



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:21 PM UTC

PDB ID : 3ADA / pdb_00003ada
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

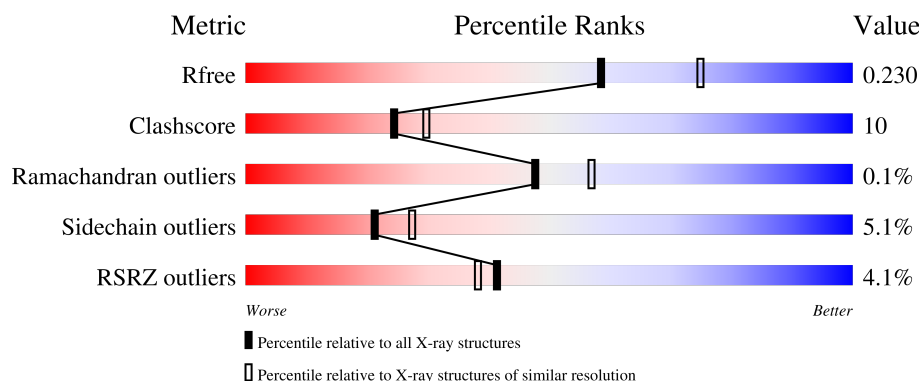
1 Overall quality at a glance

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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% 78% 18% .
2	B	399	4% 80% 16% ..
3	C	203	3% 71% 21% ..
4	D	99	5% 77% 11% .. 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

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
1	A	963	Total	C	N	O	S	0	0	0
			7229	4507	1287	1413	22			

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

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

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

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

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

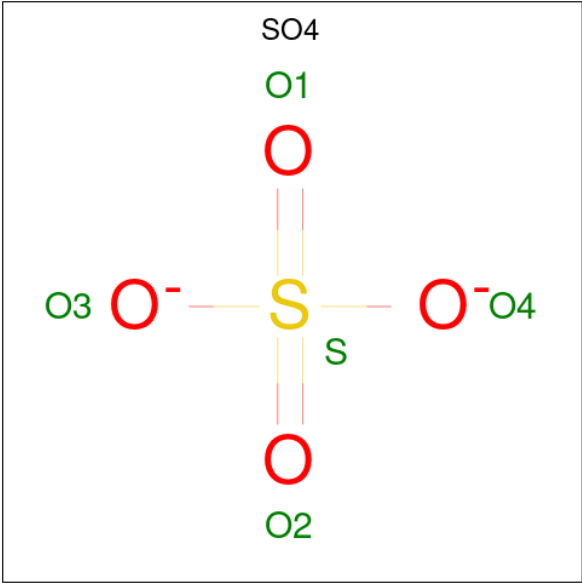
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	91	Total	C	N	O	S	0	0	0
			749	476	135	133	5			

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



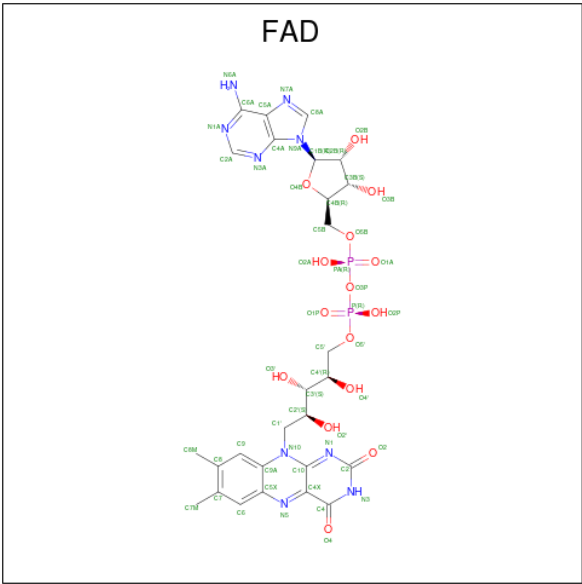
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

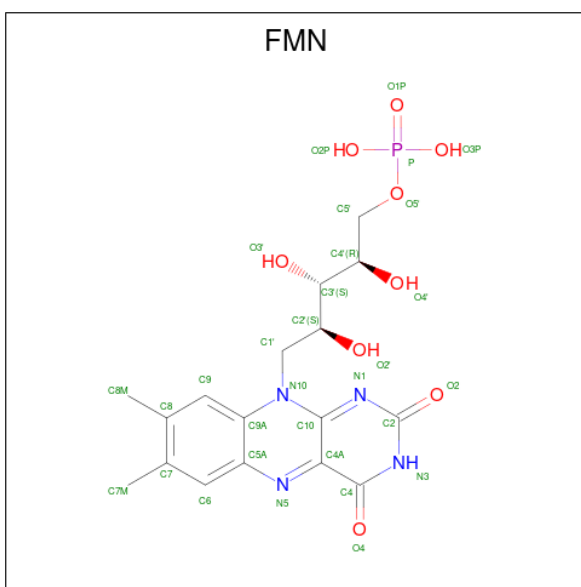
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



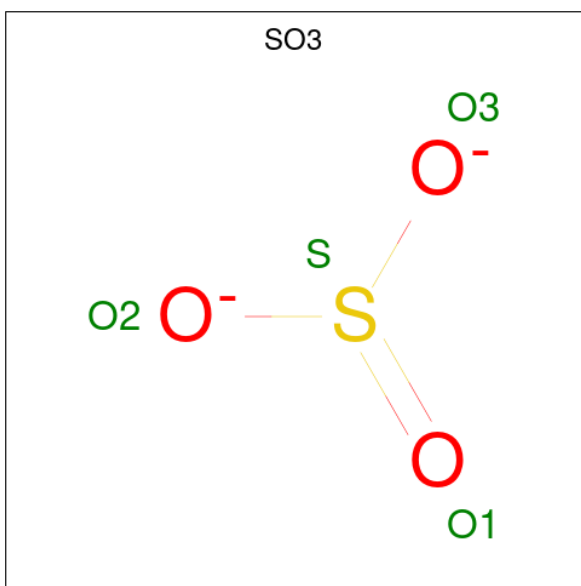
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 8 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

- Molecule 9 is SULFITE ION (CCD ID: SO3) (formula: O₃S).



