WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Dec 18, 2023 – 08:41 AM EST

PDB ID	:	1VRQ
Title	:	Crystal Structure of Heterotetrameric Sarcosine Oxidase from Corynebacterium sp. U-96 in complex with Folinic Acid
Authors	:	Ida, K.; Moriguchi, T.; Suzuki, H.
Deposited on	:	2005-04-27
Resolution	:	2.20 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), 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 ⓘ

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

The reported resolution of this entry is 2.20 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.
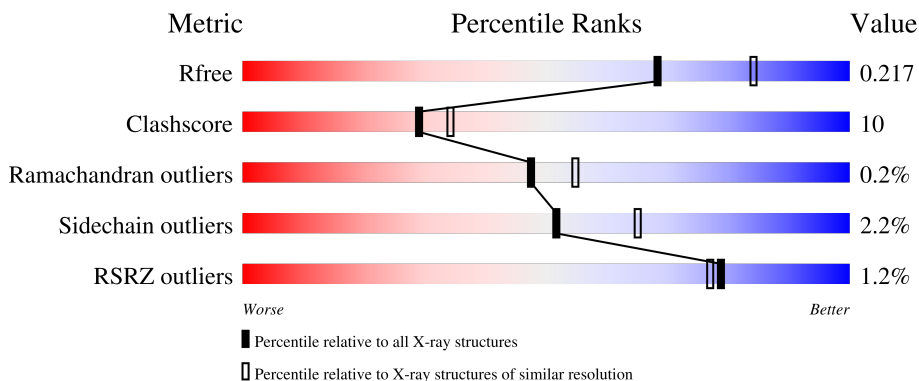
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	964	83% ... 16% ·
2	B	404	78% ... 21% ·
3	C	206	75% ... 19% ... 5%
4	D	99	84% ... 7% · 8%

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
10	DMG	B	1005	-	-	X	-
5	SO4	A	2002	-	-	X	-
9	FMN	B	1004	-	-	X	-

2 Entry composition ⓘ

There are 12 unique types of molecules in this entry. The entry contains 13880 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 Sarcosine oxidase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	963	Total	C	N	O	S	0	0	0
			7229	4507	1287	1413	22			

- Molecule 2 is a protein called Sarcosine oxidase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	0	0
			3093	1972	537	574	10			

- Molecule 3 is a protein called Sarcosine oxidase gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	195	Total	C	N	O	S	0	0	0
			1433	902	257	271	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	201	HIS	-	expression tag	UNP Q50LE9
C	202	HIS	-	expression tag	UNP Q50LE9
C	203	HIS	-	expression tag	UNP Q50LE9
C	204	HIS	-	expression tag	UNP Q50LE9
C	205	HIS	-	expression tag	UNP Q50LE9
C	206	HIS	-	expression tag	UNP Q50LE9

- Molecule 4 is a protein called Sarcosine oxidase delta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	91	Total	C	N	O	S	0	0	0
			749	476	135	133	5			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0
5	B	1	Total 5	O 4	S 1	0	0
5	B	1	Total 5	O 4	S 1	0	0
5	C	1	Total 5	O 4	S 1	0	0
5	D	1	Total 5	O 4	S 1	0	0
5	D	1	Total 5	O 4	S 1	0	0

- Molecule 6 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD)

(formula: $C_{21}H_{27}N_7O_{14}P_2$).

NAD
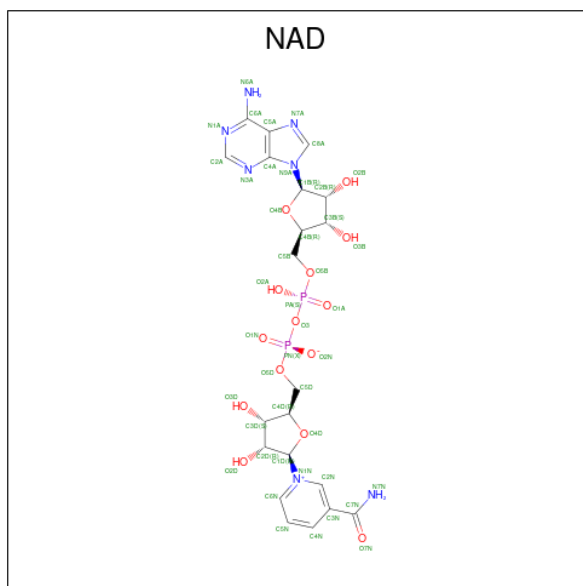
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	44	21	7	14	2	0	0

- Molecule 7 is N-{[4-({[(6R)-2-amino-5-formyl-4-oxo-1,4,5,6,7,8-hexahydropteridin-6-yl]methyl}amino)phenyl]carbonyl}-L-glutamic acid (three-letter code: FON) (formula: $C_{20}H_{23}N_7O_7$).
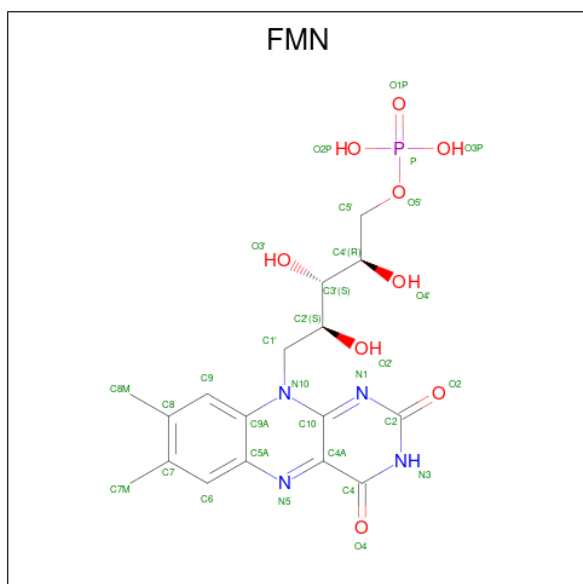

