WORLDWIDE
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 03:40 PM JST

PDB ID	:	7VIW
Title	:	Dark adapted MmCPDII during oxidized to semiquinone TR-SFX studies
Authors	:	Maestre-Reyna, M.; Yang, C.-H.; Huang, W.-C.; Nango, E.; Ngura Putu, E.P.G.; Franz-Badur, S.; Wu, W.-J.; Wu, H.-Y.; Wang, P.-H.; Hosokawa, Y.; Saft, M.; Emmerich, H.-J.; Liao, J.-H.; Lee, C.-C.; Huang, K.-F.; Chang, Y.-K.; Weng, J.-H.; Royant, A.; Gad, W.; Pang, A.H.; Chang, C.-W.; Sugahara, M.; Owada, S.; Joti, Y.; Yamashita, A.; Tanaka, R.; Tanaka, T.; Luo, F.J.; Tono, K.; Kiontke, S.; Yamamoto, J.; Iwata, S.; Essen, L.-O.; Bessho, Y.; Tsai, M.-D.
Deposited on	:	2021-09-28
Resolution	:	1.74 Å(reported)

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

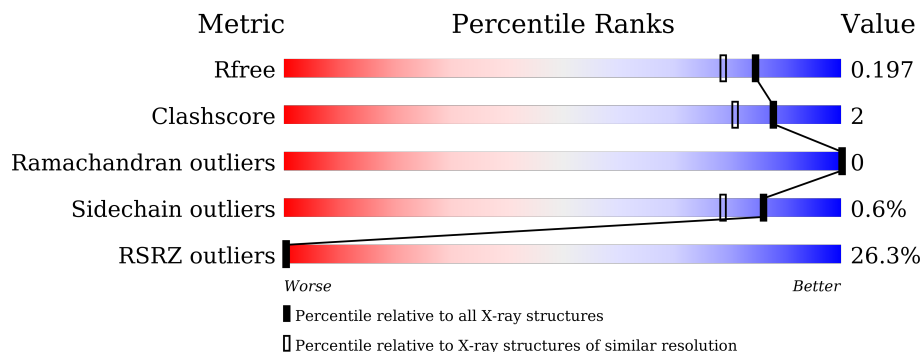|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	Percentile Ranks	Value
Rfree		0.197
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		0.6%
RSRZ outliers		26.3%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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 <=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	482	24% 88% 5% 7%

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

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 3803 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 DNA photolyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	449	3551	2303	577	656	15	0	8	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP Q8PYK9
A	-16	GLY	-	expression tag	UNP Q8PYK9
A	-15	SER	-	expression tag	UNP Q8PYK9
A	-14	SER	-	expression tag	UNP Q8PYK9
A	-13	HIS	-	expression tag	UNP Q8PYK9
A	-12	HIS	-	expression tag	UNP Q8PYK9
A	-11	HIS	-	expression tag	UNP Q8PYK9
A	-10	HIS	-	expression tag	UNP Q8PYK9
A	-9	HIS	-	expression tag	UNP Q8PYK9
A	-8	HIS	-	expression tag	UNP Q8PYK9
A	-7	SER	-	expression tag	UNP Q8PYK9
A	-6	SER	-	expression tag	UNP Q8PYK9
A	-5	GLY	-	expression tag	UNP Q8PYK9
A	-4	LEU	-	expression tag	UNP Q8PYK9
A	-3	VAL	-	expression tag	UNP Q8PYK9
A	-2	PRO	-	expression tag	UNP Q8PYK9
A	-1	ARG	-	expression tag	UNP Q8PYK9
A	0	GLY	-	expression tag	UNP Q8PYK9
A	1	SER	-	expression tag	UNP Q8PYK9
A	2	HIS	-	expression tag	UNP Q8PYK9
A	377	THR	MET	engineered mutation	UNP Q8PYK9