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

- Molecule 10 is ZINC ION (CCD ID: 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

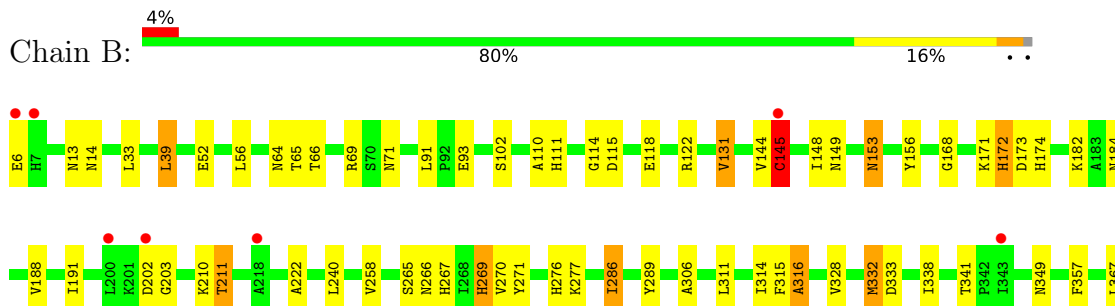
3 Residue-property plots [i](#)

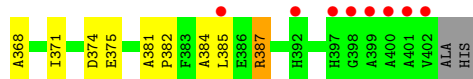
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: SARCOSINE OXIDASE ALPHA SUBUNIT

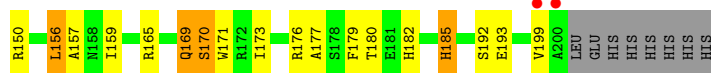
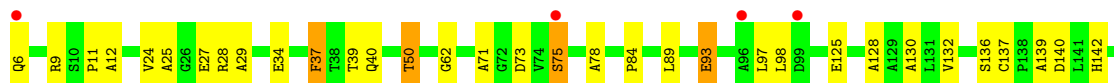


• Molecule 2: SARCOSINE OXIDASE BETA SUBUNIT

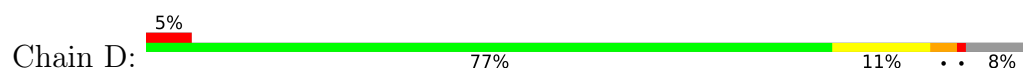




● Molecule 3: SARCOSINE OXIDASE GAMMA SUBUNIT



● Molecule 4: SARCOSINE OXIDASE DELTA SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	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) 99.6 (69.98-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.82 (at 2.20Å)	Xtriage
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 (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13493	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, NAD, FMN, SO4, SO3, ZN

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	1.40	36/7361 (0.5%)	1.20	29/10017 (0.3%)
2	B	1.31	9/3136 (0.3%)	1.20	15/4266 (0.4%)
3	C	1.65	15/1461 (1.0%)	1.36	9/1998 (0.5%)
4	D	1.22	3/772 (0.4%)	1.19	7/1040 (0.7%)
All	All	1.40	63/12730 (0.5%)	1.22	60/17321 (0.3%)

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	145	CYS	CB-SG	15.46	2.32	1.81
2	B	145	CYS	CA-CB	9.85	1.71	1.53
1	A	409	VAL	CA-CB	9.15	1.63	1.54
2	B	144	VAL	CA-C	8.24	1.62	1.52
1	A	375	ALA	CA-CB	8.23	1.63	1.53
4	D	6	CYS	CA-CB	8.04	1.65	1.53
2	B	145	CYS	N-CA	7.48	1.56	1.46
1	A	135	ALA	CA-CB	7.47	1.63	1.53
2	B	316	ALA	CA-CB	7.08	1.64	1.53
3	C	130	ALA	CA-CB	6.98	1.64	1.53
1	A	81	HIS	CA-C	-6.72	1.44	1.52
3	C	132	VAL	CA-CB	6.72	1.64	1.54
4	D	74	VAL	CA-CB	6.68	1.61	1.55
1	A	458	ALA	CA-CB	6.64	1.64	1.53
3	C	128	ALA	CA-CB	6.52	1.63	1.53
1	A	246	LEU	CA-C	-6.51	1.44	1.52
3	C	185	HIS	CA-C	6.49	1.61	1.52
2	B	65	THR	CA-CB	6.45	1.63	1.53
1	A	232	SER	N-CA	6.34	1.53	1.46
1	A	226	PRO	CA-C	6.18	1.60	1.52
3	C	25	ALA	CA-CB	6.06	1.62	1.53
4	D	63	CYS	CA-CB	6.02	1.63	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	131	VAL	CA-CB	5.98	1.62	1.54
3	C	75	SER	N-CA	5.91	1.53	1.46
3	C	159	ILE	CA-CB	5.87	1.60	1.55
1	A	231	VAL	CA-CB	-5.72	1.47	1.53
1	A	233	ARG	CA-C	5.71	1.60	1.52
1	A	788	ALA	CA-CB	5.65	1.62	1.53
1	A	217	GLN	N-CA	5.63	1.53	1.46
1	A	114	PRO	C-O	-5.61	1.17	1.24
2	B	188	VAL	CA-CB	5.57	1.59	1.54
1	A	425	ALA	CA-CB	5.55	1.61	1.53
1	A	204	VAL	C-O	5.54	1.29	1.23
3	C	139	ALA	CA-C	-5.53	1.45	1.53
3	C	24	VAL	CA-CB	5.43	1.63	1.55
1	A	120	TYR	CA-C	5.40	1.59	1.52
1	A	213	ILE	C-O	5.39	1.30	1.24
2	B	191	ILE	CA-CB	5.38	1.60	1.53
1	A	730	VAL	CA-CB	5.34	1.60	1.53
3	C	28	ARG	CA-C	-5.32	1.46	1.53
1	A	696	ALA	CA-CB	-5.32	1.45	1.53
3	C	165	ARG	NE-CZ	5.31	1.38	1.33
3	C	150	ARG	CA-C	-5.27	1.46	1.52
1	A	318	ILE	CA-CB	5.27	1.60	1.53
1	A	592	VAL	CA-CB	5.26	1.60	1.53
1	A	436	ALA	N-CA	5.24	1.52	1.46
1	A	533	ALA	N-CA	-5.22	1.40	1.46
1	A	553	TYR	C-O	5.21	1.30	1.24
3	C	29	ALA	CA-CB	5.21	1.62	1.53
1	A	124	VAL	C-O	5.20	1.29	1.23
3	C	173	ILE	CA-C	-5.15	1.46	1.52
3	C	140	ASP	CA-C	5.14	1.59	1.52
1	A	400	ILE	CG1-CD1	5.13	1.71	1.51
1	A	388	SER	N-CA	5.12	1.52	1.46
1	A	477	HIS	CA-C	5.11	1.59	1.52
1	A	179	ALA	C-O	-5.10	1.18	1.24
1	A	386	LEU	N-CA	5.09	1.52	1.46
1	A	900	VAL	CA-CB	5.06	1.60	1.54
1	A	201	ARG	CA-C	-5.05	1.46	1.52
1	A	225	GLY	C-O	5.04	1.30	1.24
1	A	525	GLY	CA-C	5.03	1.57	1.52
1	A	57	LEU	CA-C	-5.02	1.45	1.52
1	A	554	THR	CA-C	5.01	1.57	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	145	CYS	CA-CB-SG	11.33	140.47	114.40
2	B	144	VAL	N-CA-C	10.33	120.13	110.42
2	B	145	CYS	N-CA-C	-9.28	91.41	108.85
3	C	132	VAL	N-CA-C	-8.80	103.27	111.45
1	A	12	ALA	CA-C-N	-8.35	108.92	122.20
1	A	12	ALA	C-N-CA	-8.35	108.92	122.20
1	A	225	GLY	CA-C-N	-8.08	111.26	119.99
1	A	225	GLY	C-N-CA	-8.08	111.26	119.99
2	B	145	CYS	N-CA-CB	7.97	125.26	110.27
2	B	258	VAL	CB-CA-C	-7.92	103.19	110.63
1	A	901	THR	CA-C-N	7.16	127.21	119.90
1	A	901	THR	C-N-CA	7.16	127.21	119.90
3	C	179	PHE	N-CA-C	-7.13	104.16	112.92
1	A	113	ASP	CA-C-N	-6.98	112.50	120.04
1	A	113	ASP	C-N-CA	-6.98	112.50	120.04
3	C	62	GLY	N-CA-C	-6.48	101.04	112.77
1	A	117	ASP	CA-C-N	-6.31	113.68	121.00
1	A	117	ASP	C-N-CA	-6.31	113.68	121.00
1	A	296	TYR	CA-C-N	-6.27	112.02	118.85
1	A	296	TYR	C-N-CA	-6.27	112.02	118.85
1	A	19	ASP	N-CA-C	-6.25	105.29	113.17
2	B	66	THR	N-CA-C	6.11	120.53	113.38
2	B	266	ASN	N-CA-C	6.09	119.18	111.69
2	B	144	VAL	CA-C-O	-5.90	114.34	121.18
2	B	387	ARG	NE-CZ-NH1	-5.84	115.66	121.50
1	A	696	ALA	N-CA-C	5.80	118.09	111.02
4	D	88	ARG	CA-C-N	-5.75	114.40	120.66
4	D	88	ARG	C-N-CA	-5.75	114.40	120.66
2	B	14	ASN	CA-C-N	-5.72	114.07	120.14
2	B	14	ASN	C-N-CA	-5.72	114.07	120.14
4	D	6	CYS	N-CA-C	-5.72	101.24	109.48
1	A	459	GLY	N-CA-C	-5.70	101.65	111.57
2	B	269	HIS	N-CA-C	5.62	117.38	108.67
4	D	9	CYS	CB-CA-C	5.60	118.96	109.55
1	A	70	GLU	N-CA-C	5.58	117.64	109.71
3	C	159	ILE	CA-C-N	5.57	125.85	119.83
3	C	159	ILE	C-N-CA	5.57	125.85	119.83
4	D	6	CYS	N-CA-CB	5.52	119.61	109.73
3	C	75	SER	CB-CA-C	-5.46	101.41	110.68
1	A	214	LEU	CA-CB-CG	-5.44	97.25	116.30
3	C	137	CYS	CA-C-N	5.43	125.90	120.04
3	C	137	CYS	C-N-CA	5.43	125.90	120.04
1	A	32	SER	CB-CA-C	-5.41	100.61	109.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	693	THR	N-CA-C	-5.39	105.49	111.36
1	A	426	SER	CB-CA-C	-5.37	101.72	110.85
1	A	404	VAL	CA-C-N	-5.37	114.43	119.85
1	A	404	VAL	C-N-CA	-5.37	114.43	119.85
1	A	225	GLY	N-CA-C	-5.32	101.48	112.34
1	A	24	LEU	N-CA-C	-5.25	100.94	108.60
4	D	62	GLY	CA-C-N	5.23	128.02	120.38
4	D	62	GLY	C-N-CA	5.23	128.02	120.38
3	C	37	PHE	N-CA-C	5.14	118.83	112.24
1	A	509	LYS	N-CA-C	-5.12	104.97	111.11
2	B	341	THR	CA-C-N	-5.12	114.44	120.12
2	B	341	THR	C-N-CA	-5.12	114.44	120.12
2	B	277	LYS	N-CA-C	-5.07	106.35	112.54
1	A	456	VAL	CA-C-N	-5.03	114.77	119.85
1	A	456	VAL	C-N-CA	-5.03	114.77	119.85
1	A	61	ARG	CA-C-N	-5.02	117.60	121.82
1	A	61	ARG	C-N-CA	-5.02	117.60	121.82

