



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2023 – 01:48 PM EDT

PDB ID : 3ADA  
Title : Heterotetrameric Sarcosine Oxidase from *Corynebacterium* sp. U-96 in complex with sulfite  
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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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

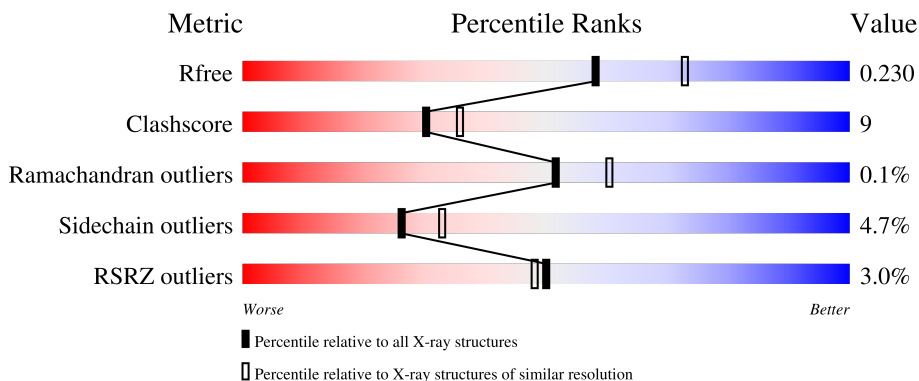
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

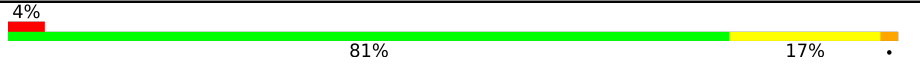



The reported resolution of this entry is 2.20 Å.

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  $\geq 3$ , 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	 4% 81% 17% .
2	B	399	 2% 82% 15% ..
3	C	203	 78% 15% . .
4	D	99	 80% 9% .. 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	ZN	D	100	-	-	X	-
6	SO4	A	2562	-	-	X	-
8	FMN	B	4	-	-	X	-
9	SO3	B	6244	-	-	X	-

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 13493 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
			Total	C	N	O	S			
1	A	963	7229	4507	1287	1413	22	0	0	0

- Molecule 2 is a protein called SARCOSINE OXIDASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	397	3057	1948	532	567	10	0	0	0

- Molecule 3 is a protein called SARCOSINE OXIDASE GAMMA SUBUNIT.

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

- Molecule 4 is a protein called SARCOSINE OXIDASE DELTA SUBUNIT.

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

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

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



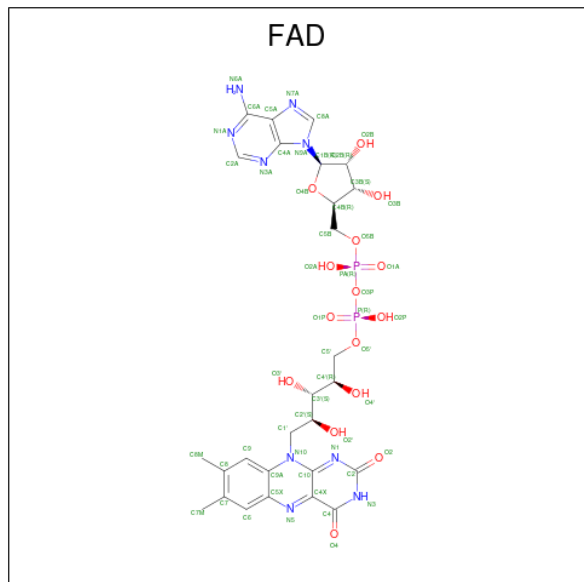
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	A	1	5	4	1	0	0
6	A	1	5	4	1	0	0
6	A	1	5	4	1	0	0

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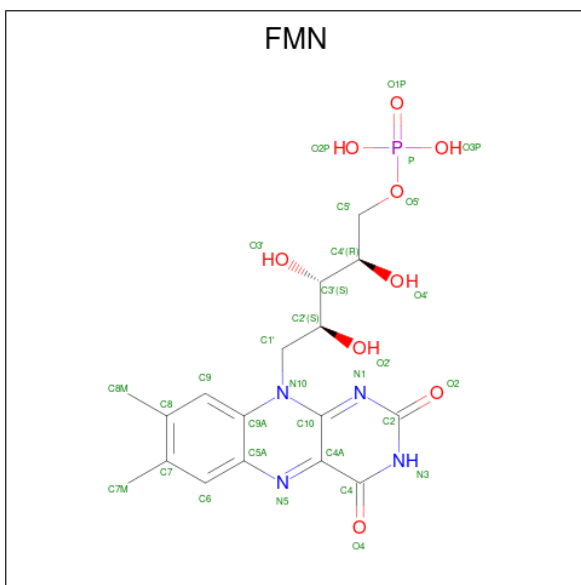
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



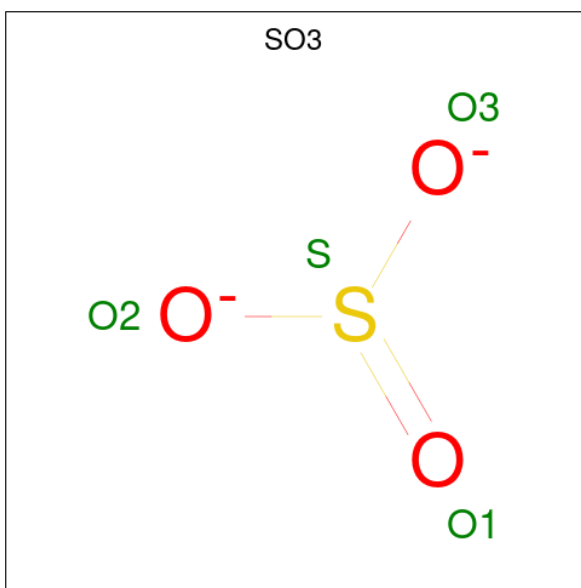
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
7	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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



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

- Molecule 9 is SULFITE ION (three-letter code: SO<sub>3</sub>) (formula: O<sub>3</sub>S).



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

- 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.

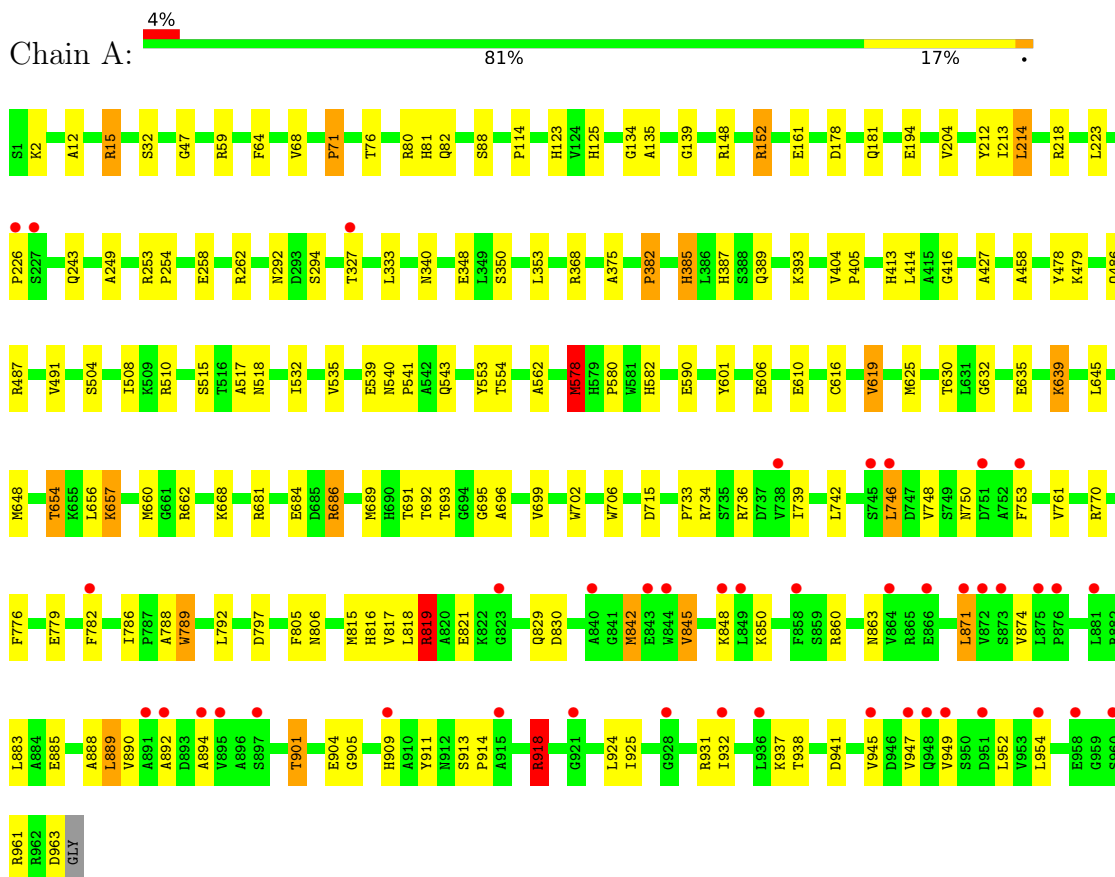
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	552	Total 552	O 552	0	0
11	B	139	Total 139	O 139	0	0
11	C	114	Total 114	O 114	0	0
11	D	47	Total 47	O 47	0	0