FON
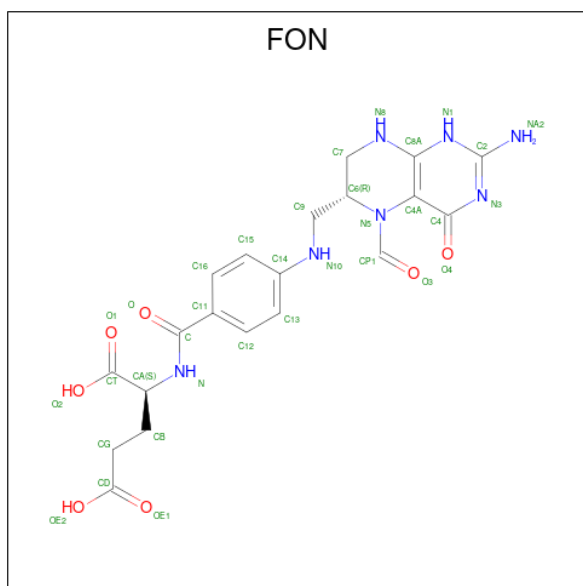
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	34	20	7	7	0	0

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).
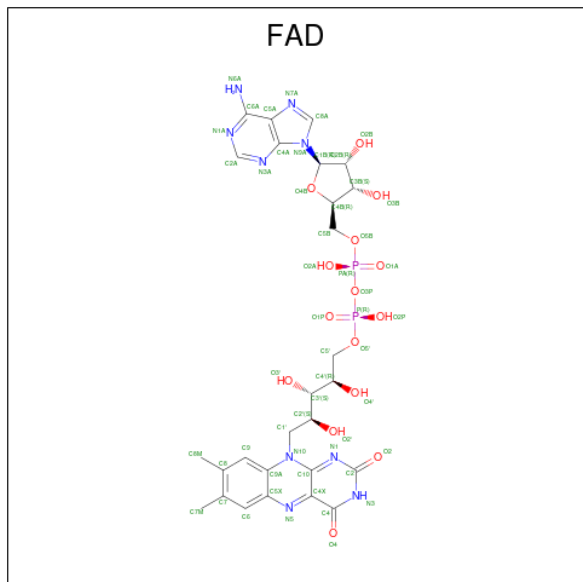
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	B	1	53	27	9	15	2	0	0

- Molecule 9 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	B	1	31	17	4	9	1	0	0

• Molecule 10 is N,N-DIMETHYLGLYCINE (three-letter code: DMG) (formula: $C_4H_9NO_2$).
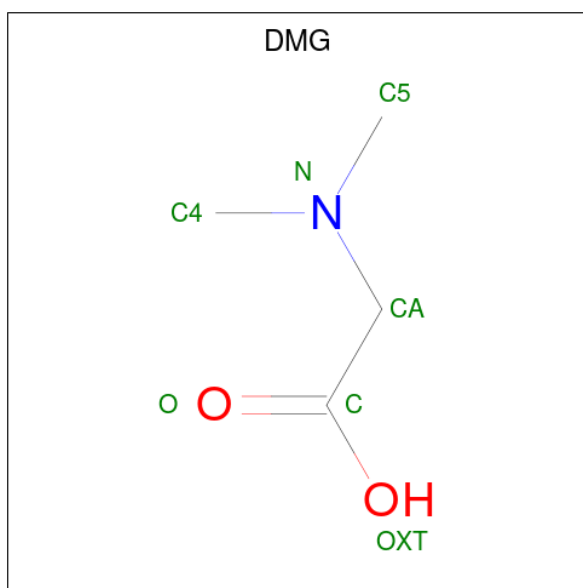
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	B	1	7	4	1	2	0	0

• Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
11	D	1	1	1	0	0

• Molecule 12 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	673	Total 673	O 673	0	0
12	B	229	Total 229	O 229	0	0
12	C	147	Total 147	O 147	0	0
12	D	92	Total 92	O 92	0	0

