



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 07:56 am BST

PDB ID : 2GAG  
Title : Heterotetrameric sarcosine: structure of a diflavin metaloenzyme at 1.85 Å resolution  
Authors : Chen, Z.W.; Hassan-Abdulah, A.; Zhao, G.; Jorns, M.S.; Mathews, F.S.  
Deposited on : 2006-03-08  
Resolution : 1.85 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

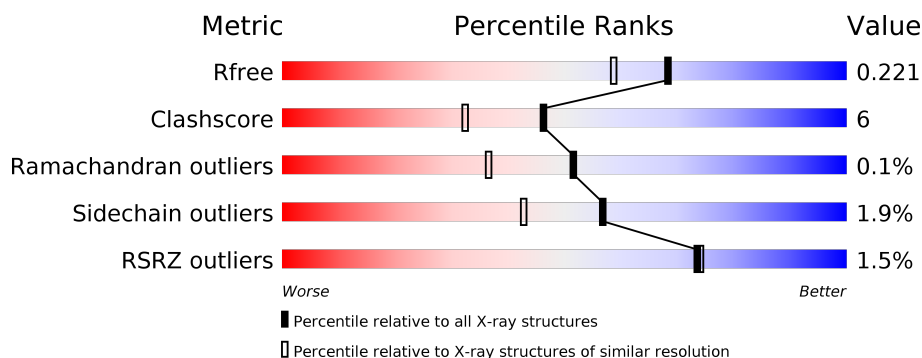
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	A	965	<div> <div>2%</div> <div>88% 11% .</div> </div>
2	B	405	<div> <div>3%</div> <div>83% 17%</div> </div>
3	C	210	<div> <div></div> <div>78% 12% 10%</div> </div>
4	D	99	<div> <div>2%</div> <div>80% 10% . 8%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	FMN	B	502	X	-	-	-
5	FOA	B	503	-	-	X	-

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 14136 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 heterotetrameric sarcosine oxidase alpha-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	965	Total	C	N	O	S	0	0	0
			7261	4520	1294	1428	19			

- Molecule 2 is a protein called heterotetrameric sarcosine oxidase beta-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	403	Total	C	N	O	S	0	0	0
			3098	1969	542	576	11			

- Molecule 3 is a protein called heterotetrameric sarcosine oxidase gamma-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	190	Total	C	N	O	S	0	0	0
			1396	877	248	266	5			

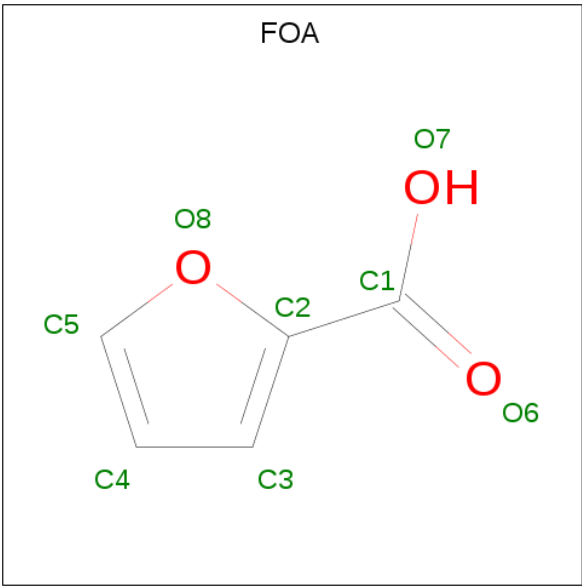
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	203	LEU	-	CLONING ARTIFACT	GB 63146667
C	204	GLU	-	CLONING ARTIFACT	GB 63146667
C	205	HIS	-	EXPRESSION TAG	GB 63146667
C	206	HIS	-	EXPRESSION TAG	GB 63146667
C	207	HIS	-	EXPRESSION TAG	GB 63146667
C	208	HIS	-	EXPRESSION TAG	GB 63146667
C	209	HIS	-	EXPRESSION TAG	GB 63146667
C	210	HIS	-	EXPRESSION TAG	GB 63146667

- Molecule 4 is a protein called heterotetrameric sarcosine oxidase delta-subunit.

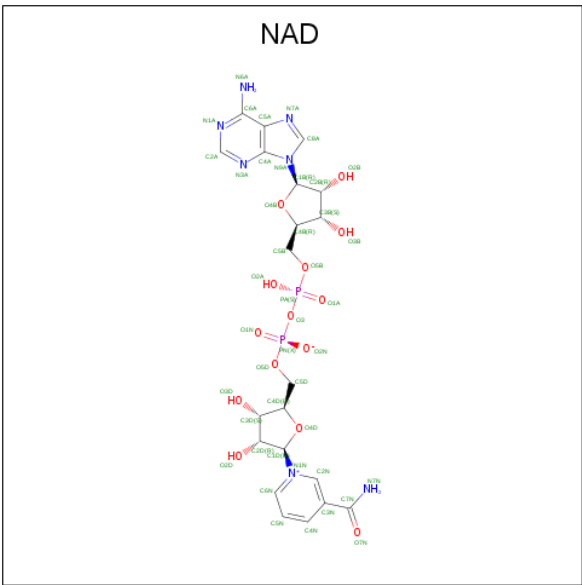
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	91	Total	C	N	O	S	0	0	0
			747	480	134	128	5			

- Molecule 5 is 2-FUROIC ACID (three-letter code: FOA) (formula: C<sub>5</sub>H<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	5	3		
5	B	1	Total	C	O	0	0
			8	5	3		

- Molecule 6 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



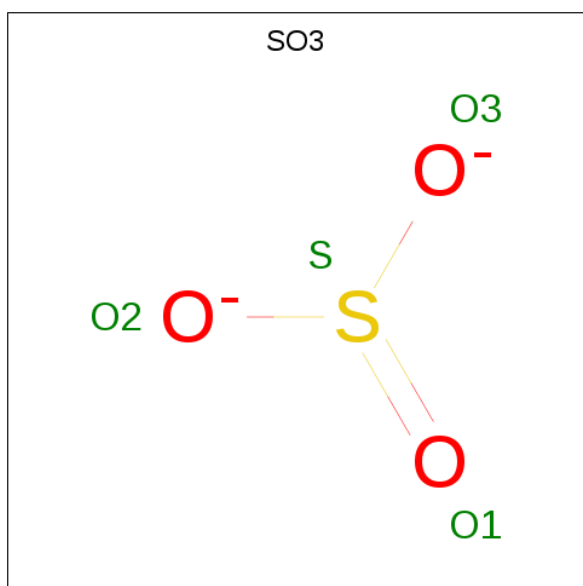
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



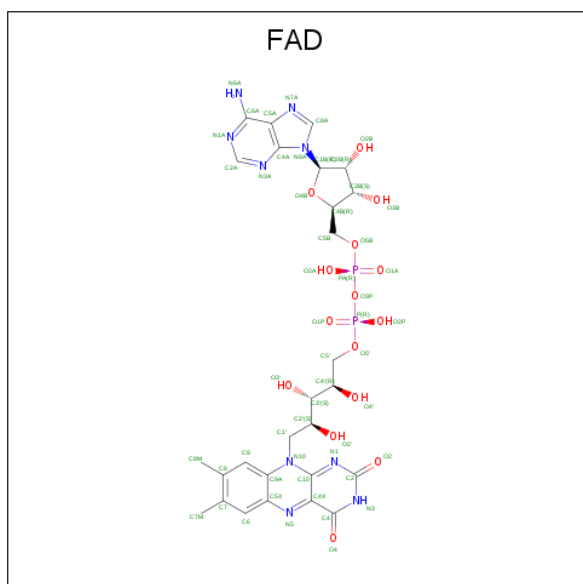
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is SULFITE ION (three-letter code: SO3) (formula:  $O_3S$ ).



