



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 12, 2021 – 12:11 pm BST

PDB ID : 6Z5F
Title : CRYSTAL STRUCTURE OF RAT PEROXISOMAL MULTIFUNCTIONAL ENZYME TYPE-1 (RPMFE1) COMPLEXED WITH 3-KETODECANOYL-COA AND OXIDISED NICOTINAMIDE ADENINE DINUCLEOTIDE
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Deposited on : 2020-05-26
Resolution : 2.25 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.18
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) : 2.18

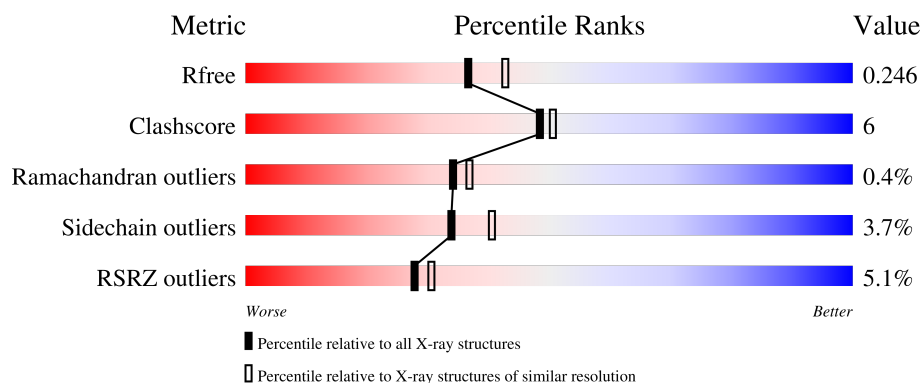
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 $\leq 5\%$. 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	742	<div> <div>3%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>
1	BBB	742	<div> <div>7%</div> <div>80%</div> <div>16%</div> <div>..</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11503 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 Peroxisomal bifunctional enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	718	Total	C	N	O	S	0	4	0
			5535	3541	968	1003	23			
1	BBB	714	Total	C	N	O	S	0	3	0
			5515	3531	965	996	23			

There are 40 discrepancies between the modelled and reference sequences:

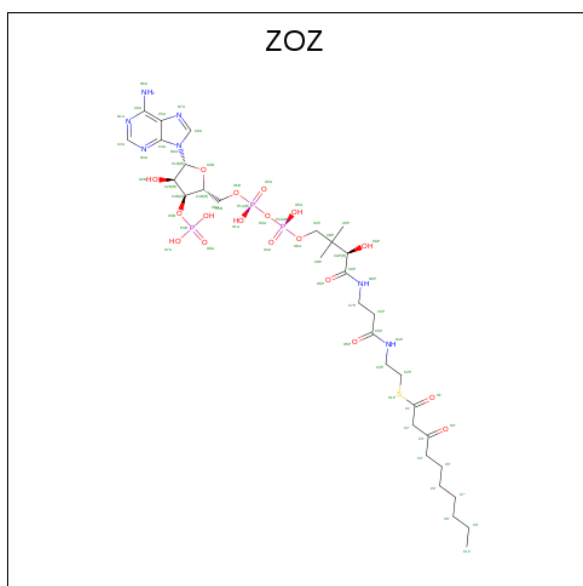
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-19	MET	-	initiating methionine	UNP P07896
AAA	-18	GLY	-	expression tag	UNP P07896
AAA	-17	SER	-	expression tag	UNP P07896
AAA	-16	SER	-	expression tag	UNP P07896
AAA	-15	HIS	-	expression tag	UNP P07896
AAA	-14	HIS	-	expression tag	UNP P07896
AAA	-13	HIS	-	expression tag	UNP P07896
AAA	-12	HIS	-	expression tag	UNP P07896
AAA	-11	HIS	-	expression tag	UNP P07896
AAA	-10	HIS	-	expression tag	UNP P07896
AAA	-9	SER	-	expression tag	UNP P07896
AAA	-8	SER	-	expression tag	UNP P07896
AAA	-7	GLY	-	expression tag	UNP P07896
AAA	-6	LEU	-	expression tag	UNP P07896
AAA	-5	VAL	-	expression tag	UNP P07896
AAA	-4	PRO	-	expression tag	UNP P07896
AAA	-3	ARG	-	expression tag	UNP P07896
AAA	-2	GLY	-	expression tag	UNP P07896
AAA	-1	SER	-	expression tag	UNP P07896
AAA	0	HIS	-	expression tag	UNP P07896
BBB	-19	MET	-	initiating methionine	UNP P07896
BBB	-18	GLY	-	expression tag	UNP P07896
BBB	-17	SER	-	expression tag	UNP P07896
BBB	-16	SER	-	expression tag	UNP P07896
BBB	-15	HIS	-	expression tag	UNP P07896

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-14	HIS	-	expression tag	UNP P07896
BBB	-13	HIS	-	expression tag	UNP P07896
BBB	-12	HIS	-	expression tag	UNP P07896
BBB	-11	HIS	-	expression tag	UNP P07896
BBB	-10	HIS	-	expression tag	UNP P07896
BBB	-9	SER	-	expression tag	UNP P07896
BBB	-8	SER	-	expression tag	UNP P07896
BBB	-7	GLY	-	expression tag	UNP P07896
BBB	-6	LEU	-	expression tag	UNP P07896
BBB	-5	VAL	-	expression tag	UNP P07896
BBB	-4	PRO	-	expression tag	UNP P07896
BBB	-3	ARG	-	expression tag	UNP P07896
BBB	-2	GLY	-	expression tag	UNP P07896
BBB	-1	SER	-	expression tag	UNP P07896
BBB	0	HIS	-	expression tag	UNP P07896

- Molecule 2 is 3-KETO-DECANOYL-COA (three-letter code: ZOZ) (formula: $C_{31}H_{52}N_7O_{18}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	S	0	0
			60	31	7	18	3	1		
2	AAA	1	Total	C	N	O	P	S	0	0
			60	31	7	18	3	1		
2	BBB	1	Total	C	N	O	P	S	0	0
			60	31	7	18	3	1		

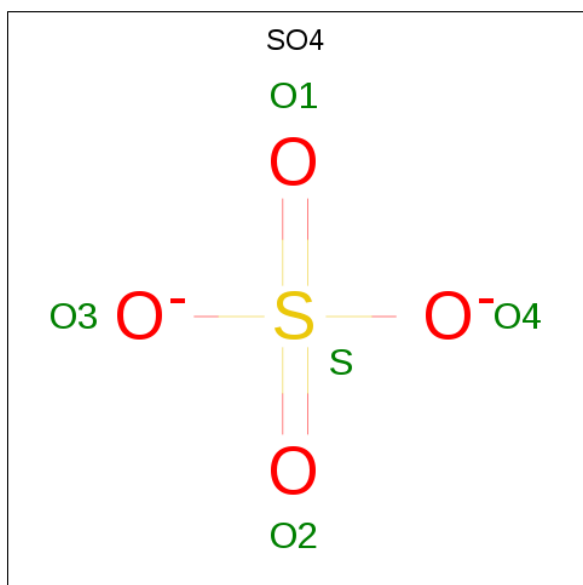
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- The image displays the chemical structure of NADH (Nicotinamide Adenine Dinucleotide). It consists of a nicotinamide ring (top) linked to a ribose sugar, which is connected via a pyrophosphate bridge to another ribose sugar, which is in turn linked to an adenine ring (bottom). The structure is color-coded: the nicotinamide ring is blue, the ribose sugars are green, the pyrophosphate bridge is red, and the adenine ring is blue. The structure is labeled with various atoms and groups, including NH₂, N, C, O, P, and H.

GOL

The diagram shows the skeletal structure of 1,2,3-propanetriol (glycerol). It consists of a three-carbon chain. The first carbon (C1) is bonded to a hydroxyl group (HO, O1). The second carbon (C2) is bonded to a hydroxyl group (OH, O2). The third carbon (C3) is bonded to a hydroxyl group (OH, O3). The atoms are labeled with green text: C1, C2, C3 for the carbons and O1, O2, O3 for the oxygens. The hydroxyl groups are written in red text as HO and OH.

