



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:03 PM UTC

PDB ID : 7VJJ / pdb_00007vjj
Title : class II photolyase MmCPDII semiquinone to fully reduced TR-SFX studies (30 us time-point)
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Deposited on : 2021-09-28
Resolution : 2.10 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)

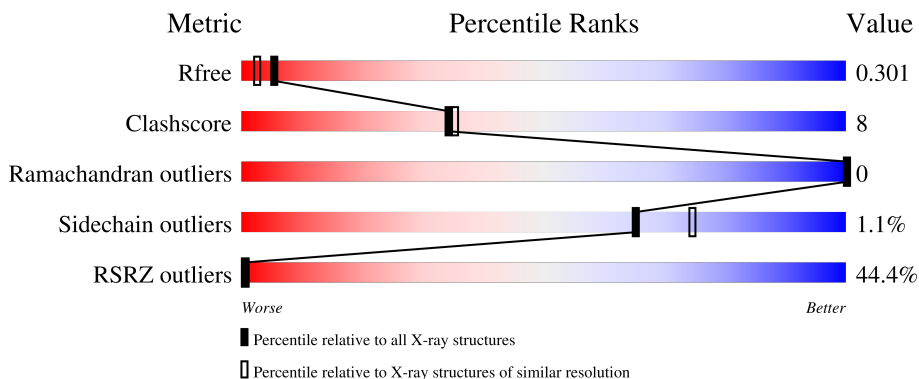
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	482	42% 78% 16% 6%

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

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3881 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.

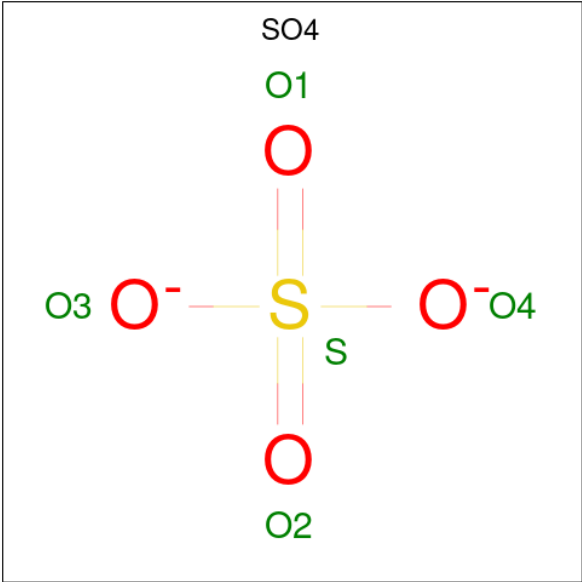
- Molecule 1 is a protein called DNA photolyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	10	0
			3590	2328	588	658	16			

There are 21 discrepancies between the modelled and reference sequences:

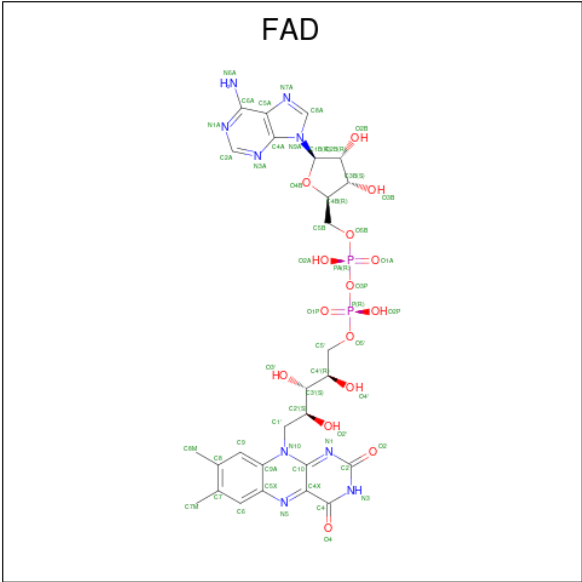
Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP Q8PYK9
A	-16	GLY	-	expression tag	UNP Q8PYK9
A	-15	SER	-	expression tag	UNP Q8PYK9
A	-14	SER	-	expression tag	UNP Q8PYK9
A	-13	HIS	-	expression tag	UNP Q8PYK9
A	-12	HIS	-	expression tag	UNP Q8PYK9
A	-11	HIS	-	expression 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 (CCD ID: SO4) (formula: O₄S).