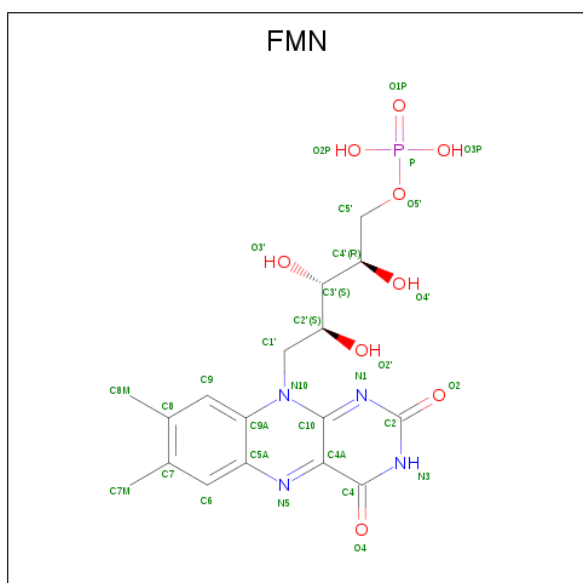
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	O	S	0	0
			4	3	1		

- Molecule 9 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 10 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



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

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

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

- Molecule 12 is water.

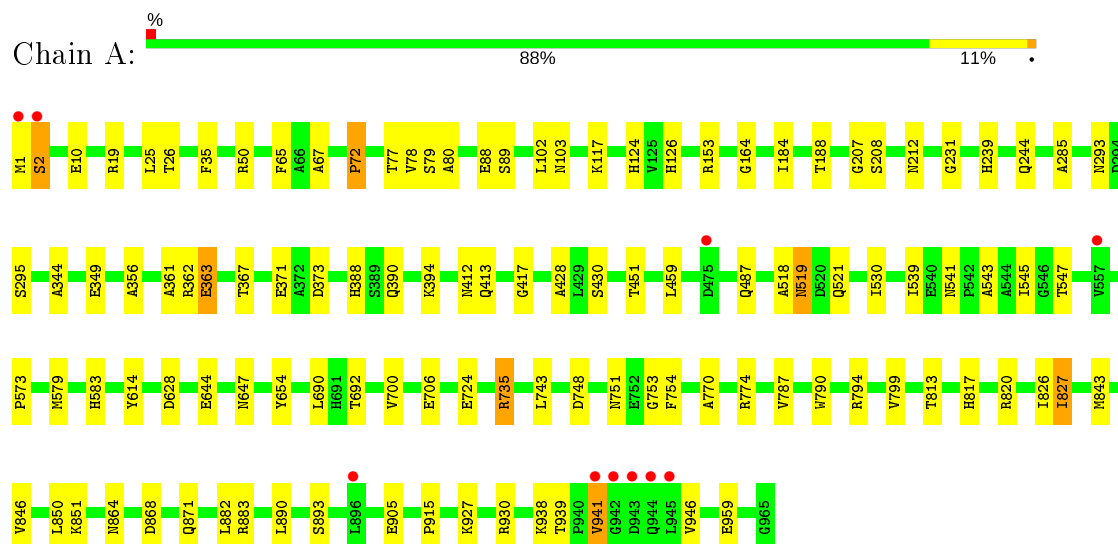
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	876	Total	O	0	0
			876	876		
12	B	313	Total	O	0	0
			313	313		
12	C	175	Total	O	0	0
			175	175		
12	D	115	Total	O	0	0
			115	115		



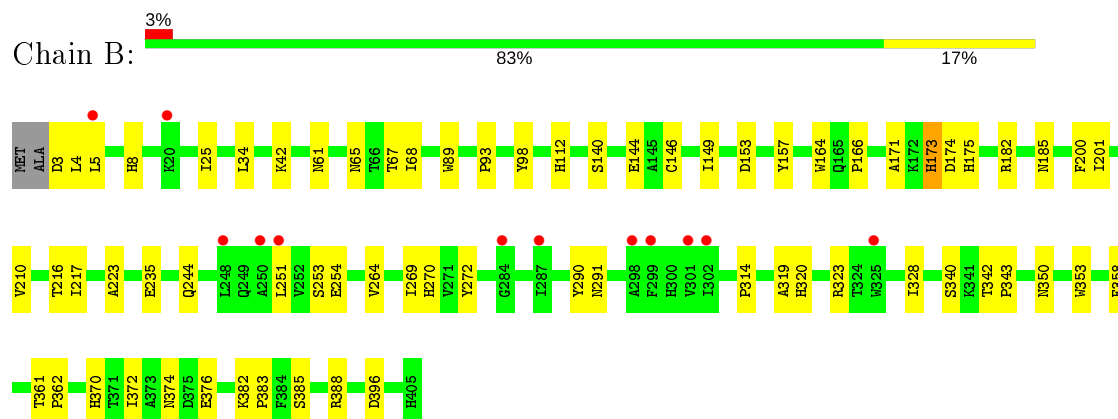
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

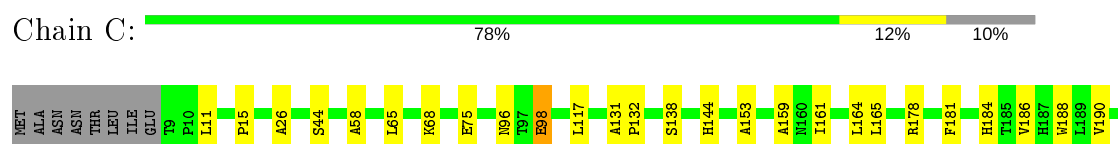
- Molecule 1: heterotetrameric sarcosine oxidase alpha-subunit

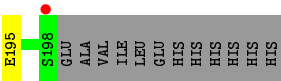


- Molecule 2: heterotetrameric sarcosine oxidase beta-subunit

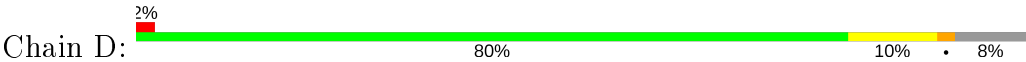


- Molecule 3: heterotetrameric sarcosine oxidase gamma-subunit





● Molecule 4: heterotetrameric sarcosine oxidase delta-subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.19Å 132.41Å 197.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.85 48.93 – 1.85	Depositor EDS
% Data completeness (in resolution range)	91.8 (40.00-1.85) 91.7 (48.93-1.85)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.82 (at 1.84Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.189 , 0.230 0.181 , 0.221	Depositor DCC
$R_{free}$ test set	7931 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.3	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 60.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14136	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: GOL, ZN, NAD, FMN, SO3, FOA, FAD

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	0.47	0/7389	0.71	1/10052 (0.0%)
2	B	0.47	0/3179	0.73	3/4323 (0.1%)
3	C	0.48	0/1426	0.70	1/1954 (0.1%)
4	D	0.56	0/773	0.73	0/1047
All	All	0.48	0/12767	0.71	5/17376 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	319	ALA	N-CA-C	-6.72	92.87	111.00
1	A	2	SER	N-CA-C	6.29	127.98	111.00
2	B	269	ILE	N-CA-C	-5.83	95.27	111.00
3	C	164	LEU	N-CA-C	-5.20	96.95	111.00
2	B	270	HIS	N-CA-C	5.16	124.93	111.00

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	A	7261	0	7143	91	0
2	B	3098	0	3013	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1396	0	1385	17	0
4	D	747	0	710	10	0
5	A	8	0	3	0	0
5	B	8	0	3	4	0
6	A	44	0	26	0	0
7	A	6	0	8	1	0
8	B	4	0	0	1	0
9	B	53	0	31	2	0
10	B	31	0	15	1	0
11	D	1	0	0	0	0
12	A	876	0	0	12	0
12	B	313	0	0	5	0
12	C	175	0	0	1	0
12	D	115	0	0	0	0
All	All	14136	0	12337	157	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.