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	7229	0	7104	140	0
2	B	3057	0	2982	63	0
3	C	1433	0	1434	30	0
4	D	749	0	708	19	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0
All	All	13493	0	12304	247	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (247) 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
2:B:172:HIS:NE2	8:B:4:FMN:HM83	1.05	1.36
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
2:B:276:HIS:HE1	11:B:452:HOH:O	1.31	1.11
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:63:CYS:SG	10:D:100:ZN:ZN	1.49	1.00
2:B:172:HIS:CD2	8:B:4:FMN:HM83	1.99	0.97
4:D:2:MET:HE2	4:D:78:PHE:HE1	1.27	0.97
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	0.94
2:B:172:HIS:NE2	8:B:4:FMN:HM81	1.81	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:2:MET:HE1	4:D:78:PHE:CE1	2.17	0.78
2:B:172:HIS:CE1	8:B:4:FMN:C8M	2.65	0.78
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
4:D:2:MET:HE2	4:D:78:PHE:CE1	2.12	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
1:A:648:MET:HE2	1:A:648:MET:HA	1.72	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:GLN:HG3	11:A:1155:HOH:O	1.97	0.64
2:B:332:MET:HA	2:B:332:MET:HE2	1.80	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
4:D:79:LYS:NZ	11:D:824:HOH:O	2.32	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
1:A:689:MET:HE1	1:A:699:VAL:HG11	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: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
1:A:830:ASP:CG	1:A:909:HIS:HE2	2.13	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:ARG:HD3	1:A:748:VAL:O	2.09	0.53
1:A:829:GLN:CD	1:A:909:HIS:CE1	2.87	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:815:MET:C	1:A:815:MET:HE2	2.35	0.51
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
3:C:169:GLN:HE21	3:C:171:TRP:NE1	1.89	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
1:A:689:MET:HE2	1:A:691:THR:HG22	1.92	0.49
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
4:D:2:MET:HE1	4:D:71:ARG:HD3	1.95	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
4:D:2:MET:HE1	4:D:71:ARG:CD	2.43	0.48
3:C:176:ARG:HD3	11:C:545:HOH:O	2.13	0.48
3:C:192:SER:O	3:C:193:GLU:C	2.55	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: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
2:B:71:ASN:O	2:B:122:ARG:HD2	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:689:MET:HE1	1:A:699:VAL:CG1	2.46	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:830:ASP:CG	1:A:909:HIS:NE2	2.74	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:815:MET:HE1	1:A:826:ILE:HD11	1.97	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:69:ARG:HD2	2:B:71:ASN:OD1	2.17	0.44
3:C:177:ALA:O	3:C:180:THR:OG1	2.29	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
1:A:940:VAL:O	1:A:941:ASP:C	2.61	0.44
2:B:357:PHE:HB3	7:B:1:FAD:C2	2.48	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
3:C:89:LEU:HD23	3:C:89:LEU:C	2.43	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
1:A:956:ASP:O	1:A:957:PRO:C	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:136:SER:OG	3:C:156:LEU:HD22	2.18	0.43
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
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
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
1:A:479:LYS:HB3	1:A:479:LYS:HE3	1.89	0.42
1:A:776:PHE:CE2	1:A:815:MET:HE3	2.55	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
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
3:C:84:PRO:HG3	4:D:8:ASN:CG	2.46	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
2:B:315:PHE:O	2:B:316:ALA:C	2.63	0.41
1:A:816:HIS:O	1:A:819:ARG:HD3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:932:ILE:H	1:A:932:ILE:HG12	1.77	0.40
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
4:D:2:MET:HE2	4:D:2:MET:HB3	1.96	0.40
1:A:819:ARG:HH22	1:A:909:HIS:CE1	2.39	0.40
3:C:12:ALA:HB3	3:C:34:GLU:CD	2.47	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%)	43	51
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%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	941	ASP
1	A	71	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	747/747 (100%)	707 (95%)	40 (5%)	20	25
2	B	314/315 (100%)	302 (96%)	12 (4%)	29	40
3	C	143/151 (95%)	132 (92%)	11 (8%)	12	13
4	D	75/81 (93%)	73 (97%)	2 (3%)	39	53
All	All	1279/1294 (99%)	1214 (95%)	65 (5%)	21	27