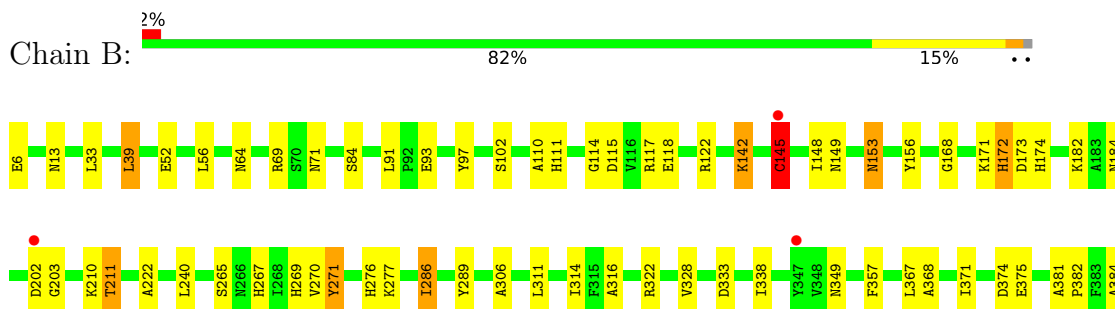
### 3 Residue-property plots

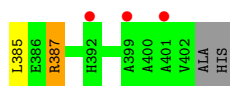
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



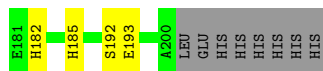
- Molecule 2: SARCOSINE OXIDASE BETA SUBUNIT





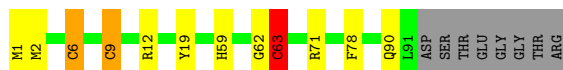
- Molecule 3: SARCOSINE OXIDASE GAMMA SUBUNIT

Chain C: 78% 15%



- Molecule 4: SARCOSINE OXIDASE DELTA SUBUNIT

Chain D: 80% 9% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	198.80Å 198.80Å 197.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	69.98 – 2.20 69.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (69.98-2.20) 99.7 (69.98-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.82 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.189 , 0.232 0.186 , 0.230	Depositor DCC
$R_{free}$ test set	5786 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.8	Xtrriage
Anisotropy	0.088	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13493	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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: SO3, NAD, SO4, FAD, ZN, FMN

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	1.12	9/7361 (0.1%)	0.95	14/10017 (0.1%)
2	B	1.19	6/3136 (0.2%)	0.92	8/4266 (0.2%)
3	C	1.29	3/1461 (0.2%)	1.11	5/1998 (0.3%)
4	D	1.07	3/772 (0.4%)	0.95	4/1040 (0.4%)
All	All	1.16	21/12730 (0.2%)	0.97	31/17321 (0.2%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	145	CYS	CB-SG	29.42	2.32	1.82
2	B	145	CYS	CA-CB	7.83	1.71	1.53
4	D	63	CYS	CB-SG	6.72	1.93	1.82
1	A	212	TYR	CD2-CE2	6.52	1.49	1.39
4	D	6	CYS	CB-SG	6.07	1.92	1.82
1	A	348	GLU	CB-CG	5.91	1.63	1.52
1	A	458	ALA	CA-CB	5.82	1.64	1.52
2	B	316	ALA	CA-CB	5.71	1.64	1.52
1	A	553	TYR	CG-CD1	5.69	1.46	1.39
3	C	130	ALA	CA-CB	5.68	1.64	1.52
4	D	6	CYS	CA-CB	5.43	1.65	1.53
1	A	375	ALA	CA-CB	5.29	1.63	1.52
1	A	135	ALA	CA-CB	5.26	1.63	1.52
3	C	128	ALA	CA-CB	5.25	1.63	1.52
3	C	125	GLU	CB-CG	-5.22	1.42	1.52
2	B	271	TYR	CE1-CZ	5.19	1.45	1.38
1	A	258	GLU	CG-CD	5.18	1.59	1.51
2	B	145	CYS	N-CA	5.17	1.56	1.46
2	B	277	LYS	CE-NZ	5.09	1.61	1.49
1	A	350	SER	CB-OG	5.07	1.48	1.42
1	A	788	ALA	CA-CB	5.00	1.62	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	145	CYS	CA-CB-SG	14.70	140.47	114.00
1	A	15	ARG	NE-CZ-NH2	-10.18	115.21	120.30
3	C	176	ARG	NE-CZ-NH2	-9.58	115.51	120.30
2	B	387	ARG	NE-CZ-NH1	-9.28	115.66	120.30
2	B	145	CYS	N-CA-CB	8.15	125.26	110.60
1	A	214	LEU	CA-CB-CG	-7.85	97.25	115.30
1	A	487	ARG	NE-CZ-NH2	-7.67	116.46	120.30
2	B	145	CYS	N-CA-C	-7.25	91.41	111.00
1	A	59	ARG	NE-CZ-NH2	-7.07	116.76	120.30
2	B	322	ARG	NE-CZ-NH1	-6.95	116.83	120.30
1	A	15	ARG	NE-CZ-NH1	6.79	123.69	120.30
3	C	176	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	A	152	ARG	NE-CZ-NH1	6.74	123.67	120.30
4	D	12	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	819	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	A	12	ALA	C-N-CA	-6.37	108.92	122.30
2	B	387	ARG	NE-CZ-NH2	6.28	123.44	120.30
3	C	28	ARG	NE-CZ-NH2	-5.94	117.33	120.30
3	C	172	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	148	ARG	NE-CZ-NH1	-5.85	117.37	120.30
2	B	142	LYS	CD-CE-NZ	-5.83	98.29	111.70
3	C	165	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	262	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	918	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	214	LEU	CB-CG-CD1	5.37	120.12	111.00
2	B	117	ARG	NE-CZ-NH2	-5.32	117.64	120.30
4	D	1	MET	CG-SD-CE	-5.17	91.92	100.20
1	A	578	MET	CG-SD-CE	-5.08	92.07	100.20
4	D	9	CYS	CA-CB-SG	5.08	123.14	114.00
1	A	625	MET	CG-SD-CE	5.06	108.29	100.20
4	D	6	CYS	N-CA-CB	5.00	119.61	110.60

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	134	0
2	B	3057	0	2982	62	0
3	C	1433	0	1434	26	0
4	D	749	0	708	15	0
5	A	44	0	26	4	0
6	A	30	0	0	5	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	11	0
9	B	4	0	0	2	0
10	D	1	0	0	4	0
11	A	552	0	0	22	0
11	B	139	0	0	6	0
11	C	114	0	0	5	0
11	D	47	0	0	1	0
All	All	13493	0	12304	233	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 9.