All (157) 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:A:1:MET:HB3	1:A:285:ALA:HB3	1.47	0.94
1:A:647:ASN:HD21	1:A:654:TYR:H	1.16	0.94
2:B:173:HIS:HD1	2:B:174:ASP:H	1.21	0.88
2:B:350:ASN:HD21	2:B:353:TRP:HE1	1.26	0.82
2:B:61:ASN:HD21	2:B:328:ILE:H	1.30	0.80
1:A:78:VAL:HG13	1:A:102:LEU:HD11	1.66	0.76
2:B:42:LYS:O	2:B:42:LYS:HD3	1.85	0.76
1:A:2:SER:HB3	12:A:2433:HOH:O	1.88	0.74
1:A:820:ARG:HD3	1:A:827:ILE:HD13	1.70	0.74
1:A:117:LYS:HG3	12:A:2016:HOH:O	1.89	0.72
2:B:350:ASN:ND2	2:B:353:TRP:HE1	1.89	0.71
1:A:88:GLU:OE2	2:B:320:HIS:HE1	1.75	0.69
1:A:207:GLY:HA2	1:A:390:GLN:HE22	1.59	0.68
12:A:2006:HOH:O	3:C:184:HIS:HD2	1.76	0.67
1:A:244:GLN:HE22	1:A:412:ASN:HD22	1.43	0.67
2:B:254:GLU:OE2	2:B:320:HIS:HD2	1.78	0.65
2:B:173:HIS:HD1	2:B:174:ASP:N	1.94	0.63
1:A:751:ASN:ND2	1:A:774:ARG:HH12	1.96	0.63
2:B:68:ILE:HD12	5:B:503:FOA:H3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:ARG:HD3	1:A:827:ILE:CD1	2.28	0.62
2:B:374:ASN:HB3	2:B:376:GLU:HG2	1.82	0.61
1:A:244:GLN:HE22	1:A:412:ASN:ND2	1.98	0.61
1:A:521:GLN:HE22	2:B:323:ARG:HD2	1.65	0.61
2:B:182:ARG:HD3	12:B:2444:HOH:O	1.99	0.61
2:B:140:SER:O	2:B:144:GLU:HG3	2.00	0.61
1:A:124:HIS:ND1	1:A:239:HIS:HE1	1.98	0.61
1:A:647:ASN:HD21	1:A:654:TYR:N	1.95	0.61
1:A:293:ASN:HD22	1:A:295:SER:H	1.48	0.60
1:A:388:HIS:HE1	1:A:394:LYS:O	1.84	0.60
12:A:2016:HOH:O	2:B:314:PRO:HB3	2.02	0.60
1:A:67:ALA:HB3	7:A:998:GOL:H31	1.85	0.59
1:A:735:ARG:HH21	1:A:735:ARG:HA	1.67	0.59
1:A:541:ASN:HD21	1:A:543:ALA:HB3	1.69	0.58
1:A:794:ARG:NH1	3:C:11:LEU:HD23	2.19	0.58
1:A:871:GLN:HE21	1:A:930:ARG:H	1.51	0.58
1:A:539:ILE:CD1	1:A:545:ILE:HD11	2.33	0.58
1:A:817:HIS:HE1	12:A:1630:HOH:O	1.87	0.57
2:B:112:HIS:HD2	2:B:157:TYR:O	1.87	0.57
2:B:340:SER:HB2	12:B:1249:HOH:O	2.04	0.57
1:A:212:ASN:ND2	1:A:413:GLN:HE21	2.03	0.56
2:B:42:LYS:C	2:B:42:LYS:HD3	2.25	0.56
1:A:770:ALA:HB2	1:A:787:VAL:HG12	1.88	0.55
2:B:272:TYR:CE1	5:B:503:FOA:H4	2.41	0.55
1:A:126:HIS:HD2	12:A:1008:HOH:O	1.90	0.55
1:A:208:SER:H	1:A:390:GLN:NE2	2.05	0.55
1:A:1:MET:O	1:A:285:ALA:HB3	2.06	0.54
3:C:96:ASN:OD1	3:C:98:GLU:HG3	2.07	0.54
1:A:871:GLN:NE2	1:A:930:ARG:H	2.05	0.54
1:A:363:GLU:HG2	12:A:2025:HOH:O	2.08	0.54
1:A:743:LEU:HD11	1:A:799:VAL:HG22	1.89	0.54
1:A:487:GLN:NE2	1:A:518:ALA:HB1	2.23	0.54
2:B:254:GLU:OE2	2:B:320:HIS:CD2	2.60	0.54
1:A:583:HIS:HE1	1:A:628:ASP:OD2	1.91	0.53
1:A:2:SER:HA	1:A:373:ASP:OD2	2.09	0.53
2:B:201:ILE:HD11	2:B:216:THR:HG23	1.90	0.53
1:A:647:ASN:ND2	1:A:654:TYR:H	1.98	0.53
1:A:843:MET:O	1:A:846:VAL:HG12	2.09	0.53
1:A:188:THR:HG21	12:A:1979:HOH:O	2.08	0.53
1:A:826:ILE:O	1:A:827:ILE:HD12	2.09	0.53
1:A:868:ASP:HB2	1:A:927:LYS:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ARG:HD3	3:C:144:HIS:CD2	2.44	0.52
1:A:724:GLU:HG3	3:C:178:ARG:HD2	1.91	0.52
1:A:539:ILE:HD12	1:A:545:ILE:HD11	1.91	0.52
1:A:751:ASN:HD22	1:A:774:ARG:HH12	1.57	0.52
8:B:504:SO3:S	10:B:502:FMN:N5	2.83	0.52
1:A:541:ASN:ND2	1:A:543:ALA:HB3	2.25	0.51
1:A:692:THR:HG21	1:A:700:VAL:HG11	1.92	0.51
2:B:290:TYR:HA	4:D:19:TYR:CD2	2.45	0.50
4:D:90:GLU:HG3	4:D:91:ILE:HG12	1.93	0.50
1:A:882:LEU:C	1:A:882:LEU:HD23	2.32	0.50
2:B:251:LEU:HD12	2:B:251:LEU:C	2.33	0.49
2:B:361:THR:HB	2:B:362:PRO:HD3	1.94	0.49
2:B:358:PHE:HB3	9:B:501:FAD:C2	2.42	0.49
4:D:90:GLU:O	4:D:90:GLU:HG3	2.12	0.49
1:A:1:MET:HB3	1:A:285:ALA:CB	2.31	0.49
1:A:1:MET:CB	1:A:285:ALA:HB3	2.32	0.48
1:A:519:ASN:ND2	1:A:519:ASN:C	2.67	0.48
1:A:893:SER:HB2	1:A:938:LYS:NZ	2.28	0.48
2:B:146:CYS:SG	2:B:149:ILE:HG13	2.55	0.47
3:C:159:ALA:O	3:C:184:HIS:HE1	1.97	0.47
2:B:25:ILE:HD11	2:B:217:ILE:HG22	1.96	0.47
1:A:293:ASN:ND2	1:A:295:SER:H	2.11	0.47
4:D:47:GLN:OE1	4:D:49:LYS:HE3	2.15	0.46
2:B:3:ASP:O	2:B:5:LEU:HD12	2.14	0.46
1:A:735:ARG:HA	1:A:735:ARG:NH2	2.31	0.46
1:A:1:MET:O	1:A:285:ALA:CB	2.64	0.46
4:D:56:ARG:HG2	4:D:68:ASN:ND2	2.30	0.46
2:B:244:GLN:NE2	2:B:291:ASN:HD21	2.13	0.46
2:B:385:SER:O	2:B:388:ARG:HG2	2.16	0.46
1:A:65:PHE:HB3	1:A:72:PRO:HD2	1.98	0.46
1:A:813:THR:O	1:A:817:HIS:CD2	2.69	0.46
2:B:382:LYS:N	2:B:383:PRO:CD	2.79	0.45
1:A:539:ILE:HD13	1:A:545:ILE:HD11	1.98	0.45
2:B:65:ASN:HA	9:B:501:FAD:C6	2.47	0.45
2:B:67:THR:HB	2:B:171:ALA:O	2.16	0.45
1:A:388:HIS:HD2	12:A:1037:HOH:O	1.99	0.45
3:C:44:SER:HB2	3:C:117:LEU:HD12	1.98	0.45
2:B:370:HIS:HD2	12:B:2101:HOH:O	1.99	0.45
1:A:231:GLY:O	3:C:195:GLU:HB2	2.16	0.45
4:D:59:HIS:CE1	4:D:62:GLY:HA3	2.52	0.45
2:B:164:TRP:NE1	2:B:166:PRO:HG3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:THR:CB	12:A:2407:HOH:O	2.66	0.44
3:C:58:ALA:HA	3:C:65:LEU:HG	1.99	0.44
1:A:706:GLU:HG3	4:D:66:TRP:CZ2	2.53	0.44
2:B:342:THR:HB	2:B:343:PRO:CD	2.48	0.44
1:A:50:ARG:HH11	1:A:50:ARG:HG3	1.82	0.44
1:A:77:THR:HA	1:A:89:SER:HA	1.98	0.44
1:A:905:GLU:O	1:A:927:LYS:HG3	2.17	0.44
1:A:361:ALA:O	1:A:362:ARG:HB2	2.18	0.43
1:A:864:ASN:HB2	12:A:2032:HOH:O	2.18	0.43
1:A:530:ILE:HD11	1:A:547:THR:HA	2.00	0.43
1:A:344:ALA:HA	1:A:349:GLU:O	2.19	0.43
1:A:417:GLY:HA2	1:A:428:ALA:HA	2.01	0.43
2:B:8:HIS:HE1	2:B:175:HIS:CE1	2.36	0.43
2:B:185:ASN:ND2	12:B:2012:HOH:O	2.51	0.43
2:B:272:TYR:CD1	5:B:503:FOA:H4	2.54	0.43
1:A:941:VAL:HG11	1:A:946:VAL:CG2	2.49	0.43
1:A:573:PRO:HA	3:C:184:HIS:CD2	2.54	0.42
3:C:26:ALA:HB2	3:C:190:VAL:HG13	2.01	0.42
4:D:4:ILE:HB	4:D:17:PHE:CE2	2.54	0.42
1:A:164:GLY:HA3	1:A:184:ILE:HD13	2.02	0.42
3:C:161:ILE:HD13	3:C:181:PHE:HB3	2.01	0.42
2:B:201:ILE:HD11	2:B:216:THR:CG2	2.49	0.42
2:B:235:GLU:OE1	4:D:49:LYS:HE2	2.19	0.42
1:A:430:SER:HA	1:A:451:THR:HG23	2.01	0.42
1:A:941:VAL:HG13	1:A:946:VAL:HG13	2.01	0.42
3:C:186:VAL:O	3:C:190:VAL:HG23	2.20	0.42
2:B:68:ILE:HD12	5:B:503:FOA:C3	2.49	0.42
3:C:15:PRO:HG3	12:C:1062:HOH:O	2.19	0.42
1:A:356:ALA:HB2	1:A:367:THR:HG22	2.02	0.42
1:A:212:ASN:HD21	1:A:413:GLN:HE21	1.67	0.42
1:A:692:THR:HB	12:A:2407:HOH:O	2.20	0.42
2:B:149:ILE:HD11	2:B:264:VAL:HG21	2.01	0.42
1:A:487:GLN:HE22	1:A:519:ASN:H	1.67	0.42
1:A:890:LEU:HD23	1:A:939:THR:HB	2.01	0.42
2:B:200:PHE:CD1	2:B:210:VAL:HG12	2.55	0.42
1:A:79:SER:O	1:A:80:ALA:C	2.59	0.41
2:B:253:SER:HA	2:B:320:HIS:O	2.21	0.41
1:A:690:LEU:N	1:A:690:LEU:HD12	2.35	0.41
3:C:138:SER:HB3	3:C:188:TRP:CZ2	2.55	0.41
1:A:614:TYR:CZ	1:A:915:PRO:HB3	2.56	0.41
2:B:89:TRP:O	2:B:93:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:THR:HB	1:A:103:ASN:HD22	1.85	0.41
1:A:820:ARG:HD2	1:A:820:ARG:C	2.40	0.41
1:A:850:LEU:HA	1:A:850:LEU:HD23	1.82	0.41
1:A:748:ASP:OD2	1:A:753:GLY:HA3	2.21	0.41
1:A:941:VAL:HG22	1:A:941:VAL:O	2.19	0.41
2:B:374:ASN:CB	2:B:376:GLU:HG2	2.50	0.41
3:C:153:ALA:HA	3:C:165:LEU:O	2.21	0.41
1:A:19:ARG:HA	1:A:35:PHE:CD1	2.55	0.41
1:A:743:LEU:CD1	1:A:799:VAL:HG22	2.50	0.41
2:B:223:ALA:HB2	2:B:372:ILE:HD11	2.03	0.41
3:C:131:ALA:HB3	3:C:132:PRO:HD3	2.01	0.41
4:D:49:LYS:HA	4:D:49:LYS:HD3	1.92	0.41
1:A:941:VAL:CG1	1:A:946:VAL:HG22	2.51	0.40
1:A:459:LEU:HD12	1:A:459:LEU:HA	1.79	0.40
2:B:153:ASP:HB3	12:B:1747:HOH:O	2.21	0.40

