



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:09 AM UTC

PDB ID : 1AOG / pdb_00001aog
Title : TRYPANOSOMA CRUZI TRYPANOTHIONE REDUCTASE (OXIDIZED FORM)
Authors : Bond, C.S.; Zhang, Y.; Hunter, W.N.
Deposited on : 1997-07-03
Resolution : 2.30 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

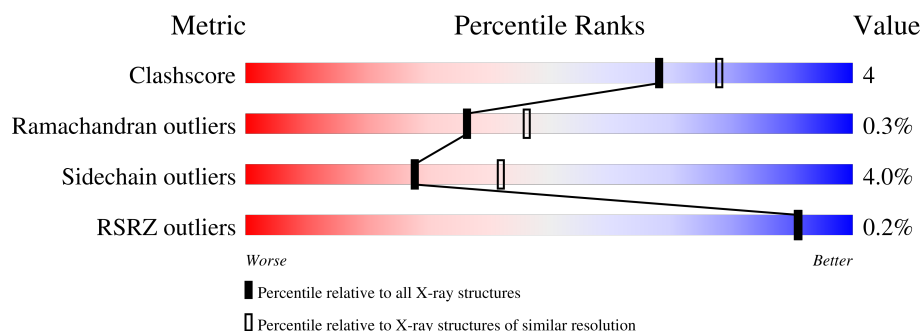
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	485	
1	B	485	

2 Entry composition [i](#)

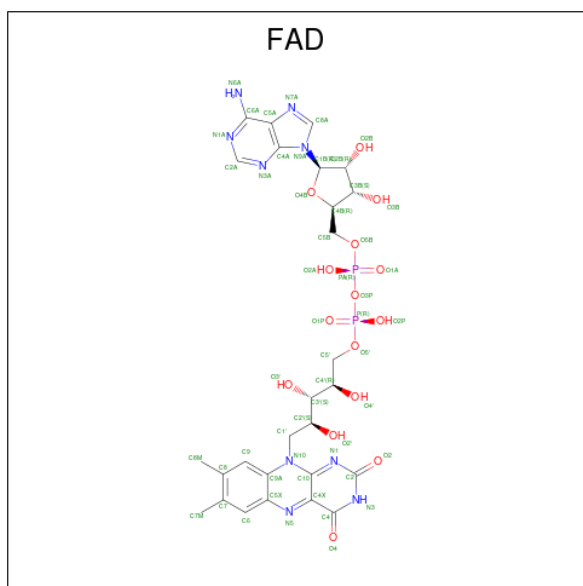
There are 4 unique types of molecules in this entry. The entry contains 7988 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRYPANOTHIONE REDUCTASE.

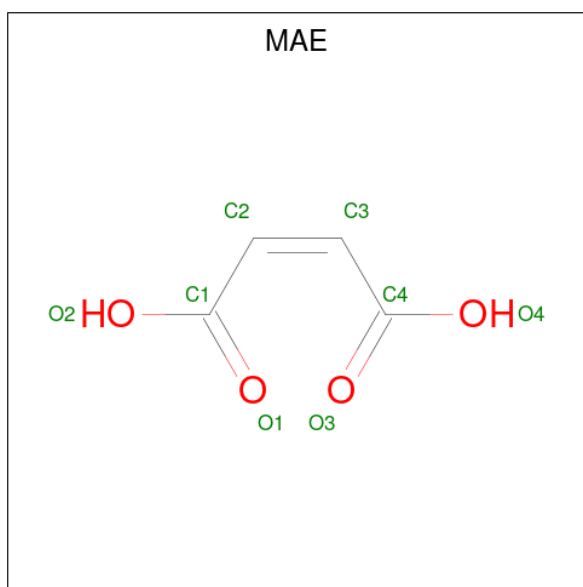
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3731	2373	635	702	21			
1	B	483	Total	C	N	O	S	0	0	0
			3716	2364	632	699	21			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is MALEIC ACID (CCD ID: MAE) (formula: $C_4H_4O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	4	4		
3	A	1	Total	C	O	0	0
			8	4	4		

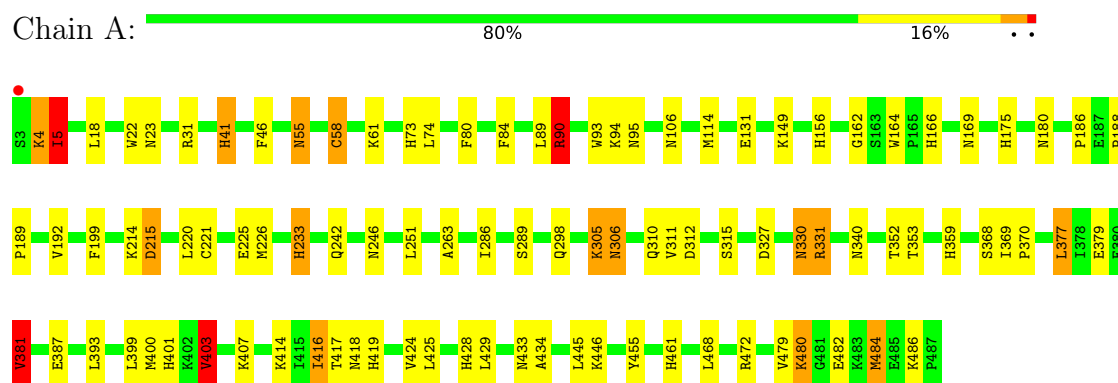
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	249	Total	O	0	0
			249	249		
4	B	170	Total	O	0	0
			170	170		