All (233) 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:4:FMN:C8M	1.73	1.48
1:A:819:ARG:HH12	1:A:909:HIS:CE1	1.44	1.35
1:A:696:ALA:HB3	6:A:2562:SO4:O3	1.22	1.27
9:B:6244:SO3:S	9:B:6244:SO3:O2	1.99	1.21
2:B:145:CYS:CB	2:B:145:CYS:SG	2.32	1.18
1:A:696:ALA:CB	6:A:2562:SO4:O3	1.92	1.16
1:A:736:ARG:NH2	1:A:963:ASP:O	1.79	1.15
4:D:6:CYS:SG	4:D:63:CYS:SG	2.44	1.14
4:D:9:CYS:SG	4:D:63:CYS:SG	2.46	1.13
4:D:2:MET:HE1	4:D:78:PHE:CE1	1.84	1.13
2:B:172:HIS:CE1	8:B:4:FMN:HM83	1.83	1.12
2:B:276:HIS:HE1	11:B:452:HOH:O	1.31	1.11
2:B:172:HIS:NE2	8:B:4:FMN:HM83	0.77	1.10
1:A:819:ARG:NH1	1:A:909:HIS:CE1	2.18	1.10
1:A:889:LEU:HD23	1:A:925:ILE:HD11	1.29	1.10
2:B:267:HIS:HD2	11:B:434:HOH:O	1.35	1.08
1:A:15:ARG:HD2	1:A:161:GLU:OE2	1.55	1.07
4:D:2:MET:HE1	4:D:78:PHE:HE1	1.22	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:63:CYS:SG	10:D:100:ZN:ZN	1.49	1.00
2:B:172:HIS:CD2	8:B:4:FMN:HM83	1.97	0.99
3:C:169:GLN:NE2	3:C:171:TRP:HE1	1.61	0.97
1:A:15:ARG:CD	1:A:161:GLU:OE2	2.13	0.96
3:C:169:GLN:HE21	3:C:171:TRP:HE1	1.04	0.96
4:D:2:MET:CE	4:D:78:PHE:CE1	2.50	0.93
4:D:9:CYS:HG	10:D:100:ZN:ZN	0.81	0.87
1:A:696:ALA:HB1	11:A:1259:HOH:O	1.75	0.85
2:B:93:GLU:HG2	11:B:617:HOH:O	1.76	0.85
4:D:2:MET:CE	4:D:78:PHE:HE1	1.88	0.85
1:A:918:ARG:HG3	1:A:918:ARG:HH11	1.41	0.84
1:A:249:ALA:HB1	11:A:966:HOH:O	1.80	0.81
1:A:292:ASN:HD22	1:A:294:SER:H	1.26	0.81
3:C:93:GLU:HG3	11:C:537:HOH:O	1.81	0.80
1:A:830:ASP:OD1	1:A:909:HIS:CD2	2.35	0.79
2:B:286:ILE:HD11	2:B:328:VAL:CG2	2.13	0.79
3:C:37:PHE:O	3:C:93:GLU:HG2	1.84	0.78
1:A:504:SER:O	1:A:508:ILE:HG12	1.84	0.77
3:C:50:THR:HG22	11:C:227:HOH:O	1.83	0.77
1:A:696:ALA:HB3	6:A:2562:SO4:S	2.25	0.76
3:C:37:PHE:O	3:C:93:GLU:CG	2.34	0.75
1:A:80:ARG:NH2	11:A:1487:HOH:O	2.20	0.74
1:A:821:GLU:OE2	1:A:913:SER:HB2	1.88	0.74
1:A:68:VAL:HG21	1:A:554:THR:HG21	1.70	0.74
1:A:292:ASN:ND2	1:A:294:SER:H	1.85	0.73
1:A:249:ALA:HB2	5:A:965:NAD:PA	2.29	0.73
1:A:2:LYS:HE2	1:A:47:GLY:HA3	1.71	0.72
1:A:249:ALA:HB2	5:A:965:NAD:O3	1.89	0.72
1:A:945:VAL:HG13	11:A:1089:HOH:O	1.88	0.72
2:B:286:ILE:HD11	2:B:328:VAL:HG21	1.69	0.72
2:B:333:ASP:OD2	2:B:387:ARG:NH1	2.21	0.72
1:A:657:LYS:HE3	1:A:660:MET:HG3	1.73	0.71
1:A:889:LEU:HD23	1:A:925:ILE:CD1	2.16	0.71
11:A:1436:HOH:O	3:C:185:HIS:HD2	1.74	0.70
1:A:510:ARG:HH21	8:B:4:FMN:C5'	2.06	0.69
1:A:226:PRO:HB2	11:A:1205:HOH:O	1.91	0.69
1:A:819:ARG:NH1	1:A:909:HIS:ND1	2.33	0.68
1:A:860:ARG:HH21	1:A:863:ASN:HD21	1.41	0.68
1:A:931:ARG:O	1:A:949:VAL:CG2	2.41	0.68
1:A:510:ARG:HH21	8:B:4:FMN:H5'1	1.58	0.68
4:D:9:CYS:SG	10:D:100:ZN:ZN	1.83	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:LYS:HG3	1:A:715:ASP:OD2	1.95	0.67
1:A:249:ALA:CB	5:A:965:NAD:O2A	2.42	0.67
1:A:15:ARG:HD3	1:A:161:GLU:OE2	1.94	0.66
1:A:82:GLN:CG	11:A:1155:HOH:O	2.43	0.66
1:A:931:ARG:O	1:A:949:VAL:HG21	1.96	0.65
2:B:149:ASN:HD21	2:B:153:ASN:HD21	1.42	0.65
3:C:11:PRO:HD2	3:C:34:GLU:OE2	1.96	0.65
4:D:63:CYS:HG	10:D:100:ZN:ZN	1.09	0.64
1:A:82:GLN:HG3	11:A:1155:HOH:O	1.97	0.64
1:A:888:ALA:O	1:A:938:THR:HG23	2.00	0.62
2:B:111:HIS:HD2	2:B:156:TYR:O	1.82	0.61
1:A:243:GLN:OE1	1:A:413:HIS:HE1	1.84	0.60
11:A:1249:HOH:O	3:C:182:HIS:HD2	1.84	0.60
2:B:387:ARG:HG3	2:B:387:ARG:HH11	1.67	0.60
1:A:382:PRO:HG2	1:A:404:VAL:HG12	1.84	0.59
2:B:114:GLY:O	2:B:118:GLU:HG2	2.02	0.59
2:B:6:GLU:HB2	11:B:504:HOH:O	2.01	0.59
1:A:742:LEU:HD21	1:A:797:ASP:HB3	1.83	0.59
3:C:125:GLU:HG3	3:C:170:SER:HB3	1.85	0.59
2:B:172:HIS:HD1	2:B:173:ASP:H	1.50	0.59
1:A:635:GLU:OE2	1:A:686:ARG:NH1	2.36	0.58
1:A:819:ARG:CZ	1:A:909:HIS:CE1	2.86	0.58
1:A:689:MET:HE2	1:A:699:VAL:HG11	1.85	0.58
1:A:689:MET:CE	1:A:699:VAL:HG11	2.33	0.58
1:A:830:ASP:OD1	1:A:909:HIS:HD2	1.82	0.58
1:A:892:ALA:HA	1:A:937:LYS:HD2	1.84	0.57
1:A:125:HIS:HD2	11:A:1065:HOH:O	1.87	0.57
1:A:746:LEU:HD23	11:A:1347:HOH:O	2.05	0.57
3:C:37:PHE:O	3:C:93:GLU:HG3	2.05	0.57
2:B:64:ASN:HA	7:B:1:FAD:C6	2.35	0.56
1:A:883:LEU:HD11	1:A:947:VAL:HG11	1.87	0.56
2:B:384:ALA:O	2:B:387:ARG:HD3	2.05	0.56
1:A:578:MET:HB2	1:A:582:HIS:CE1	2.41	0.56
1:A:387:HIS:HE1	1:A:393:LYS:O	1.89	0.55
3:C:71:ALA:O	3:C:78:ALA:HA	2.06	0.55
1:A:582:HIS:CD2	1:A:601:TYR:OH	2.60	0.55
1:A:368:ARG:HD2	11:A:1365:HOH:O	2.07	0.55
2:B:172:HIS:HD1	2:B:173:ASP:N	2.06	0.55
2:B:39:LEU:HD13	2:B:368:ALA:CB	2.37	0.54
2:B:102:SER:O	2:B:168:GLY:HA3	2.08	0.54
1:A:830:ASP:OD2	1:A:909:HIS:NE2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:MET:O	1:A:845:VAL:HG12	2.07	0.54
2:B:153:ASN:HD22	2:B:153:ASN:H	1.55	0.54
3:C:11:PRO:HG3	11:C:245:HOH:O	2.07	0.54
1:A:616:CYS:SG	1:A:817:VAL:HG11	2.48	0.54
1:A:68:VAL:CG2	1:A:554:THR:HG21	2.38	0.53
1:A:736:ARG:HD3	1:A:748:VAL:O	2.09	0.53
2:B:13:ASN:HD22	2:B:184:ASN:HD21	1.56	0.53
1:A:909:HIS:HB3	1:A:911:TYR:CE1	2.44	0.52
1:A:632:GLY:HA3	1:A:696:ALA:HB2	1.92	0.51
1:A:194:GLU:O	1:A:194:GLU:HG3	2.10	0.51
1:A:539:GLU:HG3	11:A:1273:HOH:O	2.10	0.51
1:A:830:ASP:CG	1:A:909:HIS:HE2	2.13	0.51
1:A:654:THR:OG1	11:A:1390:HOH:O	2.19	0.50
1:A:580:PRO:HG2	3:C:9:ARG:HH12	1.76	0.50
1:A:770:ARG:NH2	11:A:1383:HOH:O	2.44	0.50
3:C:73:ASP:OD2	3:C:75:SER:HB2	2.10	0.50
1:A:178:ASP:HB2	1:A:181:GLN:HE21	1.76	0.50
1:A:616:CYS:HB2	1:A:914:PRO:HG2	1.93	0.50
2:B:202:ASP:OD1	2:B:203:GLY:N	2.45	0.50
2:B:270:VAL:HG22	2:B:271:TYR:N	2.27	0.50
2:B:39:LEU:HD13	2:B:368:ALA:HA	1.94	0.50
3:C:40:GLN:HA	3:C:89:LEU:O	2.11	0.49
2:B:381:ALA:N	2:B:382:PRO:CD	2.75	0.49