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	963/965 (100%)	934 (97%)	28 (3%)	1 (0%)	51	36
2	B	401/405 (99%)	385 (96%)	16 (4%)	0	100	100
3	C	188/210 (90%)	181 (96%)	7 (4%)	0	100	100
4	D	89/99 (90%)	86 (97%)	3 (3%)	0	100	100
All	All	1641/1679 (98%)	1586 (97%)	54 (3%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	PRO

### 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	749/749 (100%)	734 (98%)	15 (2%)	55	40
2	B	319/320 (100%)	314 (98%)	5 (2%)	62	49
3	C	143/161 (89%)	140 (98%)	3 (2%)	53	38
4	D	74/79 (94%)	72 (97%)	2 (3%)	44	29
All	All	1285/1309 (98%)	1260 (98%)	25 (2%)	57	43

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	25	LEU
1	A	363	GLU
1	A	371	GLU
1	A	519	ASN
1	A	579	MET
1	A	644	GLU
1	A	735	ARG
1	A	754	PHE
1	A	790	TRP
1	A	827	ILE
1	A	851	LYS
1	A	883	ARG
1	A	941	VAL
1	A	959	GLU
2	B	4	LEU
2	B	34	LEU
2	B	98	TYR
2	B	173	HIS
2	B	396	ASP
3	C	68	LYS

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Mol	Chain	Res	Type
3	C	75	GLU
3	C	98	GLU
4	D	90	GLU
4	D	91	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	126	HIS
1	A	201	GLN
1	A	212	ASN
1	A	239	HIS
1	A	260	ASN
1	A	277	ASN
1	A	293	ASN
1	A	382	ASN
1	A	388	HIS
1	A	390	GLN
1	A	412	ASN
1	A	487	GLN
1	A	519	ASN
1	A	521	GLN
1	A	583	HIS
1	A	647	ASN
1	A	751	ASN
1	A	817	HIS
1	A	830	GLN
1	A	871	GLN
1	A	916	ASN
2	B	15	ASN
2	B	44	HIS
2	B	61	ASN
2	B	109	ASN
2	B	112	HIS
2	B	127	ASN
2	B	185	ASN
2	B	244	GLN
2	B	249	GLN
2	B	260	HIS
2	B	320	HIS
2	B	350	ASN