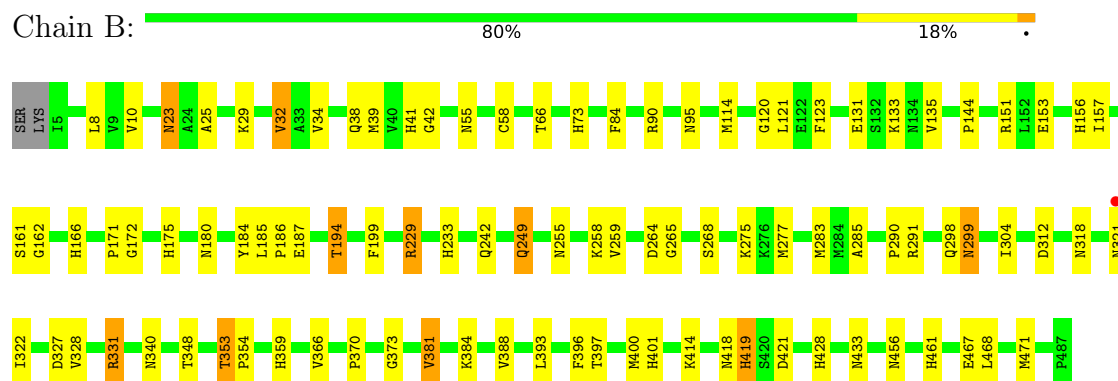
3 Residue-property plots [i](#)

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: TRYPANOTHIONE REDUCTASE



• Molecule 1: TRYPANOTHIONE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	92.81Å 92.81Å 156.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30 8.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.5 (8.00-2.30) 91.8 (8.00-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 2.30Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.189 , (Not available) 0.173 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.042 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7988	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAE, 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	0.90	15/3808 (0.4%)	1.65	65/5159 (1.3%)
1	B	0.88	14/3793 (0.4%)	1.55	52/5140 (1.0%)
All	All	0.89	29/7601 (0.4%)	1.60	117/10299 (1.1%)

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
1	A	0	1
1	B	0	1
All	All	0	2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	403	VAL	CA-CB	8.02	1.65	1.54
1	A	166	HIS	CD2-NE2	-7.69	1.29	1.37
1	B	166	HIS	CD2-NE2	-6.95	1.30	1.37
1	B	359	HIS	CD2-NE2	-6.81	1.30	1.37
1	B	419	HIS	CD2-NE2	-6.78	1.30	1.37
1	B	461	HIS	CD2-NE2	-6.74	1.30	1.37
1	B	175	HIS	CD2-NE2	-6.69	1.30	1.37
1	B	41	HIS	CD2-NE2	-6.51	1.30	1.37
1	A	215	ASP	CA-CB	6.48	1.73	1.53
1	A	461	HIS	CD2-NE2	-6.38	1.30	1.37
1	B	156	HIS	CD2-NE2	-6.38	1.30	1.37
1	A	41	HIS	CD2-NE2	-6.34	1.30	1.37
1	B	381	VAL	CA-CB	6.33	1.63	1.54
1	A	156	HIS	CD2-NE2	-6.30	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	HIS	CD2-NE2	-6.29	1.30	1.37
1	B	428	HIS	CD2-NE2	-6.27	1.30	1.37
1	A	233	HIS	CD2-NE2	-6.27	1.30	1.37
1	B	233	HIS	CD2-NE2	-6.18	1.31	1.37
1	A	419	HIS	CD2-NE2	-5.98	1.31	1.37
1	A	428	HIS	CD2-NE2	-5.97	1.31	1.37
1	B	401	HIS	CD2-NE2	-5.86	1.31	1.37
1	A	175	HIS	CD2-NE2	-5.78	1.31	1.37
1	A	401	HIS	CD2-NE2	-5.73	1.31	1.37
1	A	73	HIS	CD2-NE2	-5.71	1.31	1.37
1	A	416	ILE	CA-CB	5.57	1.62	1.54
1	B	73	HIS	CD2-NE2	-5.55	1.31	1.37
1	A	381	VAL	CA-CB	5.51	1.62	1.54
1	B	120	GLY	C-O	5.23	1.30	1.24
1	B	73	HIS	CG-ND1	-5.19	1.32	1.38