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).
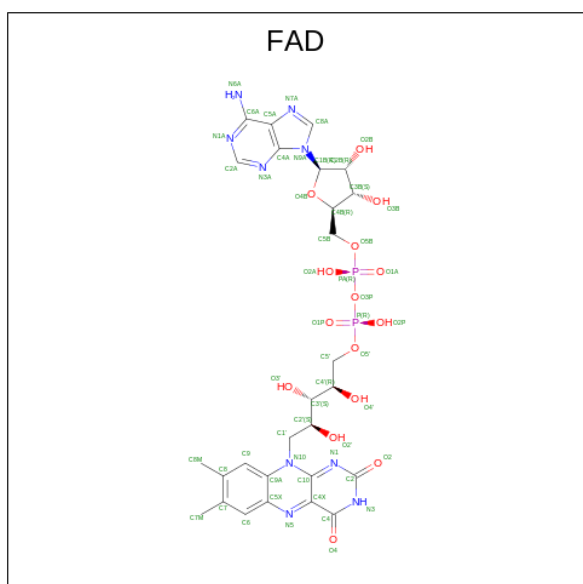
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	178	Total 179	O 179	0	1

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: DNA photolyase
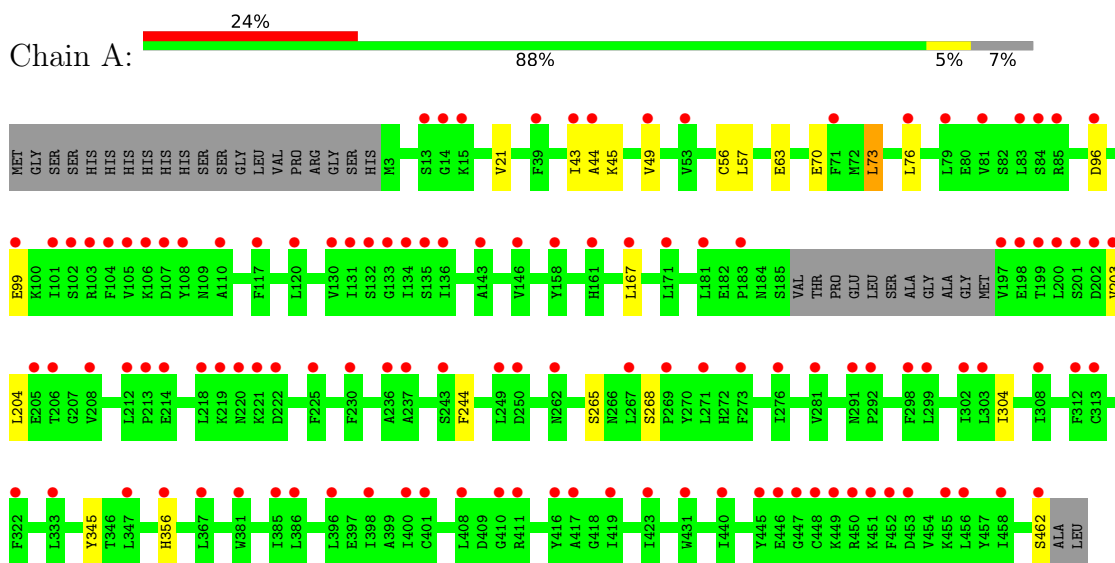
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	70.50Å 70.50Å 246.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.49 – 1.74 38.75 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.49-1.74) 100.0 (38.75-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 1.74Å)	Xtriage
Refinement program	PHENIX (1.19_4092: ???)	Depositor
R, R_{free}	0.163 , 0.199 0.165 , 0.197	Depositor DCC
R_{free} test set	3199 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	39.2	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 61.4	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3803	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, 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	0.63	3/3673 (0.1%)	0.68	1/4992 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56[A]	CYS	CB-SG	-6.49	1.71	1.82
1	A	56[B]	CYS	CB-SG	-6.49	1.71	1.82
1	A	63	GLU	CB-CG	5.71	1.63	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ASP	CB-CG-OD1	5.51	123.26	118.30

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	3551	0	3331	13	0
2	A	20	0	0	1	0
3	A	53	0	29	1	0
4	A	179	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3803	0	3360	14	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 2.