3 Residue-property plots ⓘ

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: Sarcosine oxidase alpha subunit
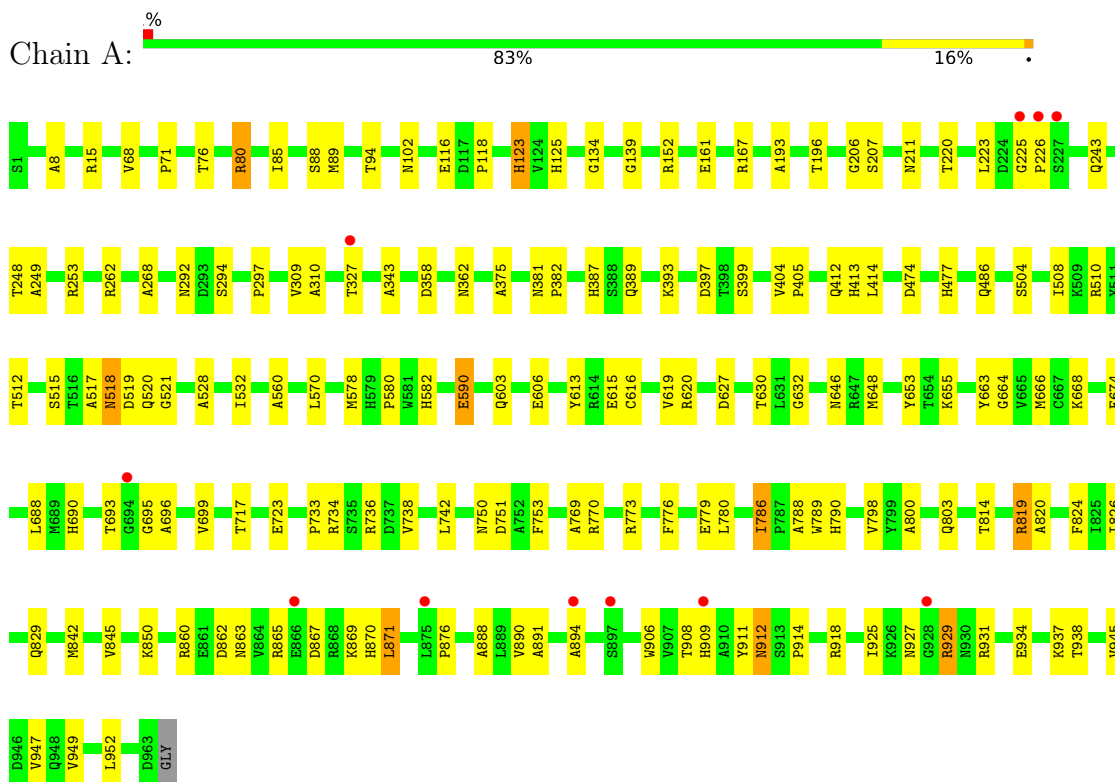
• Molecule 2: Sarcosine oxidase beta subunit
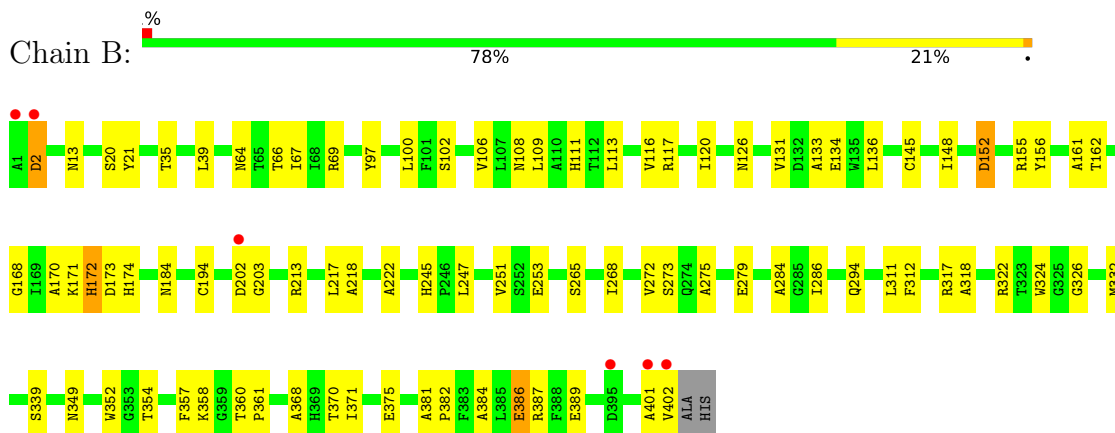
• Molecule 3: Sarcosine oxidase gamma subunit

Chain C:

• Molecule 4: Sarcosine oxidase delta subunit

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	199.40Å 199.40Å 197.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	99.50 – 2.20 99.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (99.50-2.20) 100.0 (99.70-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.04 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.192 , 0.224 0.185 , 0.217	Depositor DCC
R_{free} test set	11676 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13880	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: FMN, NAD, FAD, ZN, SO4, FON, DMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#|Z| > 5$	RMSZ	$\#|Z| > 5$
1	A	0.36	0/7361	0.58	0/10017
2	B	0.35	0/3173	0.57	1/4318 (0.0%)
3	C	0.38	0/1461	0.58	0/1998
4	D	0.38	0/772	0.57	0/1040
All	All	0.36	0/12767	0.57	1/17373 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	318	ALA	N-CA-C	-5.47	96.23	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7229	0	7104	148	0
2	B	3093	0	3023	70	0
3	C	1433	0	1434	26	0
4	D	749	0	706	6	0
5	A	40	0	0	4	0
5	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	5	0	0	0	0
5	D	10	0	0	0	0
6	A	44	0	26	5	0
7	A	34	0	21	7	0
8	B	53	0	31	7	0
9	B	31	0	19	10	0
10	B	7	0	8	7	0
11	D	1	0	0	0	0
12	A	673	0	0	14	0
12	B	229	0	0	5	0
12	C	147	0	0	1	0
12	D	92	0	0	1	0
All	All	13880	0	12372	242	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 242 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:HIS:NE2	9:B:1004:FMN:HM83	1.52	1.24
2:B:172:HIS:HE2	9:B:1004:FMN:C8M	1.63	1.09
10:B:1005:DMG:H43	10:B:1005:DMG:O	1.53	1.04
2:B:172:HIS:HE2	9:B:1004:FMN:HM83	0.90	1.01
1:A:819:ARG:HG2	1:A:824:PHE:HB2	1.50	0.91

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	A	961/964 (100%)	929 (97%)	31 (3%)	1 (0%)	51	60
2	B	400/404 (99%)	386 (96%)	12 (3%)	2 (0%)	29	31
3	C	193/206 (94%)	183 (95%)	9 (5%)	1 (0%)	29	31
4	D	89/99 (90%)	84 (94%)	5 (6%)	0	100	100
All	All	1643/1673 (98%)	1582 (96%)	57 (4%)	4 (0%)	47	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	401	ALA
3	C	199	VAL
1	A	71	PRO
2	B	203	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	A	747/747 (100%)	731 (98%)	16 (2%)	53	67
2	B	318/319 (100%)	310 (98%)	8 (2%)	47	60
3	C	143/154 (93%)	140 (98%)	3 (2%)	53	67
4	D	75/81 (93%)	74 (99%)	1 (1%)	69	81
All	All	1283/1301 (99%)	1255 (98%)	28 (2%)	52	65

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	912	ASN
4	D	90	GLN
2	B	97	TYR
3	C	94	ASN
2	B	2	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43

such sidechains are listed below:

Mol	Chain	Res	Type
2	B	14	ASN
2	B	349	ASN
2	B	111	HIS
2	B	266	ASN
3	C	102	GLN

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 ⓘ

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	$\#|Z| > 2$
5	SO4	B	2006	-	4,4,4	0.24	0	6,6,6	0.10	0
8	FAD	B	1001	-	53,58,58	1.16	2 (3%)	68,89,89	1.41	9 (13%)
9	FMN	B	1004	-	33,33,33	1.36	2 (6%)	48,50,50	1.40	9 (18%)
5	SO4	A	2009	-	4,4,4	0.27	0	6,6,6	0.08	0
5	SO4	A	2011	-	4,4,4	0.38	0	6,6,6	0.11	0
5	SO4	A	2013	-	4,4,4	0.38	0	6,6,6	0.12	0
5	SO4	D	2005	-	4,4,4	0.27	0	6,6,6	0.16	0
5	SO4	A	2010	-	4,4,4	0.29	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	SO4	A	2003	-	4,4,4	0.29	0	6,6,6	0.07	0
6	NAD	A	1002	-	42,48,48	1.51	5 (11%)	50,73,73	1.20	4 (8%)
7	FON	A	1003	-	34,36,36	2.19	11 (32%)	36,50,50	2.53	11 (30%)
5	SO4	A	2007	-	4,4,4	0.24	0	6,6,6	0.14	0
5	SO4	D	2012	-	4,4,4	0.38	0	6,6,6	0.11	0
5	SO4	C	2001	-	4,4,4	0.29	0	6,6,6	0.15	0
10	DMG	B	1005	-	6,6,6	1.10	0	7,7,7	1.39	0
5	SO4	A	2008	-	4,4,4	0.27	0	6,6,6	0.13	0
5	SO4	A	2002	-	4,4,4	0.20	0	6,6,6	0.17	0
5	SO4	B	2004	-	4,4,4	0.25	0	6,6,6	0.10	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
8	FAD	B	1001	-	-	3/30/50/50	0/6/6/6
9	FMN	B	1004	-	-	3/18/18/18	0/3/3/3
6	NAD	A	1002	-	-	5/26/62/62	0/5/5/5
7	FON	A	1003	-	-	3/24/37/37	0/2/3/3
10	DMG	B	1005	-	-	3/4/4/4	-

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1003	FON	C7-N8	7.88	1.58	1.44
6	A	1002	NAD	O7N-C7N	6.40	1.36	1.24
9	B	1004	FMN	C4A-N5	5.03	1.40	1.30
8	B	1001	FAD	C4X-N5	5.01	1.40	1.30
6	A	1002	NAD	C2N-N1N	4.74	1.40	1.35

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1003	FON	C8A-C4A-C4	6.98	119.90	114.44
7	A	1003	FON	C4A-N5-C6	-6.88	107.11	119.31
7	A	1003	FON	C6-C9-N10	-6.39	95.57	112.23
8	B	1001	FAD	N3A-C2A-N1A	-5.08	120.74	128.68
6	A	1002	NAD	N3A-C2A-N1A	-5.03	120.82	128.68

There are no chirality outliers.
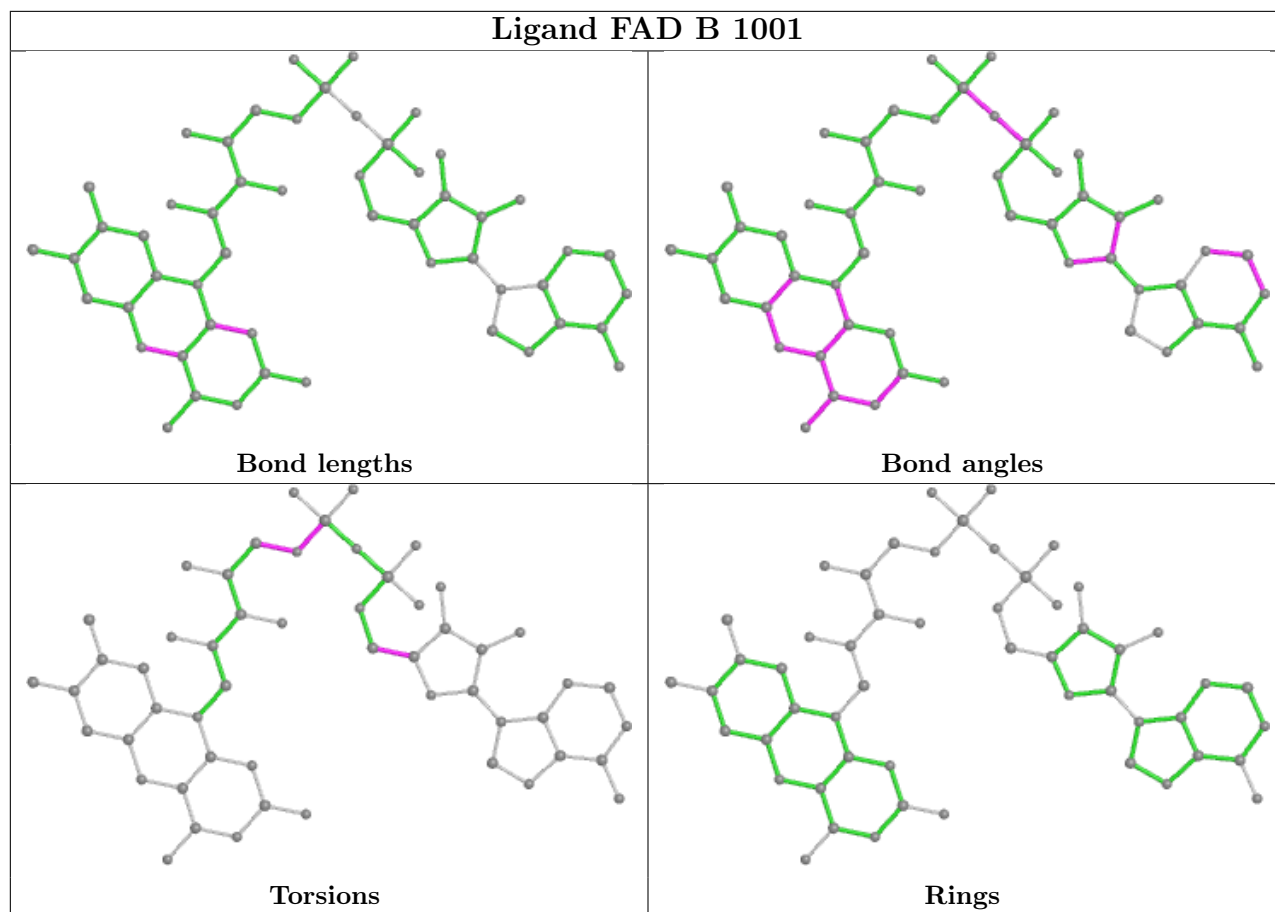
5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1002	NAD	C5D-O5D-PN-O1N
9	B	1004	FMN	C5'-O5'-P-O1P
9	B	1004	FMN	C5'-O5'-P-O2P
9	B	1004	FMN	C5'-O5'-P-O3P
7	A	1003	FON	N-CA-CT-O1