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	GLU	CA-CB-CG	19.49	153.08	114.10
1	A	480	LYS	CG-CD-CE	16.96	150.30	111.30
1	A	214	LYS	CA-C-N	-13.95	104.10	122.79
1	A	214	LYS	C-N-CA	-13.95	104.10	122.79
1	A	306	ASN	CA-CB-CG	10.98	123.58	112.60
1	A	225	GLU	CB-CG-CD	9.71	129.11	112.60
1	A	215	ASP	CB-CA-C	9.50	126.26	111.72
1	B	353	THR	CB-CA-C	9.43	120.59	109.47
1	A	359	HIS	CB-CG-CD2	-8.86	119.68	131.20
1	A	433	ASN	CB-CG-ND2	8.65	129.38	116.40
1	A	4	LYS	N-CA-C	8.35	128.59	110.80
1	A	5	ILE	N-CA-C	8.26	126.52	109.34
1	B	95	ASN	OD1-CG-ND2	-8.13	114.47	122.60
1	A	225	GLU	CB-CA-C	-7.94	97.35	110.85
1	B	401	HIS	CA-CB-CG	-7.91	105.89	113.80
1	A	340	ASN	OD1-CG-ND2	-7.69	114.91	122.60
1	B	359	HIS	CB-CG-CD2	-7.65	121.26	131.20
1	A	4	LYS	O-C-N	7.62	132.72	122.59
1	B	249	GLN	CA-CB-CG	7.56	129.23	114.10
1	A	106	ASN	OD1-CG-ND2	-7.42	115.18	122.60
1	A	298	GLN	CG-CD-NE2	7.27	127.30	116.40
1	A	330	ASN	OD1-CG-ND2	-7.08	115.52	122.60
1	A	215	ASP	CA-CB-CG	7.06	119.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	ARG	CB-CG-CD	-6.99	95.22	111.30
1	B	38	GLN	OE1-CD-NE2	-6.93	115.67	122.60
1	B	166	HIS	CB-CG-CD2	-6.92	122.21	131.20
1	A	215	ASP	CA-C-O	6.81	131.33	121.86
1	B	175	HIS	CB-CG-CD2	-6.78	122.39	131.20
1	A	401	HIS	CA-CB-CG	-6.73	107.07	113.80
1	B	275	LYS	CG-CD-CE	6.67	126.63	111.30
1	A	246	ASN	OD1-CG-ND2	-6.62	115.98	122.60
1	B	199	PHE	CA-CB-CG	6.58	120.38	113.80
1	A	5	ILE	N-CA-CB	-6.48	100.54	111.23
1	A	90	ARG	CA-CB-CG	6.45	127.01	114.10
1	B	84	PHE	CA-CB-CG	6.40	120.20	113.80
1	B	401	HIS	CB-CG-CD2	-6.35	122.94	131.20
1	A	180	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	A	306	ASN	OD1-CG-ND2	-6.31	116.29	122.60
1	B	229	ARG	CG-CD-NE	-6.31	98.13	112.00
1	A	305	LYS	CA-CB-CG	6.30	126.70	114.10
1	A	359	HIS	CB-CG-ND1	6.30	132.15	122.70
1	B	55	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	B	90	ARG	CA-CB-CG	6.26	126.63	114.10
1	A	312	ASP	CA-CB-CG	6.25	118.85	112.60
1	B	291	ARG	CA-CB-CG	6.25	126.59	114.10
1	A	199	PHE	CA-CB-CG	6.22	120.02	113.80
1	B	299	ASN	OD1-CG-ND2	-6.14	116.46	122.60
1	B	95	ASN	CB-CG-ND2	6.06	125.49	116.40
1	A	46	PHE	CA-CB-CG	-6.00	107.80	113.80
1	B	318	ASN	OD1-CG-ND2	-5.98	116.62	122.60
1	A	4	LYS	CA-C-N	5.97	132.71	121.97
1	A	4	LYS	C-N-CA	5.97	132.71	121.97
1	B	456	ASN	OD1-CG-ND2	-5.95	116.65	122.60
1	A	434	ALA	CA-C-N	5.79	125.47	119.05
1	A	434	ALA	C-N-CA	5.79	125.47	119.05
1	A	4	LYS	CA-C-O	5.78	128.78	120.51
1	A	5	ILE	CA-C-O	-5.77	113.57	120.78
1	A	369	ILE	CA-C-O	-5.76	116.96	120.88
1	B	359	HIS	CB-CG-ND1	5.76	131.33	122.70
1	A	379	GLU	N-CA-C	5.75	117.55	111.28
1	B	373	GLY	O-C-N	-5.72	118.91	123.49
1	A	169	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	B	23	ASN	CA-CB-CG	5.72	118.32	112.60
1	B	249	GLN	CB-CG-CD	-5.71	102.90	112.60
1	A	225	GLU	N-CA-CB	5.69	118.58	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	418	ASN	N-CA-C	-5.68	99.87	108.67
1	A	149	LYS	N-CA-C	-5.65	106.05	113.12
1	B	353	THR	CA-C-N	5.63	125.81	119.90
1	B	353	THR	C-N-CA	5.63	125.81	119.90
1	A	369	ILE	N-CA-C	-5.62	102.58	108.15
1	B	131	GLU	N-CA-C	-5.61	104.65	112.45
1	B	461	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	B	433	ASN	OD1-CG-ND2	-5.58	117.02	122.60
1	A	461	HIS	CB-CG-CD2	-5.57	123.96	131.20
1	B	249	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	A	486	LYS	CA-C-O	-5.56	114.56	120.23
1	A	289	SER	CA-C-N	5.56	125.57	119.90
1	A	289	SER	C-N-CA	5.56	125.57	119.90
1	B	166	HIS	CB-CG-ND1	5.56	131.03	122.70
1	B	366	VAL	N-CA-C	-5.54	99.66	107.75
1	B	156	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	B	38	GLN	CG-CD-NE2	5.51	124.66	116.40
1	A	263	ALA	N-CA-C	5.48	117.96	111.33
1	B	55	ASN	CB-CG-ND2	5.47	124.61	116.40
1	A	353	THR	CA-C-N	5.46	125.73	119.83
1	A	353	THR	C-N-CA	5.46	125.73	119.83
1	B	264	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	95	ASN	CA-CB-CG	-5.42	107.18	112.60
1	B	194	THR	CB-CA-C	5.42	119.07	110.19
1	B	255	ASN	CA-C-N	5.41	125.67	119.83
1	B	255	ASN	C-N-CA	5.41	125.67	119.83
1	A	331	ARG	O-C-N	-5.35	115.47	122.59
1	B	265	GLY	N-CA-C	-5.35	107.16	114.64
1	A	58	CYS	N-CA-C	5.34	117.52	111.11
1	B	255	ASN	OD1-CG-ND2	-5.34	117.25	122.60
1	A	22	TRP	CE2-CD2-CG	-5.32	100.82	107.20
1	B	187	GLU	CA-CB-CG	5.27	124.63	114.10
1	A	418	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	A	149	LYS	N-CA-CB	-5.24	102.40	110.42
1	A	306	ASN	CB-CG-ND2	5.23	124.25	116.40
1	A	225	GLU	N-CA-C	5.22	117.05	111.36
1	A	93	TRP	CE2-CD2-CG	-5.21	100.95	107.20
1	A	55	ASN	N-CA-C	5.20	119.68	112.45
1	A	84	PHE	CA-CB-CG	5.18	118.98	113.80
1	B	340	ASN	OD1-CG-ND2	-5.12	117.48	122.60
1	A	23	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	A	433	ASN	OD1-CG-ND2	-5.10	117.50	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	312	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	249	GLN	CB-CA-C	-5.08	101.47	109.80
1	B	340	ASN	CB-CG-ND2	5.07	124.01	116.40
1	A	131	GLU	N-CA-C	-5.07	105.41	112.45
1	B	291	ARG	CA-C-O	5.05	127.05	121.39
1	A	298	GLN	CB-CG-CD	5.04	121.17	112.60
1	B	421	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	180	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	B	397	THR	N-CA-C	-5.01	102.00	109.42
1	A	164	TRP	CB-CG-CD1	-5.00	119.39	126.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	ASP	Mainchain
1	B	299	ASN	Sidechain