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Mol	Chain	Res	Type
2	B	370	HIS
2	B	374	ASN
2	B	393	HIS
3	C	77	GLN
3	C	184	HIS
3	C	187	HIS
4	D	68	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	NAD	A	999	-	42,48,48	2.62	17 (40%)	50,73,73	2.10	11 (22%)
8	SO3	B	504	-	1,3,3	0.65	0	0,3,3	0.00	-
5	FOA	B	503	-	1,8,8	0.01	0	1,10,10	1.41	0
9	FAD	B	501	-	51,58,58	3.13	21 (41%)	60,89,89	2.20	14 (23%)
5	FOA	A	997	-	1,8,8	0.54	0	1,10,10	1.58	0
7	GOL	A	998	-	5,5,5	0.35	0	5,5,5	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	FMN	B	502	2	31,33,33	3.74	12 (38%)	40,50,50	4.19	23 (57%)

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
6	NAD	A	999	-	-	4/26/62/62	0/5/5/5
5	FOA	B	503	-	-	0/0/4/4	0/1/1/1
9	FAD	B	501	-	-	3/30/50/50	0/6/6/6
5	FOA	A	997	-	-	0/0/4/4	0/1/1/1
7	GOL	A	998	-	-	4/4/4/4	-
10	FMN	B	502	2	1/1/4/4	6/18/18/18	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	502	FMN	C4A-C10	12.76	1.51	1.38
9	B	501	FAD	C4X-C10	9.46	1.48	1.38
6	A	999	NAD	C4A-N3A	7.42	1.45	1.35
10	B	502	FMN	C9A-C5A	7.36	1.57	1.42
10	B	502	FMN	C4A-N5	6.39	1.42	1.33
9	B	501	FAD	C5X-N5	5.90	1.45	1.35
9	B	501	FAD	C10-N1	5.62	1.40	1.33
10	B	502	FMN	C2-N3	5.61	1.49	1.38
10	B	502	FMN	C8-C7	5.59	1.54	1.40
9	B	501	FAD	C9A-N10	5.43	1.45	1.38
9	B	501	FAD	C4-N3	5.31	1.42	1.33
10	B	502	FMN	C4-N3	5.25	1.42	1.33
9	B	501	FAD	C2A-N3A	5.16	1.40	1.32
6	A	999	NAD	C2N-N1N	5.14	1.41	1.35
9	B	501	FAD	C4A-N3A	5.12	1.42	1.35
9	B	501	FAD	C4X-N5	5.01	1.40	1.33
9	B	501	FAD	P-O5'	-4.98	1.39	1.59
6	A	999	NAD	C2A-N1A	4.82	1.42	1.33
9	B	501	FAD	C6-C5X	4.79	1.49	1.41
6	A	999	NAD	O4B-C1B	4.76	1.47	1.41
9	B	501	FAD	C8-C7	4.70	1.52	1.40
9	B	501	FAD	C2A-N1A	4.66	1.42	1.33
9	B	501	FAD	O5B-C5B	-4.63	1.26	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	999	NAD	O4D-C1D	4.41	1.47	1.41
10	B	502	FMN	C1'-N10	4.29	1.52	1.48
6	A	999	NAD	C2D-C1D	3.93	1.59	1.53
6	A	999	NAD	C2A-N3A	3.78	1.38	1.32
6	A	999	NAD	C6N-C5N	3.76	1.47	1.38
10	B	502	FMN	C9A-N10	3.74	1.43	1.38
6	A	999	NAD	C6N-N1N	3.62	1.44	1.35
9	B	501	FAD	C2B-C1B	3.52	1.59	1.53
9	B	501	FAD	C8M-C8	-3.35	1.44	1.51
9	B	501	FAD	C5'-C4'	3.30	1.56	1.51
10	B	502	FMN	C1'-C2'	-3.10	1.31	1.50
6	A	999	NAD	C2N-C3N	3.01	1.43	1.39
6	A	999	NAD	C4N-C3N	2.90	1.44	1.39
6	A	999	NAD	C2B-C1B	-2.87	1.49	1.53
10	B	502	FMN	C4'-C3'	-2.87	1.48	1.53
9	B	501	FAD	C6-C7	2.83	1.44	1.37
6	A	999	NAD	C5D-C4D	-2.61	1.43	1.51
6	A	999	NAD	C3N-C7N	2.60	1.54	1.50
6	A	999	NAD	O5B-C5B	2.58	1.54	1.44
9	B	501	FAD	C9A-C5X	2.52	1.47	1.42
9	B	501	FAD	C2-N3	2.27	1.42	1.38
10	B	502	FMN	C8M-C8	-2.25	1.46	1.51
6	A	999	NAD	C6A-C5A	2.20	1.51	1.43
10	B	502	FMN	C4-C4A	2.20	1.45	1.41
9	B	501	FAD	C2-N1	2.15	1.42	1.38
9	B	501	FAD	C9-C9A	2.11	1.44	1.40
6	A	999	NAD	C5B-C4B	-2.03	1.45	1.51

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	502	FMN	C4-N3-C2	14.64	127.50	115.14
9	B	501	FAD	C4-N3-C2	8.67	122.46	115.14
10	B	502	FMN	C4A-N5-C5A	8.64	125.41	116.77
10	B	502	FMN	C4A-C10-N10	-7.75	112.34	120.30
6	A	999	NAD	N3A-C2A-N1A	-6.99	117.75	128.68
10	B	502	FMN	P-O5'-C5'	6.09	135.06	118.30
10	B	502	FMN	C4-C4A-C10	-5.98	115.99	119.95
10	B	502	FMN	C4A-C4-N3	-5.95	115.30	123.43
9	B	501	FAD	O4B-C1B-C2B	-5.84	98.39	106.93
9	B	501	FAD	C4X-N5-C5X	5.69	122.46	116.77
9	B	501	FAD	N3A-C2A-N1A	-5.42	120.21	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	502	FMN	C8M-C8-C7	4.97	130.92	120.74
10	B	502	FMN	C9A-N10-C10	4.94	128.38	121.91
6	A	999	NAD	C5N-C4N-C3N	4.78	126.00	120.34
10	B	502	FMN	C8M-C8-C9	-4.40	109.81	120.34
10	B	502	FMN	O4'-C4'-C3'	4.33	119.63	109.10
9	B	501	FAD	P-O5'-C5'	4.21	146.36	121.68
10	B	502	FMN	C1'-C2'-C3'	4.19	121.51	109.79
6	A	999	NAD	C6N-N1N-C2N	4.05	125.67	121.97
6	A	999	NAD	C1B-N9A-C4A	-4.02	119.57	126.64
10	B	502	FMN	O2'-C2'-C3'	4.02	118.87	109.10
6	A	999	NAD	C5A-C6A-N6A	3.73	126.01	120.35
10	B	502	FMN	C5A-C9A-N10	-3.71	115.03	117.72
10	B	502	FMN	O2'-C2'-C1'	3.63	118.33	109.59
6	A	999	NAD	C2A-N1A-C6A	3.50	124.75	118.75
10	B	502	FMN	C1'-N10-C10	-3.50	115.28	118.41
10	B	502	FMN	C4-C4A-N5	3.46	122.56	118.60
6	A	999	NAD	O5B-C5B-C4B	-3.36	97.41	108.99
10	B	502	FMN	O3'-C3'-C4'	3.32	116.84	108.81
10	B	502	FMN	C9A-C5A-N5	-3.21	117.33	122.36
6	A	999	NAD	O2D-C2D-C3D	3.13	121.95	111.82
9	B	501	FAD	C4X-C4-N3	-2.95	119.40	123.43
10	B	502	FMN	O3'-C3'-C2'	-2.79	102.06	108.81
9	B	501	FAD	C5'-C4'-C3'	-2.78	106.83	112.20
6	A	999	NAD	C5N-C6N-N1N	-2.75	116.45	120.40
10	B	502	FMN	C5'-C4'-C3'	-2.72	106.95	112.20
9	B	501	FAD	C4X-C10-N10	-2.71	117.52	120.30
9	B	501	FAD	O2P-P-O5'	2.70	120.30	107.75
9	B	501	FAD	C4-C4X-C10	-2.61	118.22	119.95
9	B	501	FAD	C2A-N1A-C6A	2.60	123.20	118.75
10	B	502	FMN	C6-C5A-N5	2.56	121.87	119.05
10	B	502	FMN	C1'-N10-C9A	-2.52	116.31	118.29
9	B	501	FAD	C4-C4X-N5	2.31	121.24	118.60
6	A	999	NAD	C3N-C2N-N1N	-2.28	118.20	120.43
9	B	501	FAD	C9A-C5X-N5	-2.27	118.81	122.36
10	B	502	FMN	O5'-C5'-C4'	2.11	114.99	109.36
9	B	501	FAD	C8M-C8-C9	-2.03	115.48	120.34
6	A	999	NAD	C4A-C5A-N7A	2.02	111.50	109.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	502	FMN	C2'