2:B:267:HIS:CD2	11:B:434:HOH:O	2.25	0.49
1:A:387:HIS:HD2	11:A:968:HOH:O	1.94	0.49
2:B:13:ASN:ND2	2:B:184:ASN:HD21	2.09	0.49
2:B:222:ALA:HB2	2:B:371:ILE:HD11	1.95	0.48
2:B:240:LEU:HD23	2:B:385:LEU:HD21	1.94	0.48
3:C:157:ALA:O	3:C:182:HIS:HE1	1.96	0.48
3:C:169:GLN:NE2	3:C:171:TRP:NE1	2.44	0.48
1:A:829:GLN:CD	1:A:909:HIS:CE1	2.87	0.48
3:C:176:ARG:HD3	11:C:545:HOH:O	2.13	0.48
1:A:510:ARG:NH2	8:B:4:FMN:C5'	2.77	0.48
1:A:696:ALA:CB	6:A:2562:SO4:S	2.96	0.47
1:A:829:GLN:HG2	1:A:909:HIS:NE2	2.29	0.47
1:A:648:MET:HE2	1:A:648:MET:HA	1.96	0.47
1:A:656:LEU:HD13	1:A:662:ARG:HB2	1.96	0.47
6:A:2562:SO4:O1	3:C:176:ARG:NH2	2.48	0.47
2:B:387:ARG:HH11	2:B:387:ARG:CG	2.26	0.47
1:A:776:PHE:O	1:A:819:ARG:HB2	2.14	0.47
2:B:64:ASN:HA	7:B:1:FAD:C5X	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:ASN:O	2:B:122:ARG:HD2	2.13	0.47
2:B:210:LYS:HE3	2:B:211:THR:O	2.14	0.47
1:A:340:ASN:HB3	1:A:353:LEU:HD22	1.97	0.47
8:B:4:FMN:N5	9:B:6244:SO3:S	2.88	0.47
1:A:82:GLN:HG2	11:A:1155:HOH:O	2.13	0.46
2:B:52:GLU:HG2	2:B:56:LEU:HA	1.97	0.46
1:A:739:ILE:HG13	1:A:782:PHE:CG	2.49	0.46
2:B:145:CYS:HB3	2:B:148:ILE:HG13	1.97	0.46
1:A:249:ALA:HB2	5:A:965:NAD:O2A	2.09	0.46
1:A:385:HIS:O	1:A:389:GLN:HG3	2.14	0.46
1:A:606:GLU:HA	1:A:610:GLU:OE1	2.16	0.46
1:A:81:HIS:NE2	1:A:226:PRO:HD2	2.31	0.46
1:A:789:TRP:CZ3	3:C:37:PHE:HA	2.51	0.46
1:A:860:ARG:NH2	1:A:863:ASN:HD21	2.11	0.46
1:A:510:ARG:NH2	8:B:4:FMN:H5'2	2.31	0.45
2:B:33:LEU:HD21	2:B:56:LEU:HD11	1.98	0.45
2:B:265:SER:O	2:B:269:HIS:HD2	1.98	0.45
1:A:152:ARG:HD3	3:C:142:HIS:CD2	2.52	0.45
1:A:733:PRO:HD3	1:A:779:GLU:OE1	2.17	0.45
1:A:889:LEU:CD2	1:A:925:ILE:HD11	2.22	0.45
2:B:265:SER:O	2:B:269:HIS:HA	2.17	0.45
2:B:286:ILE:HD11	2:B:328:VAL:HG23	1.97	0.45
1:A:510:ARG:HH21	8:B:4:FMN:H5'2	1.80	0.45
1:A:668:LYS:HD3	1:A:702:TRP:CH2	2.52	0.45
2:B:172:HIS:CE1	8:B:4:FMN:C8M	2.65	0.44
2:B:69:ARG:HD2	2:B:71:ASN:OD1	2.17	0.44
1:A:776:PHE:CZ	1:A:819:ARG:HG3	2.52	0.44
1:A:562:ALA:HB1	2:B:306:ALA:HA	2.00	0.44
2:B:357:PHE:HB3	7:B:1:FAD:C2	2.48	0.44
3:C:192:SER:O	3:C:193:GLU:C	2.55	0.44
1:A:253:ARG:HB2	1:A:254:PRO:HD2	1.98	0.44
1:A:416:GLY:HA2	1:A:427:ALA:HA	1.99	0.44
1:A:630:THR:HB	1:A:693:THR:HG23	1.98	0.44
1:A:805:PHE:O	1:A:806:ASN:HB3	2.17	0.44
1:A:871:LEU:HD13	1:A:952:LEU:HD11	1.99	0.44
2:B:171:LYS:HD2	2:B:171:LYS:HA	1.67	0.44
1:A:405:PRO:HB2	1:A:414:LEU:HD13	2.00	0.43
3:C:93:GLU:CG	11:C:537:HOH:O	2.54	0.43
1:A:656:LEU:HD23	1:A:681:ARG:HB2	2.00	0.43
1:A:689:MET:HE2	1:A:691:THR:HG22	2.00	0.43
3:C:136:SER:OG	3:C:156:LEU:HD22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:90:GLN:HG3	11:D:678:HOH:O	2.17	0.43
1:A:114:PRO:HA	2:B:314:ILE:HG13	2.00	0.43
1:A:223:LEU:HD12	1:A:226:PRO:HB3	2.00	0.43
1:A:918:ARG:HG3	1:A:918:ARG:NH1	2.18	0.43
4:D:2:MET:HE3	4:D:71:ARG:HD2	2.00	0.43
1:A:702:TRP:O	1:A:706:TRP:HD1	2.02	0.43
2:B:276:HIS:CE1	11:B:452:HOH:O	2.24	0.43
2:B:289:TYR:HA	4:D:19:TYR:CD2	2.54	0.43
1:A:890:VAL:HG22	1:A:894:ALA:HB3	2.01	0.42
2:B:142:LYS:HZ3	2:B:142:LYS:HG2	1.67	0.42
1:A:901:THR:HG23	11:A:1510:HOH:O	2.18	0.42
4:D:59:HIS:CE1	4:D:62:GLY:HA3	2.53	0.42
1:A:76:THR:HA	1:A:88:SER:HA	2.01	0.42
1:A:134:GLY:O	1:A:139:GLY:HA3	2.20	0.42
1:A:204:VAL:HG13	1:A:213:ILE:HG23	2.01	0.42
1:A:904:GLU:HG3	1:A:931:ARG:HH22	1.84	0.42
2:B:153:ASN:HD22	2:B:153:ASN:N	2.15	0.42
1:A:64:PHE:HB3	1:A:71:PRO:HD2	2.01	0.42
1:A:961:ARG:HE	1:A:961:ARG:HB3	1.68	0.42
3:C:177:ALA:O	3:C:180:THR:OG1	2.29	0.42
1:A:479:LYS:HB3	1:A:479:LYS:HE3	1.89	0.42
1:A:692:THR:OG1	1:A:695:GLY:N	2.53	0.41
2:B:286:ILE:CD1	2:B:328:VAL:HG21	2.44	0.41
2:B:374:ASP:O	2:B:375:GLU:HG2	2.19	0.41
1:A:945:VAL:CG1	11:A:1089:HOH:O	2.56	0.41
2:B:182:LYS:HD3	2:B:182:LYS:HA	1.49	0.41
2:B:349:ASN:HB2	2:B:367:LEU:HD22	2.01	0.41
1:A:478:TYR:HB3	1:A:491:VAL:HB	2.03	0.41
4:D:2:MET:HE1	4:D:78:PHE:CZ	2.48	0.41
1:A:819:ARG:NH2	1:A:909:HIS:CE1	2.89	0.41
11:A:1124:HOH:O	2:B:267:HIS:CE1	2.74	0.41
2:B:110:ALA:HB1	2:B:115:ASP:HB3	2.01	0.41
2:B:111:HIS:CE1	2:B:265:SER:OG	2.73	0.41
1:A:885:GLU:HG2	1:A:909:HIS:HA	2.01	0.41
1:A:539:GLU:O	1:A:541:PRO:HD3	2.21	0.41
1:A:540:ASN:HB3	1:A:543:GLN:HE21	1.85	0.41
1:A:938:THR:HG22	11:A:1385:HOH:O	2.20	0.41
2:B:111:HIS:HB3	2:B:156:TYR:HB3	2.03	0.41
1:A:830:ASP:CG	1:A:909:HIS:NE2	2.74	0.41
1:A:816:HIS:O	1:A:819:ARG:HD3	2.21	0.40
1:A:932:ILE:H	1:A:932:ILE:HG12	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:ILE:N	1:A:532:ILE:HD13	2.36	0.40
1:A:905:GLY:HA3	1:A:924:LEU:O	2.21	0.40
2:B:39:LEU:CD1	2:B:368:ALA:HA	2.52	0.40
1:A:486:GLN:OE1	1:A:517:ALA:HB1	2.22	0.40
2:B:387:ARG:NH1	2:B:387:ARG:HG3	2.33	0.40
1:A:515:SER:HA	11:A:974:HOH:O	2.21	0.40
1:A:619:VAL:HG21	1:A:818:LEU:CD1	2.51	0.40
1:A:750:ASN:ND2	1:A:963:ASP:OD1	2.54	0.40
1:A:776:PHE:CE2	1:A:819:ARG:HG3	2.56	0.40
1:A:819:ARG:HH22	1:A:909:HIS:CE1	2.39	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%)	930 (97%)	29 (3%)	2 (0%)	47	55
2	B	395/399 (99%)	381 (96%)	14 (4%)	0	100	100
3	C	193/203 (95%)	181 (94%)	12 (6%)	0	100	100
4	D	89/99 (90%)	86 (97%)	3 (3%)	0	100	100
All	All	1638/1665 (98%)	1578 (96%)	58 (4%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	941	ASP
1	A	71	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	747/747 (100%)	709 (95%)	38 (5%)	24	29
2	B	314/315 (100%)	302 (96%)	12 (4%)	33	42
3	C	143/151 (95%)	134 (94%)	9 (6%)	18	20
4	D	75/81 (93%)	74 (99%)	1 (1%)	69	81
All	All	1279/1294 (99%)	1219 (95%)	60 (5%)	26	33

