



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:35 pm BST

PDB ID : 3AD7  
Title : Heterotetrameric Sarcosine Oxidase from *Corynebacterium* sp. U-96 in complex with methylthio acetate  
Authors : Suzuki, H.; Moriguchi, T.; Ida, K.  
Deposited on : 2010-01-15  
Resolution : 2.20 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

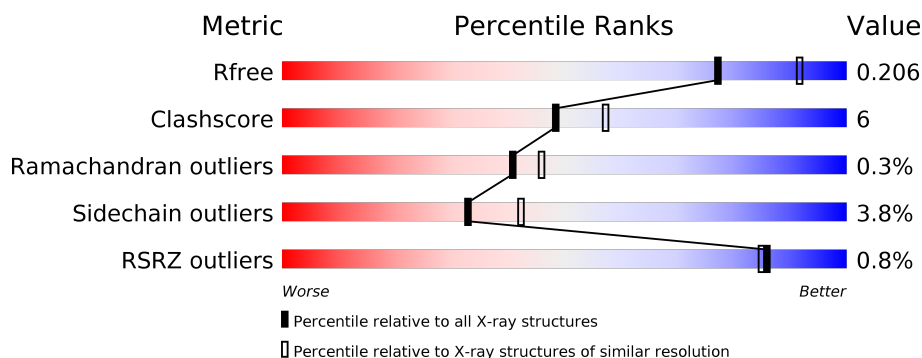
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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 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	964	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>.</div> </div> </div>
2	B	404	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>.</div> </div> </div>
3	C	203	<div> <div></div> <div> <div></div> <div>86%</div> <div>9%</div> <div>.</div> </div> </div>
4	D	99	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>.</div> <div>8%</div> </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
8	FMN	B	406	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 13623 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 Subunit alpha of sarcosine oxidase.

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 Subunit beta of sarcosine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	0	0
			3108	1981	541	576	10			

- Molecule 3 is a protein called Subunit gamma of sarcosine oxidase.

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

- Molecule 4 is a protein called Subunit delta of sarcosine oxidase.

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 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
5	A	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula:  $\text{O}_4\text{S}$ ).



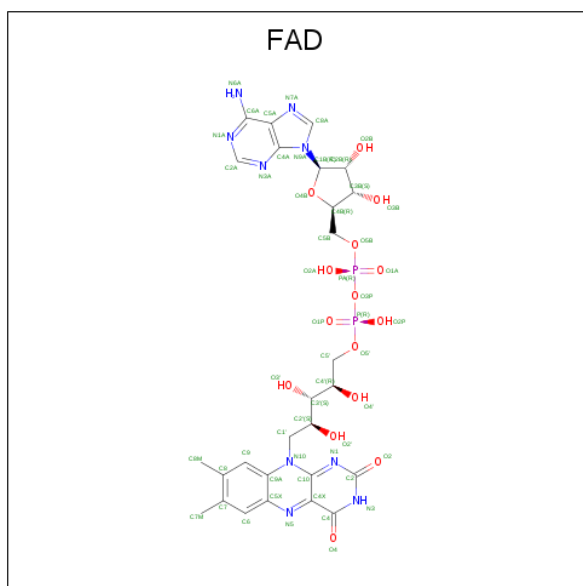
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 5	O 4	S 1	0	0
6	A	1	Total 5	O 4	S 1	0	0
6	A	1	Total 5	O 4	S 1	0	0

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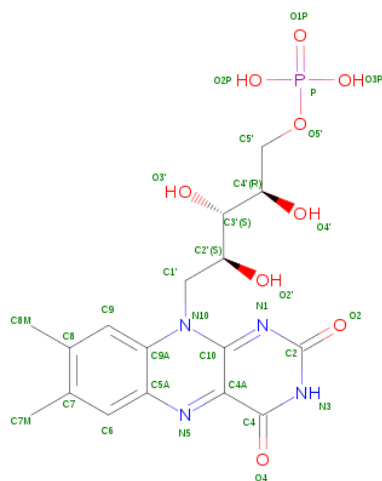
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$ ).



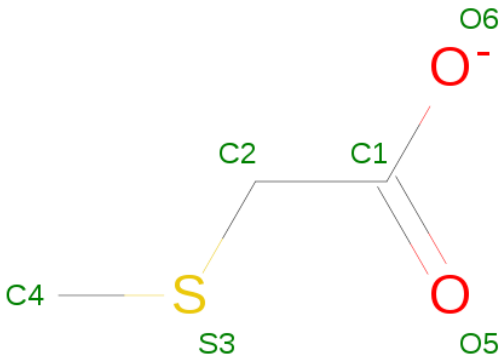
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 8 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



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

- Molecule 9 is [METHYLTHIO]ACETATE (three-letter code: MTG) (formula:  $\text{C}_3\text{H}_5\text{O}_2\text{S}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	O	S	0	0
			6	3	2	1		

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 11 is water.

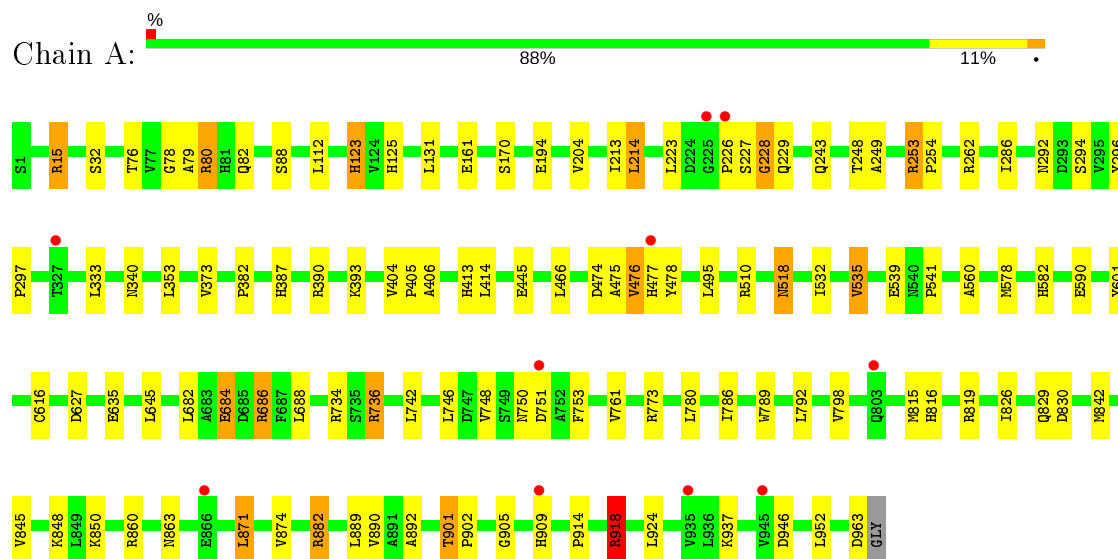
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	558	Total 558	O 558	0	0
11	B	184	Total 184	O 184	0	0
11	C	117	Total 117	O 117	0	0
11	D	65	Total 65	O 65	0	0