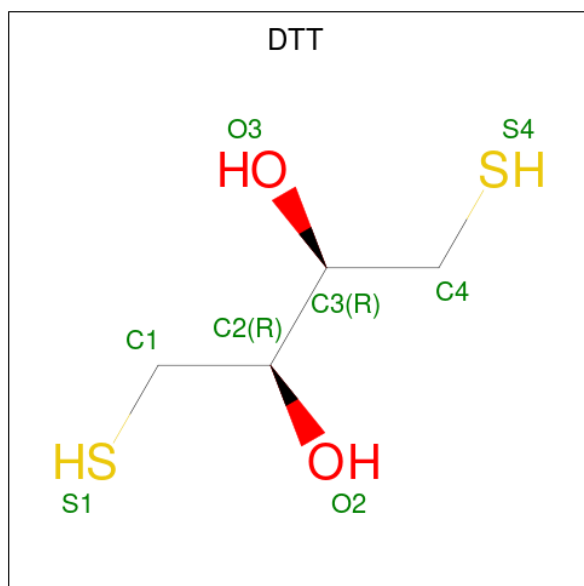
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			8	4	2	2		

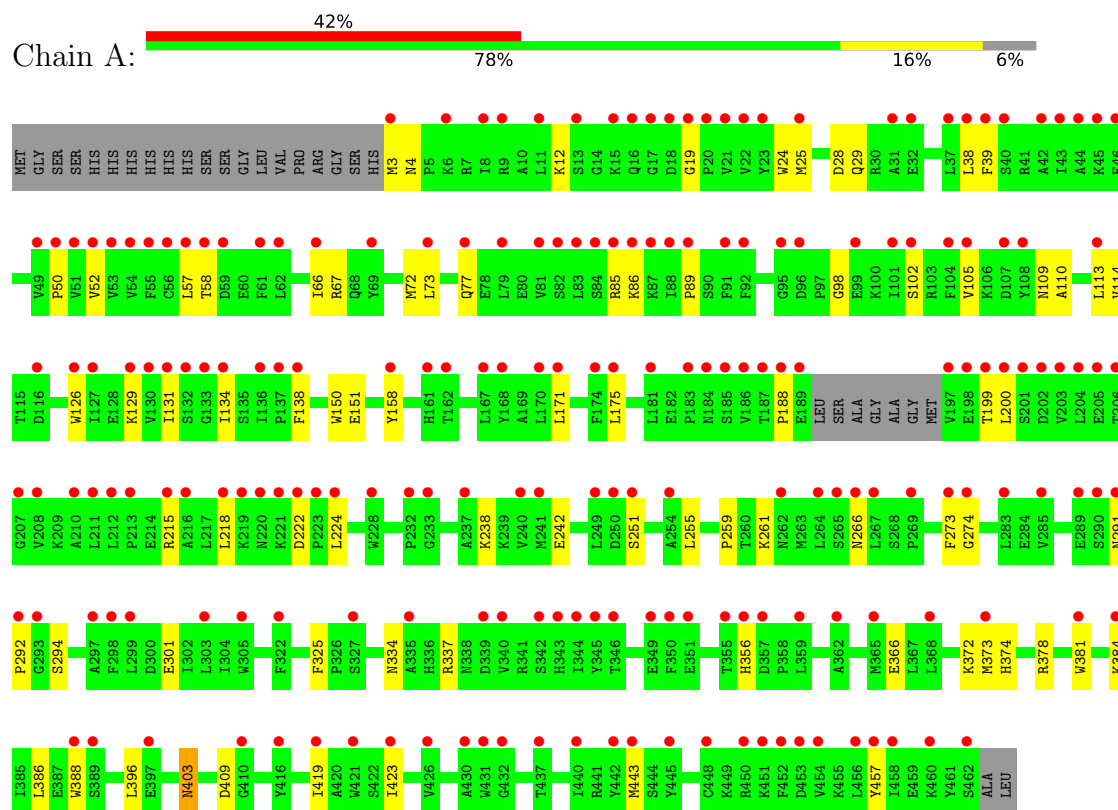
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	215	Total	O	0	0
			215	215		

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	70.52Å 70.52Å 246.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.68 – 2.10 31.68 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.68-2.10) 99.9 (31.68-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.89Å)	Xtriage
Refinement program	PHENIX (1.19_4092: ???)	Depositor
R, R_{free}	0.207 , 0.229 (Not available) , 0.301	Depositor DCC
R_{free} test set	2440 reflections (2.16%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	3881	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: DTT, 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	0.13	0/3721	0.24	0/5057

There are no bond length outliers.

There are no bond angle outliers.

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	3590	0	3375	52	0
2	A	15	0	0	1	0
3	A	53	0	26	5	0
4	A	8	0	9	1	0
5	A	215	0	0	8	0
All	All	3881	0	3410	54	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 8.