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	102	ASN
1	A	194	GLU
1	A	214	LEU
1	A	318	ILE
1	A	327	THR
1	A	333	LEU
1	A	382	PRO
1	A	385	HIS
1	A	503	GLN
1	A	532	ILE
1	A	535	VAL
1	A	544	ILE
1	A	578	MET
1	A	616	CYS
1	A	619	VAL
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	761	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	786	ILE
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	871	LEU
1	A	874	VAL
1	A	889	LEU
1	A	901	THR
1	A	918	ARG
1	A	935	VAL
1	A	938	THR
1	A	954	LEU
1	A	958	GLU
2	B	39	LEU
2	B	91	LEU
2	B	131	VAL
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	332	MET
2	B	338	ILE
3	C	6	GLN
3	C	27	GLU
3	C	39	THR
3	C	50	THR
3	C	93	GLU
3	C	97	LEU
3	C	98	LEU
3	C	156	LEU
3	C	169	GLN
3	C	170	SER
3	C	199	VAL
4	D	3	LEU
4	D	63	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	125	HIS
1	A	181	GLN
1	A	200	GLN
1	A	238	HIS
1	A	276	ASN
1	A	292	ASN
1	A	387	HIS
1	A	412	GLN
1	A	413	HIS
1	A	489	GLN
1	A	543	GLN
1	A	582	HIS
1	A	750	ASN
1	A	803	GLN
1	A	863	ASN
2	B	13	ASN
2	B	111	HIS
2	B	153	ASN
2	B	269	HIS
2	B	369	HIS
3	C	6	GLN
3	C	158	ASN
3	C	169	GLN
3	C	182	HIS
4	D	32	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	2567	-	4,4,4	0.28	0	6,6,6	0.43	0
6	SO4	A	2559	-	4,4,4	0.34	0	6,6,6	0.17	0
6	SO4	D	2566	-	4,4,4	0.33	0	6,6,6	0.09	0
8	FMN	B	4	-	33,33,33	1.94	9 (27%)	48,50,50	2.47	14 (29%)
6	SO4	A	2561	-	4,4,4	0.28	0	6,6,6	0.27	0
6	SO4	A	2562	-	4,4,4	0.55	0	6,6,6	0.78	0
6	SO4	C	2564	-	4,4,4	0.73	0	6,6,6	0.39	0
5	NAD	A	965	-	46,48,48	1.99	10 (21%)	64,73,73	1.97	20 (31%)
9	SO3	B	6244	-	1,3,3	10.78	1 (100%)	0,3,3	-	-
7	FAD	B	1	-	58,58,58	1.64	6 (10%)	85,89,89	1.71	18 (21%)
6	SO4	A	2560	-	4,4,4	0.28	0	6,6,6	0.46	0
6	SO4	A	2563	-	4,4,4	0.26	0	6,6,6	0.17	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
7	FAD	B	1	-	-	2/34/50/50	0/6/6/6
8	FMN	B	4	-	-	7/18/18/18	0/3/3/3
5	NAD	A	965	-	-	4/30/62/62	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	6244	SO3	O1-S	10.78	1.90	1.44
7	B	1	FAD	PA-O3P	-6.84	1.52	1.59
5	A	965	NAD	O7N-C7N	6.31	1.35	1.24
8	B	4	FMN	O5'-C5'	-5.92	1.22	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	965	NAD	C5A-N7A	-5.18	1.29	1.39
7	B	1	FAD	C4X-N5	5.16	1.41	1.30
8	B	4	FMN	C4A-N5	4.80	1.41	1.30
5	A	965	NAD	C4A-N9A	-4.40	1.28	1.37
5	A	965	NAD	PN-O5D	-3.47	1.45	1.59
7	B	1	FAD	C10-N1	3.06	1.39	1.33
5	A	965	NAD	O4D-C4D	3.02	1.51	1.45
5	A	965	NAD	C8A-N9A	-3.01	1.32	1.37
5	A	965	NAD	PA-O1A	-2.99	1.40	1.50
8	B	4	FMN	P-O3P	2.98	1.65	1.54
5	A	965	NAD	C2N-N1N	2.93	1.38	1.35
8	B	4	FMN	C4A-C10	-2.91	1.35	1.44
8	B	4	FMN	P-O2P	-2.62	1.45	1.54
8	B	4	FMN	C9-C8	-2.45	1.36	1.39
5	A	965	NAD	C2B-C1B	-2.29	1.46	1.53
8	B	4	FMN	C4A-C4	-2.26	1.36	1.44
8	B	4	FMN	C4'-C3'	2.24	1.57	1.53
8	B	4	FMN	C9A-C5A	-2.20	1.37	1.41
7	B	1	FAD	O3B-C3B	2.18	1.48	1.43
7	B	1	FAD	C9-C9A	2.18	1.43	1.39
7	B	1	FAD	O4B-C4B	2.13	1.49	1.45
5	A	965	NAD	C5B-C4B	2.06	1.57	1.51