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	3731	0	3743	27	0
1	B	3716	0	3725	29	0
2	A	53	0	27	0	0
2	B	53	0	31	0	0
3	A	16	0	4	0	0
4	A	249	0	0	2	0
4	B	170	0	0	2	0
All	All	7988	0	7530	55	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 4.

All (55) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:GLU:OE2	1:A:480:LYS:HD3	1.90	0.71
1:A:90:ARG:HH11	1:A:90:ARG:HB2	1.56	0.69
1:B:331:ARG:HB2	4:B:592:HOH:O	1.93	0.69
1:B:114:MET:HE3	1:B:121:LEU:HD21	1.79	0.63
1:B:171:PRO:HG2	1:B:258:LYS:HB3	1.80	0.63
1:A:305:LYS:HE3	1:A:310:GLN:HG3	1.86	0.57
1:A:5:ILE:HG23	1:A:31:ARG:NH1	2.20	0.57
1:B:172:GLY:HA3	1:B:259:VAL:O	2.05	0.56
1:B:468:LEU:HA	1:B:471:MET:HE3	1.91	0.53
1:B:10:VAL:HB	1:B:34:VAL:HG12	1.90	0.53
1:A:233:HIS:HB3	4:A:732:HOH:O	2.08	0.53
1:B:348:THR:HG23	1:B:354:PRO:HB3	1.89	0.52
4:A:706:HOH:O	1:B:400:MET:HB3	2.09	0.52
1:A:417:THR:HG22	1:A:424:VAL:HA	1.92	0.51
1:B:290:PRO:HB3	1:B:328:VAL:HA	1.91	0.51
1:A:393:LEU:HD13	1:A:414:LYS:HD2	1.93	0.50
1:B:8:LEU:HB3	1:B:32:VAL:HB	1.94	0.50
1:A:18:LEU:HD22	1:A:114:MET:HE1	1.94	0.48
1:A:41:HIS:HB3	1:A:55:ASN:OD1	2.13	0.48
1:B:157:ILE:HB	1:B:322:ILE:HG12	1.96	0.48
1:B:396:PHE:CE1	1:B:467:GLU:HG3	2.48	0.48
1:A:94:LYS:HE3	1:A:186:PRO:O	2.13	0.47
1:A:226:MET:HE1	1:A:233:HIS:CE1	2.49	0.47
1:A:189:PRO:HB2	1:A:192:VAL:HB	1.97	0.47
1:A:5:ILE:HG23	1:A:31:ARG:HH12	1.79	0.47
1:A:479:VAL:HB	1:A:484:MET:HE2	1.97	0.46
1:B:39:MET:SD	1:B:123:PHE:CE2	3.09	0.45
1:B:8:LEU:O	1:B:32:VAL:HA	2.16	0.45
1:A:311:VAL:HB	1:A:315:SER:HA	1.98	0.45
1:B:133:LYS:O	1:B:321:ASN:ND2	2.49	0.45
1:A:400:MET:HG3	1:B:66:THR:HG21	1.98	0.44
1:A:429:LEU:HD21	1:A:468:LEU:HD21	1.98	0.44
1:B:39:MET:SD	1:B:123:PHE:HE2	2.40	0.44
1:A:188:PRO:HA	1:A:189:PRO:HD3	1.82	0.44
1:A:221:CYS:HA	1:A:251:LEU:O	2.18	0.44
1:A:242:GLN:OE1	1:A:370:PRO:HG2	2.18	0.44
1:B:249:GLN:HE22	1:B:277:MET:HE1	1.83	0.43
1:B:393:LEU:HD23	1:B:414:LYS:HD2	2.00	0.43
1:A:74:LEU:HD13	1:A:89:LEU:HD11	2.00	0.43
1:A:377:LEU:HG	1:A:381:VAL:HG22	2.00	0.43
1:B:162:GLY:HA2	1:B:327:ASP:HB2	2.00	0.43
1:B:135:VAL:HG22	1:B:153:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:HIS:HD2	4:B:578:HOH:O	2.03	0.42
1:B:388:VAL:HG22	1:B:419:HIS:HB3	2.02	0.42
1:B:25:ALA:O	1:B:29:LYS:HA	2.21	0.41
1:A:399:LEU:O	1:A:403:VAL:HG13	2.19	0.41
1:B:242:GLN:OE1	1:B:370:PRO:HG3	2.20	0.41
1:B:283:MET:HE3	1:B:285:ALA:HB2	2.03	0.41
1:A:455:TYR:HB2	1:A:472:ARG:NH1	2.36	0.41
1:A:479:VAL:O	1:A:482:GLU:HG2	2.21	0.41
1:B:185:LEU:HA	1:B:186:PRO:HD3	1.89	0.41
1:B:42:GLY:HA2	1:B:184:TYR:CZ	2.56	0.41
1:A:80:PHE:CZ	1:A:403:VAL:HG22	2.56	0.40
1:A:162:GLY:HA2	1:A:327:ASP:HB2	2.03	0.40
1:B:353:THR:HA	1:B:354:PRO:HD3	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	483/485 (100%)	466 (96%)	15 (3%)	2 (0%)	30	38
1	B	481/485 (99%)	464 (96%)	16 (3%)	1 (0%)	43	55
All	All	964/970 (99%)	930 (96%)	31 (3%)	3 (0%)	36	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	4	LYS
1	B	144	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	406/406 (100%)	387 (95%)	19 (5%)	23	35
1	B	404/406 (100%)	391 (97%)	13 (3%)	34	51
All	All	810/812 (100%)	778 (96%)	32 (4%)	28	42

