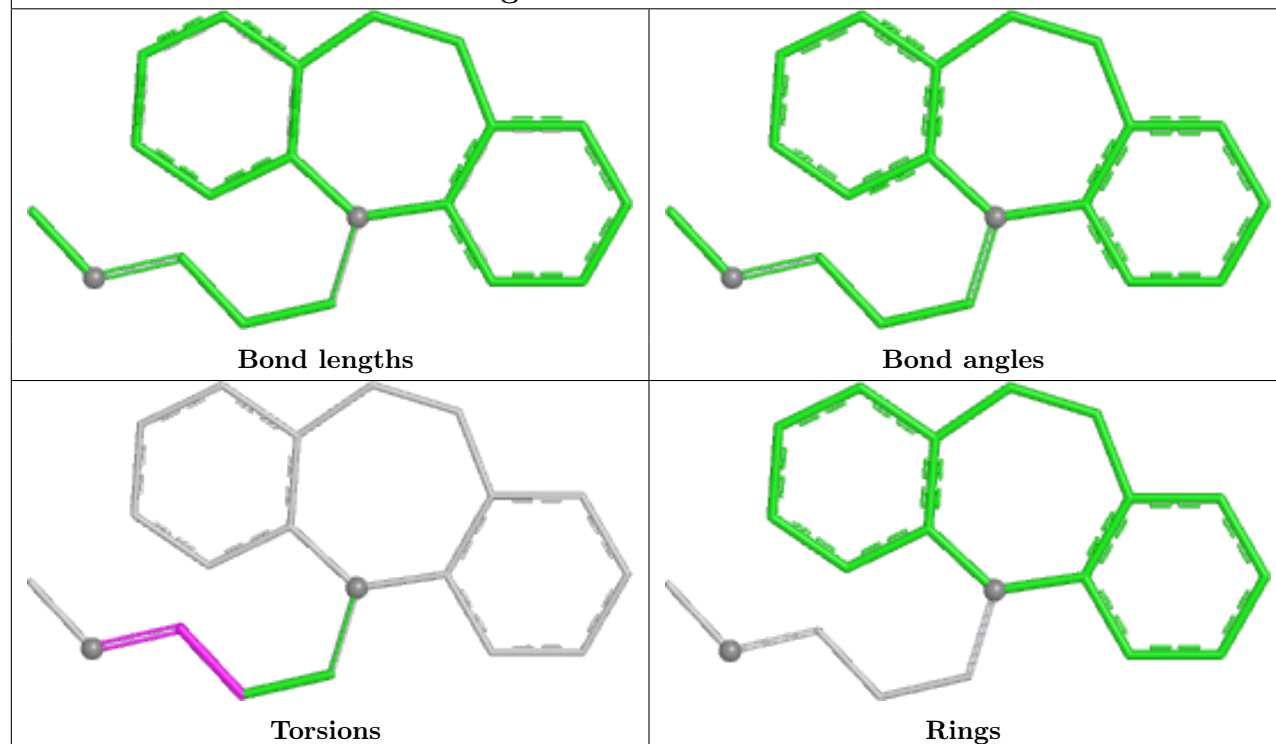
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	202	DSM	1	0
2	BBB	201	DSM	1	0