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



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

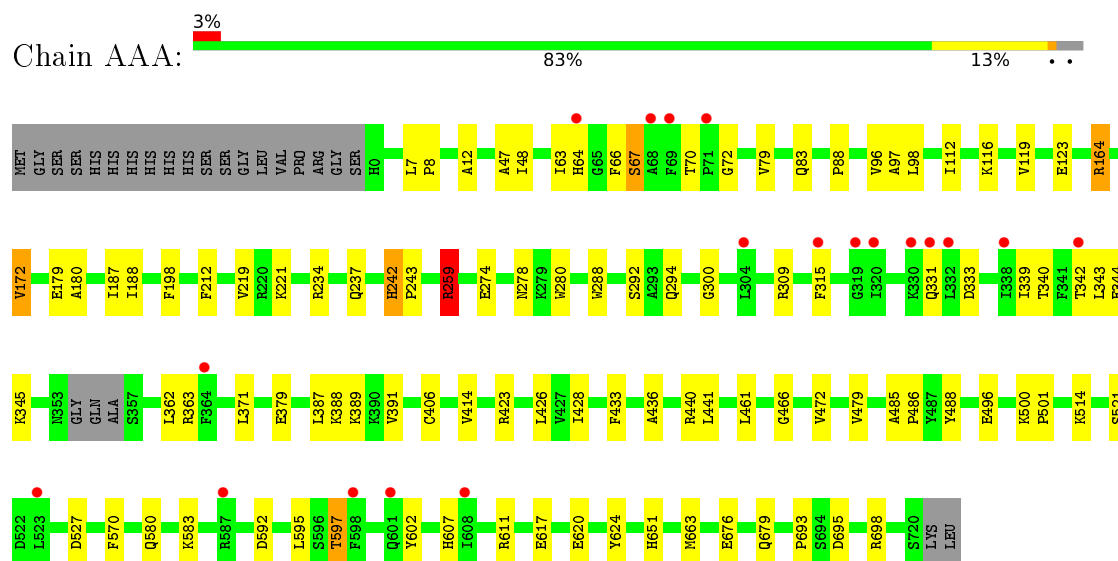
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	123	Total	O	0	0
			123	123		
6	BBB	40	Total	O	0	0
			40	40		

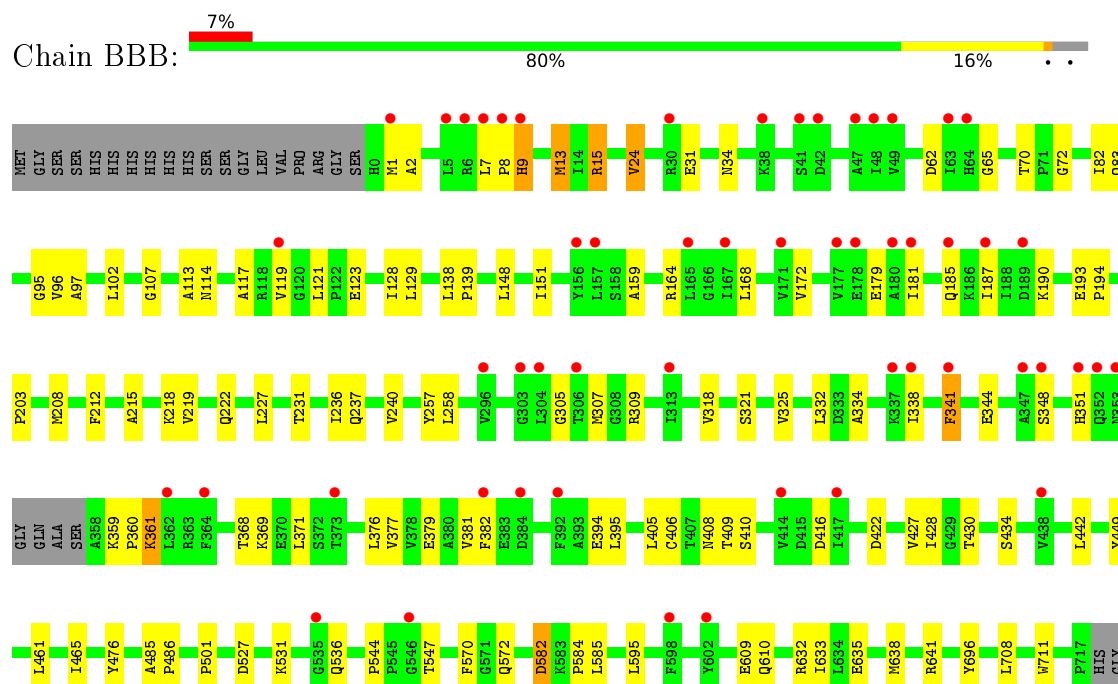
3 Residue-property plots [i](#)

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: Peroxisomal bifunctional enzyme



- Molecule 1: Peroxisomal bifunctional enzyme



SER
LYS
LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.16Å 125.98Å 223.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.63 – 2.25 62.55 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (62.63-2.25) 100.0 (62.55-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.209 , 0.246 0.209 , 0.246	Depositor DCC
R_{free} test set	4429 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11503	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ZOZ, GOL, NAD, 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	0.35	0/5675	0.69	1/7687 (0.0%)
1	BBB	0.34	3/5651 (0.1%)	0.62	1/7654 (0.0%)
All	All	0.34	3/11326 (0.0%)	0.66	2/15341 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	15[A]	ARG	CZ-NH2	6.50	1.41	1.33
1	BBB	15[B]	ARG	CZ-NH2	6.50	1.41	1.33
1	BBB	13	MET	SD-CE	5.08	2.06	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	13	MET	CG-SD-CE	-7.27	88.56	100.20
1	AAA	259	ARG	CG-CD-NE	6.43	125.30	111.80

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	5535	0	5652	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BBB	5515	0	5637	77	0
2	AAA	120	0	0	2	0
2	BBB	60	0	0	1	0
3	AAA	44	0	26	1	0
3	BBB	44	0	26	0	0
4	AAA	12	0	16	1	0
5	AAA	5	0	0	0	0
5	BBB	5	0	0	0	0
6	AAA	123	0	0	0	0
6	BBB	40	0	0	0	0
All	All	11503	0	11357	136	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 136 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:13:MET:CE	1:BBB:13:MET:SD	2.06	1.43
1:BBB:15[B]:ARG:HH21	1:BBB:15[B]:ARG:HG2	1.09	1.13
1:BBB:15[B]:ARG:HH21	1:BBB:15[B]:ARG:CG	1.79	0.96
1:AAA:172:VAL:HG21	1:AAA:179:GLU:HG2	1.49	0.93
1:BBB:379:GLU:OE2	1:BBB:381:VAL:HG22	1.79	0.82

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	718/742 (97%)	687 (96%)	29 (4%)	2 (0%)	41	46
1	BBB	713/742 (96%)	680 (95%)	29 (4%)	4 (1%)	25	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1431/1484 (96%)	1367 (96%)	58 (4%)	6 (0%)	34 37

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	67	SER
1	AAA	607	HIS
1	BBB	9	HIS
1	BBB	409	THR
1	BBB	65	GLY

5.3.2 Protein sidechains ⓘ

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	594/609 (98%)	569 (96%)	25 (4%)	30 34
1	BBB	590/609 (97%)	570 (97%)	20 (3%)	37 45
All	All	1184/1218 (97%)	1139 (96%)	45 (4%)	34 39

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	114	ASN
1	BBB	361	LYS
1	BBB	219	VAL
1	BBB	332	LEU
1	BBB	416	ASP

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	ZOZ	BBB	902	-	53,62,62	0.55	0	65,89,89	0.92	2 (3%)
2	ZOZ	AAA	801	-	53,62,62	0.55	0	65,89,89	0.60	1 (1%)
5	SO4	AAA	805	-	4,4,4	0.36	0	6,6,6	0.07	0
4	GOL	AAA	806	-	5,5,5	0.09	0	5,5,5	0.41	0
3	NAD	AAA	802	-	42,48,48	0.84	1 (2%)	50,73,73	0.84	2 (4%)
5	SO4	BBB	903	-	4,4,4	0.39	0	6,6,6	0.05	0
2	ZOZ	AAA	804	-	53,62,62	0.59	0	65,89,89	0.94	2 (3%)
3	NAD	BBB	901	-	42,48,48	0.75	1 (2%)	50,73,73	0.92	4 (8%)
4	GOL	AAA	803	-	5,5,5	0.13	0	5,5,5	0.46	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	ZOZ	BBB	902	-	-	20/57/78/78	0/3/3/3
2	ZOZ	AAA	801	-	-	16/57/78/78	0/3/3/3
4	GOL	AAA	806	-	-	2/4/4/4	-
3	NAD	AAA	802	-	-	5/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ZOZ	AAA	804	-	-	12/57/78/78	0/3/3/3
3	NAD	BBB	901	-	-	15/26/62/62	0/5/5/5
4	GOL	AAA	803	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	802	NAD	C2N-N1N	3.60	1.39	1.35
3	BBB	901	NAD	C2N-N1N	3.19	1.38	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	804	ZOZ	C3'-C2'-C1'	5.83	124.13	112.52
2	BBB	902	ZOZ	C3'-C2'-C1'	5.67	123.80	112.52
3	AAA	802	NAD	C6N-N1N-C2N	-3.10	119.15	121.97
3	BBB	901	NAD	C6N-N1N-C2N	-3.01	119.23	121.97
3	BBB	901	NAD	C3D-C2D-C1D	2.84	105.26	100.98

There are no chirality outliers.