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	123	HIS
1	A	214	LEU
1	A	218	ARG
1	A	327	THR
1	A	333	LEU
1	A	382	PRO
1	A	385	HIS
1	A	518	ASN
1	A	535	VAL
1	A	578	MET
1	A	590	GLU
1	A	619	VAL
1	A	639	LYS
1	A	645	LEU
1	A	654	THR
1	A	657	LYS
1	A	684	GLU
1	A	686	ARG
1	A	734	ARG
1	A	746	LEU
1	A	753	PHE
1	A	761	VAL
1	A	786	ILE

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Mol	Chain	Res	Type
1	A	789	TRP
1	A	792	LEU
1	A	815	MET
1	A	819	ARG
1	A	842	MET
1	A	845	VAL
1	A	848	LYS
1	A	850	LYS
1	A	871	LEU
1	A	874	VAL
1	A	889	LEU
1	A	901	THR
1	A	918	ARG
1	A	954	LEU
2	B	39	LEU
2	B	84	SER
2	B	91	LEU
2	B	97	TYR
2	B	145	CYS
2	B	153	ASN
2	B	172	HIS
2	B	174	HIS
2	B	211	THR
2	B	286	ILE
2	B	311	LEU
2	B	338	ILE
3	C	39	THR
3	C	50	THR
3	C	93	GLU
3	C	97	LEU
3	C	98	LEU
3	C	146	PHE
3	C	150	ARG
3	C	156	LEU
3	C	170	SER
4	D	63	CYS

Sometimes 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	82	GLN

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Mol	Chain	Res	Type
1	A	102	ASN
1	A	123	HIS
1	A	125	HIS
1	A	181	GLN
1	A	238	HIS
1	A	292	ASN
1	A	362	ASN
1	A	387	HIS
1	A	413	HIS
1	A	452	GLN
1	A	503	GLN
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	13	ASN
2	B	14	ASN
2	B	111	HIS
2	B	153	ASN
2	B	269	HIS
2	B	299	HIS
2	B	344	GLN
2	B	373	HIS
3	C	6	GLN
3	C	158	ASN
3	C	169	GLN
3	C	182	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	A	2559	-	4,4,4	0.25	0	6,6,6	0.18	0
6	SO4	A	2562	-	4,4,4	0.49	0	6,6,6	0.81	0
6	SO4	A	2561	-	4,4,4	0.22	0	6,6,6	0.25	0
6	SO4	A	2560	-	4,4,4	0.17	0	6,6,6	0.45	0
8	FMN	B	4	-	33,33,33	1.94	9 (27%)	48,50,50	2.40	15 (31%)
7	FAD	B	1	-	53,58,58	1.41	5 (9%)	68,89,89	1.35	10 (14%)
6	SO4	C	2564	-	4,4,4	0.66	0	6,6,6	0.41	0
6	SO4	A	2563	-	4,4,4	0.16	0	6,6,6	0.14	0
9	SO3	B	6244	-	1,3,3	10.87	1 (100%)	0,3,3	-	-
6	SO4	A	2567	-	4,4,4	0.24	0	6,6,6	0.40	0
6	SO4	D	2566	-	4,4,4	0.22	0	6,6,6	0.12	0
5	NAD	A	965	-	42,48,48	1.85	7 (16%)	50,73,73	1.99	17 (34%)

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
7	FAD	B	1	-	-	4/30/50/50	0/6/6/6
8	FMN	B	4	-	-	7/18/18/18	0/3/3/3
5	NAD	A	965	-	-	5/26/62/62	0/5/5/5

All (22) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	6244	SO3	O1-S	10.87	1.90	1.44
5	A	965	NAD	O7N-C7N	6.13	1.35	1.24
8	B	4	FMN	O5'-C5'	-5.87	1.22	1.44
7	B	1	FAD	C4X-N5	5.73	1.41	1.30
8	B	4	FMN	C4A-N5	5.34	1.41	1.30
5	A	965	NAD	C2B-C1B	-4.92	1.46	1.53
5	A	965	NAD	PN-O5D	-3.33	1.45	1.59
7	B	1	FAD	C10-N1	3.03	1.39	1.33
5	A	965	NAD	O4D-C4D	3.00	1.51	1.45
5	A	965	NAD	PA-O1A	-2.95	1.40	1.50
8	B	4	FMN	C4A-C10	-2.88	1.35	1.44
8	B	4	FMN	P-O3P	2.87	1.65	1.54
5	A	965	NAD	C5A-N7A	-2.79	1.29	1.39
5	A	965	NAD	C2N-N1N	2.66	1.38	1.35
8	B	4	FMN	P-O2P	-2.54	1.45	1.54
7	B	1	FAD	O3B-C3B	2.29	1.48	1.43
8	B	4	FMN	C4A-C4	-2.26	1.36	1.44
8	B	4	FMN	C9-C8	-2.25	1.36	1.39
7	B	1	FAD	C9-C9A	2.16	1.43	1.39
7	B	1	FAD	O4B-C4B	2.12	1.49	1.45
8	B	4	FMN	C9A-C5A	-2.07	1.37	1.41
8	B	4	FMN	C4'-C3'	2.06	1.57	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	4	FMN	C5'-C4'-C3'	-8.34	96.09	112.20
8	B	4	FMN	O4'-C4'-C5'	-6.70	94.85	109.92
8	B	4	FMN	O5'-P-O1P	5.23	121.14	106.47
5	A	965	NAD	N3A-C2A-N1A	-4.91	121.00	128.68
5	A	965	NAD	O4B-C1B-C2B	-4.75	99.99	106.93
7	B	1	FAD	N3A-C2A-N1A	-4.43	121.76	128.68
5	A	965	NAD	O4D-C1D-C2D	-4.05	101.01	106.93
8	B	4	FMN	C9A-C5A-N5	-3.99	118.10	122.43
5	A	965	NAD	C5B-C4B-C3B	-3.91	100.51	115.18
8	B	4	FMN	C4-N3-C2	-3.64	118.92	125.64
5	A	965	NAD	C2A-N1A-C6A	3.47	124.70	118.75
5	A	965	NAD	C6N-N1N-C2N	-3.40	118.88	121.97
7	B	1	FAD	C4-N3-C2	-3.26	119.62	125.64
8	B	4	FMN	O4-C4-C4A	-3.17	118.18	126.60
5	A	965	NAD	C2N-C3N-C4N	3.12	121.79	118.26
7	B	1	FAD	C4X-C10-N10	3.10	121.02	116.48
5	A	965	NAD	C5N-C6N-N1N	3.04	124.76	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	965	NAD	C6N-C5N-C4N	-3.00	115.07	119.44
7	B	1	FAD	C10-C4X-N5	-2.84	118.82	124.86
5	A	965	NAD	C2D-C3D-C4D	-2.81	97.18	102.64
8	B	4	FMN	O2-C2-N1	-2.78	117.22	121.83
7	B	1	FAD	O4B-C1B-C2B	-2.78	102.87	106.93
7	B	1	FAD	C4A-C5A-N7A	-2.68	106.60	109.40
5	A	965	NAD	O7N-C7N-C3N	2.61	122.75	119.63
8	B	4	FMN	C4'-C3'-C2'	2.49	118.53	113.36
5	A	965	NAD	C1B-N9A-C4A	-2.45	122.33	126.64
8	B	4	FMN	C10-C4A-N5	-2.44	119.67	124.86
5	A	965	NAD	C3N-C2N-N1N	-2.43	118.05	120.43
7	B	1	FAD	C9A-C5X-N5	-2.41	119.81	122.43
5	A	965	NAD	C5A-C6A-N6A	2.35	123.92	120.35
7	B	1	FAD	O2-C2-N1	-2.30	118.02	121.83
7	B	1	FAD	C4-C4X-C10	2.24	120.56	116.79
8	B	4	FMN	C4-C4A-C10	2.23	120.54	116.79
5	A	965	NAD	C5A-C6A-N1A	-2.20	115.37	120.35
8	B	4	FMN	O3'-C3'-C2'	2.19	114.09	108.81
5	A	965	NAD	O7N-C7N-N7N	-2.15	119.52	122.58
5	A	965	NAD	C4A-C5A-N7A	-2.15	107.16	109.40
8	B	4	FMN	C5A-C9A-N10	2.13	120.16	117.95
8	B	4	FMN	C4A-C10-N10	2.08	119.53	116.48
7	B	1	FAD	C4X-C4-N3	2.04	118.38	113.19
8	B	4	FMN	O5'-C5'-C4'	2.03	114.77	109.36
8	B	4	FMN	C4A-C4-N3	2.00	118.27	113.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1	FAD	C5'-O5'-P-O1P
8	B	4	FMN	C1'-C2'-C3'-C4'
8	B	4	FMN	C3'-C4'-C5'-O5'
8	B	4	FMN	O4'-C4'-C5'-O5'
8	B	4	FMN	C2'-C3'-C4'-C5'
8	B	4	FMN	O3'-C3'-C4'-C5'
8	B	4	FMN	O2'-C2'-C3'-C4'
5	A	965	NAD	C5D-O5D-PN-O3
7	B	1	FAD	C4'-C5'-O5'-P
5	A	965	NAD	C3B-C4B-C5B-O5B
8	B	4	FMN	C2'-C3'-C4'-O4'
5	A	965	NAD	O4D-C4D-C5D-O5D