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	4	FMN	C5'-C4'-C3'	-8.55	96.09	112.22
8	B	4	FMN	O4'-C4'-C5'	-6.86	94.85	109.99
8	B	4	FMN	O5'-P-O1P	5.44	121.14	106.44
7	B	1	FAD	C5A-C4A-N3A	-5.23	119.52	126.72
5	A	965	NAD	O4B-C1B-N9A	-5.14	98.22	108.09
5	A	965	NAD	N3A-C2A-N1A	-5.01	121.00	128.58
7	B	1	FAD	N3A-C2A-N1A	-4.51	121.76	128.58
7	B	1	FAD	N9A-C8A-N7A	-4.47	107.60	113.94
8	B	4	FMN	C9A-C5A-N5	-4.10	118.10	122.45
5	A	965	NAD	C5B-C4B-C3B	-4.08	100.51	115.21
8	B	4	FMN	C4-N3-C2	-3.78	118.92	125.64
7	B	1	FAD	C4A-N9A-C8A	3.74	109.67	105.74
7	B	1	FAD	N3A-C4A-N9A	3.74	133.52	127.17
7	B	1	FAD	C5A-N7A-C8A	3.63	109.16	103.45
5	A	965	NAD	C2A-N1A-C6A	3.63	124.70	118.73
5	A	965	NAD	C5A-C4A-N3A	-3.56	121.81	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	965	NAD	C6N-N1N-C2N	-3.53	118.88	121.88
7	B	1	FAD	C4A-C5A-N7A	-3.48	106.60	110.58
7	B	1	FAD	C2A-N3A-C4A	3.43	120.21	111.83
7	B	1	FAD	C4-N3-C2	-3.39	119.62	125.64
5	A	965	NAD	C5N-C6N-N1N	3.21	124.76	120.38
7	B	1	FAD	C4X-C10-N10	3.17	121.02	116.48
8	B	4	FMN	O4-C4-C4A	-3.16	118.18	126.53
5	A	965	NAD	O4B-C1B-C2B	-3.10	99.99	106.62
5	A	965	NAD	C2N-C3N-C4N	3.04	121.79	118.26
5	A	965	NAD	C6N-C5N-C4N	-3.04	115.07	119.45
5	A	965	NAD	N9A-C8A-N7A	-3.00	109.68	113.94
5	A	965	NAD	C4A-C5A-N7A	-2.99	107.16	110.58
8	B	4	FMN	C4'-C3'-C2'	2.98	118.53	113.57
7	B	1	FAD	C10-C4X-N5	-2.93	118.82	124.81
5	A	965	NAD	C2D-C3D-C4D	-2.81	97.18	102.61
8	B	4	FMN	O2-C2-N1	-2.76	117.22	121.80
7	B	1	FAD	C4B-O4B-C1B	-2.71	103.49	109.47
5	A	965	NAD	C2A-N3A-C4A	2.67	118.34	111.83
5	A	965	NAD	O7N-C7N-C3N	2.58	122.75	119.60
8	B	4	FMN	C10-C4A-N5	-2.52	119.67	124.81
7	B	1	FAD	C9A-C5X-N5	-2.49	119.81	122.45
8	B	4	FMN	C5A-C9A-N10	2.42	120.16	117.97
5	A	965	NAD	C5A-C4A-N9A	2.39	108.42	105.81
5	A	965	NAD	O2N-PN-O3	2.38	113.70	107.27
7	B	1	FAD	O4B-C1B-N9A	-2.36	103.55	108.09
7	B	1	FAD	O2-C2-N1	-2.28	118.02	121.80
5	A	965	NAD	C5A-N7A-C8A	2.28	107.03	103.45
8	B	4	FMN	O3'-C3'-C2'	2.27	114.09	108.93
5	A	965	NAD	O7N-C7N-N7N	-2.14	119.52	122.62
8	B	4	FMN	C4A-C10-N10	2.13	119.53	116.48
7	B	1	FAD	C4-C4X-C10	2.11	120.56	116.93
8	B	4	FMN	C4-C4A-C10	2.10	120.54	116.93
5	A	965	NAD	O3-PN-O1N	-2.08	104.44	110.70
7	B	1	FAD	O3P-PA-O1A	2.03	116.81	110.70
8	B	4	FMN	O5'-C5'-C4'	2.03	114.77	109.36
7	B	1	FAD	C4X-C4-N3	2.01	118.38	113.25

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1	FAD	C5'-O5'-P-O1P

Continued on next page...

Continued from previous page...

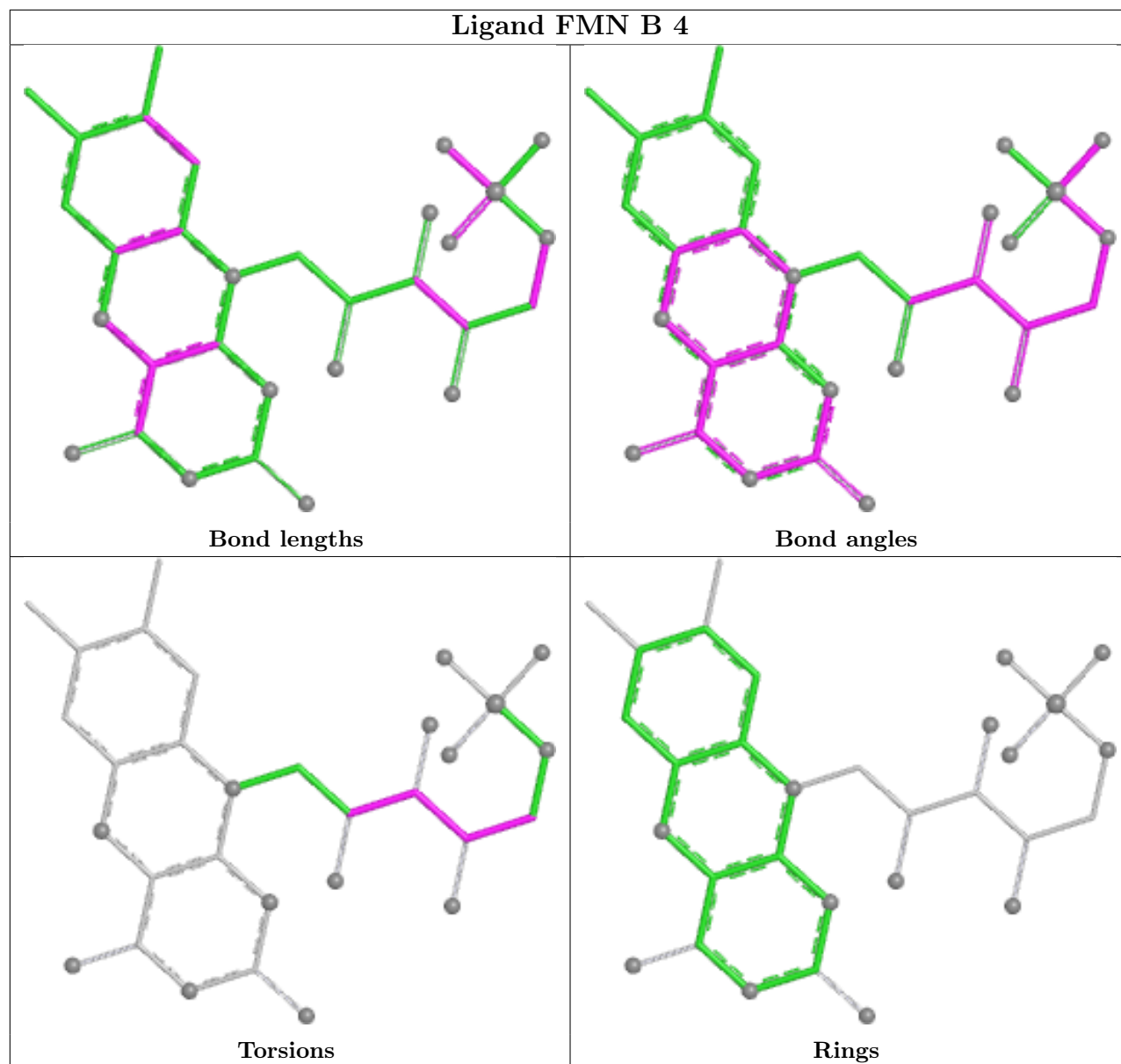
Mol	Chain	Res	Type	Atoms
8	B	4	FMN	C1'-C2'-C3'-C4'
8	B	4	FMN	C3'-C4'-C5'-O5'
8	B	4	FMN	O4'-C4'-C5'-O5'
8	B	4	FMN	C2'-C3'-C4'-C5'
8	B	4	FMN	O3'-C3'-C4'-C5'
8	B	4	FMN	O2'-C2'-C3'-C4'
8	B	4	FMN	C2'-C3'-C4'-O4'
7	B	1	FAD	C4'-C5'-O5'-P
5	A	965	NAD	C5D-O5D-PN-O1N
5	A	965	NAD	C3B-C4B-C5B-O5B
5	A	965	NAD	O4D-C4D-C5D-O5D
5	A	965	NAD	C2B-C1B-N9A-C8A