5 of 74 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	801	ZOZ	C1'-C2'-C3'-O3'
2	AAA	801	ZOZ	CAP-CBP-CCP-O6A
2	AAA	801	ZOZ	C5B-O5B-P1A-O1A
2	AAA	801	ZOZ	C5B-O5B-P1A-O2A
2	AAA	801	ZOZ	C3B-O3B-P3B-O7A

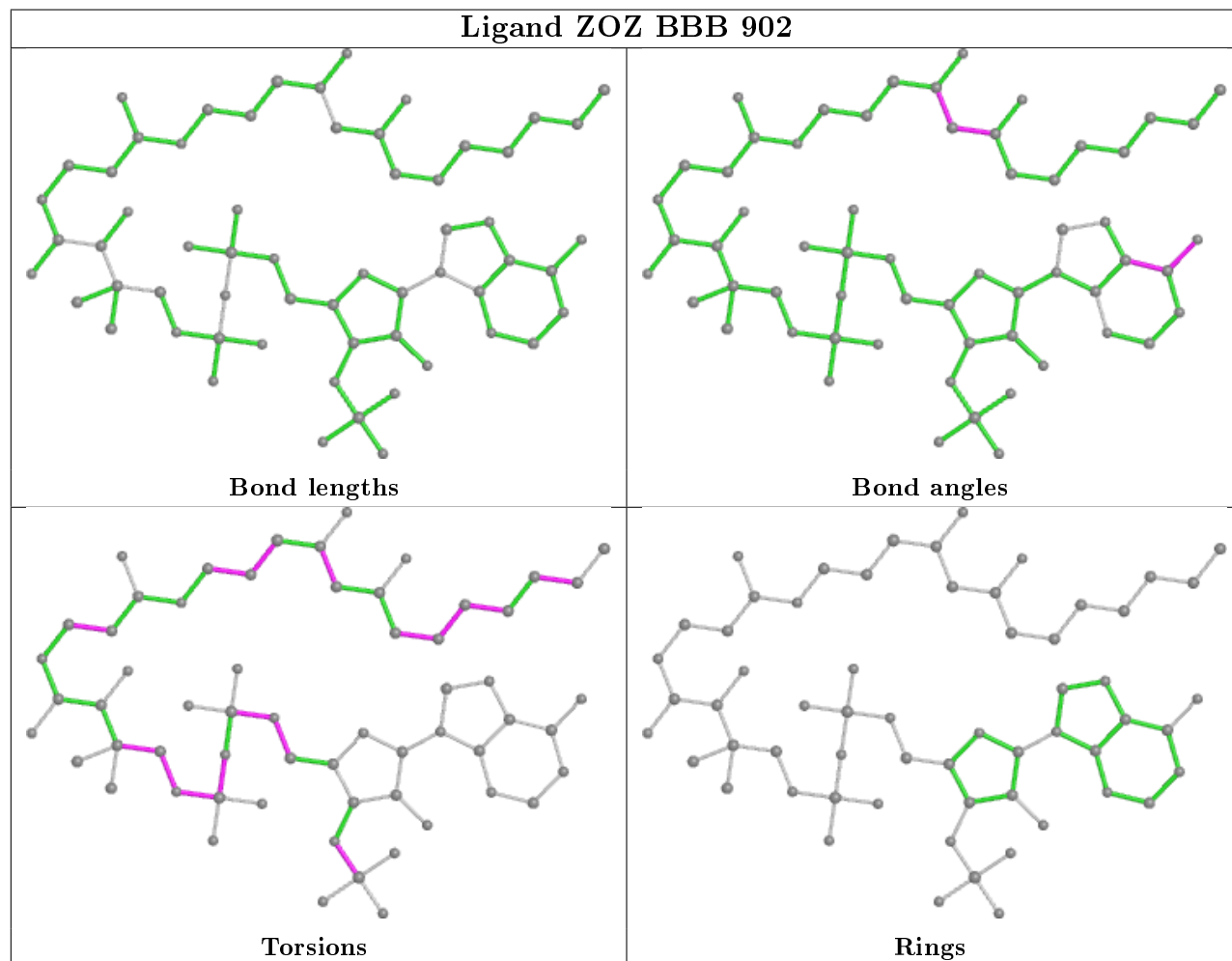
There are no ring outliers.

4 monomers are involved in 5 short contacts:

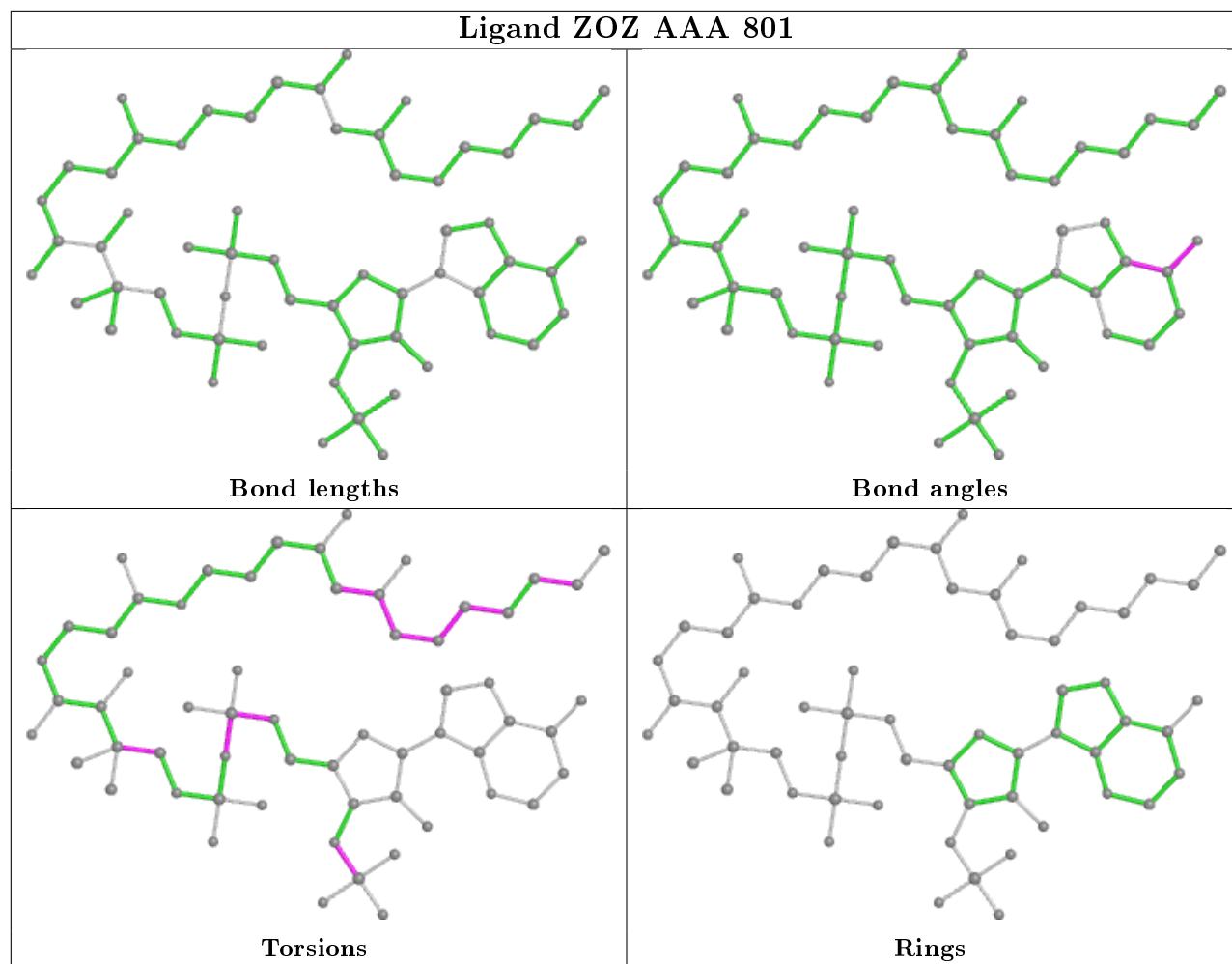
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	902	ZOZ	1	0
4	AAA	806	GOL	1	0
3	AAA	802	NAD	1	0
2	AAA	804	ZOZ	2	0