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	CYS
1	A	61	LYS
1	A	90	ARG
1	A	220	LEU
1	A	286	ILE
1	A	306	ASN
1	A	330	ASN
1	A	331	ARG
1	A	352	THR
1	A	368	SER
1	A	377	LEU
1	A	381	VAL
1	A	403	VAL
1	A	407	LYS
1	A	416	ILE
1	A	425	LEU
1	A	445	LEU
1	A	446	LYS
1	A	484	MET
1	B	23	ASN
1	B	32	VAL
1	B	58	CYS
1	B	151	ARG
1	B	161	SER
1	B	194	THR
1	B	229	ARG
1	B	268	SER

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Mol	Chain	Res	Type
1	B	298	GLN
1	B	304	ILE
1	B	331	ARG
1	B	381	VAL
1	B	384	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	69	GLN
1	A	175	HIS
1	A	180	ASN
1	A	233	HIS
1	A	246	ASN
1	A	310	GLN
1	B	69	GLN
1	B	233	HIS
1	B	246	ASN
1	B	249	GLN
1	B	419	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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
2	FAD	B	492	-	58,58,58	1.38	7 (12%)	85,89,89	1.82	10 (11%)
3	MAE	A	501	-	7,7,7	1.94	3 (42%)	8,8,8	2.14	3 (37%)
3	MAE	A	500	-	7,7,7	2.03	3 (42%)	8,8,8	3.12	4 (50%)
2	FAD	A	492	-	58,58,58	1.71	9 (15%)	85,89,89	1.98	14 (16%)

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
2	FAD	B	492	-	-	7/34/50/50	0/6/6/6
3	MAE	A	501	-	-	0/5/5/5	-
3	MAE	A	500	-	-	0/5/5/5	-
2	FAD	A	492	-	-	4/34/50/50	0/6/6/6

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	492	FAD	O2B-C2B	-6.68	1.26	1.43
2	A	492	FAD	C1'-C2'	-4.48	1.46	1.52
2	B	492	FAD	C5X-N5	-4.15	1.31	1.39
2	A	492	FAD	C9-C8	-3.65	1.34	1.39
2	B	492	FAD	C9-C8	-3.43	1.34	1.39
2	B	492	FAD	C6-C7	-3.31	1.35	1.39
2	A	492	FAD	C6-C7	-3.25	1.35	1.39
3	A	500	MAE	O2-C1	-3.24	1.22	1.30
2	A	492	FAD	C5X-N5	-3.22	1.33	1.39
2	B	492	FAD	C2'-C3'	-3.00	1.48	1.53
2	A	492	FAD	C2'-C3'	-2.90	1.48	1.53
3	A	500	MAE	O4-C4	-2.87	1.23	1.30
2	B	492	FAD	O3B-C3B	2.80	1.49	1.43
2	B	492	FAD	C3B-C4B	-2.70	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	MAE	O2-C1	-2.67	1.23	1.30
3	A	501	MAE	O4-C4	-2.54	1.23	1.30
3	A	501	MAE	C3-C4	-2.26	1.42	1.48
2	A	492	FAD	C4'-C3'	-2.23	1.49	1.53
2	A	492	FAD	C9A-N10	-2.21	1.37	1.41
2	A	492	FAD	C7M-C7	2.20	1.55	1.51
3	A	500	MAE	C3-C2	2.10	1.39	1.33
2	B	492	FAD	P-O3P	-2.02	1.57	1.59