All (14) 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:A:505:SO4:O2	4:A:601:HOH:O	1.95	0.82
1:A:57:LEU:HD13	1:A:203:VAL:HG11	1.76	0.66
1:A:167[A]:LEU:HD23	1:A:304:ILE:HD13	1.87	0.56
1:A:73[A]:LEU:HD12	1:A:76:LEU:HD12	1.89	0.55
1:A:44:ALA:HB1	1:A:49:VAL:O	2.13	0.49
1:A:57:LEU:HD21	1:A:73[A]:LEU:HD11	1.95	0.49
1:A:45:LYS:CE	4:A:763:HOH:O	2.61	0.48
1:A:21:VAL:HG21	1:A:43:ILE:HG22	1.96	0.48
1:A:244:PHE:CD1	1:A:265:SER:HA	2.51	0.46
1:A:462:SER:O	1:A:462:SER:OG	2.30	0.43
1:A:345:TYR:OH	1:A:356:HIS:ND1	2.41	0.43
1:A:73[A]:LEU:HD12	1:A:73[A]:LEU:HA	1.90	0.41
1:A:268:SER:HB3	3:A:503:FAD:H5'2	2.02	0.41
1:A:70:GLU:HG3	1:A:204:LEU:HD11	2.03	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	453/482 (94%)	444 (98%)	9 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	353/416 (85%)	349 (99%)	4 (1%)	73	59

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73[A]	LEU
1	A	73[B]	LEU
1	A	99[A]	GLU
1	A	99[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 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	SO4	A	505	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	A	501	-	4,4,4	0.72	0	6,6,6	0.83	0
2	SO4	A	502	-	4,4,4	0.16	0	6,6,6	0.25	0
3	FAD	A	503	-	53,58,58	2.50	20 (37%)	68,89,89	1.67	14 (20%)
2	SO4	A	504	-	4,4,4	0.16	0	6,6,6	0.12	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
3	FAD	A	503	-	-	3/30/50/50	0/6/6/6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	FAD	C2B-C1B	-8.43	1.41	1.53
3	A	503	FAD	O4'-C4'	-5.60	1.31	1.43
3	A	503	FAD	C3B-C4B	-5.21	1.39	1.53
3	A	503	FAD	O2-C2	4.81	1.33	1.24
3	A	503	FAD	C9A-N10	-4.64	1.33	1.41
3	A	503	FAD	O4-C4	4.12	1.31	1.23
3	A	503	FAD	O2'-C2'	-3.85	1.35	1.43
3	A	503	FAD	C2B-C3B	-3.82	1.42	1.53
3	A	503	FAD	C4'-C3'	-3.51	1.46	1.53
3	A	503	FAD	O4B-C1B	3.04	1.45	1.41
3	A	503	FAD	C6A-N6A	3.00	1.45	1.34
3	A	503	FAD	C2'-C3'	-2.93	1.47	1.53
3	A	503	FAD	C2A-N3A	2.66	1.36	1.32
3	A	503	FAD	C4-N3	-2.38	1.34	1.38
3	A	503	FAD	C1'-C2'	2.36	1.56	1.52
3	A	503	FAD	C8M-C8	2.31	1.55	1.51
3	A	503	FAD	O3'-C3'	-2.12	1.38	1.43
3	A	503	FAD	P-O5'	2.07	1.67	1.59
3	A	503	FAD	C2-N3	-2.05	1.34	1.39
3	A	503	FAD	C10-N10	-2.02	1.32	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	503	FAD	C4A-C5A-N7A	-4.58	104.62	109.40
3	A	503	FAD	N3A-C2A-N1A	-3.95	122.51	128.68
3	A	503	FAD	C4-N3-C2	-3.91	118.42	125.64
3	A	503	FAD	C4X-C4-N3	3.42	121.88	113.19
3	A	503	FAD	C4X-C10-N1	-3.31	117.05	124.73
3	A	503	FAD	C4X-C10-N10	3.22	121.19	116.48
3	A	503	FAD	C5'-C4'-C3'	-3.17	106.07	112.20
3	A	503	FAD	C5X-C9A-N10	2.66	120.70	117.95
3	A	503	FAD	C10-N1-C2	2.65	122.21	116.90
3	A	503	FAD	C1B-N9A-C4A	-2.30	122.59	126.64
3	A	503	FAD	O4-C4-C4X	-2.29	120.53	126.60
3	A	503	FAD	O2A-PA-O1A	2.24	123.33	112.24
3	A	503	FAD	C1'-C2'-C3'	2.21	115.96	109.79
3	A	503	FAD	C9A-N10-C10	-2.12	117.47	120.77