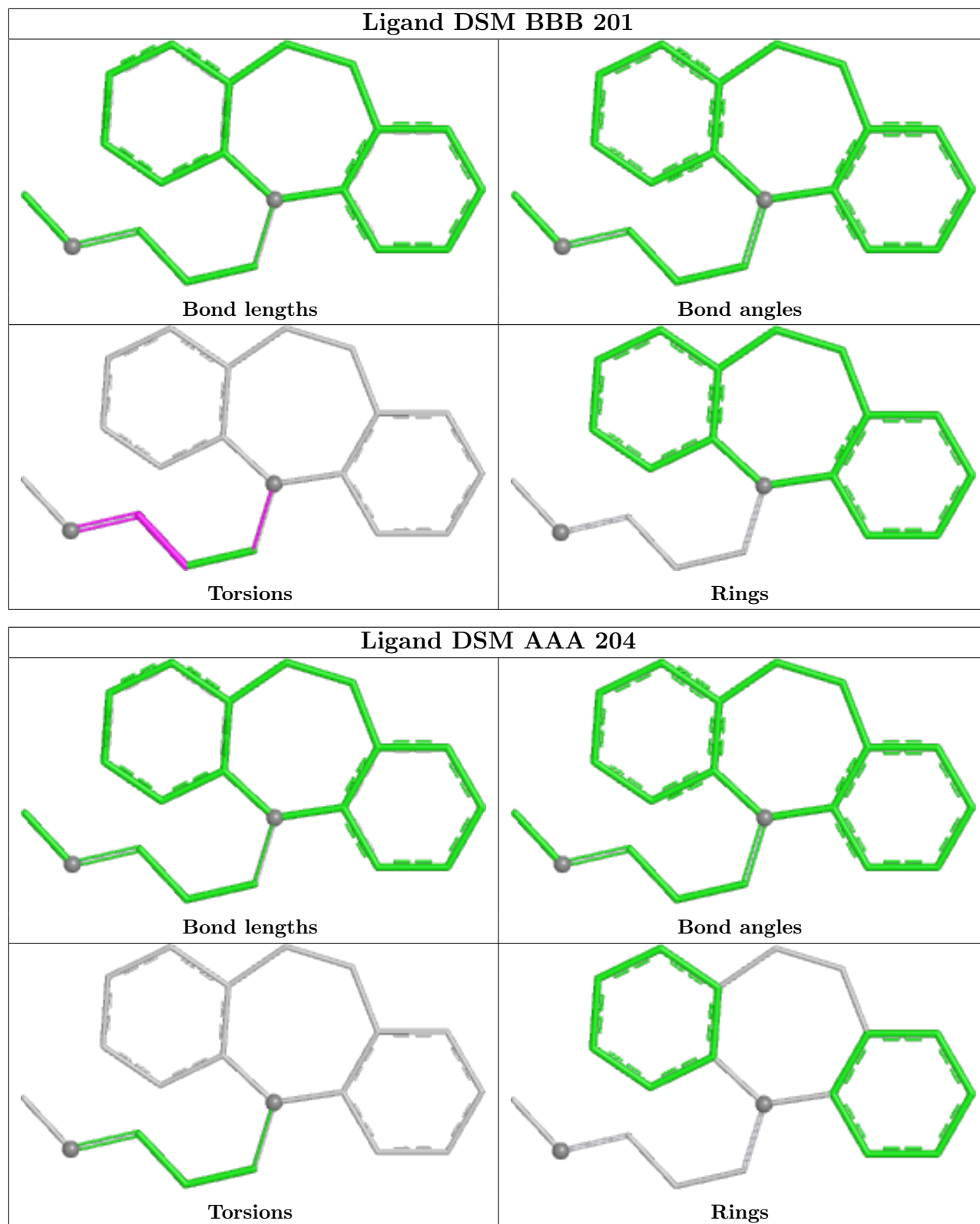
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand DSM AAA 201