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	492	FAD	C2B-C1B-N9A	9.44	136.75	113.30
2	B	492	FAD	O2A-PA-O3P	8.41	130.01	107.27
2	A	492	FAD	O3B-C3B-C4B	7.58	132.85	111.08
2	B	492	FAD	O3B-C3B-C4B	6.96	131.06	111.08
2	A	492	FAD	O2B-C2B-C3B	6.28	131.95	111.82
2	B	492	FAD	O3P-PA-O1A	-6.24	91.92	110.70
3	A	500	MAE	O2-C1-O1	-5.97	110.55	122.70
3	A	500	MAE	O4-C4-O3	-4.90	112.73	122.70
2	A	492	FAD	O3P-PA-O1A	-4.56	96.99	110.70
2	A	492	FAD	O2A-PA-O3P	4.28	118.85	107.27
2	B	492	FAD	C5B-C4B-C3B	-4.15	100.28	115.21
2	B	492	FAD	O4B-C1B-N9A	3.80	115.39	108.09
3	A	501	MAE	O2-C1-O1	-3.75	115.06	122.70
3	A	501	MAE	O4-C4-O3	-3.54	115.50	122.70
2	A	492	FAD	O4B-C1B-N9A	-3.12	102.10	108.09
2	A	492	FAD	C10-N1-C2	3.06	123.48	116.85
2	B	492	FAD	C10-N1-C2	3.03	123.41	116.85
2	B	492	FAD	O4B-C1B-C2B	-2.86	100.50	106.62
3	A	500	MAE	O4-C4-C3	2.83	126.56	116.16
2	B	492	FAD	O2B-C2B-C3B	2.57	120.05	111.82
2	A	492	FAD	C4A-N9A-C1B	2.35	132.12	126.63
2	A	492	FAD	O4'-C4'-C5'	-2.34	104.82	109.99
3	A	501	MAE	O1-C1-C2	2.33	128.22	121.06
2	A	492	FAD	O2B-C2B-C1B	2.32	118.10	110.10
2	A	492	FAD	C2B-C3B-C4B	2.29	107.03	102.61
2	B	492	FAD	C4X-C10-N1	-2.27	119.03	124.59
2	B	492	FAD	O4'-C4'-C5'	-2.21	105.11	109.99
2	A	492	FAD	C10-C4X-N5	-2.15	120.42	124.81
3	A	500	MAE	O1-C1-C2	2.10	127.51	121.06
2	A	492	FAD	C4X-C10-N1	-2.07	119.51	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	492	FAD	C2'-C1'-N10	2.01	119.68	110.20

There are no chirality outliers.

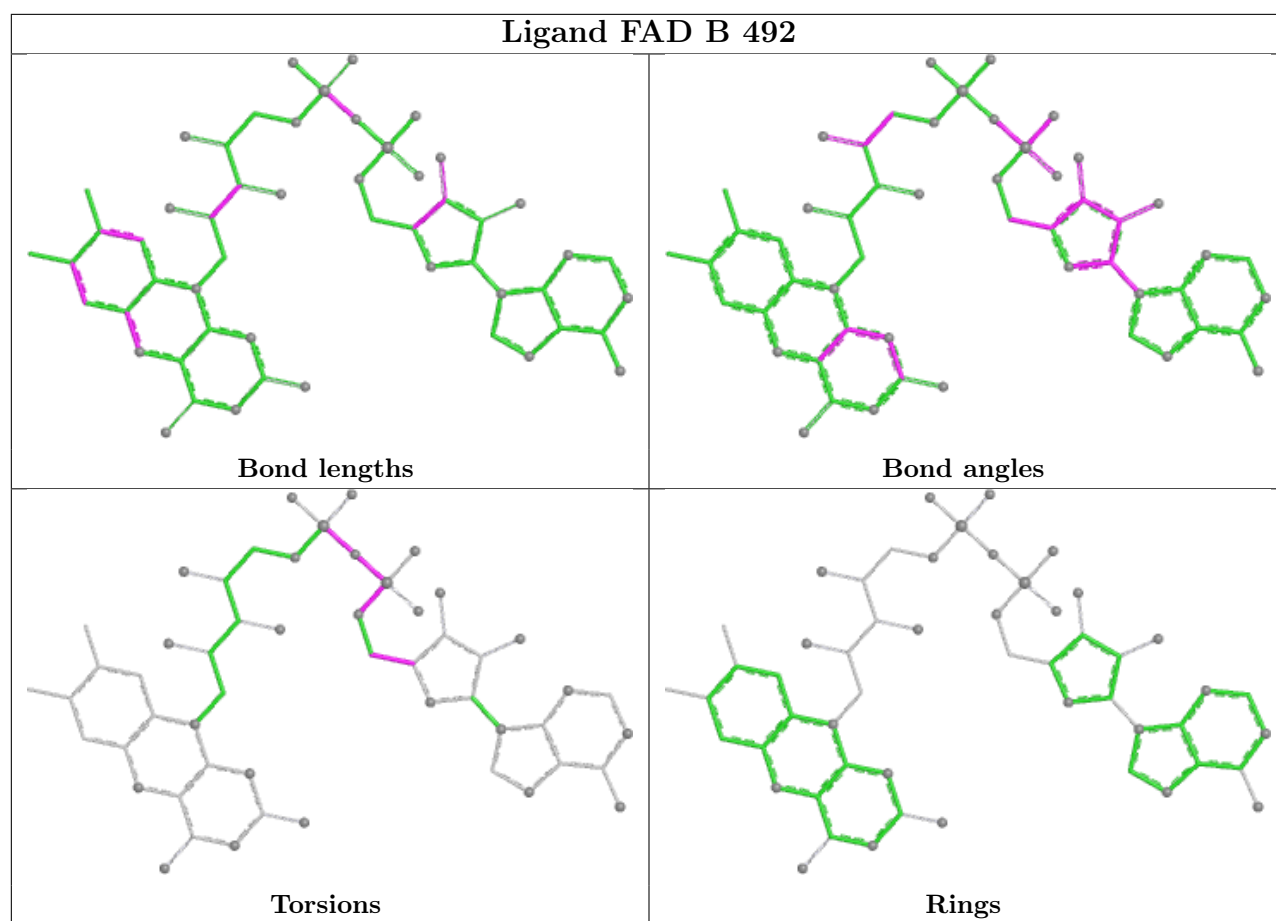
All (11) torsion outliers are listed below:

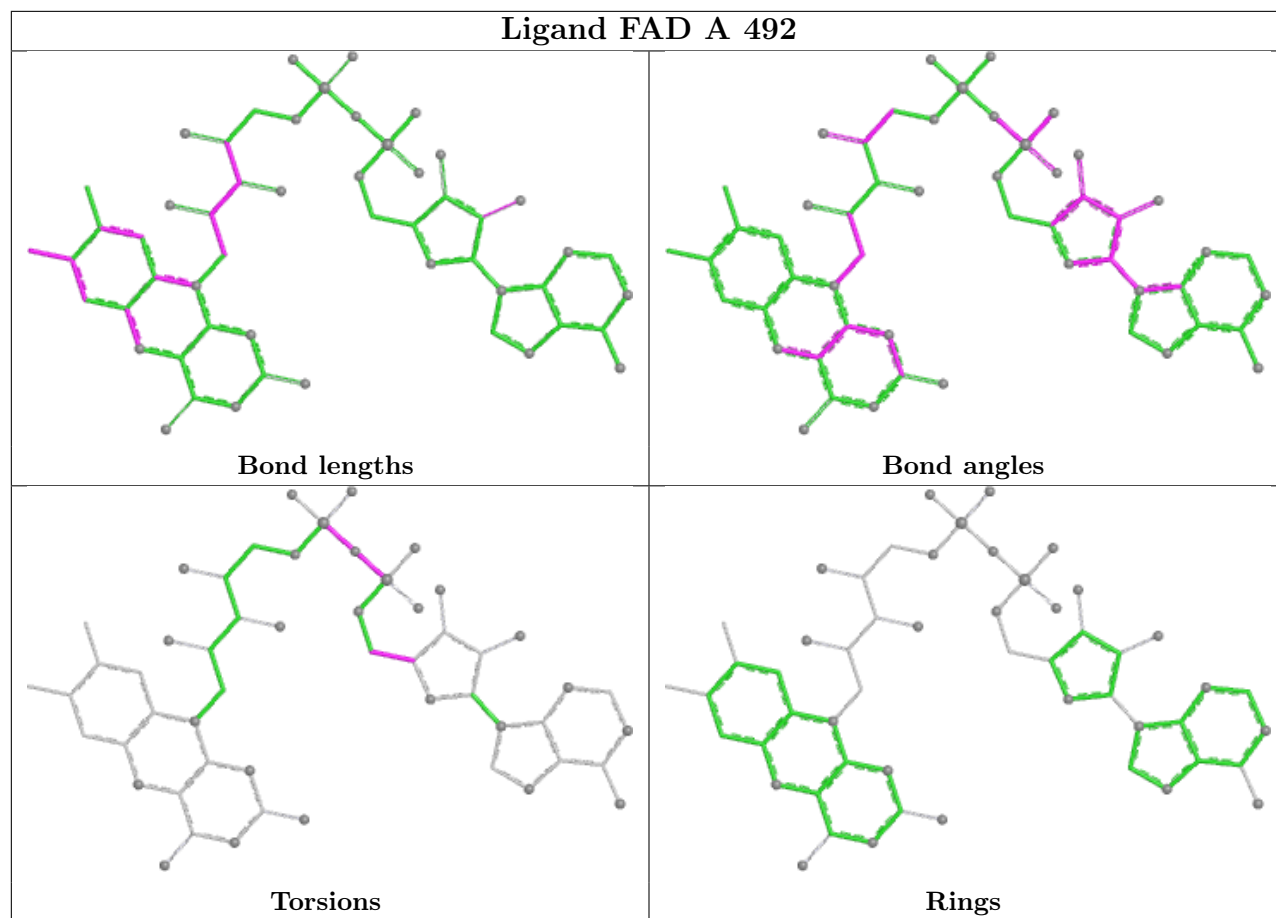
Mol	Chain	Res	Type	Atoms
2	B	492	FAD	C5B-O5B-PA-O1A
2	B	492	FAD	C3B-C4B-C5B-O5B
2	B	492	FAD	O4B-C4B-C5B-O5B
2	A	492	FAD	PA-O3P-P-O5'
2	B	492	FAD	PA-O3P-P-O5'
2	A	492	FAD	P-O3P-PA-O2A
2	B	492	FAD	C5B-O5B-PA-O2A
2	B	492	FAD	P-O3P-PA-O2A
2	A	492	FAD	O4B-C4B-C5B-O5B
2	B	492	FAD	P-O3P-PA-O1A
2	A	492	FAD	P-O3P-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	485/485 (100%)	-0.85	1 (0%) 91 91	7, 23, 51, 80	0
1	B	483/485 (99%)	-0.56	1 (0%) 91 91	6, 31, 73, 90	0
All	All	968/970 (99%)	-0.71	2 (0%) 91 91	6, 26, 68, 90	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	321	ASN	2.5
1	A	3	SER	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.