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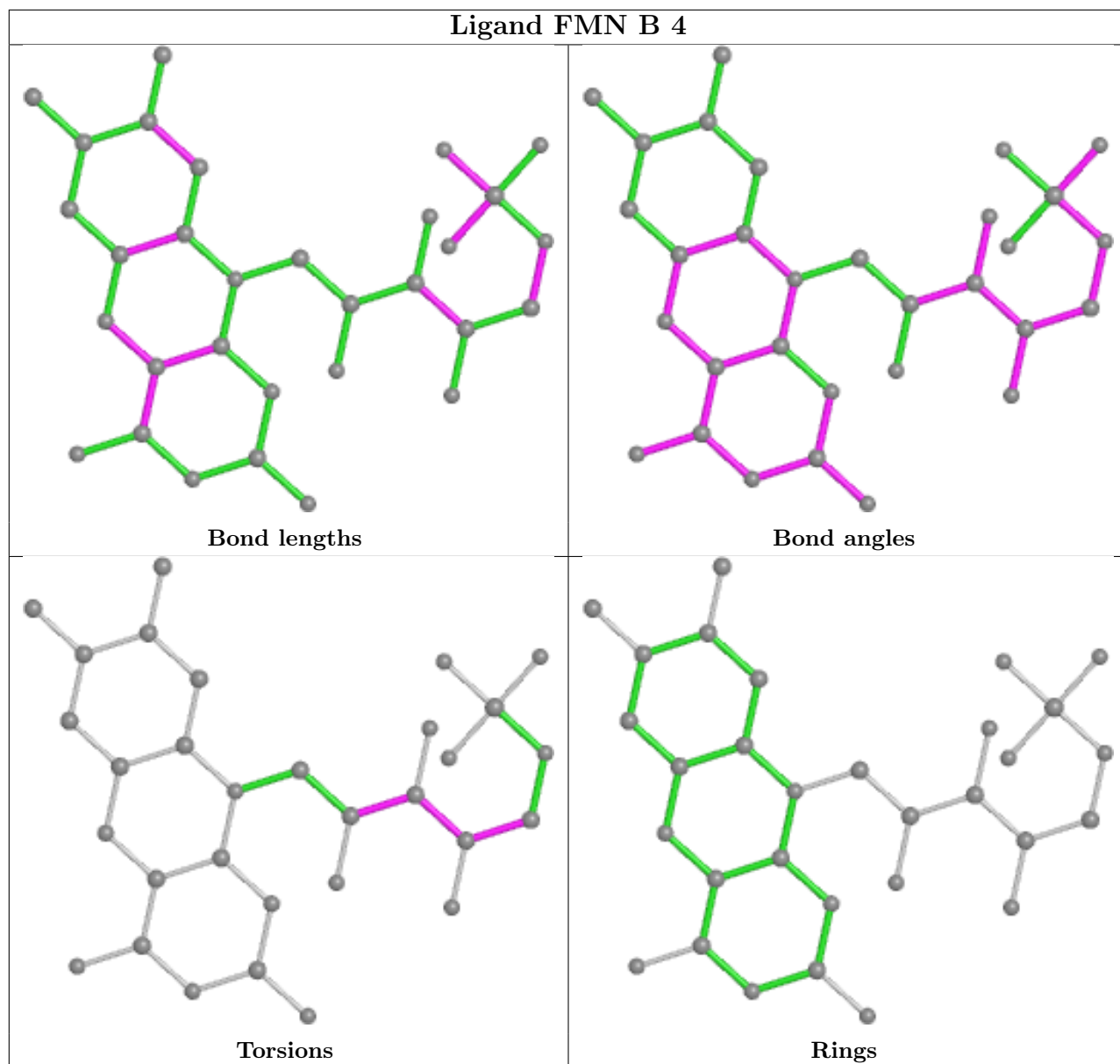
Mol	Chain	Res	Type	Atoms
7	B	1	FAD	C5'-O5'-P-O3P
5	A	965	NAD	C5D-O5D-PN-O1N
5	A	965	NAD	O4B-C4B-C5B-O5B
7	B	1	FAD	O4B-C4B-C5B-O5B

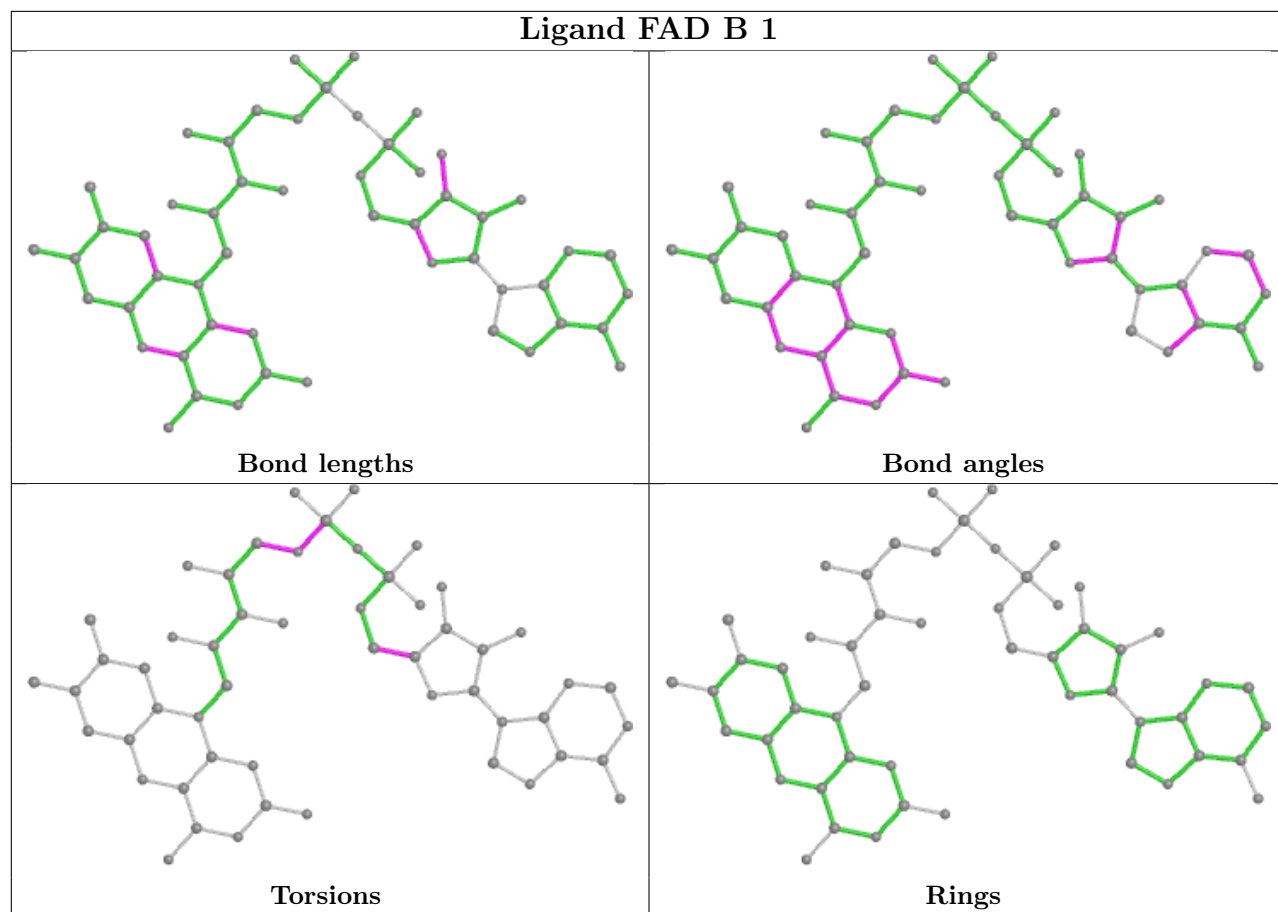
There are no ring outliers.