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	FAD	C5B-O5B-PA-O1A
3	A	503	FAD	C5B-O5B-PA-O3P
3	A	503	FAD	C4'-C5'-O5'-P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	505	SO4	1	0
3	A	503	FAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand FAD A 503

Bond lengths — Bond angles — Torsions — Rings
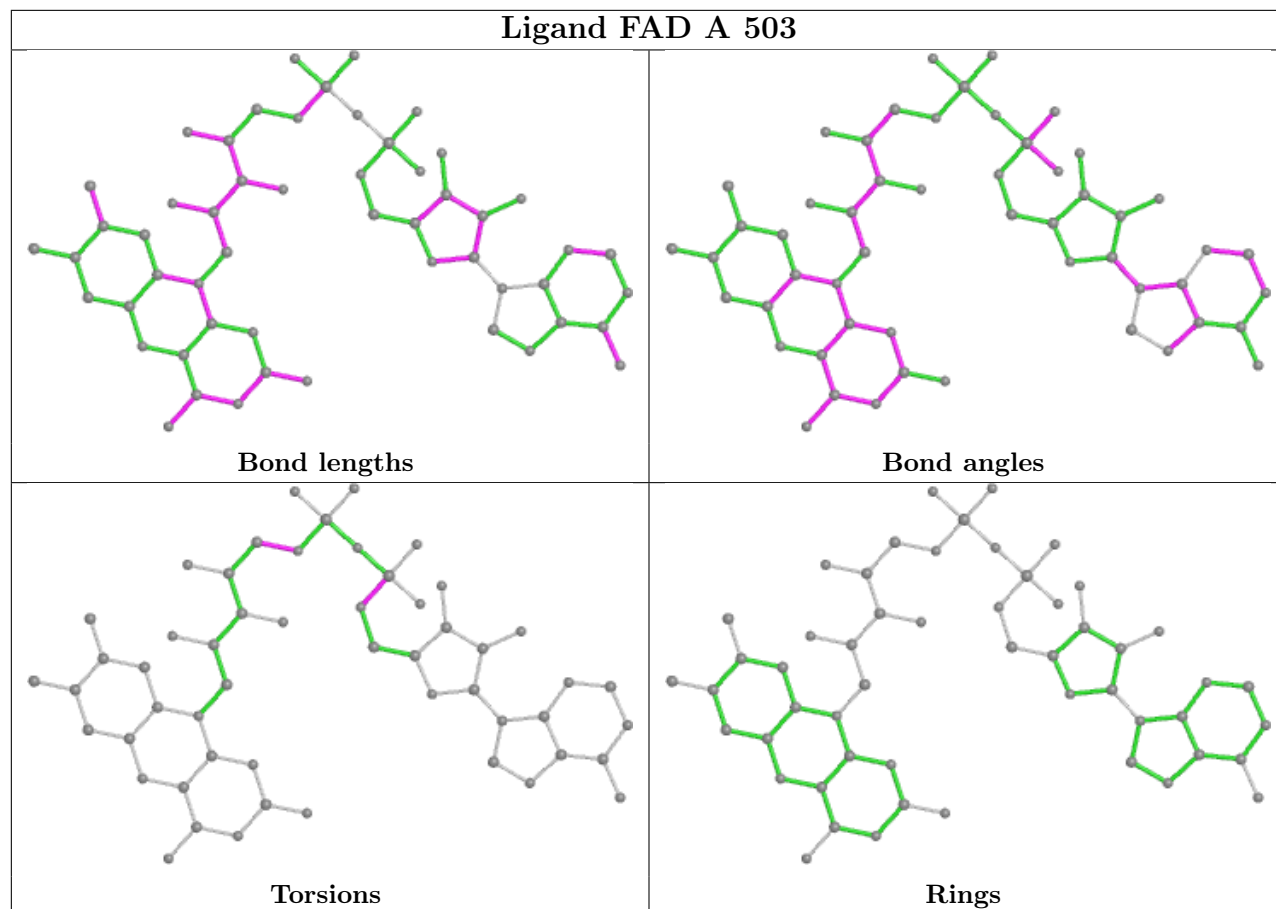
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	449/482 (93%)	1.51	118 (26%)	0	0	32, 49, 68, 115	4 (0%)