All (54) 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:158:TYR:CD1	1:A:158:TYR:CZ	2.39	1.02
1:A:39:PHE:CG	1:A:39:PHE:CE1	2.41	0.95
3:A:503:FAD:H62A	4:A:505:DTT:H2	1.57	0.69
1:A:105:VAL:HG13	1:A:110:ALA:HB3	1.80	0.64
1:A:98:GLY:HA3	1:A:129:LYS:HG2	1.80	0.63
1:A:386:LEU:HB2	1:A:423:ILE:HG12	1.83	0.61
1:A:291:ASN:HD22	1:A:292:PRO:HD2	1.67	0.59
1:A:251:SER:HB3	1:A:255:LEU:HD12	1.84	0.59
1:A:3:MET:HE1	1:A:38:LEU:HB3	1.86	0.58
1:A:255:LEU:HD22	1:A:261:LYS:HD2	1.86	0.58
1:A:85:ARG:NH1	5:A:624:HOH:O	2.38	0.55
1:A:301:GLU:HB3	3:A:503:FAD:H8A	1.88	0.55
1:A:50:PRO:HG2	1:A:188:PRO:HB3	1.88	0.55
1:A:67:ARG:NE	2:A:501:SO4:O3	2.39	0.55
1:A:12:LYS:N	5:A:601:HOH:O	2.41	0.54
1:A:291:ASN:HB3	1:A:294:SER:HB2	1.90	0.54
3:A:503:FAD:H3B	5:A:620:HOH:O	2.07	0.54
1:A:301:GLU:HB3	3:A:503:FAD:C8A	2.39	0.53
1:A:52:VAL:HG12	1:A:89:PRO:HG2	1.93	0.51
1:A:129:LYS:NZ	5:A:630:HOH:O	2.43	0.50
1:A:24:TRP:N	1:A:114:VAL:O	2.42	0.50
1:A:218[A]:LEU:HD21	1:A:222:ASP:HB2	1.95	0.49
1:A:19:GLY:HA3	1:A:109:ASN:O	2.12	0.48
1:A:77:GLN:NE2	5:A:633:HOH:O	2.46	0.48
1:A:28:ASP:HA	1:A:274:GLY:HA3	1.96	0.47
1:A:366:GLU:OE1	1:A:457:TYR:OH	2.23	0.47
1:A:373:MET:O	1:A:378:ARG:HD2	2.15	0.47
1:A:325:PHE:HZ	1:A:396:LEU:HD21	1.80	0.46
1:A:373:MET:HE1	1:A:381:TRP:CG	2.50	0.46
1:A:102:SER:HA	1:A:134:ILE:HD11	1.98	0.45
1:A:72:MET:HG3	1:A:273:PHE:CD1	2.51	0.45
1:A:66:ILE:HD12	1:A:215:ARG:HG3	1.98	0.45
1:A:171:LEU:HD22	1:A:175:LEU:HB2	1.98	0.45
1:A:86:LYS:NZ	5:A:638:HOH:O	2.48	0.45
1:A:259:PRO:HA	1:A:374:HIS:CD2	2.52	0.44
1:A:419:ILE:HD11	1:A:423:ILE:HD12	1.98	0.44
1:A:4:ASN:ND2	5:A:640:HOH:O	2.49	0.44
1:A:57:LEU:HD21	1:A:73[B]:LEU:HD11	1.99	0.44
1:A:334:ASN:OD1	1:A:337:ARG:NE	2.41	0.44
1:A:443:MET:HE3	1:A:443:MET:HB3	1.93	0.44
1:A:25:MET:SD	1:A:29:GLN:HA	2.57	0.44
1:A:378:ARG:NH2	1:A:409:ASP:OD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:HG21	1:A:126[B]:TRP:CZ2	2.52	0.44
1:A:373:MET:HG2	1:A:374:HIS:N	2.34	0.43
1:A:384:LYS:HD3	1:A:384:LYS:HA	1.75	0.43
1:A:218[B]:LEU:HG	1:A:224:LEU:HD13	2.00	0.42
1:A:150:TRP:CD1	1:A:151:GLU:HG2	2.55	0.41
1:A:386:LEU:HD13	1:A:423:ILE:HG23	2.02	0.41
1:A:238:LYS:O	1:A:242:GLU:HG3	2.20	0.41
1:A:403:ASN:OD1	3:A:503:FAD:N5	2.54	0.41
1:A:266:ASN:HA	1:A:372:LYS:HE3	2.02	0.41
1:A:138:PHE:O	5:A:601:HOH:O	2.22	0.40
1:A:356:HIS:HE1	1:A:388:TRP:CZ2	2.38	0.40
1:A:113:LEU:O	1:A:138:PHE:HA	2.22	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	459/482 (95%)	442 (96%)	17 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	359/416 (86%)	355 (99%)	4 (1%)	65 74