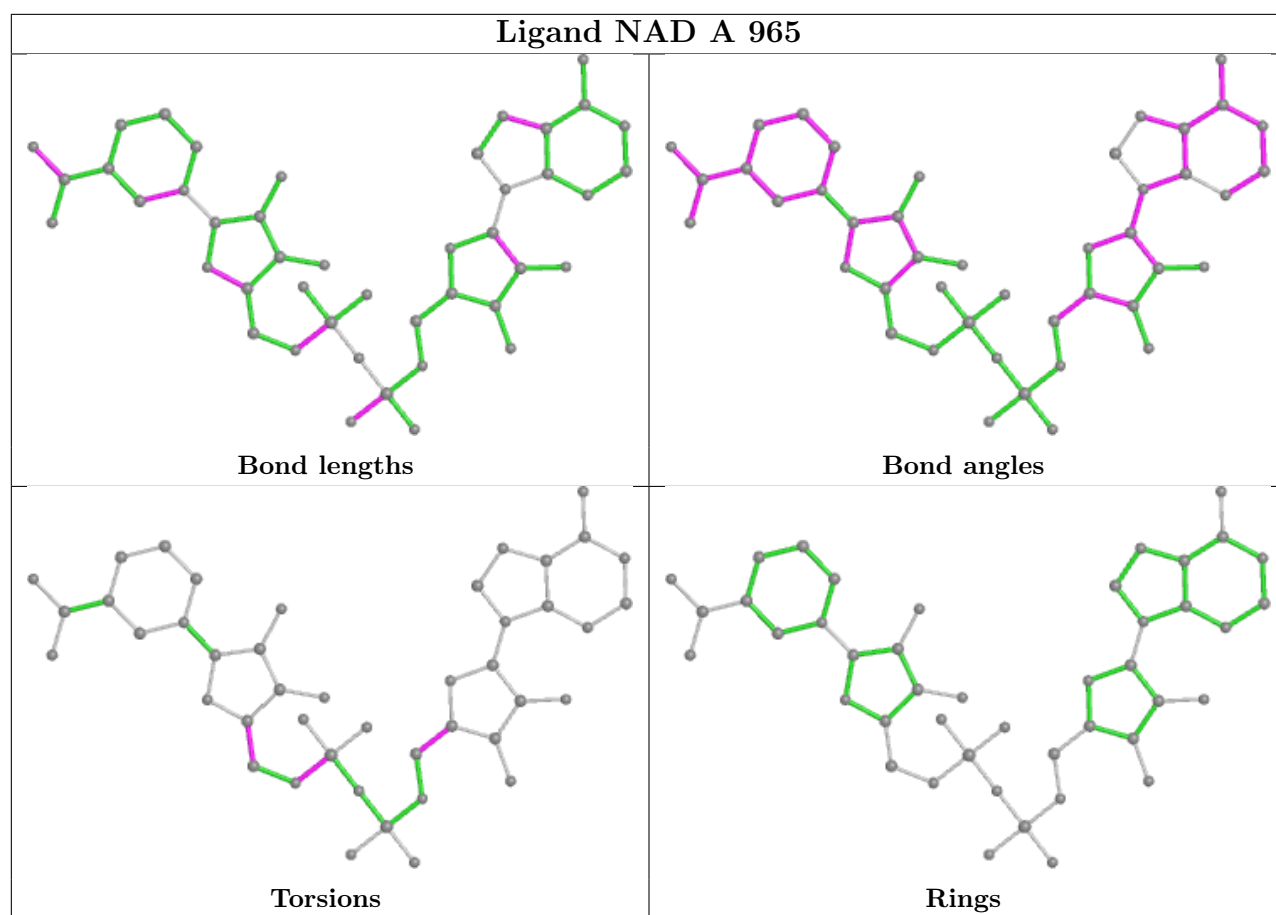
5 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2562	SO4	5	0
8	B	4	FMN	11	0
7	B	1	FAD	3	0
9	B	6244	SO3	2	0
5	A	965	NAD	4	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	963/964 (99%)	-0.05	43 (4%) 33 32	19, 35, 68, 86	0
2	B	397/399 (99%)	-0.12	6 (1%) 73 72	24, 43, 59, 76	0
3	C	195/203 (96%)	-0.26	0 100 100	24, 34, 56, 68	0
4	D	91/99 (91%)	-0.22	0 100 100	26, 37, 72, 108	0
All	All	1646/1665 (98%)	-0.10	49 (2%) 50 48	19, 38, 66, 108	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	954	LEU	4.6
1	A	849	LEU	4.2
1	A	848	LYS	4.1
1	A	897	SER	3.6
1	A	875	LEU	3.5
1	A	866	GLU	3.5
1	A	782	PHE	3.4
1	A	928	GLY	3.4
2	B	399	ALA	3.4
1	A	915	ALA	3.4
2	B	202	ASP	3.2
1	A	909	HIS	3.1
1	A	226	PRO	3.1
2	B	392	HIS	3.0
1	A	932	ILE	2.8
1	A	947	VAL	2.8
1	A	960	SER	2.8
1	A	823	GLY	2.7
1	A	948	GLN	2.7
1	A	873	SER	2.7
1	A	894	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	753	PHE	2.6
1	A	881	LEU	2.6
1	A	958	GLU	2.6
1	A	227	SER	2.5
1	A	746	LEU	2.5
1	A	891	ALA	2.4
1	A	738	VAL	2.4
1	A	892	ALA	2.4
1	A	327	THR	2.3
1	A	844	TRP	2.3
1	A	872	VAL	2.3
1	A	864	VAL	2.3
1	A	949	VAL	2.3
1	A	840	ALA	2.3
1	A	921	GLY	2.2
1	A	951	ASP	2.2
2	B	145	CYS	2.2
1	A	895	VAL	2.2
1	A	945	VAL	2.2
1	A	936	LEU	2.2
2	B	347	TYR	2.1
1	A	745	SER	2.1
1	A	843	GLU	2.1
1	A	876	PRO	2.1
1	A	751	ASP	2.1
2	B	401	ALA	2.1
1	A	858	PHE	2.1
1	A	871	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