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	VAL	16.8
1	A	218	LEU	9.0
1	A	198	GLU	7.2
1	A	220	ASN	6.7
1	A	202	ASP	6.4
1	A	222	ASP	6.3
1	A	219	LYS	6.2
1	A	450	ARG	5.1
1	A	108	TYR	5.0
1	A	431	TRP	5.0
1	A	456	LEU	4.6
1	A	462	SER	4.5
1	A	158	TYR	4.4
1	A	14	GLY	4.4
1	A	302	ILE	4.4
1	A	132	SER	4.3
1	A	203	VAL	4.2
1	A	206	THR	4.2
1	A	423	ILE	4.1
1	A	221	LYS	4.0
1	A	276	ILE	4.0
1	A	408	LEU	4.0
1	A	199	THR	3.9
1	A	44	ALA	3.9
1	A	452	PHE	3.9
1	A	291	ASN	3.9
1	A	13	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	273	PHE	3.8
1	A	419	ILE	3.7
1	A	201[A]	SER	3.7
1	A	281	VAL	3.7
1	A	120	LEU	3.6
1	A	267	LEU	3.6
1	A	396	LEU	3.5
1	A	458	ILE	3.4
1	A	303	LEU	3.4
1	A	107	ASP	3.4
1	A	104	PHE	3.4
1	A	271	LEU	3.3
1	A	161	HIS	3.3
1	A	146	VAL	3.2
1	A	292	PRO	3.2
1	A	200	LEU	3.2
1	A	400	ILE	3.1
1	A	49	VAL	3.1
1	A	83	LEU	3.0
1	A	81	VAL	3.0
1	A	71	PHE	3.0
1	A	230	PHE	3.0
1	A	447	GLY	3.0
1	A	105	VAL	3.0
1	A	130	VAL	3.0
1	A	131	ILE	2.9
1	A	39	PHE	2.9
1	A	208	VAL	2.9
1	A	356	HIS	2.8
1	A	449	LYS	2.8
1	A	205	GLU	2.8
1	A	110	ALA	2.8
1	A	446	GLU	2.8
1	A	99[A]	GLU	2.8
1	A	103	ARG	2.7
1	A	85	ARG	2.7
1	A	416	TYR	2.7
1	A	76	LEU	2.7
1	A	298	PHE	2.7
1	A	398	ILE	2.7
1	A	333	LEU	2.7
1	A	453	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	133	GLY	2.6
1	A	410	GLY	2.6
1	A	135	SER	2.6
1	A	143	ALA	2.6
1	A	250	ASP	2.6
1	A	249	LEU	2.6
1	A	448	CYS	2.5
1	A	106	LYS	2.5
1	A	102	SER	2.5
1	A	269	PRO	2.5
1	A	322	PHE	2.5
1	A	15	LYS	2.5
1	A	212	LEU	2.5
1	A	381	TRP	2.5
1	A	445	TYR	2.4
1	A	262	ASN	2.4
1	A	84	SER	2.4
1	A	181	LEU	2.4
1	A	43	ILE	2.4
1	A	411	ARG	2.4
1	A	101	ILE	2.3
1	A	136	ILE	2.3
1	A	347	LEU	2.3
1	A	386	LEU	2.3
1	A	440	ILE	2.3
1	A	367	LEU	2.3
1	A	313	CYS	2.3
1	A	117	PHE	2.3
1	A	417	ALA	2.3
1	A	79	LEU	2.2
1	A	171	LEU	2.2
1	A	455	LYS	2.2
1	A	183	PRO	2.2
1	A	213	PRO	2.2
1	A	214	GLU	2.2
1	A	385	ILE	2.2
1	A	243	SER	2.1
1	A	312	PHE	2.1
1	A	53	VAL	2.1
1	A	134	ILE	2.1
1	A	237	ALA	2.1
1	A	401	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	225	PHE	2.1
1	A	167[A]	LEU	2.1
1	A	299	LEU	2.1
1	A	308	ILE	2.1
1	A	236	ALA	2.0
1	A	451	LYS	2.0
1	A	96	ASP	2.0