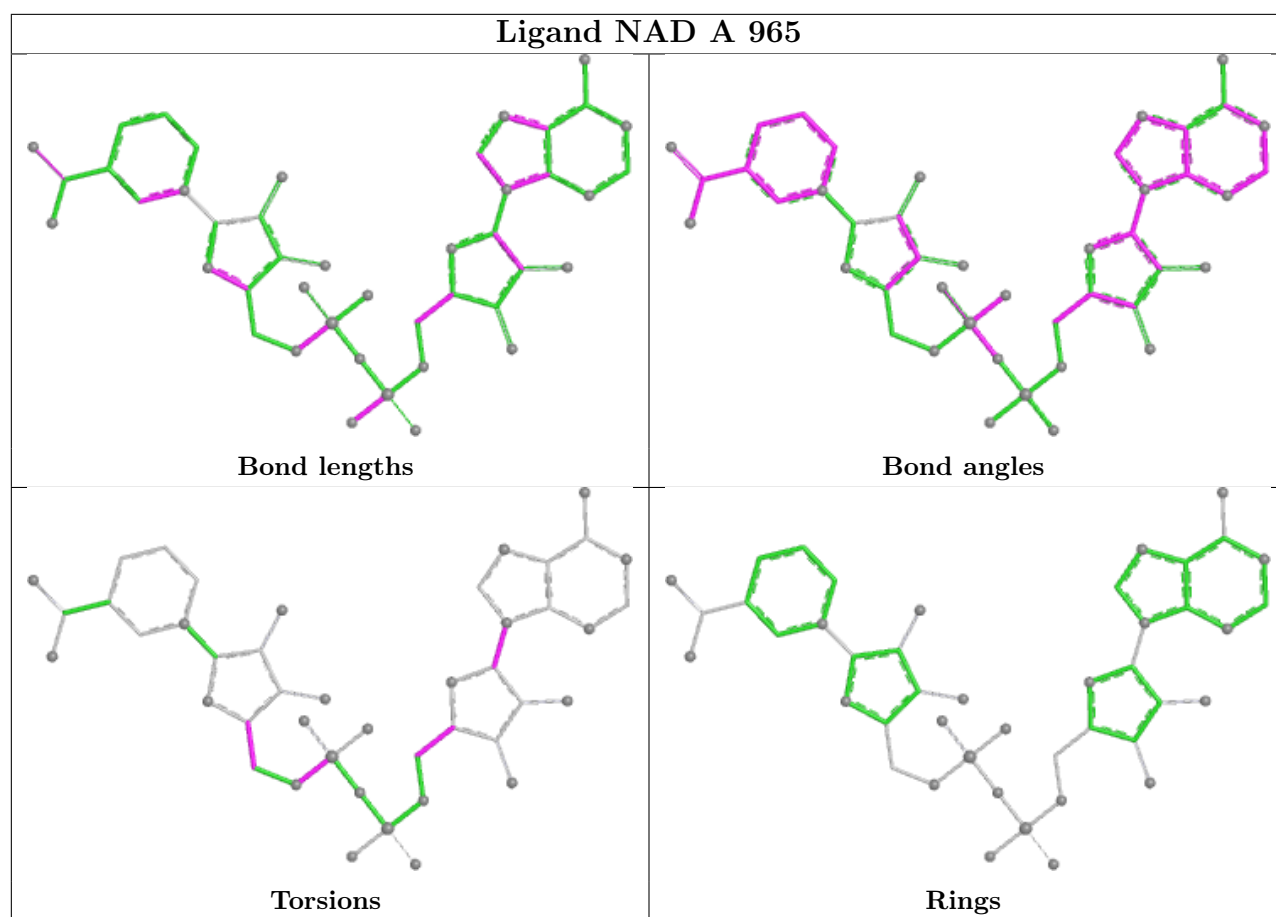
There are no ring outliers.