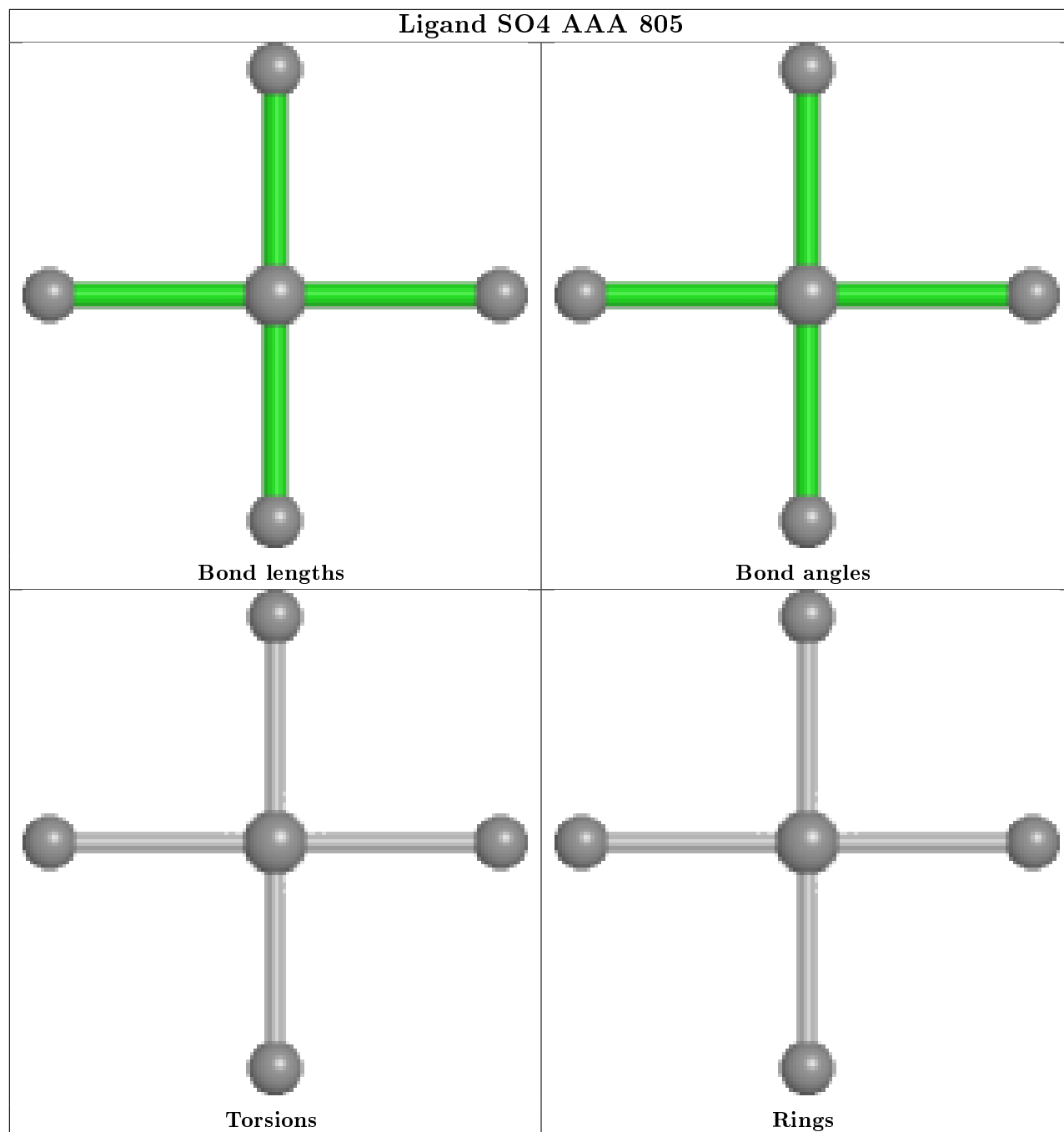
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