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	999	NAD	C5D-O5D-PN-O3
7	A	998	GOL	O1-C1-C2-C3
7	A	998	GOL	C1-C2-C3-O3
7	A	998	GOL	O2-C2-C3-O3
10	B	502	FMN	C2'-C1'-N10-C9A
10	B	502	FMN	C2'-C1'-N10-C10
10	B	502	FMN	N10-C1'-C2'-O2'
9	B	501	FAD	C4'-C5'-O5'-P
10	B	502	FMN	O2'-C2'-C3'-C4'
10	B	502	FMN	O2'-C2'-C3'-O3'
7	A	998	GOL	O1-C1-C2-O2
6	A	999	NAD	O4D-C4D-C5D-O5D
6	A	999	NAD	C3D-C4D-C5D-O5D
10	B	502	FMN	O4'-C4'-C5'-O5'
9	B	501	FAD	O4B-C4B-C5B-O5B
9	B	501	FAD	C5'-O5'-P-O1P
6	A	999	NAD	O4B-C4B-C5B-O5B

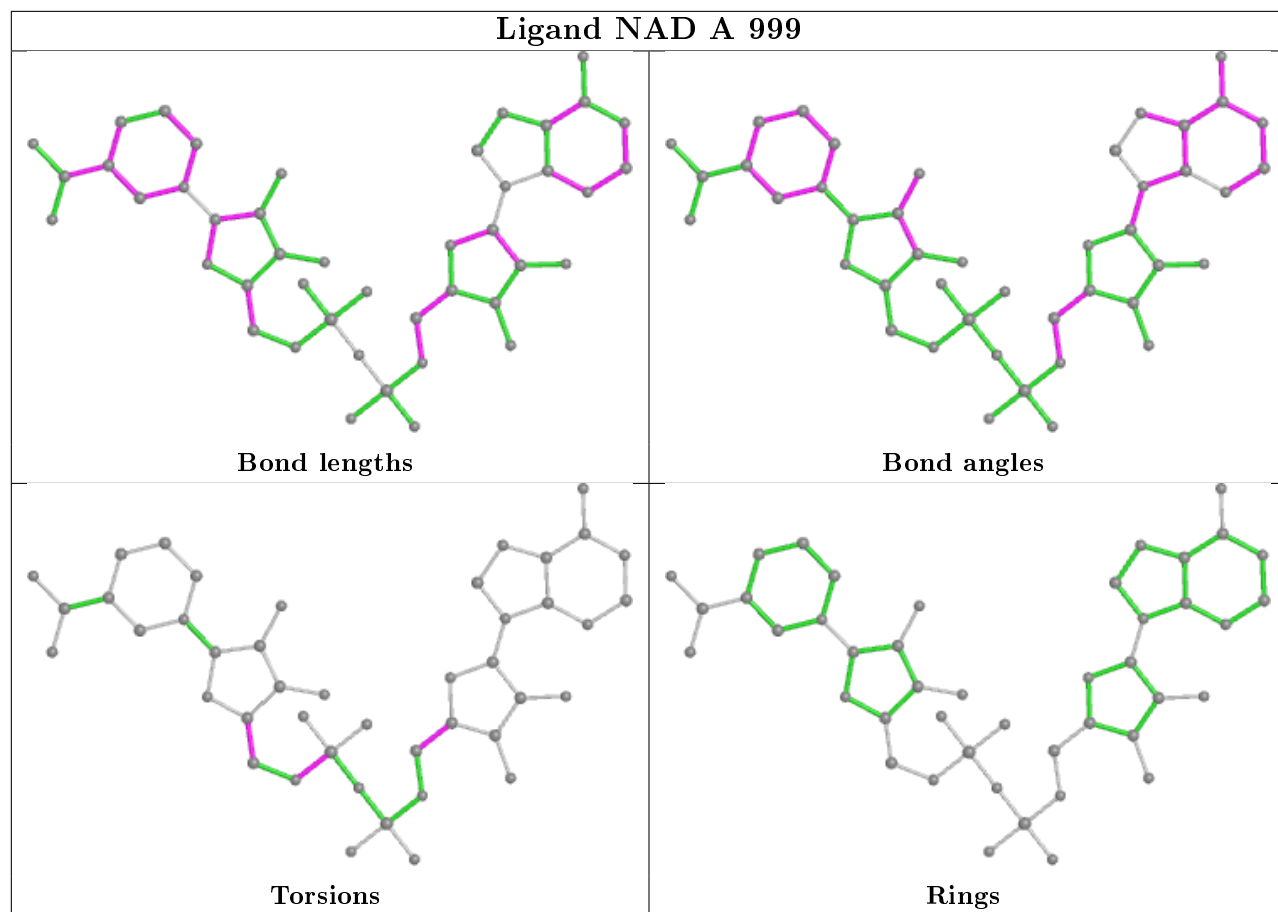
There are no ring outliers.