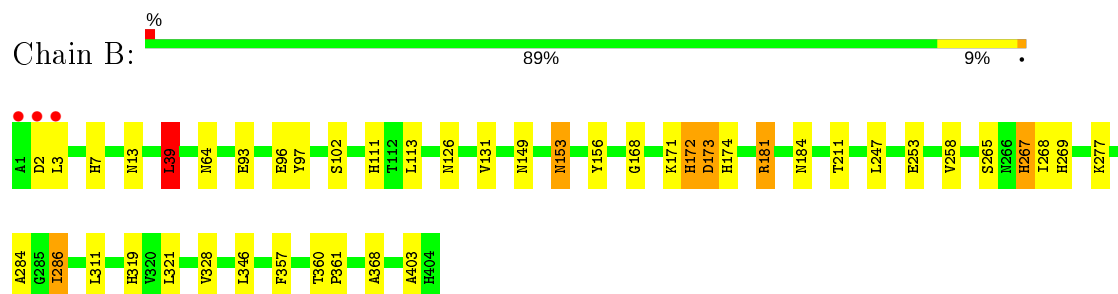
### 3 Residue-property plots [i](#)

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.

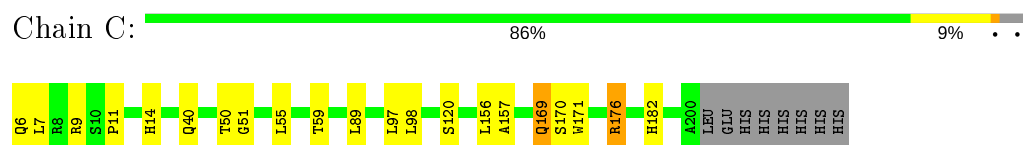
#### • Molecule 1: Subunit alpha of sarcosine oxidase



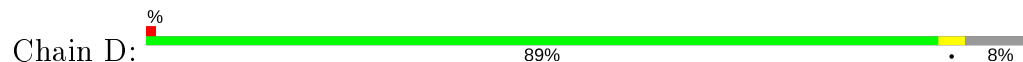
#### • Molecule 2: Subunit beta of sarcosine oxidase

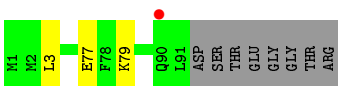


#### • Molecule 3: Subunit gamma of sarcosine oxidase



#### • Molecule 4: Subunit delta of sarcosine oxidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	198.95Å 198.95Å 196.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.53 – 2.20 39.53 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.53-2.20) 100.0 (39.53-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.22 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.170 , 0.205 0.170 , 0.206	Depositor DCC
$R_{free}$ test set	5804 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.3	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	13623	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAD, FMN, SO4, MTG, 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	0.82	0/7361	0.79	10/10017 (0.1%)
2	B	0.84	0/3189	0.74	3/4340 (0.1%)
3	C	0.88	0/1461	0.86	2/1998 (0.1%)
4	D	0.85	0/772	0.82	1/1040 (0.1%)
All	All	0.84	0/12783	0.79	16/17395 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	176	ARG	NE-CZ-NH2	-10.21	115.20	120.30
1	A	15	ARG	NE-CZ-NH2	-9.47	115.56	120.30
3	C	176	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	A	214	LEU	CA-CB-CG	-7.76	97.46	115.30
1	A	918	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	262	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	A	253	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	A	228	GLY	N-CA-C	5.85	127.73	113.10
2	B	173	ASP	CB-CG-OD1	5.83	123.55	118.30
2	B	181	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	918	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	390	ARG	NE-CZ-NH1	5.32	122.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	736	ARG	NE-CZ-NH2	-5.25	117.67	120.30
4	D	3	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	15	ARG	NE-CZ-NH1	5.13	122.86	120.30
2	B	39	LEU	CB-CG-CD1	5.12	119.69	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	268	ILE	Peptide