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

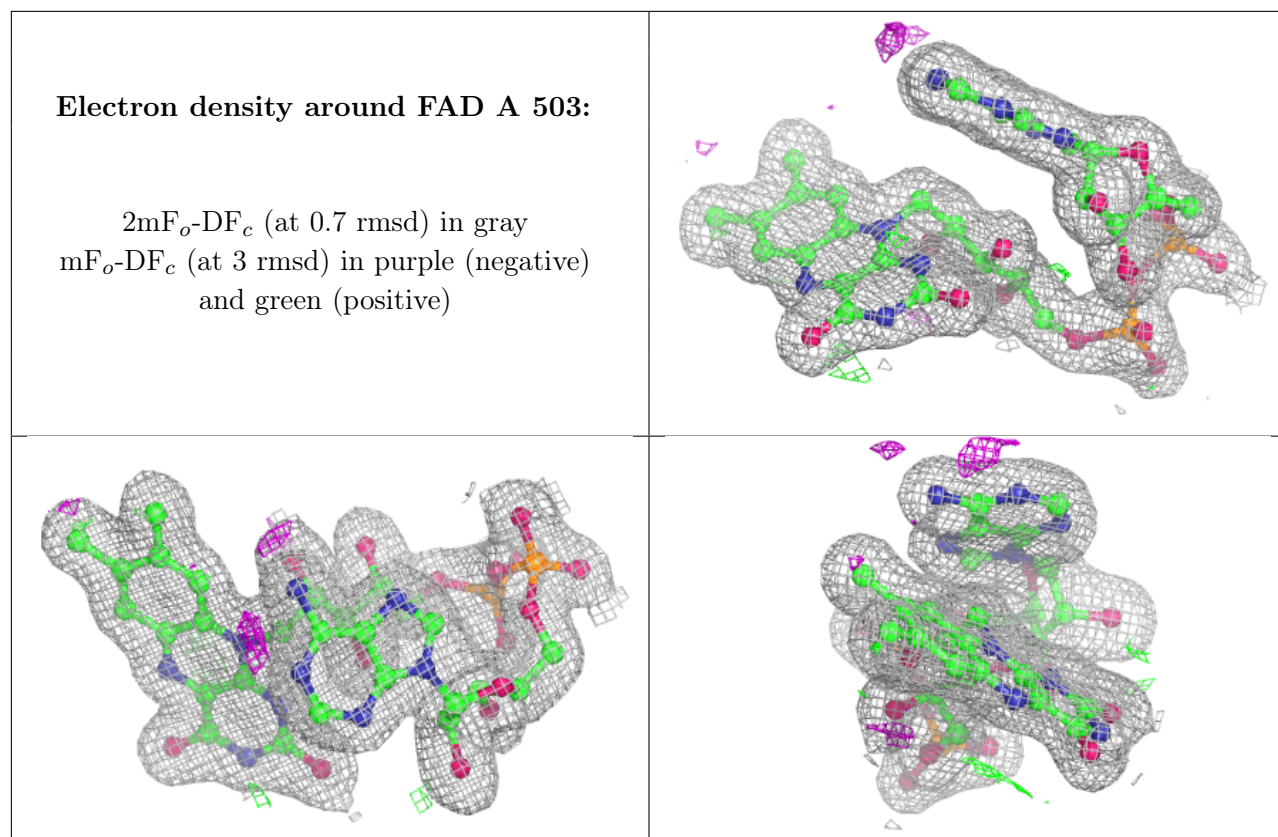There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	SO4	A	504	5/5	0.66	0.27	111,114,129,140	0
2	SO4	A	505	5/5	0.67	0.35	118,125,132,138	0
2	SO4	A	502	5/5	0.83	0.27	62,82,93,95	0
3	FAD	A	503	53/53	0.90	0.16	31,35,38,40	0
2	SO4	A	501	5/5	0.99	0.13	44,44,53,56	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 A 503:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.