There are no ring outliers.

8 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1001	FAD	7	0
9	B	1004	FMN	10	0
5	A	2011	SO4	1	0
5	A	2013	SO4	1	0
6	A	1002	NAD	5	0
7	A	1003	FON	7	0
10	B	1005	DMG	7	0
5	A	2002	SO4	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 FAD B 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand FMN B 1004

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD A 1002

Bond lengths

Bond angles

Torsions

Rings

Ligand FON A 1003

Bond lengths

Bond angles

Torsions

Rings
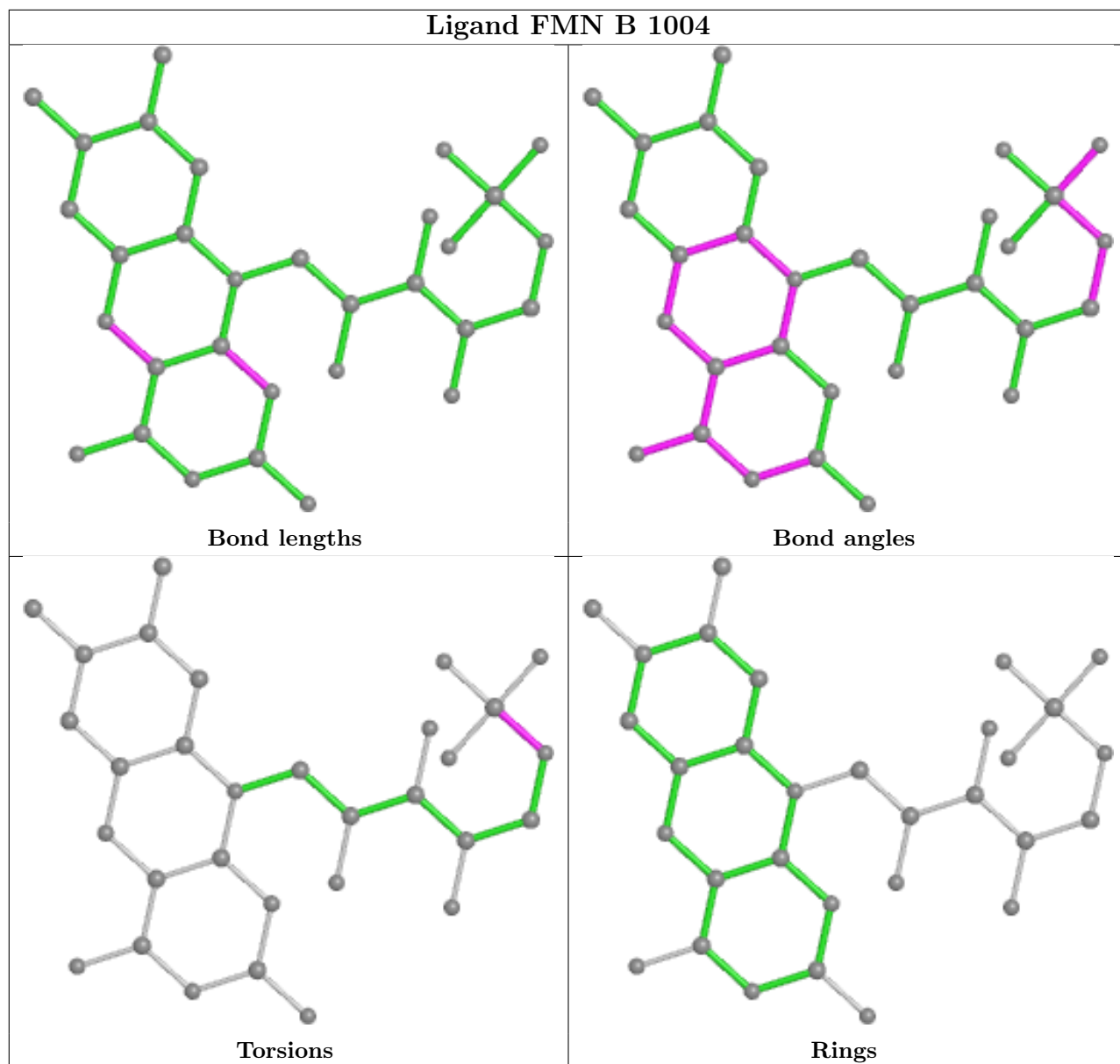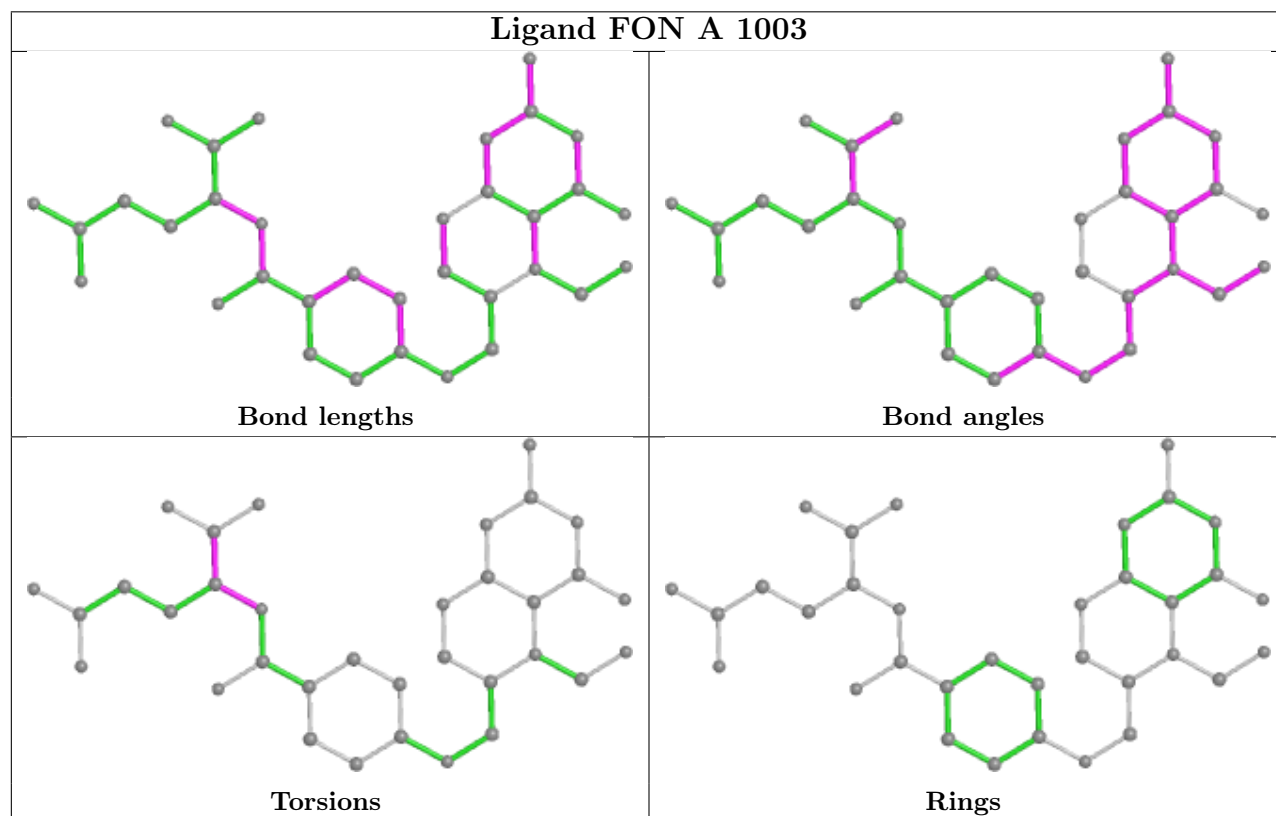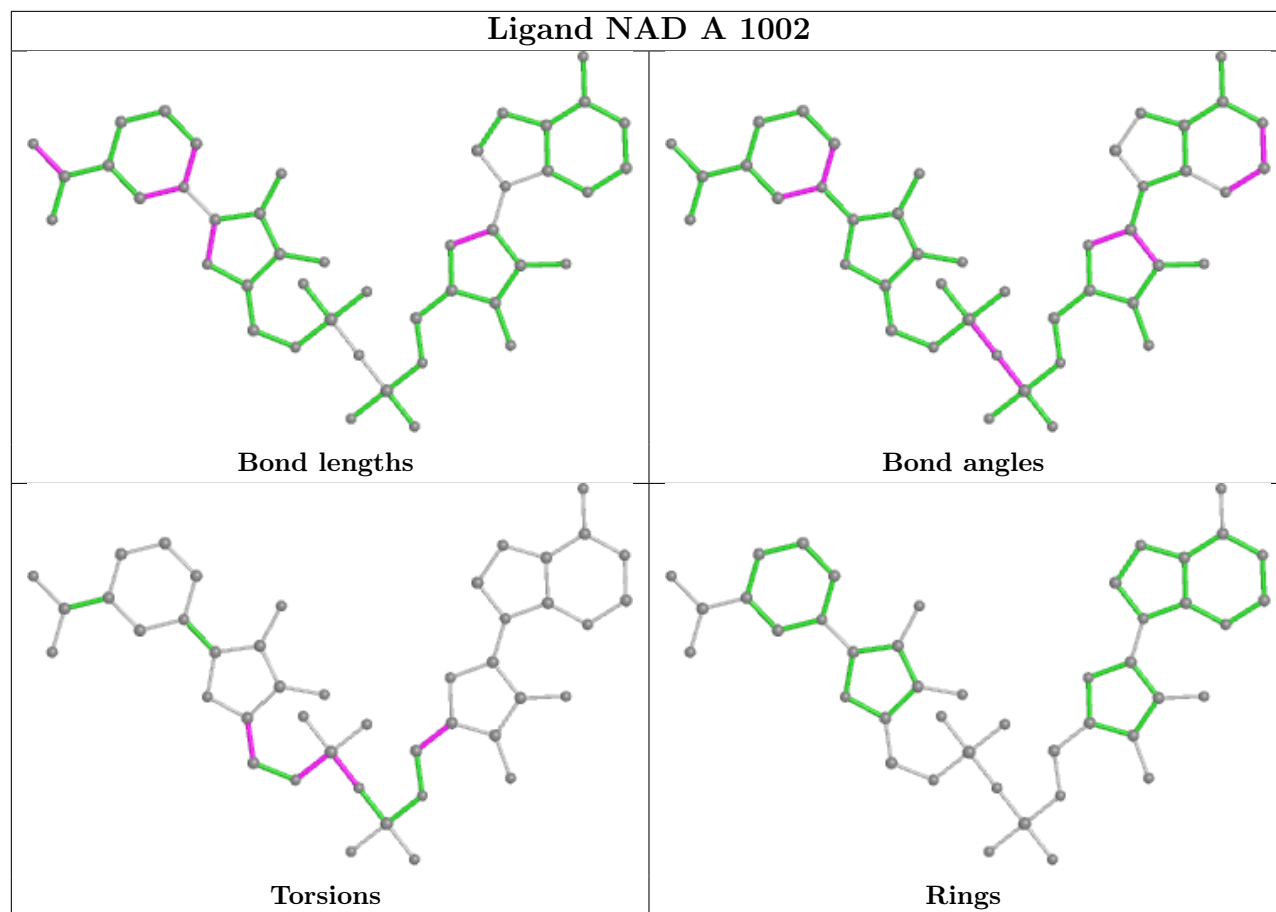
5.7 Other polymers ⓘ