## 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	100	0
2	B	3108	0	3035	41	0
3	C	1433	0	1434	12	0
4	D	749	0	706	1	0
5	A	44	0	26	4	0
6	A	25	0	0	0	0
6	B	10	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
7	B	53	0	31	3	0
8	B	31	0	19	10	0
9	B	6	0	5	0	0
10	D	1	0	0	0	0
11	A	558	0	0	12	0
11	B	184	0	0	6	0
11	C	117	0	0	2	0
11	D	65	0	0	0	0
All	All	13623	0	12360	151	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 (151) 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	8:B:406:FMN:C8M	1.79	1.44
1:A:829:GLN:HB2	1:A:909:HIS:HE1	1.10	1.17
2:B:172:HIS:NE2	8:B:406:FMN:HM83	0.82	1.14
1:A:829:GLN:HB2	1:A:909:HIS:CE1	1.87	1.10
1:A:882:ARG:HG2	1:A:882:ARG:HH11	1.14	1.07
1:A:829:GLN:OE1	1:A:909:HIS:NE2	1.88	1.04
2:B:172:HIS:CD2	8:B:406:FMN:HM83	1.93	1.02
2:B:172:HIS:CE1	8:B:406:FMN:HM83	1.95	1.01
3:C:169:GLN:NE2	3:C:171:TRP:HE1	1.61	0.97
3:C:169:GLN:HE21	3:C:171:TRP:HE1	1.03	0.96
1:A:15:ARG:HD2	1:A:161:GLU:OE2	1.74	0.88
1:A:829:GLN:CB	1:A:909:HIS:CE1	2.57	0.87
1:A:249:ALA:HB1	11:A:997:HOH:O	1.75	0.86
1:A:226:PRO:HB2	11:A:1211:HOH:O	1.75	0.85
1:A:15:ARG:CD	1:A:161:GLU:OE2	2.28	0.82
1:A:918:ARG:HG3	1:A:918:ARG:HH11	1.46	0.80
1:A:815:MET:HE2	1:A:816:HIS:HD2	1.45	0.80
2:B:149:ASN:HD21	2:B:153:ASN:HD21	1.30	0.79
1:A:510:ARG:HH21	8:B:406:FMN:C5'	1.97	0.78
2:B:93:GLU:HG2	11:B:658:HOH:O	1.84	0.76
1:A:510:ARG:NH2	8:B:406:FMN:H5'2	2.00	0.76
1:A:475:ALA:O	1:A:477:HIS:N	2.21	0.74
2:B:286:ILE:HD11	2:B:328:VAL:HG21	1.70	0.74
1:A:892:ALA:HA	1:A:937:LYS:HD2	1.70	0.73
2:B:269:HIS:CE1	2:B:403:ALA:H	2.06	0.73
1:A:882:ARG:HG2	1:A:882:ARG:NH1	1.91	0.71
1:A:474:ASP:HB3	1:A:477:HIS:CD2	2.27	0.69
1:A:292:ASN:HD22	1:A:294:SER:H	1.41	0.67
2:B:172:HIS:HD1	2:B:173:ASP:H	1.42	0.66
1:A:860:ARG:HH21	1:A:863:ASN:HD21	1.45	0.64
1:A:510:ARG:HH21	8:B:406:FMN:H5'2	1.57	0.64
1:A:750:ASN:ND2	1:A:773:ARG:HH12	1.96	0.63
1:A:82:GLN:HG2	11:A:1117:HOH:O	1.97	0.63
2:B:13:ASN:ND2	2:B:184:ASN:HD21	1.97	0.63
3:C:157:ALA:O	3:C:182:HIS:HE1	1.82	0.63
2:B:269:HIS:HE1	2:B:403:ALA:H	1.46	0.61
1:A:15:ARG:HD3	1:A:161:GLU:OE2	2.01	0.61
1:A:819:ARG:HH22	1:A:909:HIS:CG	2.18	0.61
1:A:901:THR:CG2	11:A:1137:HOH:O	2.48	0.61
1:A:125:HIS:HD2	11:A:1189:HOH:O	1.83	0.60
11:A:1272:HOH:O	3:C:182:HIS:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLN:OE1	1:A:413:HIS:HE1	1.84	0.60
1:A:292:ASN:ND2	1:A:294:SER:H	1.99	0.60
1:A:842:MET:O	1:A:845:VAL:HG12	2.01	0.60
1:A:249:ALA:HB2	5:A:965:NAD:PA	2.41	0.60
1:A:510:ARG:NH2	8:B:406:FMN:C5'	2.63	0.60
2:B:172:HIS:HD1	2:B:173:ASP:N	2.01	0.59
1:A:826:ILE:CG2	1:A:829:GLN:HG3	2.32	0.59
1:A:750:ASN:HD22	1:A:773:ARG:HH12	1.50	0.58
1:A:249:ALA:CB	5:A:965:NAD:O2A	2.52	0.58
1:A:510:ARG:HH21	8:B:406:FMN:H5'1	1.69	0.58
1:A:249:ALA:HB2	5:A:965:NAD:O3	2.03	0.58
1:A:937:LYS:NZ	1:A:946:ASP:OD2	2.36	0.57
2:B:153:ASN:HD22	2:B:153:ASN:H	1.52	0.57
1:A:475:ALA:C	1:A:477:HIS:N	2.58	0.57
1:A:736:ARG:NH2	1:A:963:ASP:O	2.28	0.57
1:A:474:ASP:HB3	1:A:477:HIS:HD2	1.68	0.56
1:A:249:ALA:HB2	5:A:965:NAD:O2A	2.06	0.56
1:A:223:LEU:HD12	1:A:226:PRO:HB3	1.89	0.55
2:B:2:ASP:HA	11:B:656:HOH:O	2.05	0.55
1:A:340:ASN:HB3	1:A:353:LEU:HD22	1.89	0.55
1:A:736:ARG:HD3	1:A:748:VAL:O	2.05	0.55
2:B:111:HIS:HD2	2:B:156:TYR:O	1.90	0.55
1:A:815:MET:CE	1:A:816:HIS:HD2	2.19	0.55
2:B:149:ASN:HD21	2:B:153:ASN:ND2	2.01	0.55
1:A:582:HIS:HE1	1:A:627:ASP:OD2	1.89	0.55
1:A:871:LEU:HD13	1:A:952:LEU:HD11	1.89	0.55
1:A:80:ARG:CG	1:A:80:ARG:HH11	2.21	0.54
2:B:360:THR:HB	2:B:361:PRO:HD3	1.89	0.54
1:A:475:ALA:C	1:A:477:HIS:H	2.10	0.54
1:A:815:MET:HE1	1:A:826:ILE:HD11	1.89	0.54
2:B:64:ASN:HA	7:B:405:FAD:C6	2.38	0.54
3:C:176:ARG:HD3	11:C:398:HOH:O	2.08	0.53
2:B:13:ASN:HD22	2:B:184:ASN:HD21	1.55	0.52
2:B:7:HIS:HE1	11:B:462:HOH:O	1.92	0.52
1:A:539:GLU:O	1:A:541:PRO:HD3	2.09	0.52
1:A:477:HIS:O	1:A:478:TYR:CD2	2.62	0.52
1:A:742:LEU:HD21	1:A:798:VAL:HG22	1.92	0.52
1:A:532:ILE:HD13	1:A:532:ILE:N	2.26	0.50
1:A:819:ARG:C	1:A:819:ARG:HD2	2.31	0.50
1:A:495:LEU:HD21	1:A:535:VAL:HG22	1.94	0.49
1:A:826:ILE:HG22	1:A:829:GLN:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:PRO:HG2	1:A:404:VAL:HG12	1.95	0.49
3:C:169:GLN:NE2	3:C:171:TRP:NE1	2.45	0.49
2:B:265:SER:O	2:B:269:HIS:HD2	1.95	0.49
2:B:39:LEU:HD13	2:B:368:ALA:HA	1.94	0.49
2:B:126:ASN:HB3	2:B:131:VAL:HG22	1.95	0.49
1:A:125:HIS:CE1	11:A:1513:HOH:O	2.66	0.48
2:B:265:SER:O	2:B:269:HIS:HA	2.13	0.48
3:C:11:PRO:HG2	3:C:120:SER:HB3	1.95	0.48
3:C:40:GLN:HA	3:C:89:LEU:O	2.12	0.48
1:A:248:THR:O	1:A:249:ALA:HB3	2.14	0.48
1:A:477:HIS:O	1:A:478:TYR:CG	2.67	0.48
1:A:901:THR:HG23	11:A:1137:HOH:O	2.13	0.48
3:C:51:GLY:HA3	11:C:213:HOH:O	2.13	0.48
1:A:905:GLY:HA3	1:A:924:LEU:O	2.14	0.47
1:A:918:ARG:CG	1:A:918:ARG:HH11	2.21	0.47
2:B:172:HIS:NE2	8:B:406:FMN:C8	2.72	0.47
1:A:582:HIS:CD2	1:A:601:TYR:OH	2.68	0.47
1:A:635:GLU:HG2	1:A:688:LEU:HD13	1.96	0.47
1:A:901:THR:HG22	11:A:1137:HOH:O	2.12	0.47
1:A:387:HIS:HD2	11:A:966:HOH:O	1.96	0.47
1:A:590:GLU:OE1	2:B:113:LEU:HD12	2.15	0.47
1:A:736:ARG:HG2	1:A:748:VAL:CG2	2.45	0.47
2:B:102:SER:O	2:B:168:GLY:HA3	2.15	0.47
2:B:181:ARG:HD2	11:B:418:HOH:O	2.16	0.46
1:A:123:HIS:HE1	1:A:560:ALA:O	1.97	0.46
2:B:247:LEU:HD13	2:B:286:ILE:HD12	1.97	0.46
1:A:80:ARG:CG	1:A:80:ARG:NH1	2.78	0.46
3:C:6:GLN:O	3:C:7:LEU:HB2	2.16	0.46
1:A:204:VAL:HG13	1:A:213:ILE:HG23	1.97	0.46
1:A:901:THR:HA	1:A:902:PRO:HD3	1.81	0.46
2:B:153:ASN:HD22	2:B:153:ASN:N	2.13	0.45
3:C:55:LEU:O	3:C:59:THR:HG23	2.17	0.45
3:C:9:ARG:HH21	3:C:14:HIS:HB3	1.80	0.45
1:A:125:HIS:HE1	11:A:1513:HOH:O	2.00	0.44
1:A:387:HIS:HE1	1:A:393:LYS:O	2.00	0.44
1:A:131:LEU:HD23	1:A:213:ILE:HG13	2.00	0.44
1:A:296:TYR:N	1:A:297:PRO:CD	2.80	0.44
2:B:277:LYS:NZ	11:B:732:HOH:O	2.16	0.44
1:A:78:GLY:O	1:A:79:ALA:C	2.55	0.44
1:A:736:ARG:HB2	1:A:780:LEU:HD21	2.00	0.43
2:B:96:GLU:O	2:B:181:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:HIS:CE1	2:B:174:HIS:HE1	2.36	0.43
1:A:684:GLU:HG3	1:A:684:GLU:O	2.19	0.42
1:A:405:PRO:HB2	1:A:414:LEU:HD13	2.00	0.42
1:A:882:ARG:NH1	1:A:882:ARG:CG	2.69	0.42
2:B:267:HIS:HD2	11:B:587:HOH:O	2.02	0.42
1:A:82:GLN:CG	11:A:1117:HOH:O	2.62	0.42
4:D:77:GLU:OE2	4:D:79:LYS:NZ	2.52	0.42
1:A:616:CYS:HB2	1:A:914:PRO:HG2	2.01	0.42
1:A:830:ASP:OD1	1:A:909:HIS:ND1	2.53	0.42
2:B:171:LYS:HE2	2:B:174:HIS:CD2	2.54	0.42
2:B:111:HIS:CE1	2:B:265:SER:OG	2.73	0.42
1:A:80:ARG:NH1	1:A:80:ARG:HG3	2.35	0.41
1:A:286:ILE:HD12	1:A:373:VAL:HB	2.03	0.41
1:A:475:ALA:O	1:A:476:VAL:C	2.57	0.41
1:A:76:THR:HA	1:A:88:SER:HA	2.01	0.41
1:A:860:ARG:NH2	1:A:863:ASN:HD21	2.16	0.41
1:A:253:ARG:HB2	1:A:254:PRO:HD2	2.03	0.41
1:A:871:LEU:HD13	1:A:952:LEU:CD1	2.50	0.41
2:B:253:GLU:OE2	2:B:319:HIS:ND1	2.41	0.41
1:A:131:LEU:CD2	1:A:213:ILE:HG13	2.51	0.41
1:A:736:ARG:HG2	1:A:748:VAL:HG23	2.03	0.41
1:A:918:ARG:HG3	1:A:918:ARG:NH1	2.22	0.41
1:A:204:VAL:HG13	1:A:213:ILE:CG2	2.51	0.41
1:A:682:LEU:HD12	1:A:686:ARG:HD2	2.04	0.40
2:B:357:PHE:HB3	7:B:405:FAD:C2	2.51	0.40
2:B:64:ASN:HA	7:B:405:FAD:C5X	2.52	0.40
1:A:112:LEU:HD12	2:B:258:VAL:HG21	2.04	0.40
1:A:518:ASN:HA	2:B:321:LEU:HD11	2.02	0.40