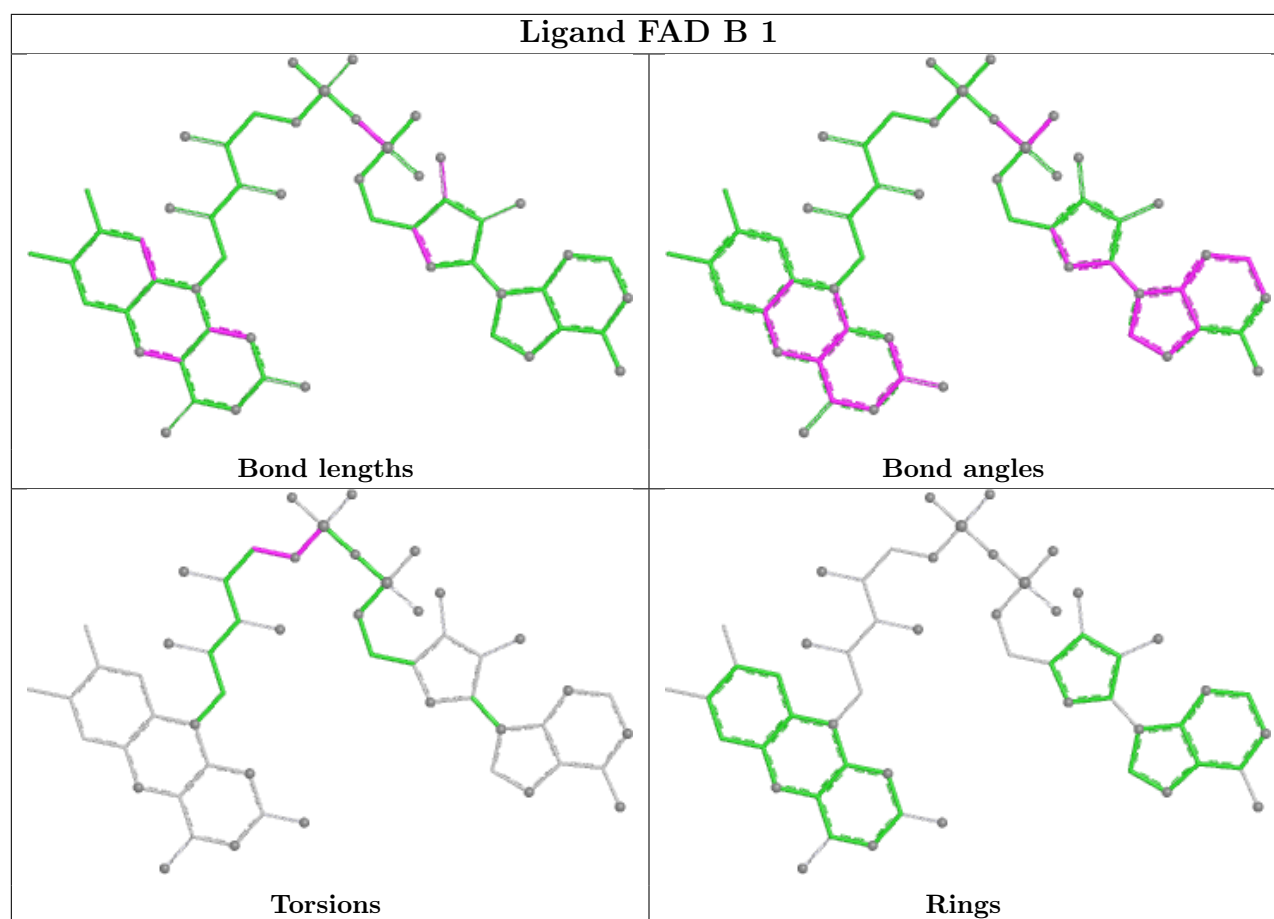
5 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	4	FMN	11	0
6	A	2562	SO4	5	0
5	A	965	NAD	4	0
9	B	6244	SO3	2	0
7	B	1	FAD	3	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	963/964 (99%)	0.15	42 (4%) 39 36	19, 35, 68, 86	0
2	B	397/399 (99%)	0.29	15 (3%) 44 41	24, 43, 59, 76	0
3	C	195/203 (96%)	0.28	6 (3%) 51 48	24, 34, 56, 68	0
4	D	91/99 (91%)	0.20	5 (5%) 30 27	26, 37, 72, 108	0
All	All	1646/1665 (98%)	0.20	68 (4%) 41 38	19, 38, 66, 108	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	91	LEU	6.4
3	C	200	ALA	5.6
2	B	401	ALA	5.0
1	A	226	PRO	4.9
2	B	402	VAL	4.6
1	A	327	THR	4.0
1	A	746	LEU	3.9
1	A	944	LEU	3.6
2	B	399	ALA	3.4
2	B	400	ALA	3.3
2	B	397	HIS	3.3
2	B	392	HIS	3.2
1	A	225	GLY	3.2
1	A	895	VAL	3.1
4	D	87	ALA	3.1
1	A	864	VAL	3.1
2	B	202	ASP	3.0
2	B	7	HIS	3.0
1	A	909	HIS	2.9
1	A	782	PHE	2.9
3	C	96	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	899	GLY	2.8
1	A	616	CYS	2.8
1	A	227	SER	2.8
1	A	694	GLY	2.8
1	A	896	ALA	2.8
1	A	945	VAL	2.8
2	B	200	LEU	2.7
1	A	963	ASP	2.6
1	A	755	PHE	2.6
1	A	658	VAL	2.6
1	A	768	GLU	2.6
1	A	753	PHE	2.6
1	A	824	PHE	2.5
2	B	6	GLU	2.5
1	A	915	ALA	2.5
1	A	938	THR	2.4
3	C	199	VAL	2.4
1	A	932	ILE	2.4
2	B	398	GLY	2.4
1	A	734	ARG	2.4
1	A	894	ALA	2.3
1	A	798	VAL	2.3
1	A	900	VAL	2.3
1	A	881	LEU	2.3
1	A	501	GLY	2.3
1	A	584	ALA	2.3
1	A	803	GLN	2.3
2	B	343	ILE	2.3
3	C	6	GLN	2.3
1	A	626	LEU	2.2
3	C	99	ASP	2.2
1	A	641	ALA	2.2
1	A	911	TYR	2.2
4	D	29	GLU	2.2
4	D	90	GLN	2.2
2	B	145	CYS	2.2
1	A	848	LYS	2.2
2	B	218	ALA	2.2
1	A	849	LEU	2.1
1	A	941	ASP	2.1
1	A	955	PHE	2.1
1	A	921	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	75	SER	2.0
1	A	83	ALA	2.0
2	B	385	LEU	2.0
4	D	88	ARG	2.0
1	A	891	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