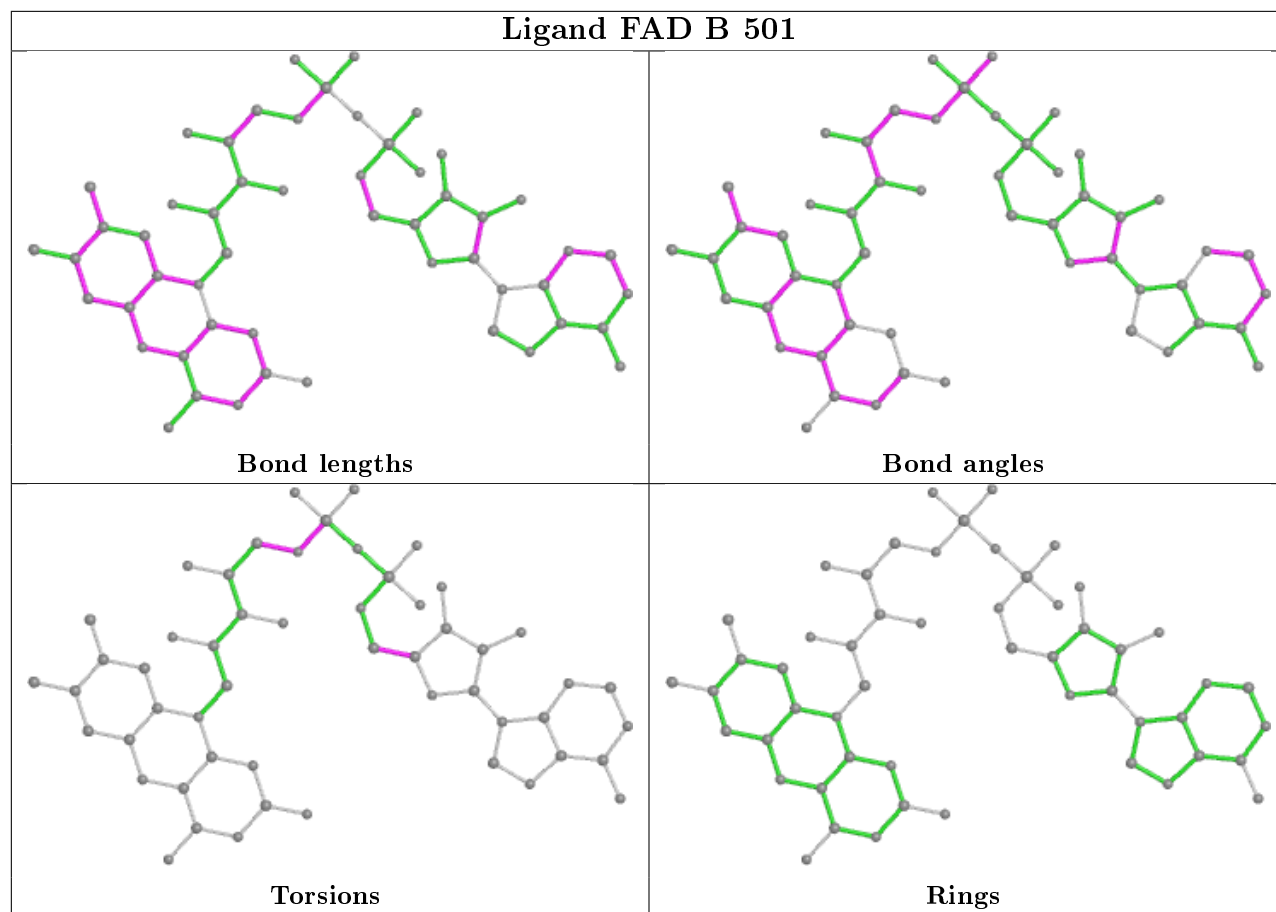
5 monomers are involved in 8 short contacts:

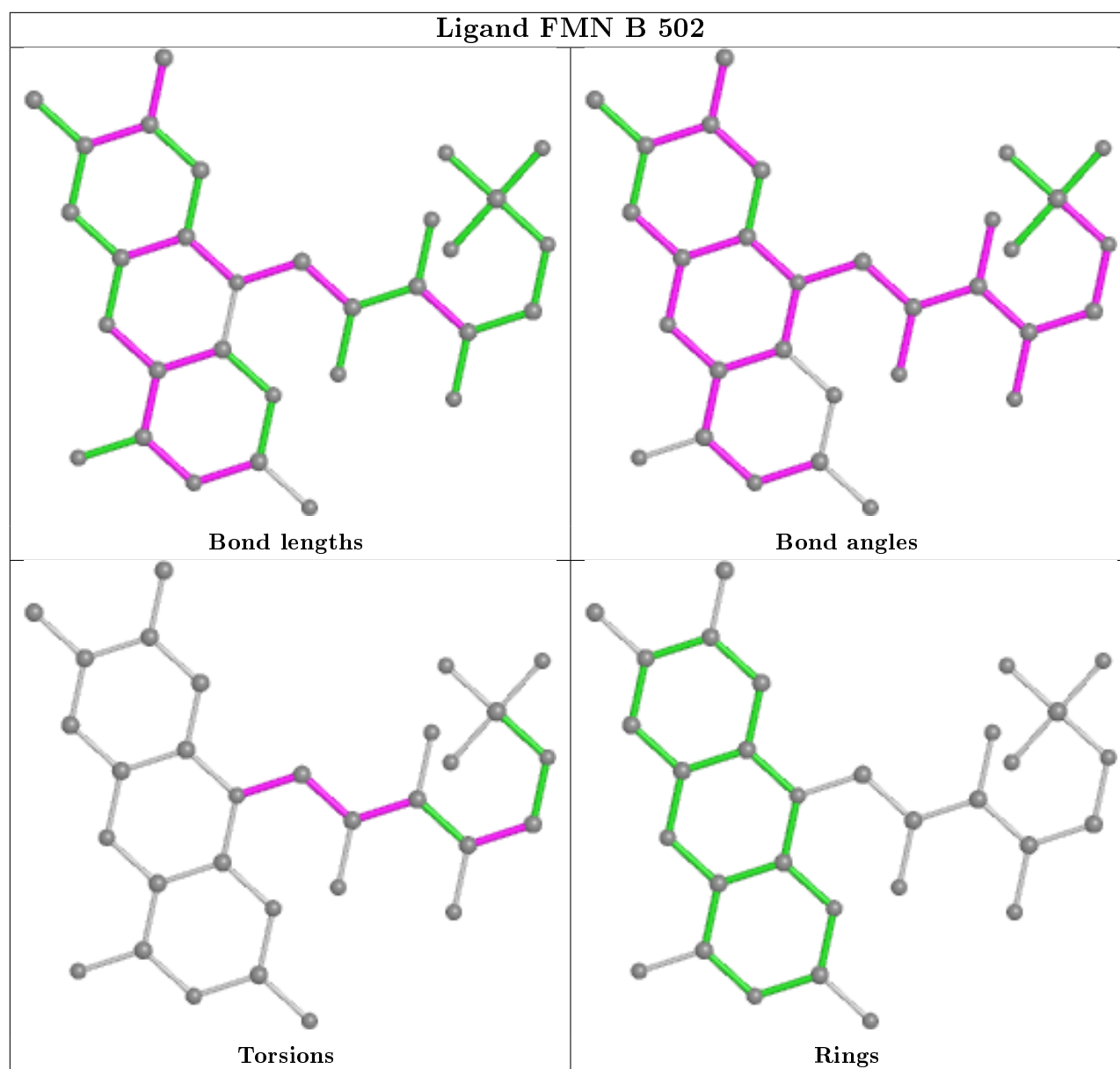
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	504	SO3	1	0
5	B	503	FOA	4	0
9	B	501	FAD	2	0
7	A	998	GOL	1	0
10	B	502	FMN	1	0

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.









## 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	A	965/965 (100%)	-0.17	10 (1%) 82 82	17, 27, 44, 75	0
2	B	403/405 (99%)	0.02	12 (2%) 50 48	17, 28, 43, 58	0
3	C	190/210 (90%)	-0.19	1 (0%) 91 91	19, 27, 41, 64	0
4	D	91/99 (91%)	-0.08	2 (2%) 62 61	17, 25, 39, 77	0
All	All	1649/1679 (98%)	-0.12	25 (1%) 73 74	17, 27, 43, 77	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	8.5
4	D	91	ILE	8.3
1	A	942	GLY	7.9
1	A	896	LEU	5.1
4	D	90	GLU	4.9
1	A	943	ASP	4.6
1	A	941	VAL	3.8
1	A	944	GLN	3.3
3	C	198	SER	3.3
2	B	248	LEU	3.2
2	B	299	PHE	3.2
2	B	302	ILE	2.9
2	B	250	ALA	2.7
1	A	557	VAL	2.6
2	B	301	VAL	2.6
1	A	945	LEU	2.5
2	B	325	TRP	2.4
2	B	287	ILE	2.4
1	A	475	ASP	2.3
2	B	20	LYS	2.2
1	A	2	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	284	GLY	2.1
2	B	251	LEU	2.1
2	B	298	ALA	2.1
2	B	5	LEU	2.1