## Ligand DSM AAA 202





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

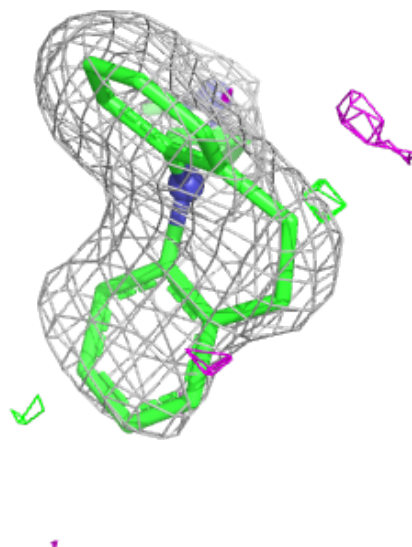
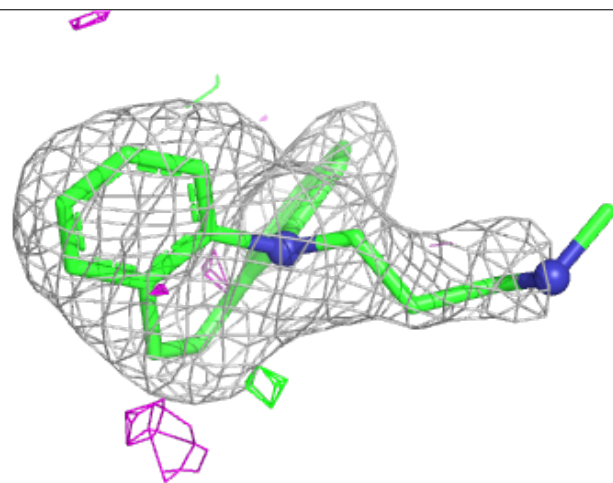
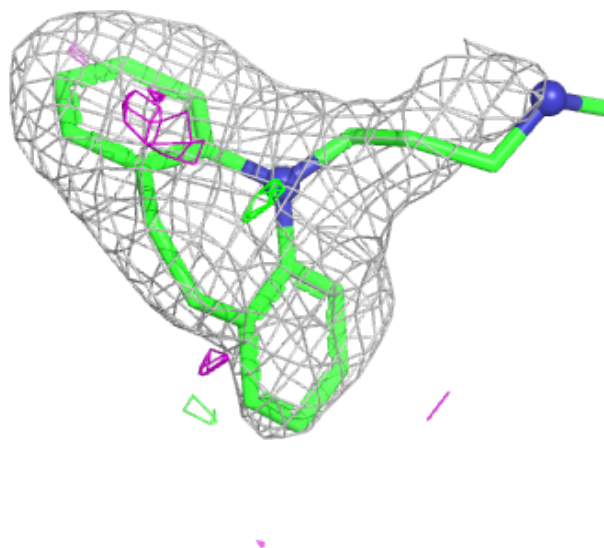
### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

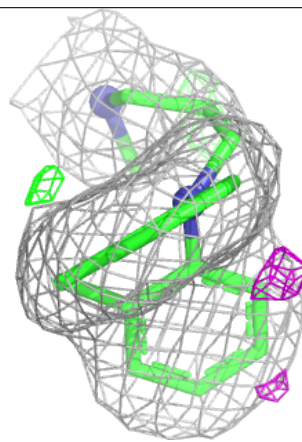
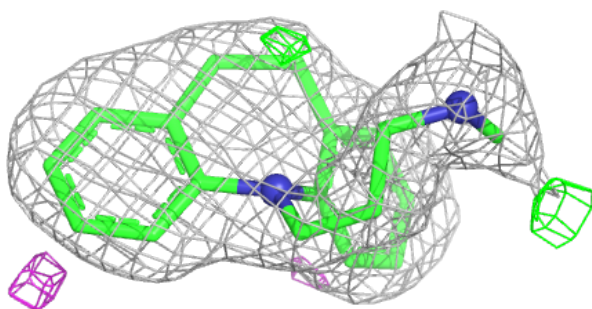
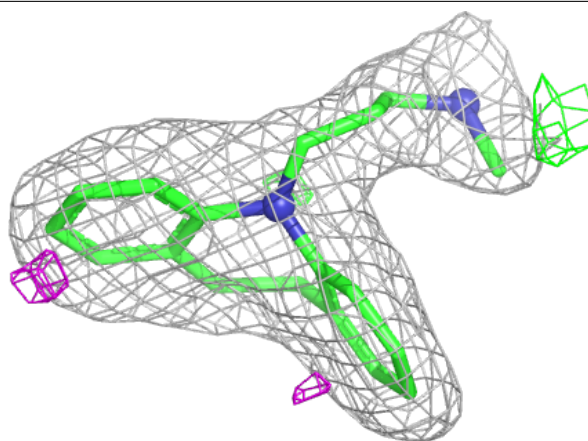
**Electron density around DSM AAA 201:**