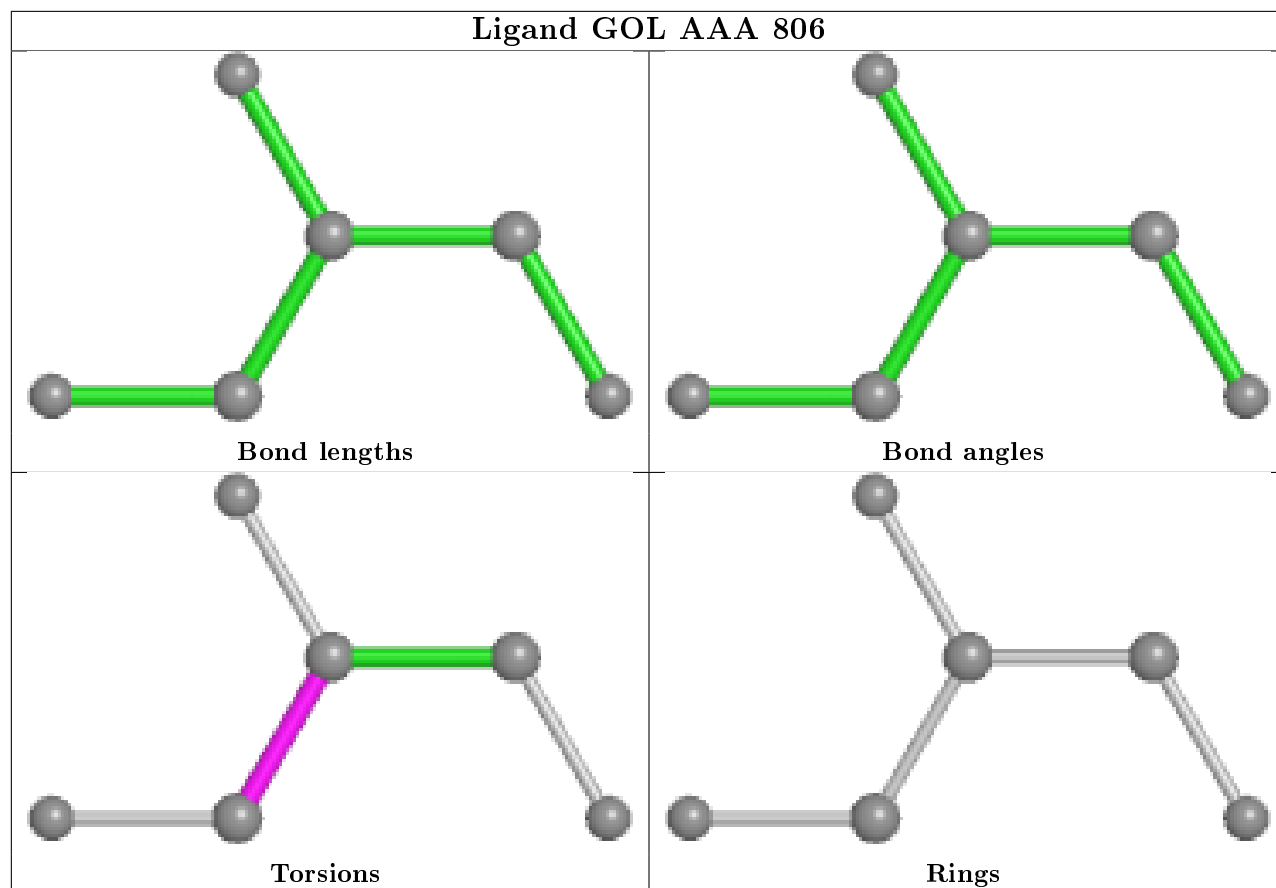


Ligand ZOZ AAA 801

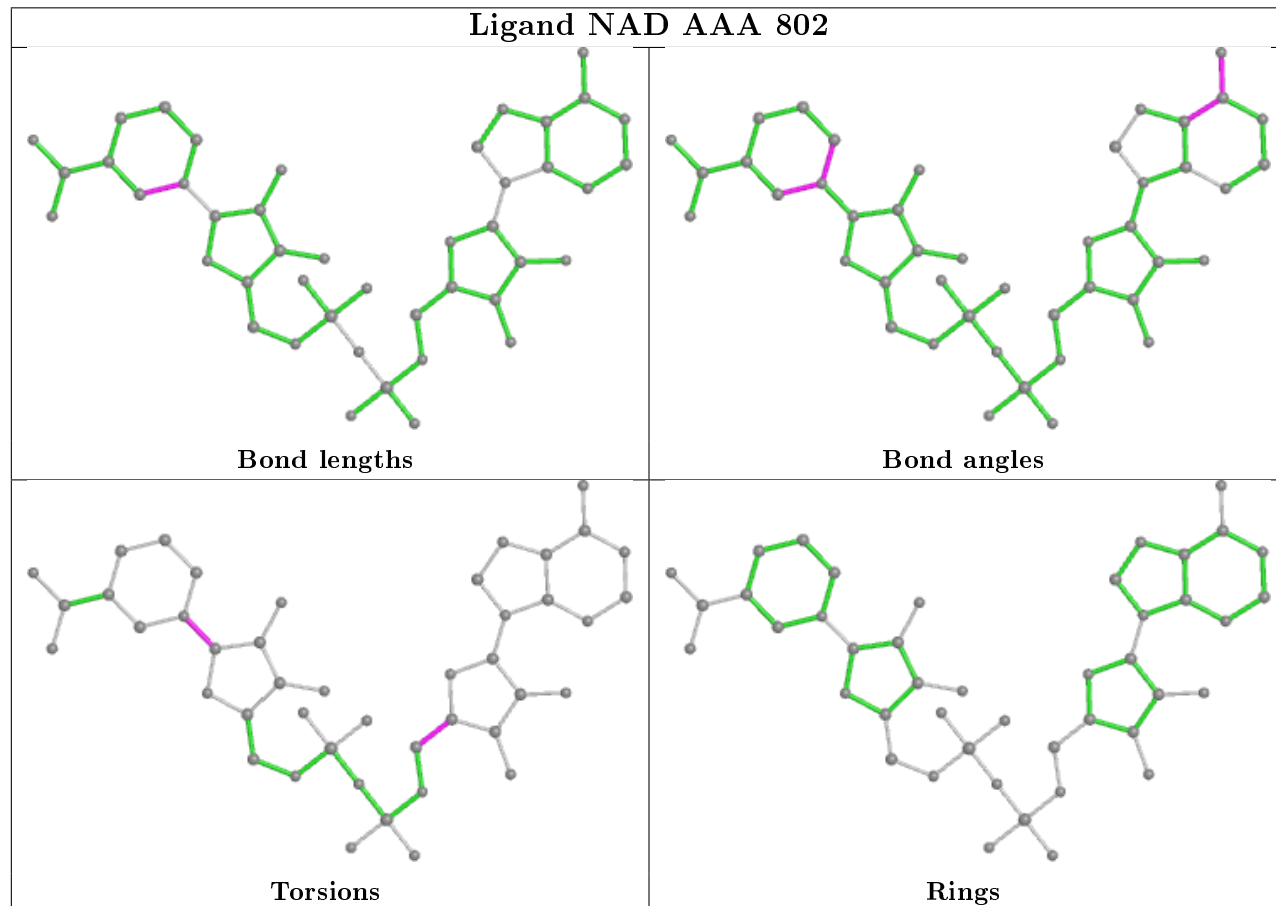


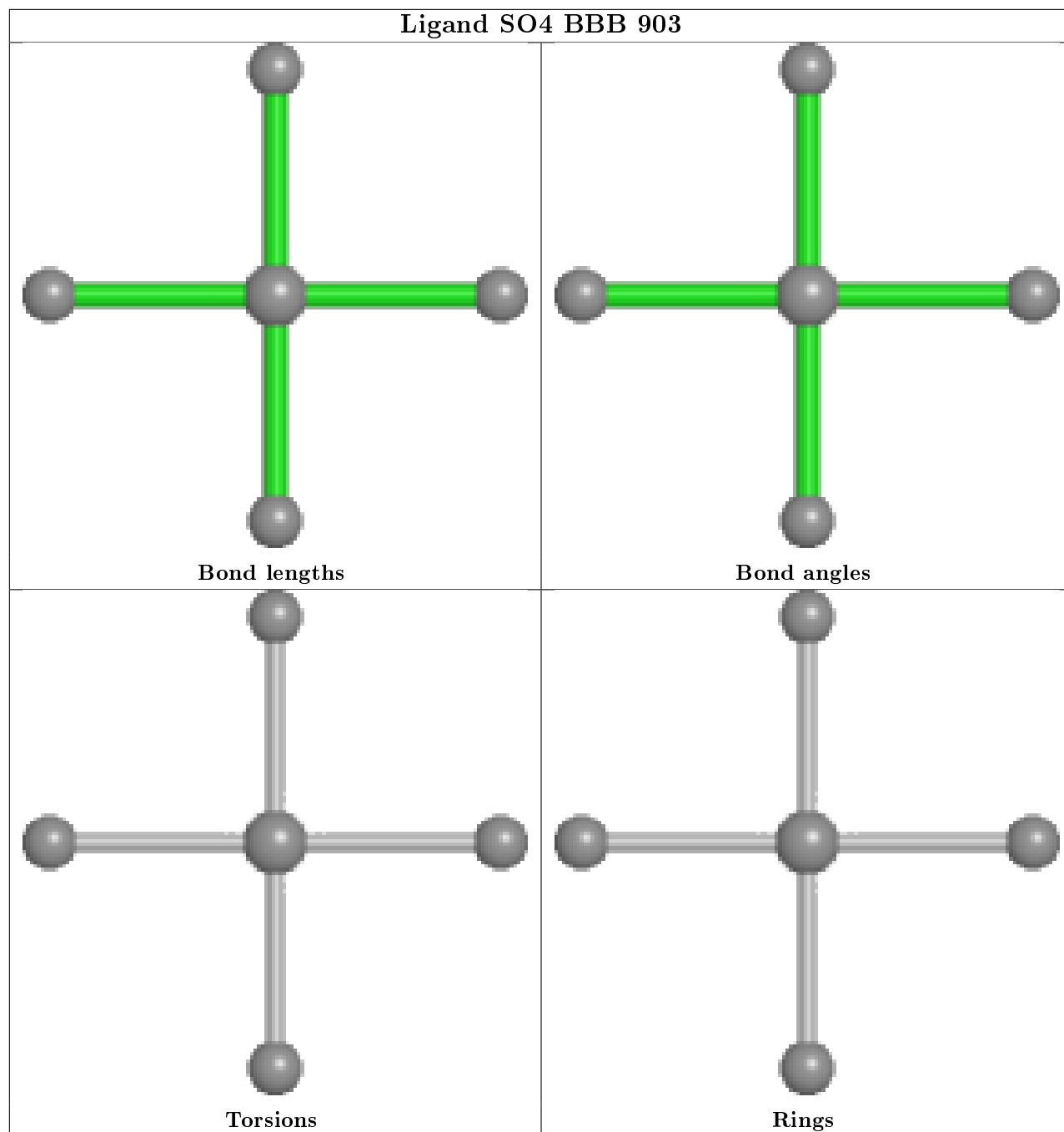


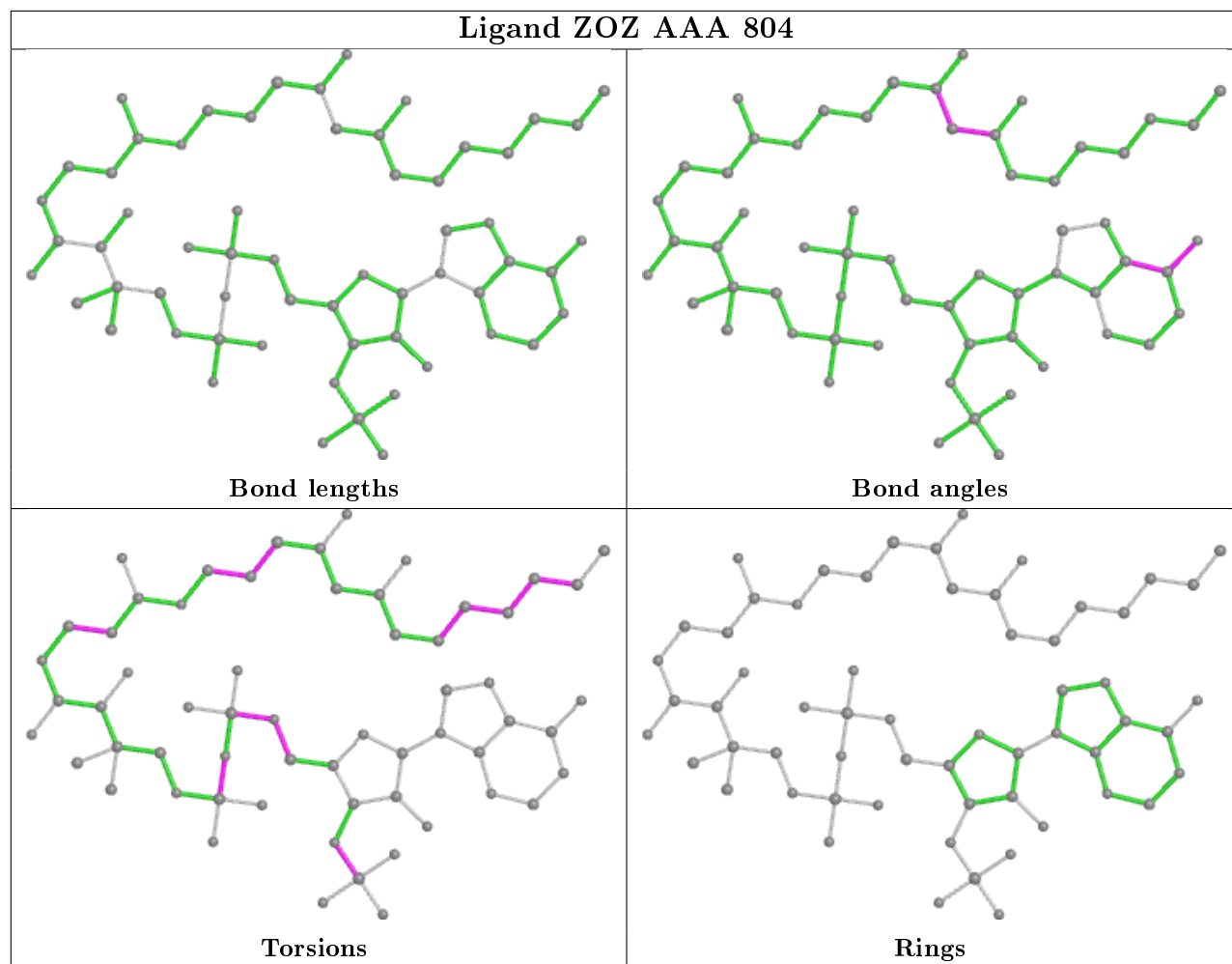
Ligand GOL AAA 806

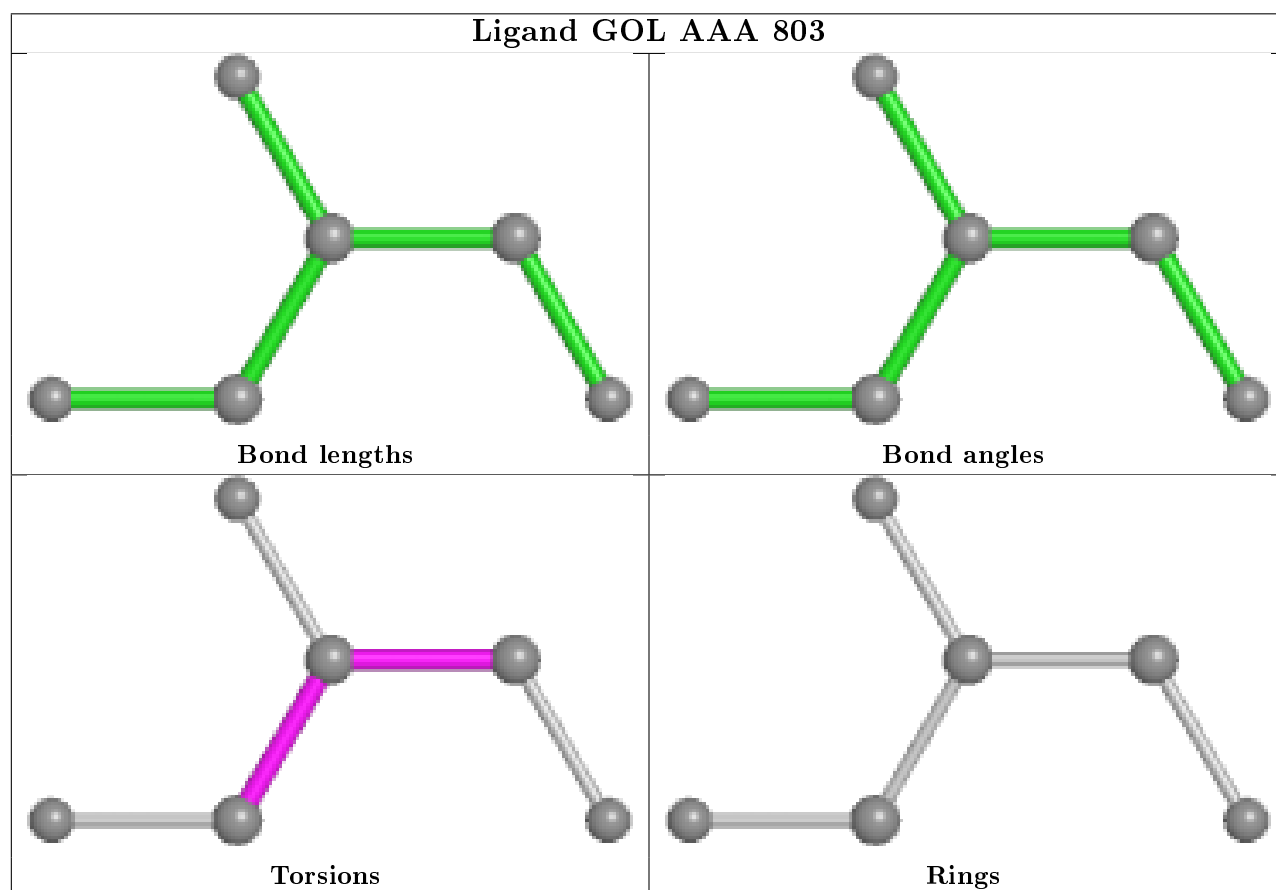
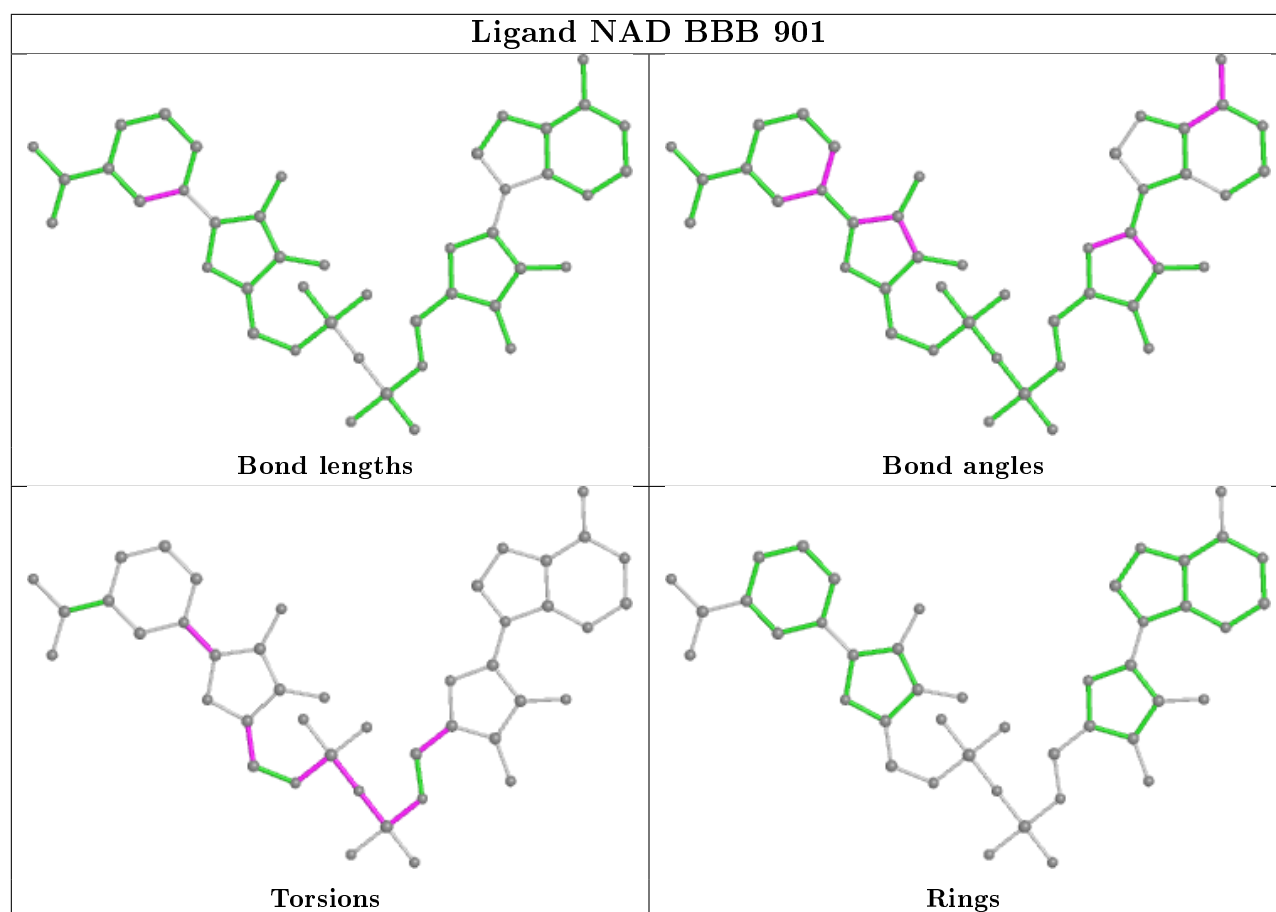


Ligand NAD AAA 802









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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	718/742 (96%)	0.31	19 (2%) 56 59	30, 57, 112, 189	0
1	BBB	714/742 (96%)	0.42	54 (7%) 13 15	49, 82, 134, 210	0
All	All	1432/1484 (96%)	0.36	73 (5%) 28 30	30, 70, 127, 210	0

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	5	LEU	5.6
1	BBB	341	PHE	4.4
1	AAA	71	PRO	4.2
1	BBB	438	VAL	3.8
1	BBB	347	ALA	3.8

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](#)