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	A	961/964 (100%)	936 (97%)	21 (2%)	4 (0%)	34	37
2	B	402/404 (100%)	392 (98%)	9 (2%)	1 (0%)	47	55
3	C	193/203 (95%)	187 (97%)	6 (3%)	0	100	100
4	D	89/99 (90%)	88 (99%)	1 (1%)	0	100	100
All	All	1645/1670 (98%)	1603 (97%)	37 (2%)	5 (0%)	41	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	SER
1	A	476	VAL
1	A	228	GLY
1	A	406	ALA
2	B	284	ALA

### 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%)	714 (96%)	33 (4%)	28	35
2	B	319/319 (100%)	309 (97%)	10 (3%)	40	51
3	C	143/151 (95%)	137 (96%)	6 (4%)	30	38
4	D	75/81 (93%)	75 (100%)	0	100	100
All	All	1284/1298 (99%)	1235 (96%)	49 (4%)	33	42

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	80	ARG
1	A	123	HIS
1	A	170	SER
1	A	194	GLU
1	A	214	LEU

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Mol	Chain	Res	Type
1	A	229	GLN
1	A	333	LEU
1	A	445	GLU
1	A	466	LEU
1	A	518	ASN
1	A	535	VAL
1	A	578	MET
1	A	645	LEU
1	A	684	GLU
1	A	686	ARG
1	A	734	ARG
1	A	746	LEU
1	A	751	ASP
1	A	753	PHE
1	A	761	VAL
1	A	786	ILE
1	A	789	TRP
1	A	792	LEU
1	A	848	LYS
1	A	850	LYS
1	A	871	LEU
1	A	874	VAL
1	A	882	ARG
1	A	889	LEU
1	A	890	VAL
1	A	901	THR
1	A	918	ARG
2	B	3	LEU
2	B	39	LEU
2	B	97	TYR
2	B	153	ASN
2	B	172	HIS
2	B	211	THR
2	B	267	HIS
2	B	286	ILE
2	B	311	LEU
2	B	346	LEU
3	C	50	THR
3	C	97	LEU
3	C	98	LEU
3	C	156	LEU
3	C	169	GLN

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Mol	Chain	Res	Type
3	C	170	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	123	HIS
1	A	125	HIS
1	A	181	GLN
1	A	229	GLN
1	A	292	ASN
1	A	387	HIS
1	A	413	HIS
1	A	477	HIS
1	A	486	GLN
1	A	518	ASN
1	A	540	ASN
1	A	543	GLN
1	A	582	HIS
1	A	750	ASN
1	A	816	HIS
1	A	863	ASN
1	A	912	ASN
2	B	7	HIS
2	B	13	ASN
2	B	14	ASN
2	B	111	HIS
2	B	153	ASN
2	B	267	HIS
2	B	269	HIS
2	B	344	GLN
2	B	369	HIS
3	C	6	GLN
3	C	40	GLN
3	C	158	ASN
3	C	169	GLN
3	C	182	HIS