## 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

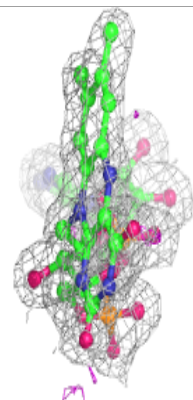
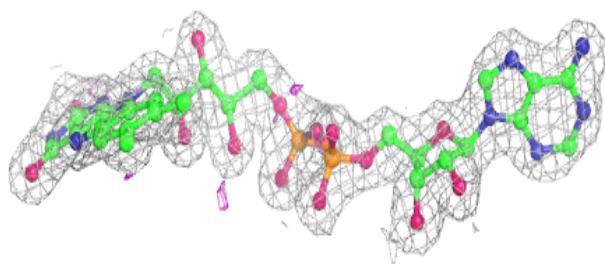
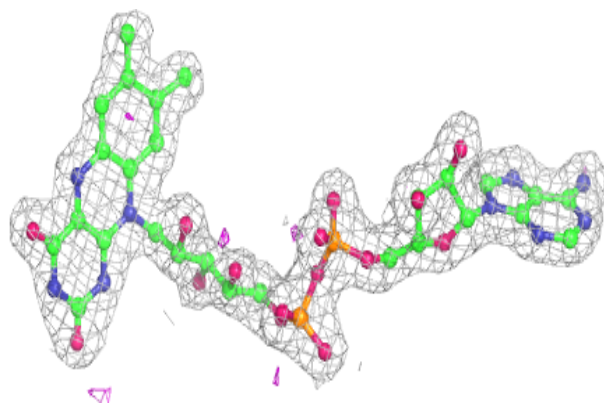
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	GOL	A	998	6/6	0.81	0.23	50,53,56,57	0
5	FOA	A	997	8/8	0.95	0.10	28,32,38,39	0
5	FOA	B	503	8/8	0.95	0.15	21,30,33,33	0
8	SO3	B	504	4/4	0.97	0.10	45,49,53,54	0
9	FAD	B	501	53/53	0.97	0.08	16,24,29,30	0
6	NAD	A	999	44/44	0.98	0.08	17,21,27,29	0
10	FMN	B	502	31/31	0.98	0.11	16,21,25,26	0
11	ZN	D	101	1/1	1.00	0.09	21,21,21,21	0

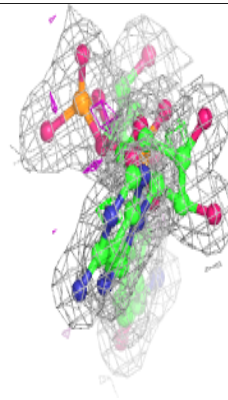
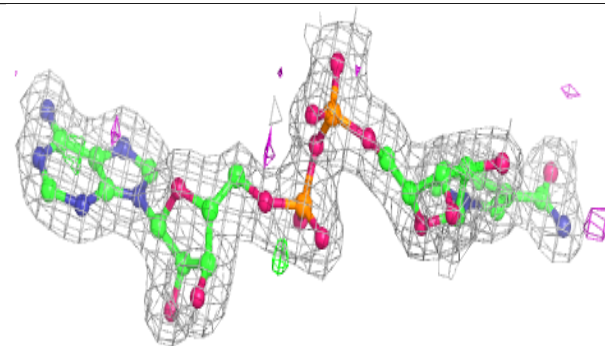
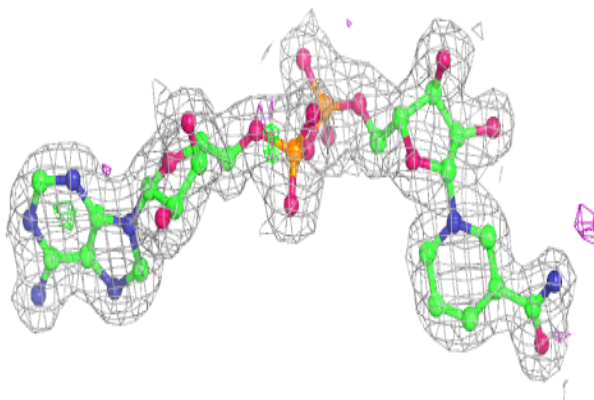
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

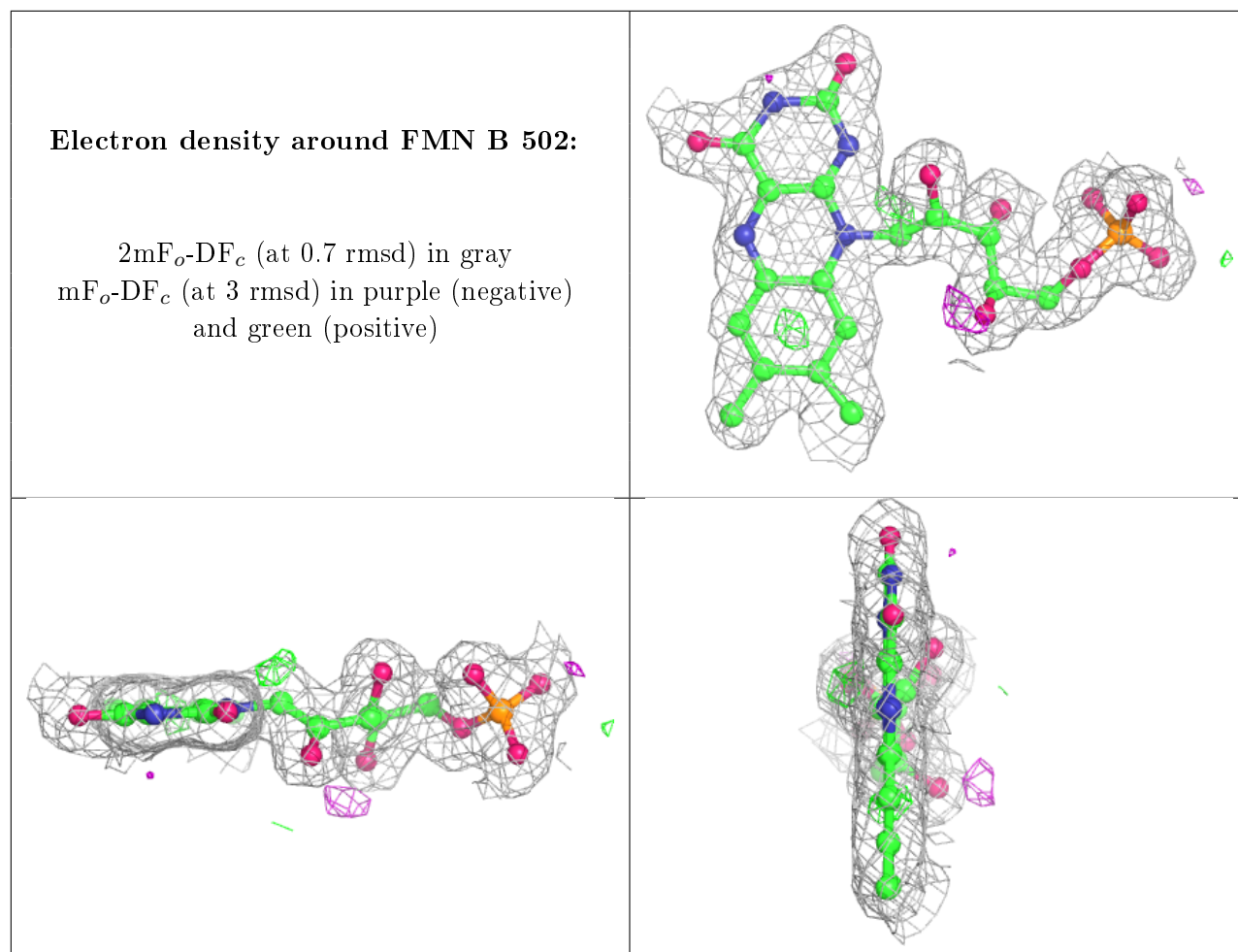
**Electron density around FAD B 501:**

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

**Electron density around NAD A 999:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.