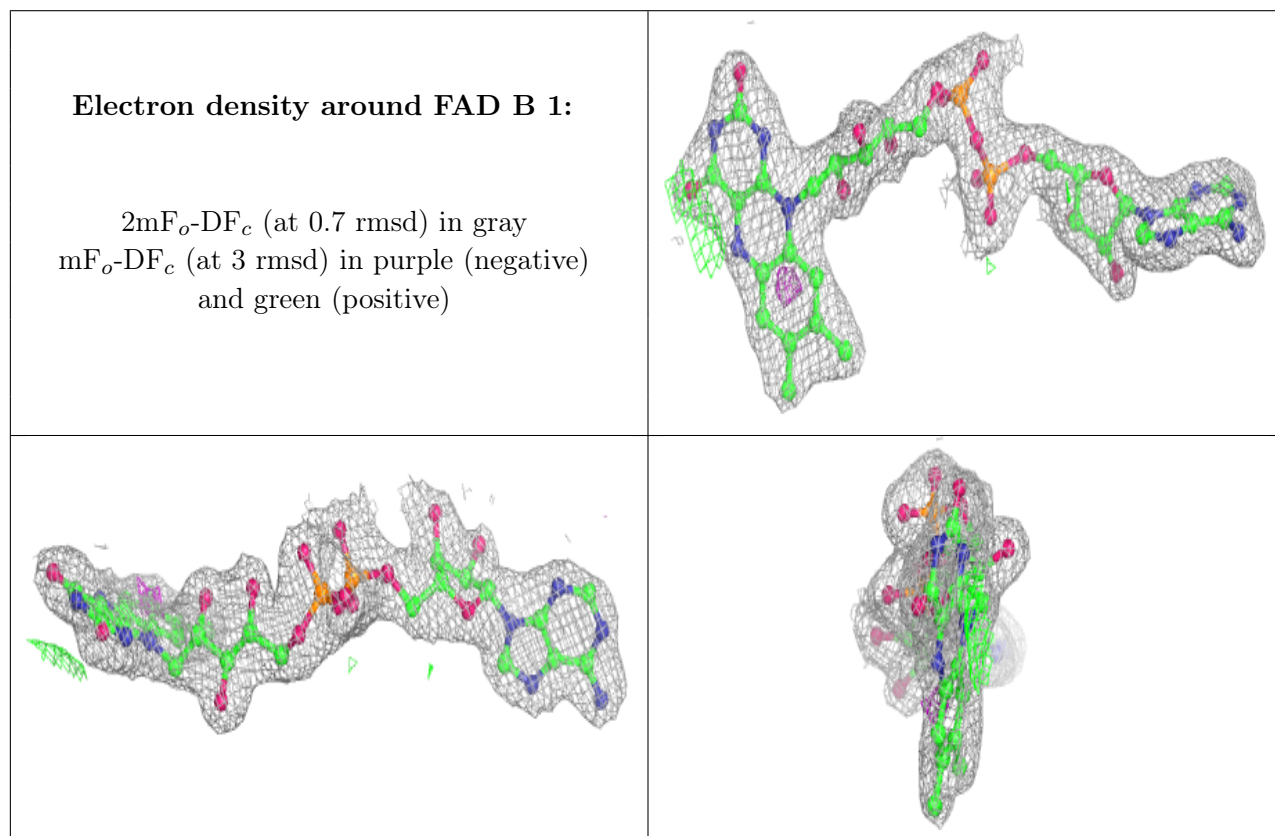
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



median, 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.

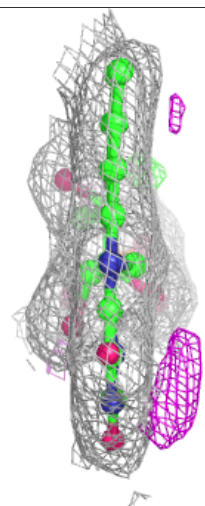
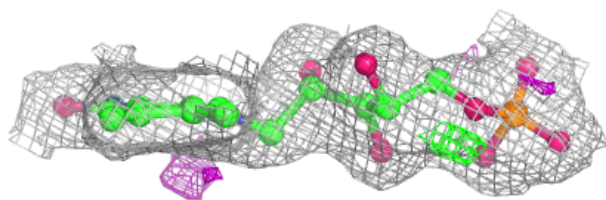
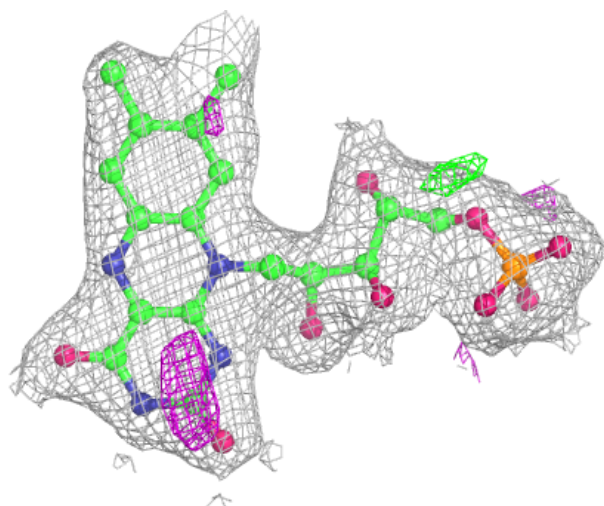
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	A	2562	5/5	0.92	0.13	44,44,73,102	0
6	SO4	A	2560	5/5	0.95	0.22	61,66,79,103	0
9	SO3	B	6244	4/4	0.95	0.13	56,59,62,73	0
6	SO4	A	2559	5/5	0.97	0.10	70,75,108,121	0
6	SO4	A	2563	5/5	0.97	0.29	78,80,92,294	0
6	SO4	D	2566	5/5	0.97	0.09	74,78,102,105	0
7	FAD	B	1	53/53	0.97	0.12	26,39,53,56	0
6	SO4	A	2561	5/5	0.97	0.14	44,55,84,100	0
8	FMN	B	4	31/31	0.98	0.10	21,27,32,42	0
6	SO4	C	2564	5/5	0.98	0.20	41,45,59,64	0
6	SO4	A	2567	5/5	0.99	0.07	44,46,61,72	0
5	NAD	A	965	44/44	0.99	0.11	12,21,27,31	0
10	ZN	D	100	1/1	0.99	0.05	32,32,32,32	0

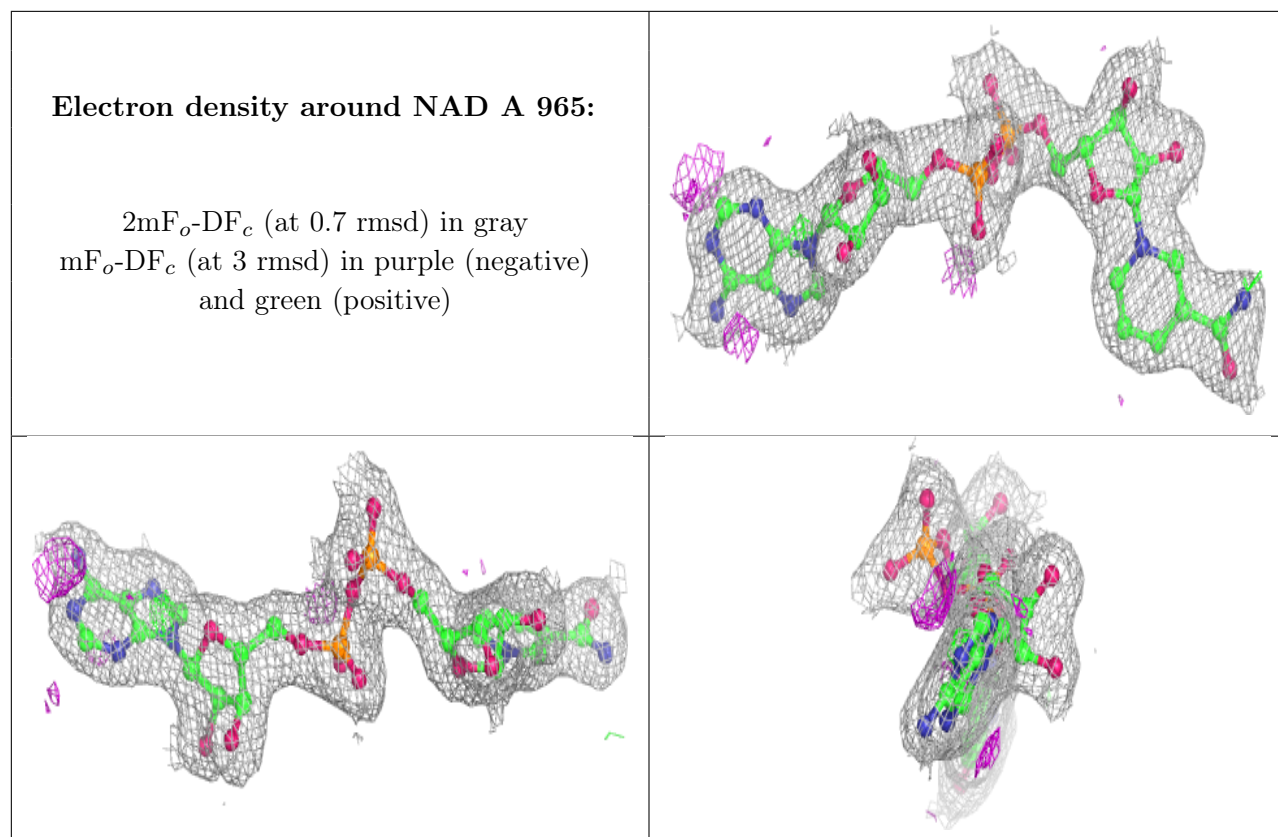
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



**Electron density around FMN B 4:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.