### 5.3.3 RNA ⓘ

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 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	SO4	C	2564	-	4,4,4	0.36	0	6,6,6	0.33	0
6	SO4	A	2567	-	4,4,4	0.11	0	6,6,6	0.40	0
6	SO4	A	2563	-	4,4,4	0.16	0	6,6,6	0.32	0
9	MTG	B	801	-	2,5,5	0.14	0	1,5,5	0.81	0
5	NAD	A	965	-	42,48,48	1.72	5 (11%)	50,73,73	1.60	7 (14%)
6	SO4	A	2571	-	4,4,4	0.18	0	6,6,6	0.44	0
6	SO4	D	2566	-	4,4,4	0.17	0	6,6,6	0.18	0
7	FAD	B	405	-	51,58,58	1.64	9 (17%)	60,89,89	1.58	10 (16%)
6	SO4	B	2569	-	4,4,4	0.10	0	6,6,6	0.44	0
8	FMN	B	406	-	31,33,33	2.22	11 (35%)	40,50,50	2.38	12 (30%)
6	SO4	A	2559	-	4,4,4	0.20	0	6,6,6	0.15	0
6	SO4	B	2568	-	4,4,4	0.16	0	6,6,6	0.34	0
6	SO4	A	2560	-	4,4,4	0.28	0	6,6,6	0.40	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
5	NAD	A	965	-	-	4/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FAD	B	405	-	-	3/30/50/50	0/6/6/6
9	MTG	B	801	-	-	0/1/3/3	-
8	FMN	B	406	-	-	9/18/18/18	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	965	NAD	O7N-C7N	6.93	1.37	1.24
8	B	406	FMN	C4-N3	5.76	1.43	1.33
7	B	405	FAD	C10-N1	5.53	1.40	1.33
5	A	965	NAD	C2N-N1N	5.28	1.41	1.35
8	B	406	FMN	O5'-C5'	-5.06	1.25	1.44
7	B	405	FAD	C4X-N5	5.06	1.40	1.33
8	B	406	FMN	C4A-N5	4.51	1.39	1.33
7	B	405	FAD	C4-N3	4.36	1.40	1.33
8	B	406	FMN	C10-N1	3.65	1.37	1.33
8	B	406	FMN	C8M-C8	3.32	1.57	1.51
5	A	965	NAD	C2B-C1B	-3.23	1.48	1.53
5	A	965	NAD	O4B-C1B	3.05	1.45	1.41
8	B	406	FMN	C9A-C5A	-2.48	1.37	1.42
7	B	405	FAD	O4'-C4'	2.45	1.48	1.43
7	B	405	FAD	C2-N3	2.39	1.42	1.38
7	B	405	FAD	C9A-N10	2.39	1.41	1.38
8	B	406	FMN	C4-C4A	-2.36	1.37	1.41
8	B	406	FMN	C7M-C7	2.30	1.55	1.51
8	B	406	FMN	C5A-N5	2.28	1.39	1.35
7	B	405	FAD	C5X-N5	2.27	1.39	1.35
7	B	405	FAD	C2A-N3A	2.22	1.35	1.32
7	B	405	FAD	C1'-N10	2.09	1.50	1.48
8	B	406	FMN	C1'-N10	2.09	1.50	1.48
5	A	965	NAD	C6N-N1N	2.08	1.40	1.35
8	B	406	FMN	P-O3P	2.07	1.62	1.54

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	406	FMN	C5'-C4'-C3'	-6.33	99.98	112.20
8	B	406	FMN	O4'-C4'-C5'	-6.23	95.92	109.92
5	A	965	NAD	O4B-C1B-C2B	-5.93	98.26	106.93
8	B	406	FMN	C4-N3-C2	5.33	119.64	115.14
7	B	405	FAD	C4X-N5-C5X	5.20	121.97	116.77
8	B	406	FMN	O5'-P-O1P	4.57	119.29	106.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	405	FAD	C4-N3-C2	4.55	118.98	115.14
7	B	405	FAD	N3A-C2A-N1A	-4.41	121.79	128.68
5	A	965	NAD	N3A-C2A-N1A	-4.40	121.80	128.68
8	B	406	FMN	C5A-C9A-N10	4.08	120.67	117.72
7	B	405	FAD	C10-C4X-N5	-3.54	118.81	121.26
5	A	965	NAD	C6N-N1N-C2N	-3.26	119.00	121.97
5	A	965	NAD	O4D-C1D-C2D	-3.20	102.25	106.93
7	B	405	FAD	C1'-N10-C9A	3.15	120.77	118.29
8	B	406	FMN	C4A-C4-N3	-3.07	119.24	123.43
8	B	406	FMN	P-O5'-C5'	3.04	126.67	118.30
5	A	965	NAD	C4A-C5A-N7A	-2.85	106.42	109.40
7	B	405	FAD	C4X-C4-N3	-2.71	119.73	123.43
8	B	406	FMN	C4A-N5-C5A	2.68	119.45	116.77
7	B	405	FAD	C4A-C5A-N7A	-2.41	106.88	109.40
5	A	965	NAD	O7N-C7N-C3N	2.41	122.51	119.63
7	B	405	FAD	C5'-C4'-C3'	-2.39	107.58	112.20
7	B	405	FAD	O4B-C1B-C2B	-2.35	103.50	106.93
8	B	406	FMN	C9A-C5A-N5	-2.23	118.88	122.36
5	A	965	NAD	C2A-N1A-C6A	2.15	122.44	118.75
7	B	405	FAD	C6-C5X-C9A	2.15	121.87	119.05
8	B	406	FMN	O3'-C3'-C2'	2.13	113.96	108.81
8	B	406	FMN	O2'-C2'-C3'	-2.13	103.93	109.10
8	B	406	FMN	C8M-C8-C9	-2.02	115.50	120.34

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	406	FMN	C1'-C2'-C3'-C4'
8	B	406	FMN	O3'-C3'-C4'-C5'
8	B	406	FMN	C3'-C4'-C5'-O5'
8	B	406	FMN	C5'-O5'-P-O3P
8	B	406	FMN	C2'-C3'-C4'-C5'
8	B	406	FMN	O2'-C2'-C3'-C4'
8	B	406	FMN	C2'-C3'-C4'-O4'
7	B	405	FAD	C4'-C5'-O5'-P
8	B	406	FMN	O4'-C4'-C5'-O5'
5	A	965	NAD	O4D-C4D-C5D-O5D
5	A	965	NAD	PA-O3-PN-O5D
8	B	406	FMN	C5'-O5'-P-O2P
5	A	965	NAD	O4B-C4B-C5B-O5B
5	A	965	NAD	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
7	B	405	FAD	C5'-O5'-P-O1P
7	B	405	FAD	O4B-C4B-C5B-O5B