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 ⓘ

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	A	963/964 (99%)	-0.41	11 (1%)	80	79	12, 26, 44, 66	0
2	B	402/404 (99%)	-0.45	6 (1%)	73	72	13, 26, 43, 71	0
3	C	195/206 (94%)	-0.50	2 (1%)	82	81	16, 23, 44, 71	0
4	D	91/99 (91%)	-0.52	0	100	100	15, 23, 43, 56	0
All	All	1651/1673 (98%)	-0.43	19 (1%)	79	77	12, 25, 44, 71	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	200	ALA	8.6
2	B	402	VAL	6.3
1	A	226	PRO	5.8
1	A	225	GLY	4.8
2	B	1	ALA	4.4

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

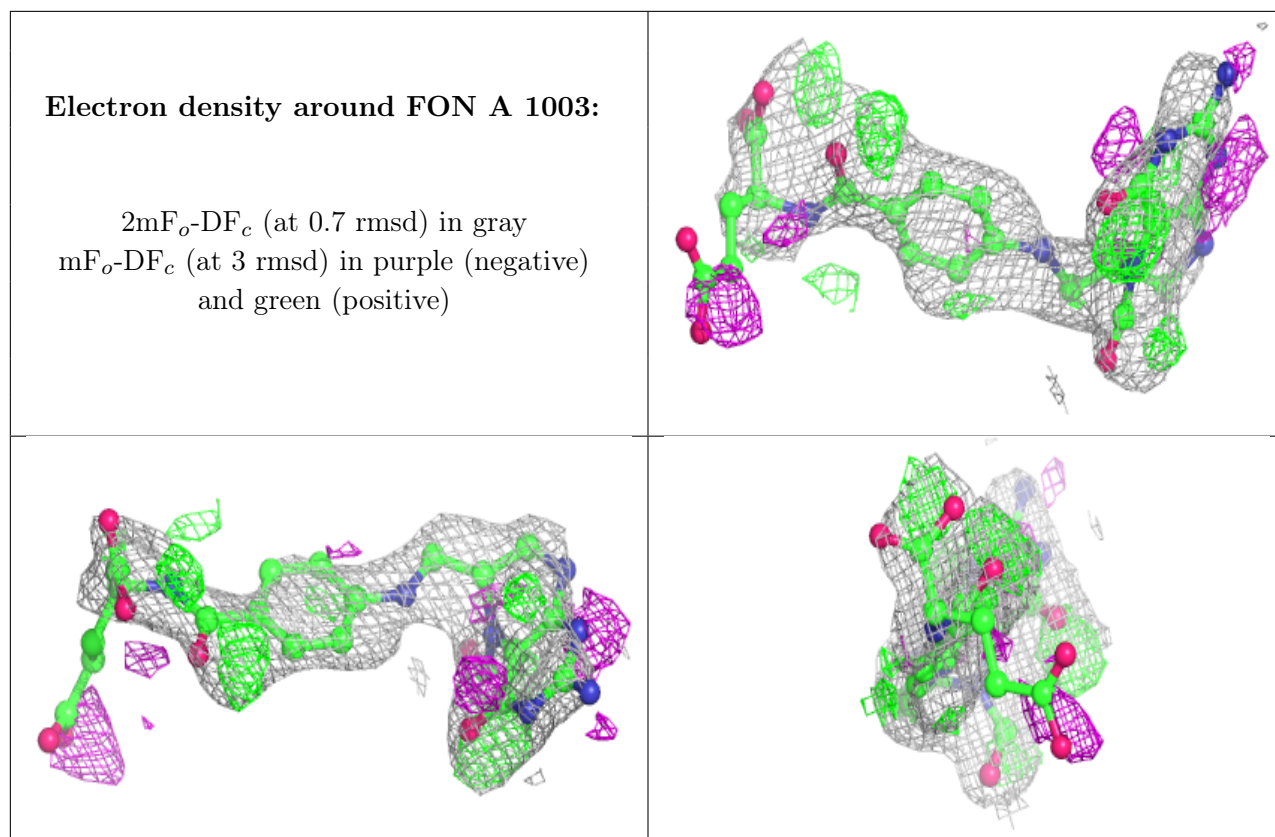There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å²)	Q<0.9
7	FON	A	1003	34/34	0.67	0.40	57,61,75,76	0
5	SO4	D	2012	5/5	0.72	0.36	85,86,86,88	0
5	SO4	A	2007	5/5	0.83	0.32	71,73,75,77	0
5	SO4	A	2010	5/5	0.87	0.36	81,81,81,82	0
5	SO4	D	2005	5/5	0.87	0.27	74,76,77,78	0
5	SO4	A	2013	5/5	0.88	0.30	74,76,77,77	0
5	SO4	A	2011	5/5	0.89	0.33	81,82,82,82	0
10	DMG	B	1005	7/7	0.89	0.23	52,53,54,54	0
5	SO4	A	2003	5/5	0.92	0.20	56,59,60,61	0
5	SO4	B	2006	5/5	0.92	0.14	72,73,74,74	0
9	FMN	B	1004	31/31	0.95	0.15	13,19,25,26	0
5	SO4	A	2008	5/5	0.95	0.20	66,66,67,68	0
8	FAD	B	1001	53/53	0.96	0.11	14,21,30,33	0
5	SO4	C	2001	5/5	0.96	0.17	53,54,55,57	0
5	SO4	A	2002	5/5	0.96	0.14	43,44,46,47	0
5	SO4	B	2004	5/5	0.97	0.08	69,69,70,70	0
6	NAD	A	1002	44/44	0.98	0.10	11,16,24,28	0
5	SO4	A	2009	5/5	0.99	0.08	47,49,51,52	0
11	ZN	D	1006	1/1	1.00	0.12	22,22,22,22	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.
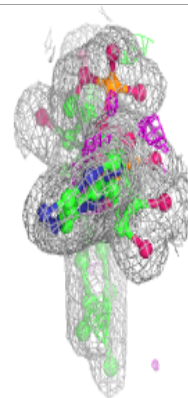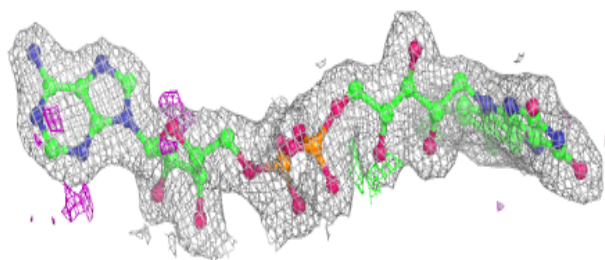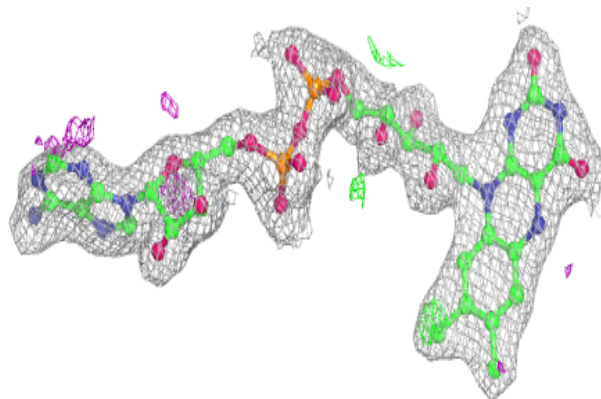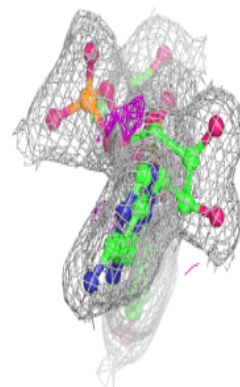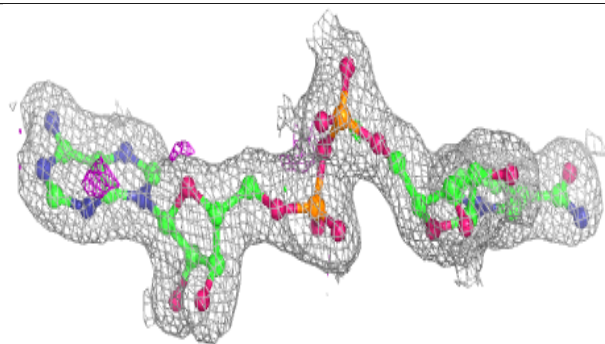
Electron density around FON A 1003:

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

Electron density around FMN B 1004:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
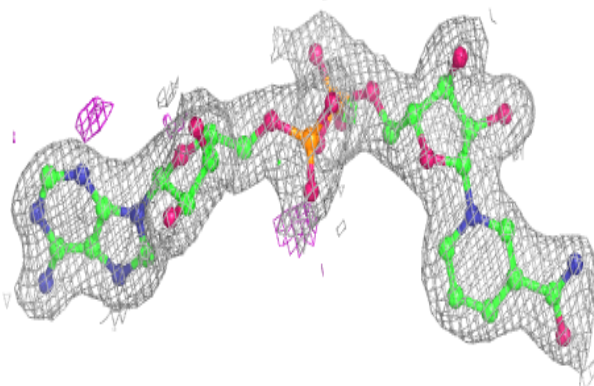and green (positive)
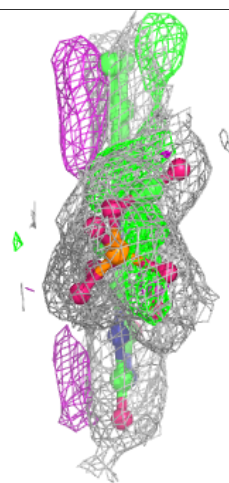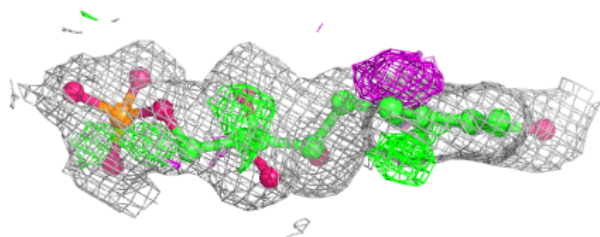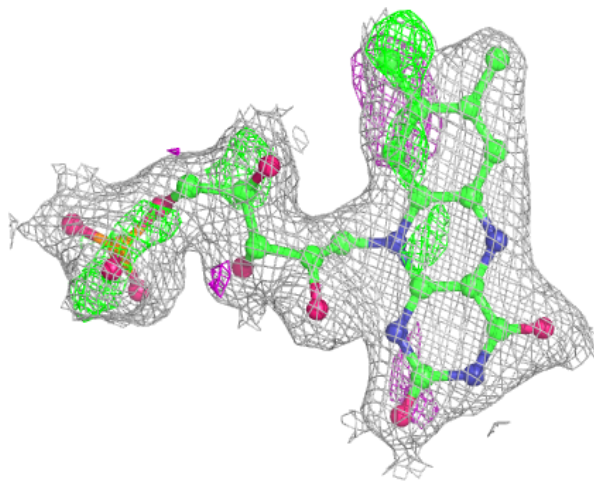
Electron density around FAD B 1001:

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

Electron density around NAD A 1002:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.