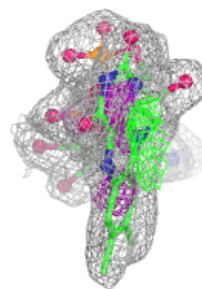
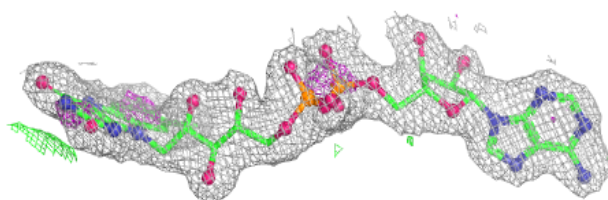
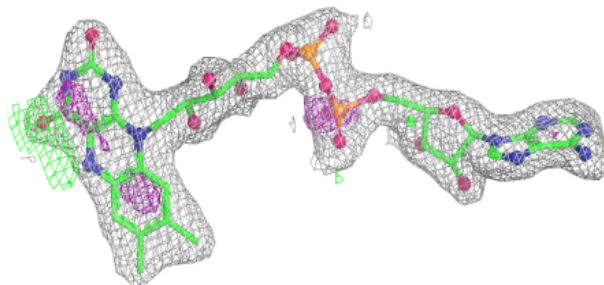
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	D	2566	5/5	0.83	0.08	74,78,102,105	0
6	SO4	A	2560	5/5	0.84	0.09	61,66,79,103	0
6	SO4	A	2562	5/5	0.84	0.12	44,44,73,102	0
6	SO4	A	2559	5/5	0.84	0.14	70,75,108,121	0
6	SO4	A	2563	5/5	0.85	0.15	78,80,92,294	0
9	SO3	B	6244	4/4	0.87	0.19	56,59,62,73	0
6	SO4	A	2561	5/5	0.91	0.07	44,55,84,100	0
6	SO4	C	2564	5/5	0.94	0.19	41,45,59,64	0
7	FAD	B	1	53/53	0.95	0.08	26,39,53,56	0
6	SO4	A	2567	5/5	0.96	0.08	44,46,61,72	0
8	FMN	B	4	31/31	0.97	0.06	21,27,32,42	0
5	NAD	A	965	44/44	0.98	0.04	12,21,27,31	0
10	ZN	D	100	1/1	0.99	0.09	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.

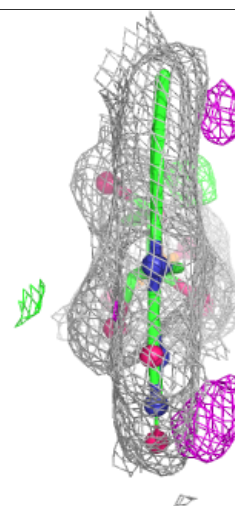
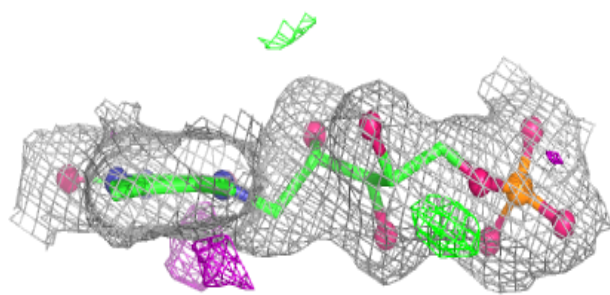
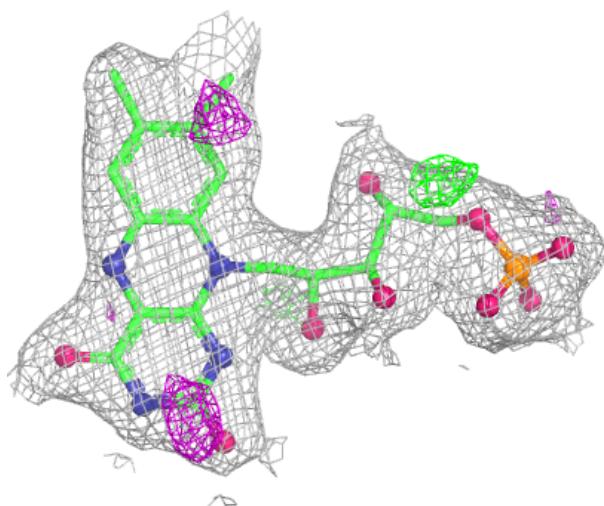
Electron density around FAD B 1:

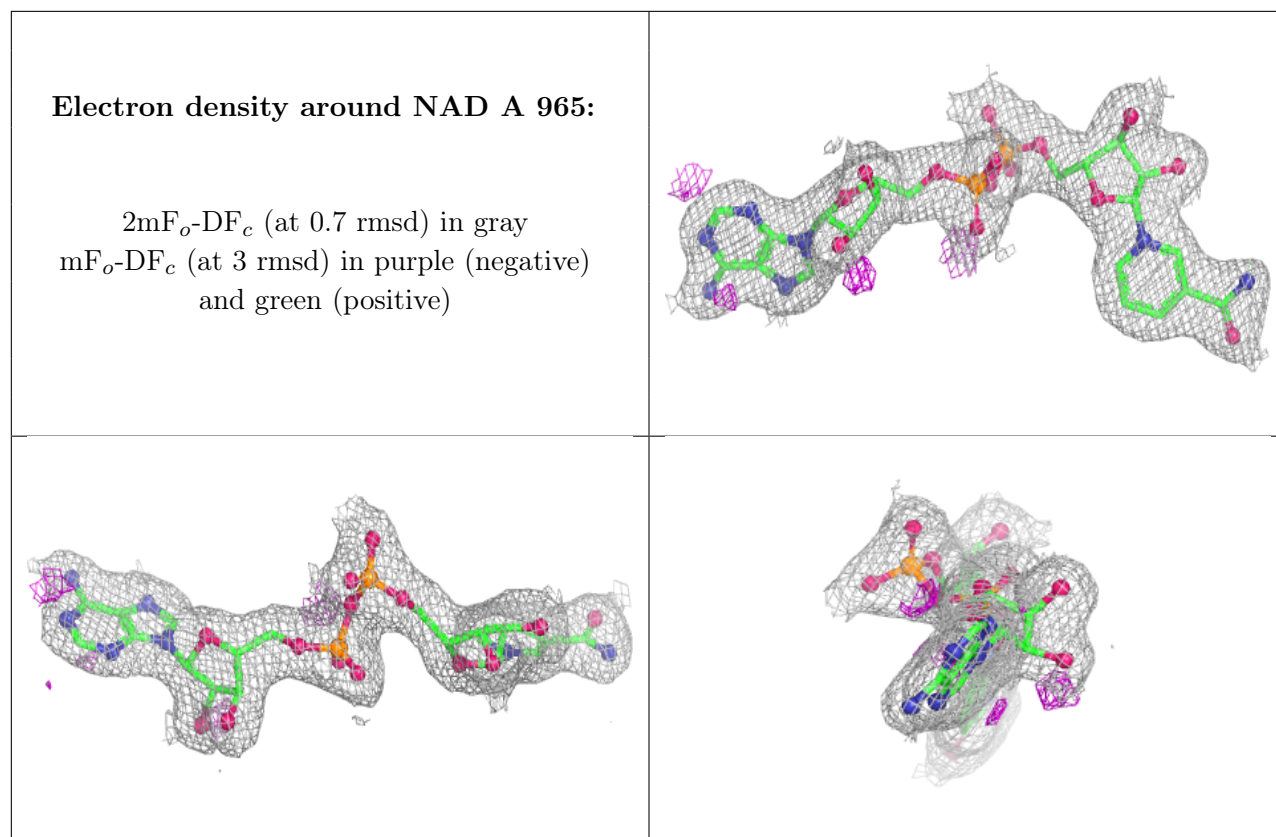
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN B 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.