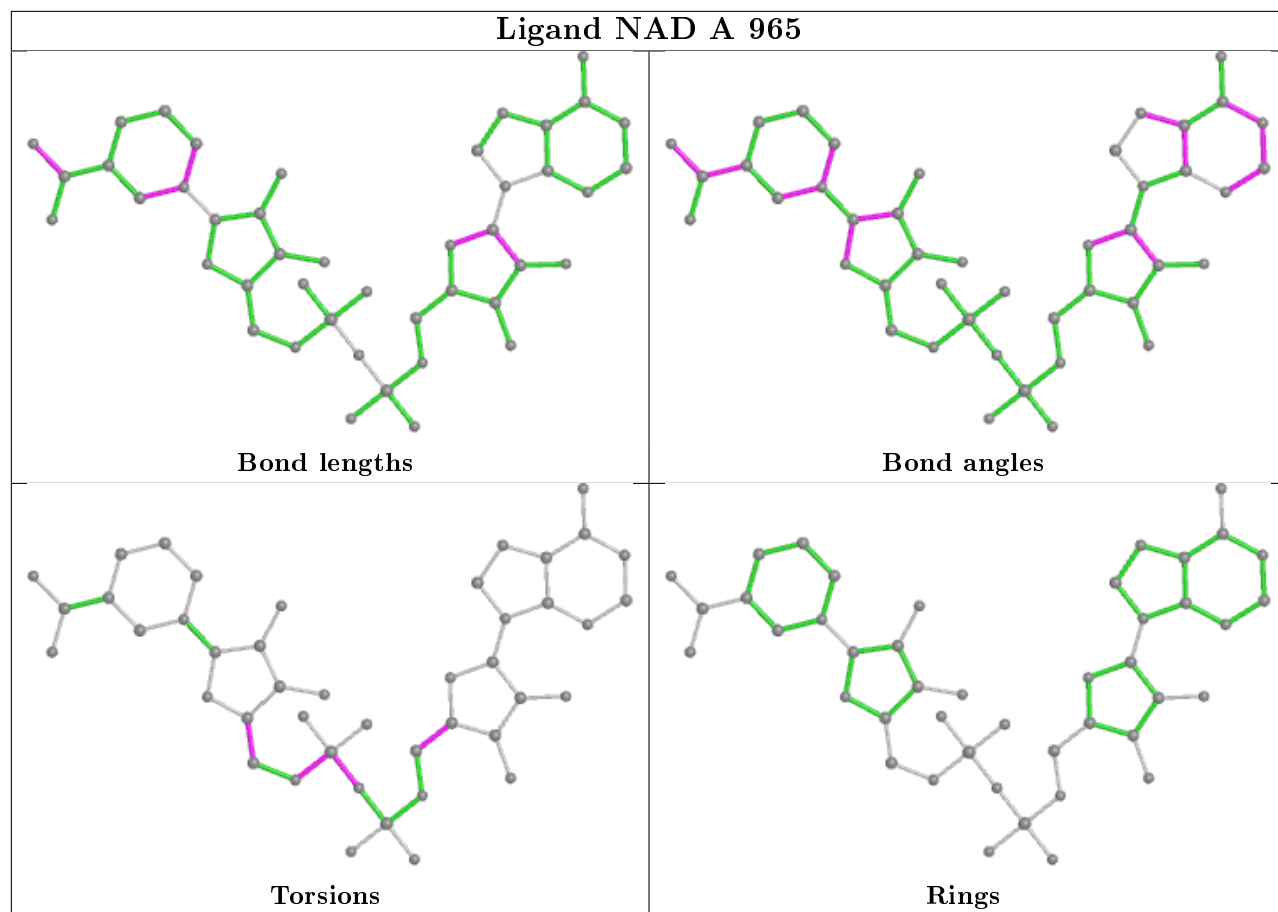
There are no ring outliers.

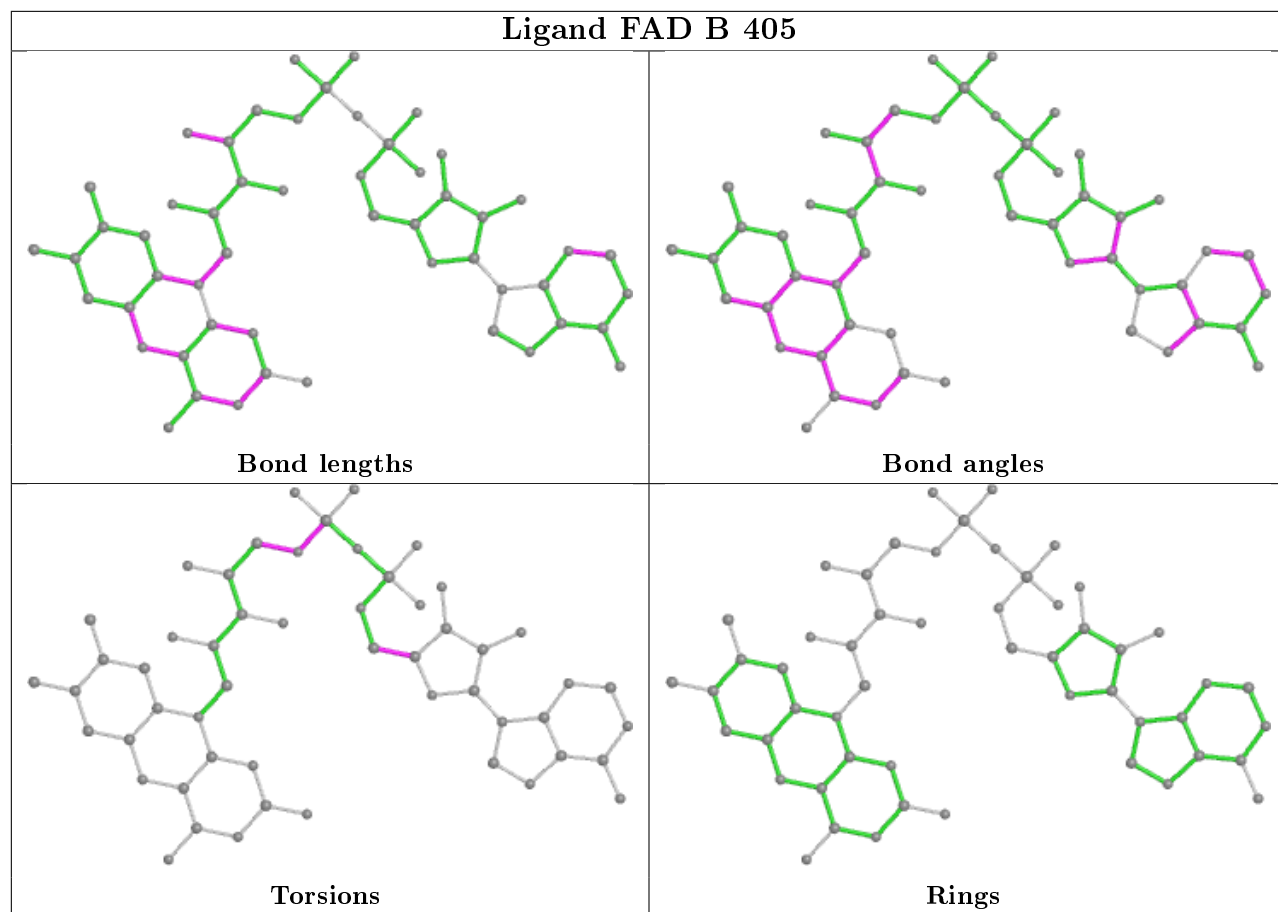
3 monomers are involved in 17 short contacts:

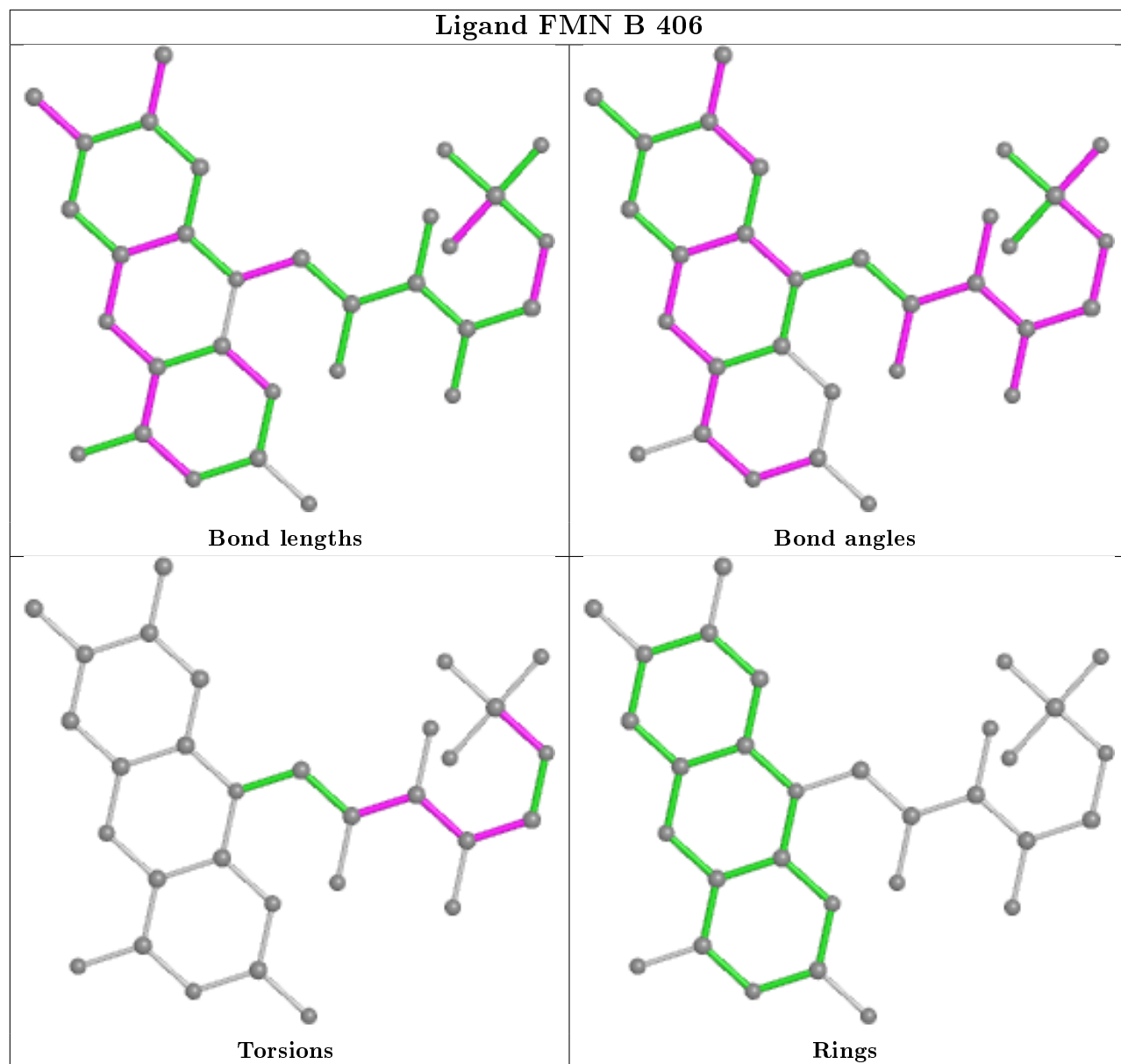
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	965	NAD	4	0
7	B	405	FAD	3	0
8	B	406	FMN	10	0

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 [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, 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	963/964 (99%)	-0.53	10 (1%) 82 81	13, 26, 43, 61	0
2	B	404/404 (100%)	-0.59	3 (0%) 87 86	14, 26, 41, 64	0
3	C	195/203 (96%)	-0.71	0 100 100	16, 24, 41, 55	0
4	D	91/99 (91%)	-0.67	1 (1%) 80 79	18, 23, 42, 52	0
All	All	1653/1670 (98%)	-0.57	14 (0%) 86 85	13, 25, 43, 64	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	3	LEU	5.4
2	B	1	ALA	5.4
2	B	2	ASP	4.2
1	A	226	PRO	3.0
1	A	327	THR	2.9
1	A	909	HIS	2.7
1	A	866	GLU	2.6
4	D	90	GLN	2.6
1	A	477	HIS	2.6
1	A	945	VAL	2.4
1	A	803	GLN	2.4
1	A	751	ASP	2.4
1	A	225	GLY	2.2
1	A	935	VAL	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 ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