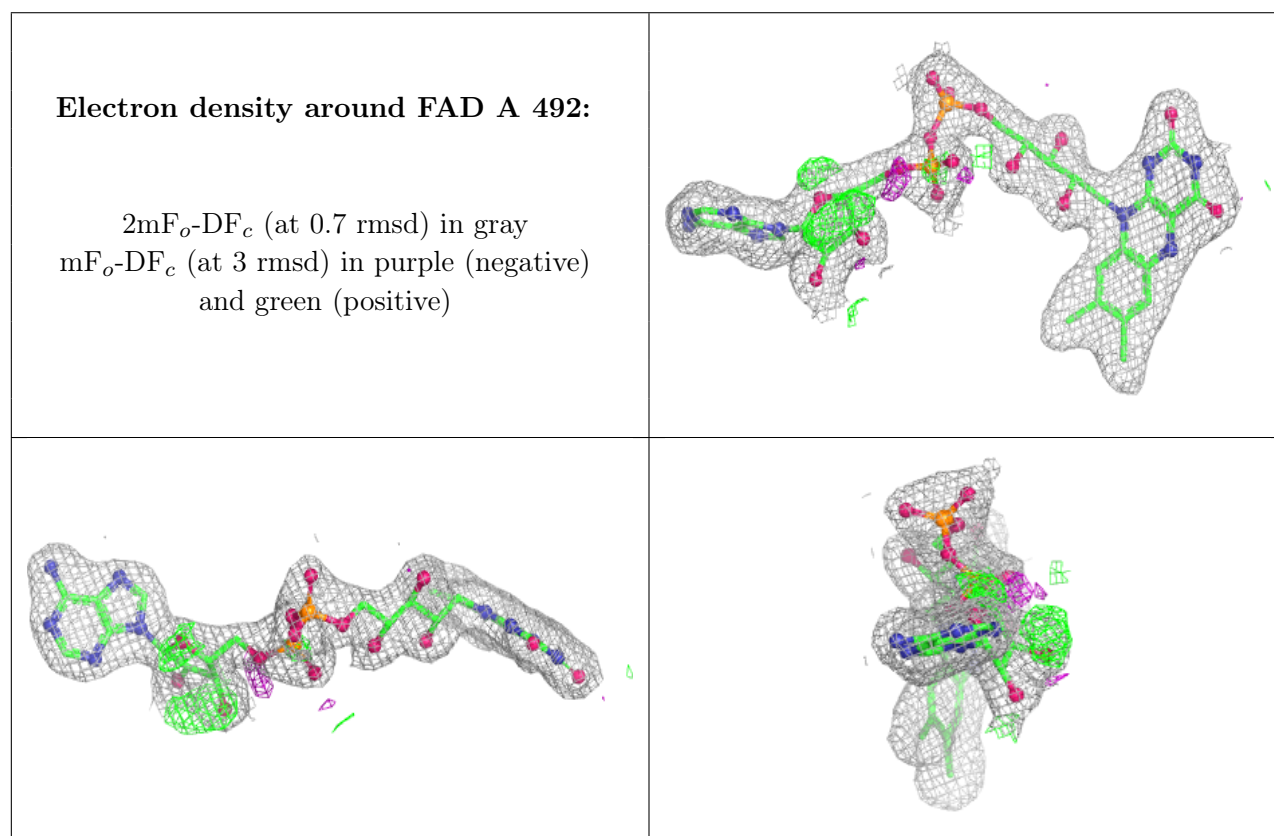
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAE	A	501	8/8	0.79	0.11	67,69,74,79	0
3	MAE	A	500	8/8	0.92	0.07	31,37,39,39	0
2	FAD	A	492	53/53	0.98	0.04	3,14,21,25	0

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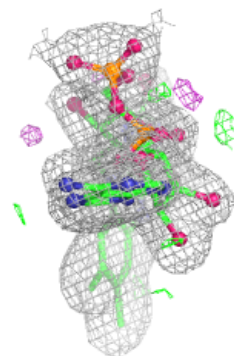
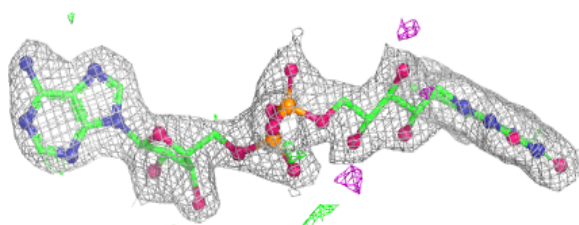
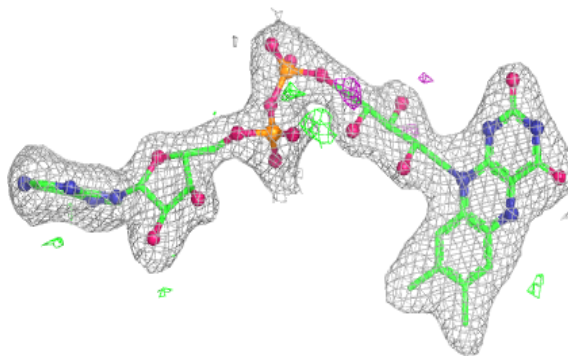
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	B	492	53/53	0.98	0.04	10,20,39,42	0

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 492:

$2mF_o-DF_c$ (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.