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



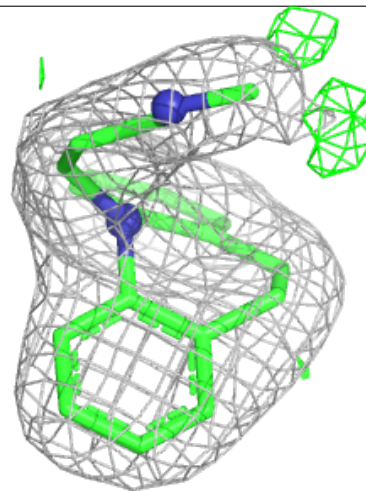
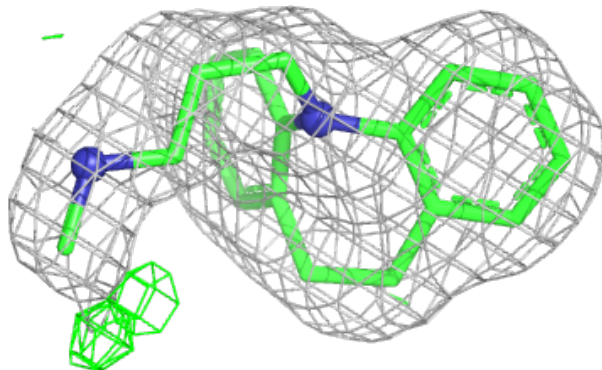
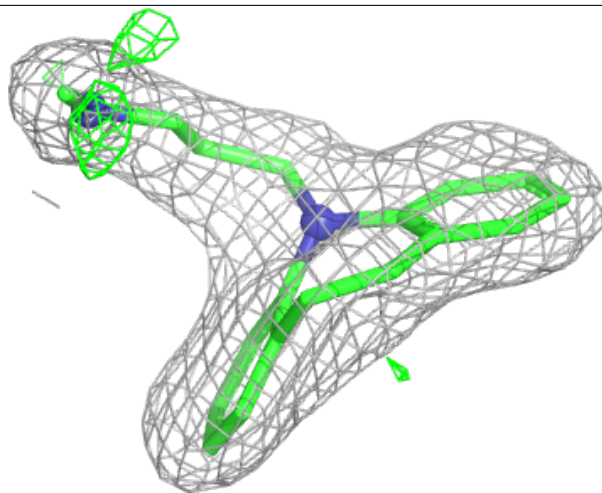
**Electron density around DSM AAA 202:**

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



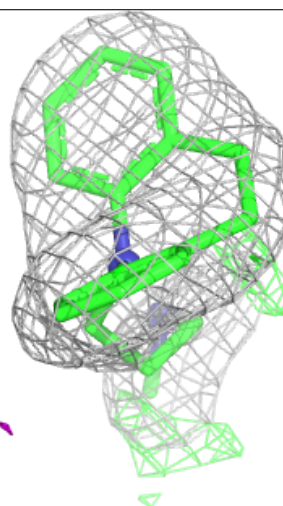
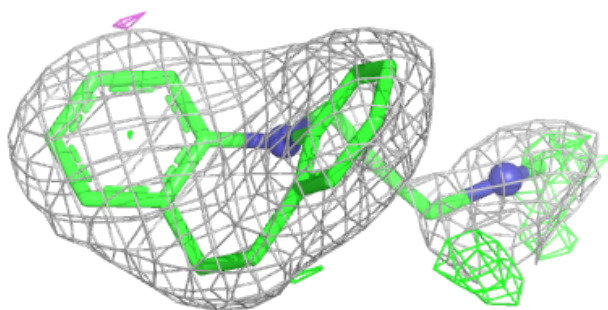
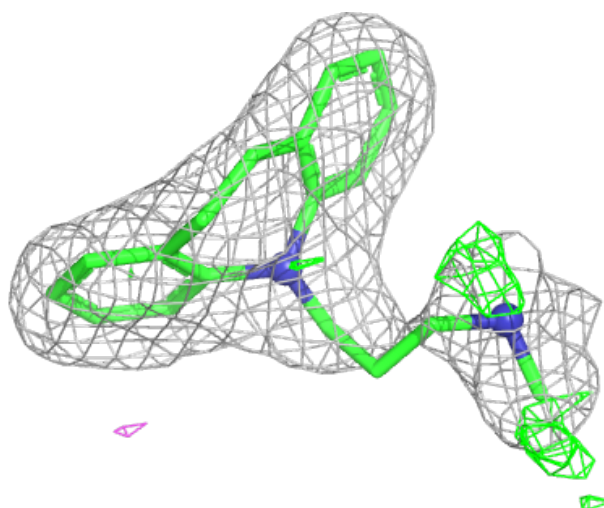
**Electron density around DSM AAA 204:**

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



**Electron density around DSM 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)



## 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.