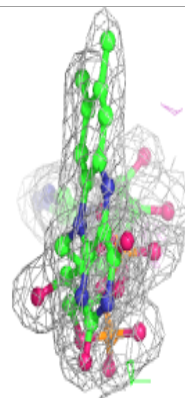
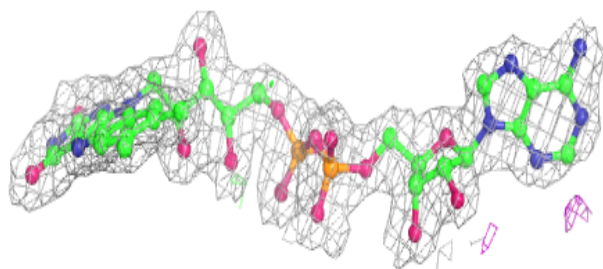
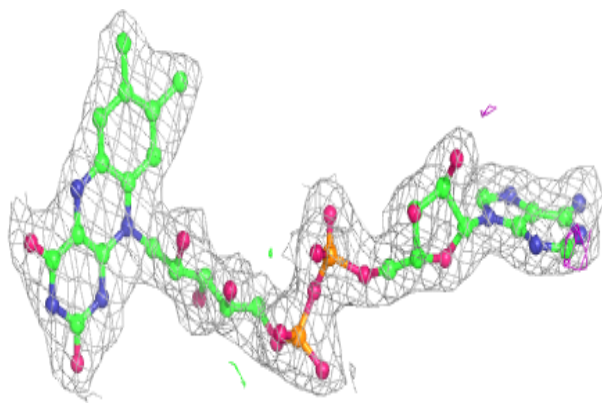
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
9	MTG	B	801	6/6	0.92	0.18	48,49,50,54	0
6	SO4	A	2563	5/5	0.93	0.37	84,84,84,85	0
6	SO4	A	2571	5/5	0.96	0.19	70,70,70,71	0
6	SO4	D	2566	5/5	0.96	0.21	89,89,90,90	0
7	FAD	B	405	53/53	0.97	0.10	19,24,27,28	0
6	SO4	B	2568	5/5	0.97	0.07	64,65,67,67	0
6	SO4	A	2560	5/5	0.97	0.12	49,50,52,52	0
8	FMN	B	406	31/31	0.98	0.12	12,15,21,23	0
6	SO4	C	2564	5/5	0.98	0.17	35,35,38,38	0
6	SO4	B	2569	5/5	0.98	0.20	59,60,61,61	0
6	SO4	A	2559	5/5	0.99	0.10	54,56,57,57	0
5	NAD	A	965	44/44	0.99	0.11	11,16,21,26	0
6	SO4	A	2567	5/5	0.99	0.06	33,34,38,40	0
10	ZN	D	100	1/1	1.00	0.06	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.

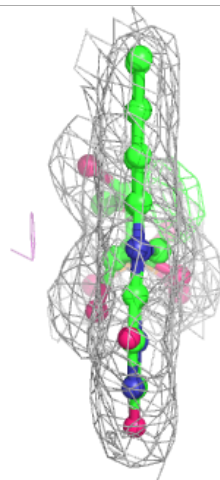
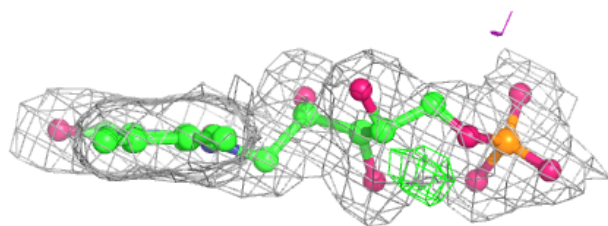
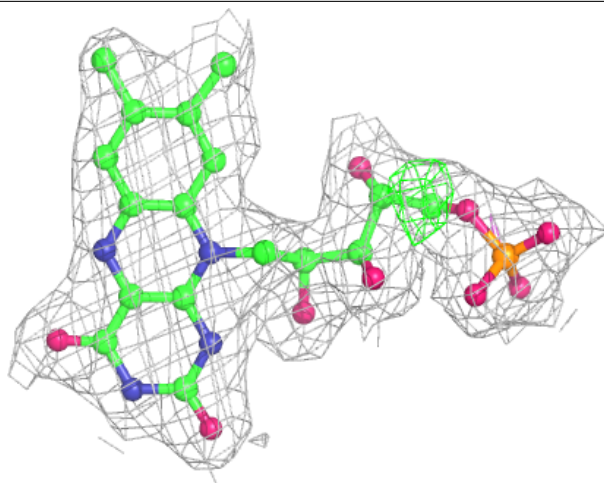
**Electron density around FAD B 405:**

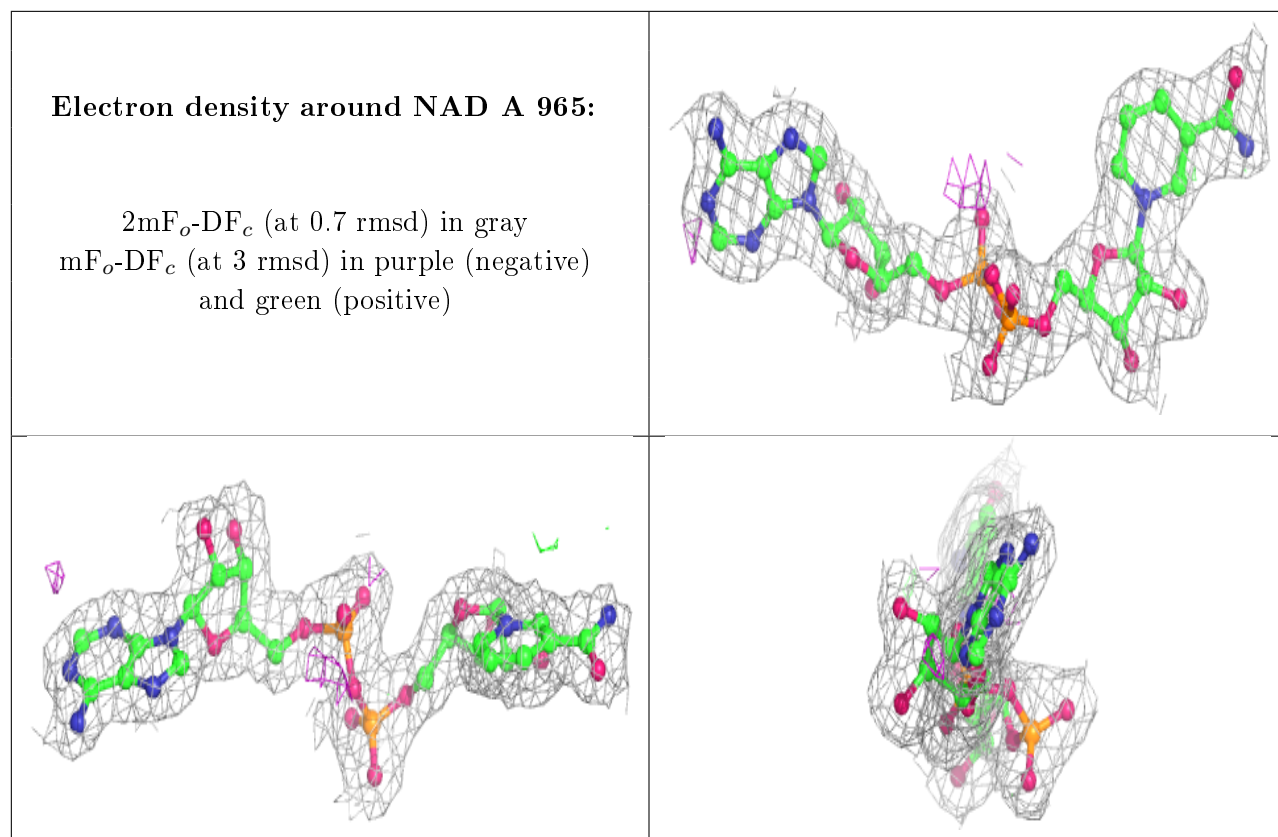
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FMN B 406:**

$2mF_o-DF_c$  (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.