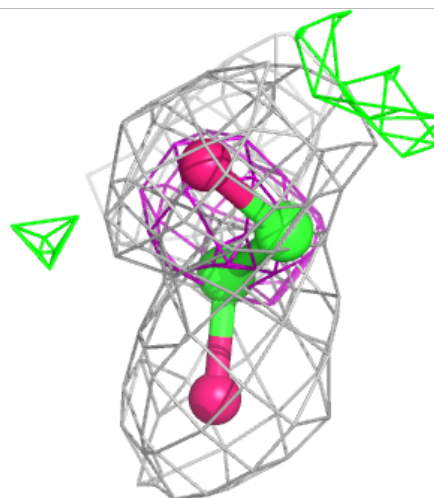
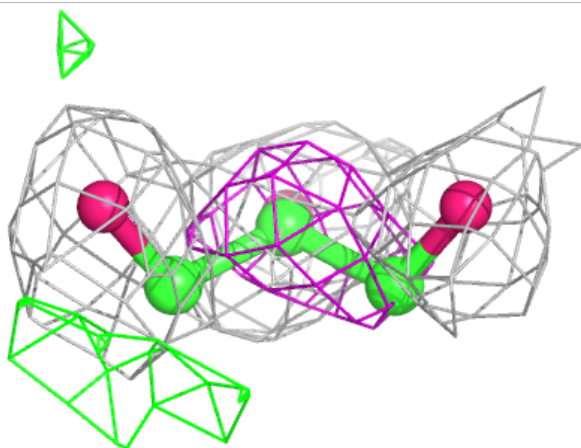
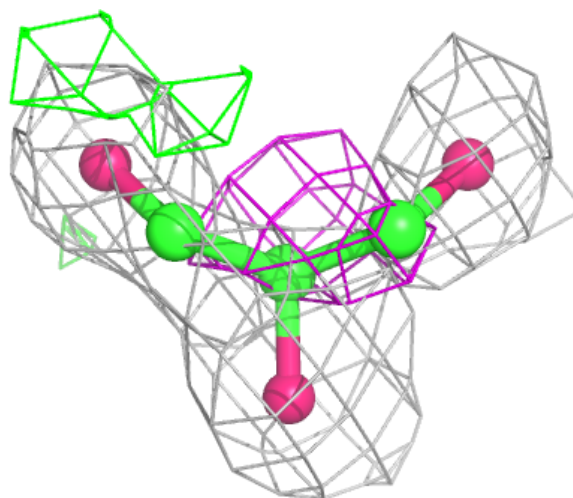
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	AAA	803	6/6	0.64	0.26	59,66,72,73	0
2	ZOZ	AAA	801	60/60	0.65	0.39	114,178,212,216	0
4	GOL	AAA	806	6/6	0.67	0.23	102,108,110,112	0
2	ZOZ	AAA	804	60/60	0.74	0.24	63,114,138,141	0
2	ZOZ	BBB	902	60/60	0.80	0.22	71,126,168,171	0
5	SO4	BBB	903	5/5	0.86	0.11	137,137,143,143	0
3	NAD	BBB	901	44/44	0.91	0.28	97,105,115,118	0
3	NAD	AAA	802	44/44	0.93	0.14	67,79,89,92	0
5	SO4	AAA	805	5/5	0.96	0.12	85,88,90,94	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.

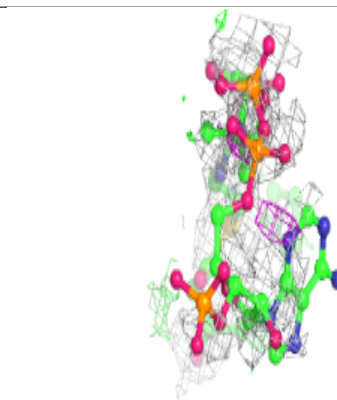
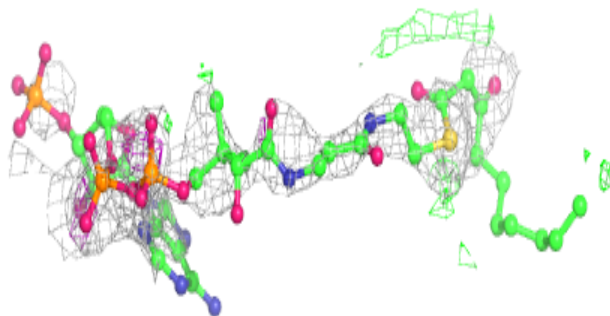
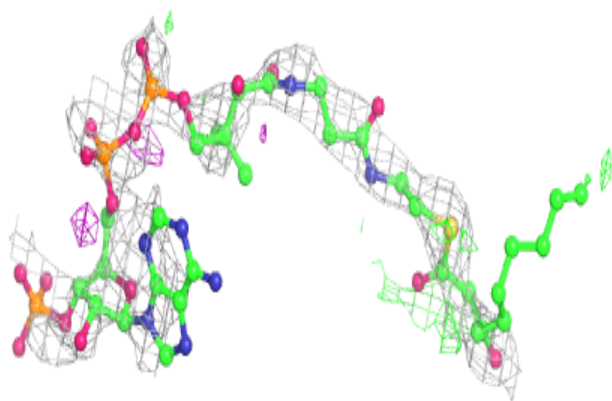
Electron density around GOL AAA 803:

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



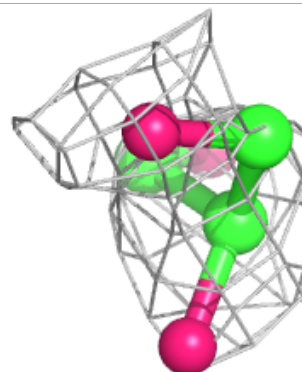
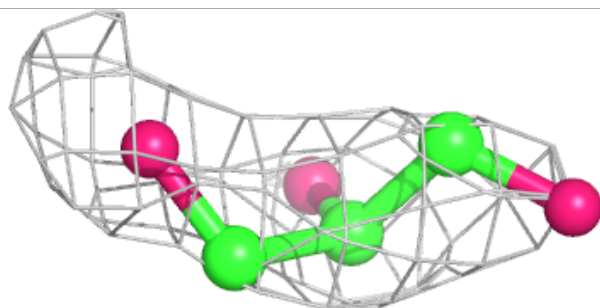
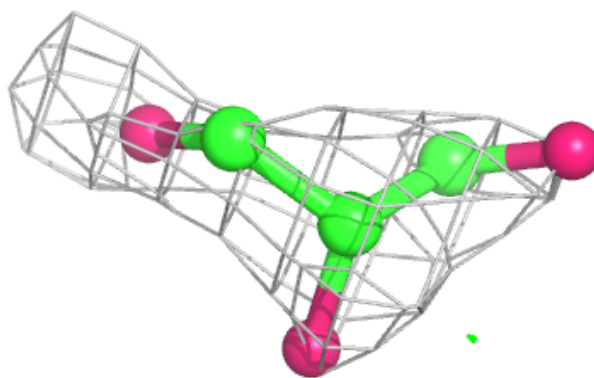
Electron density around ZOZ AAA 801:

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



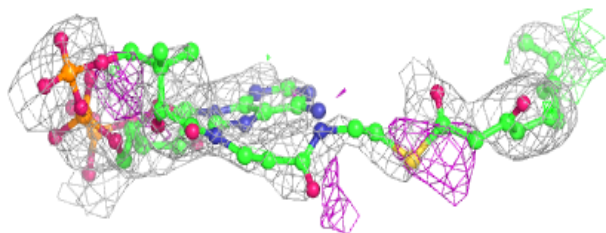
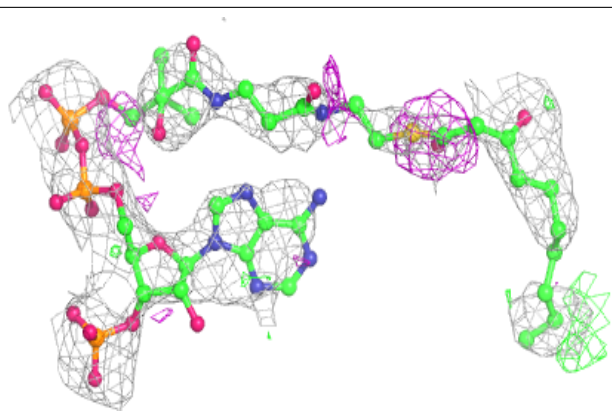
Electron density around GOL AAA 806:

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

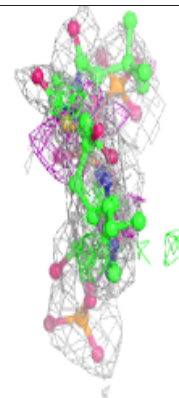
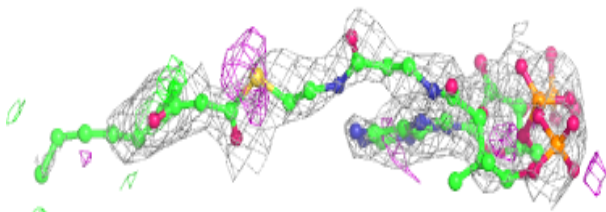
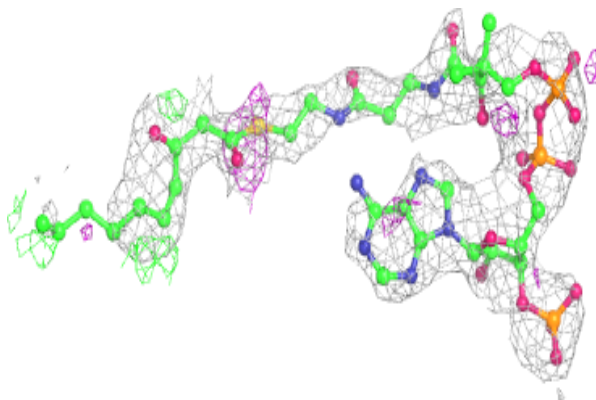


Electron density around ZOZ AAA 804:

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

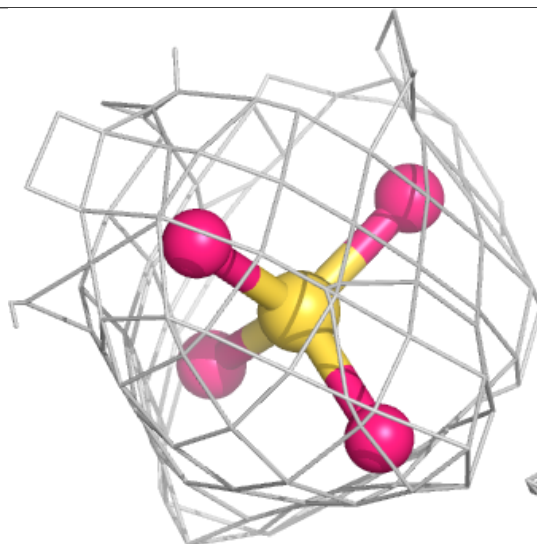
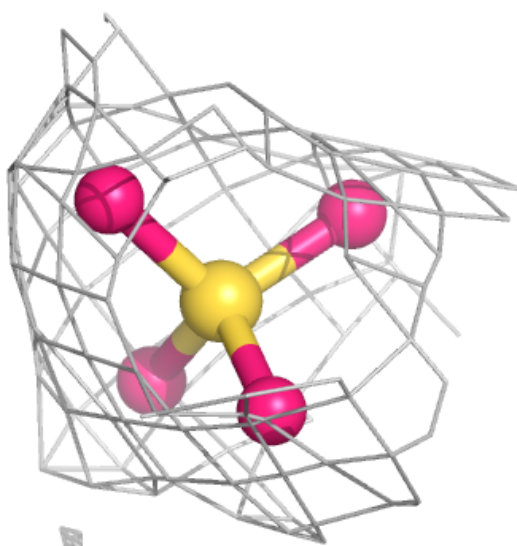
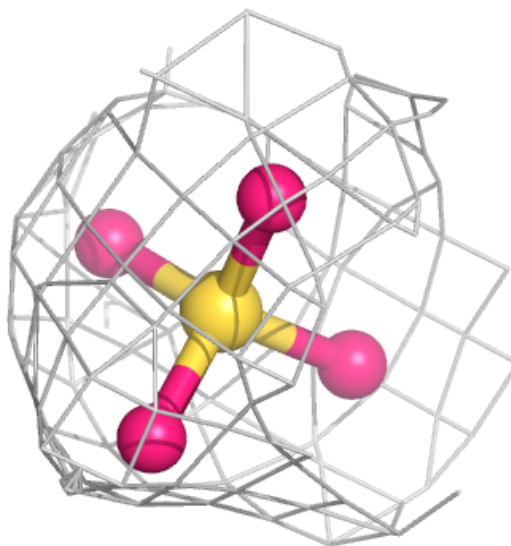
**Electron density around ZOZ BBB 902:**

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



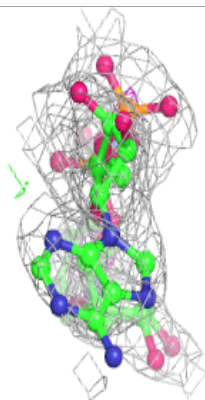
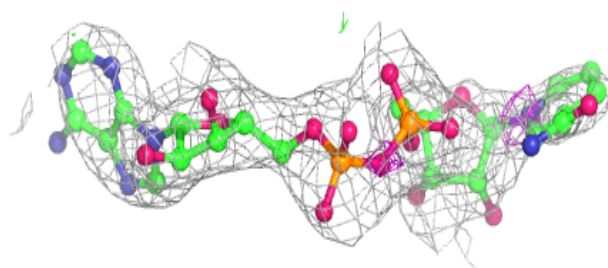
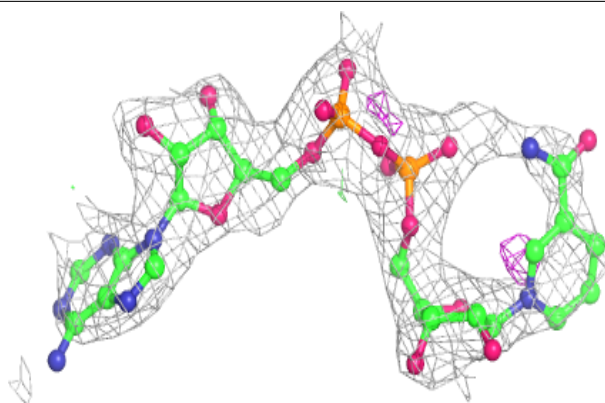
Electron density around SO4 BBB 903:

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

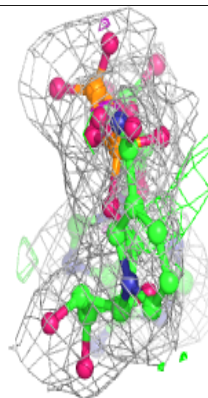
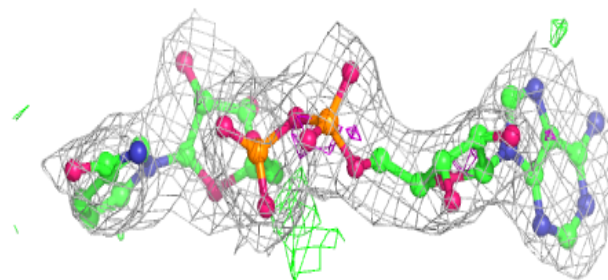
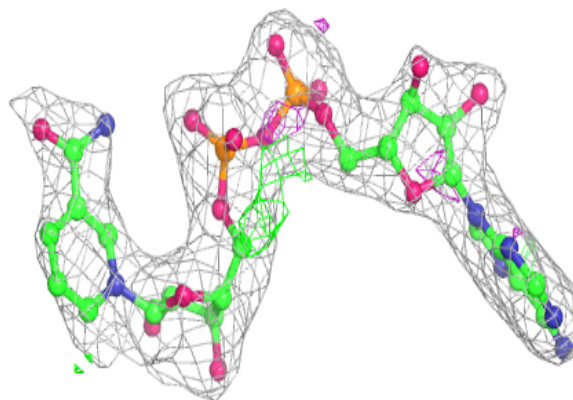


Electron density around NAD BBB 901:

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

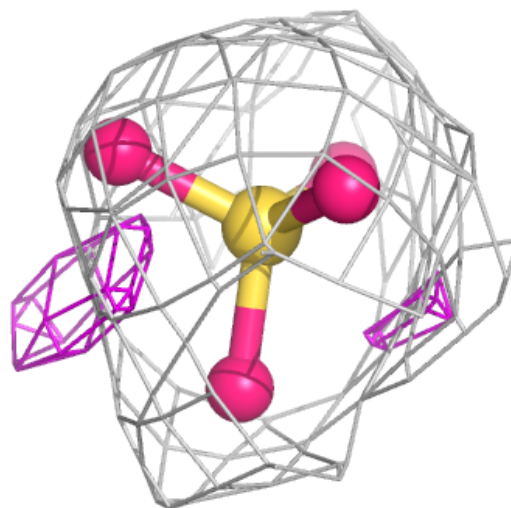
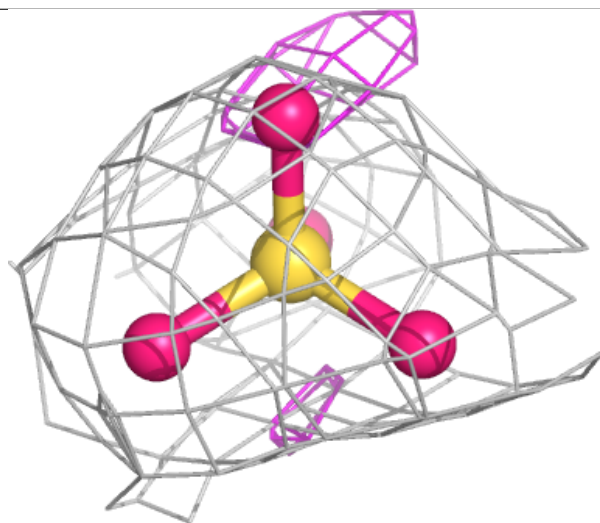
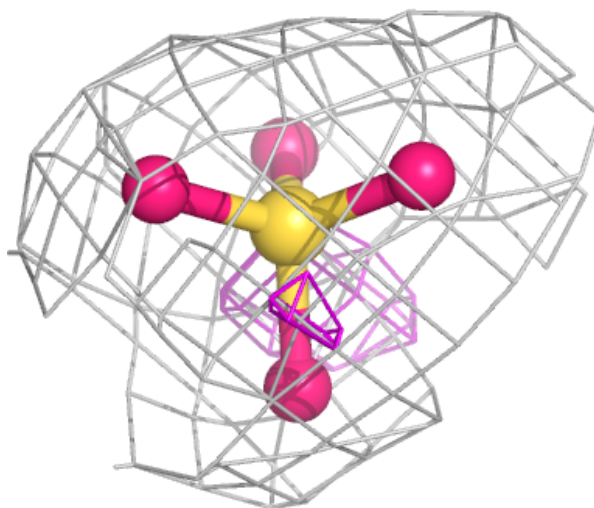
**Electron density around NAD AAA 802:**

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



Electron density around SO4 AAA 805:

$2mF_o - DF_c$ (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.