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

Mol	Chain	Res	Type
1	A	131	ILE
1	A	199	THR
1	A	200	LEU
1	A	403	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	220	ASN
1	A	279	GLN
1	A	291	ASN
1	A	343	HIS
1	A	403	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 ⓘ

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
3	FAD	A	503	-	58,58,58	3.54	28 (48%)	85,89,89	2.07	23 (27%)
2	SO4	A	501	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	A	504	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	A	502	-	4,4,4	0.24	0	6,6,6	0.07	0
4	DTT	A	505	-	7,7,7	0.89	0	4,8,8	2.66	2 (50%)

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
4	DTT	A	505	-	-	5/8/8/8	-
3	FAD	A	503	-	-	4/34/50/50	0/6/6/6

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	FAD	PA-O3P	8.29	1.68	1.59
3	A	503	FAD	P-O3P	7.48	1.67	1.59
3	A	503	FAD	O2'-C2'	-7.42	1.27	1.43
3	A	503	FAD	O4'-C4'	-6.82	1.29	1.43
3	A	503	FAD	C3B-C4B	-6.75	1.35	1.53
3	A	503	FAD	C4'-C3'	-6.52	1.42	1.53
3	A	503	FAD	C9A-N10	-6.25	1.30	1.41
3	A	503	FAD	O4-C4	5.99	1.34	1.23
3	A	503	FAD	C8A-N9A	-5.94	1.27	1.37
3	A	503	FAD	C2'-C3'	-5.85	1.43	1.53
3	A	503	FAD	C2B-C1B	-5.79	1.35	1.53
3	A	503	FAD	C2B-C3B	-5.59	1.38	1.53
3	A	503	FAD	O2-C2	5.49	1.35	1.24
3	A	503	FAD	C6A-N6A	4.52	1.45	1.34
3	A	503	FAD	C4-N3	-4.30	1.30	1.38
3	A	503	FAD	O3'-C3'	-3.53	1.34	1.43
3	A	503	FAD	C1B-N9A	-3.49	1.36	1.46
3	A	503	FAD	C4A-N9A	-3.49	1.30	1.37
3	A	503	FAD	P-O5'	2.95	1.70	1.59
3	A	503	FAD	PA-O5B	2.71	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	FAD	C2-N3	-2.71	1.33	1.39
3	A	503	FAD	C10-N10	-2.65	1.31	1.37
3	A	503	FAD	C5B-C4B	-2.65	1.43	1.51
3	A	503	FAD	PA-O2A	2.49	1.66	1.55
3	A	503	FAD	C8M-C8	2.46	1.55	1.51
3	A	503	FAD	P-O2P	2.30	1.66	1.55
3	A	503	FAD	C5A-C4A	2.22	1.43	1.39
3	A	503	FAD	C5X-N5	-2.12	1.35	1.39

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	FAD	C4A-N9A-C8A	8.17	114.32	105.74
3	A	503	FAD	N3A-C4A-N9A	5.79	137.02	127.17
3	A	503	FAD	C5A-C4A-N3A	-5.77	118.77	126.72
3	A	503	FAD	C4A-C5A-N7A	-4.47	105.47	110.58
4	A	505	DTT	C2-C1-S1	4.25	126.31	114.43
3	A	503	FAD	N3A-C2A-N1A	-3.97	122.58	128.58
3	A	503	FAD	C5X-N5-C4X	-3.87	111.82	118.09
3	A	503	FAD	N9A-C8A-N7A	-3.60	108.83	113.94
3	A	503	FAD	C4X-C10-N10	3.52	121.52	116.48
3	A	503	FAD	C4X-C10-N1	-3.43	116.18	124.59
3	A	503	FAD	C2A-N3A-C4A	3.33	119.97	111.83
3	A	503	FAD	C4X-C4-N3	3.01	120.91	113.25
3	A	503	FAD	C4-N3-C2	-2.93	120.44	125.64
3	A	503	FAD	C5X-C9A-N10	2.78	120.48	117.97
3	A	503	FAD	C4B-O4B-C1B	-2.76	103.38	109.47
4	A	505	DTT	O2-C2-C3	-2.72	103.86	109.57
3	A	503	FAD	C9A-N10-C10	-2.56	116.85	120.75
3	A	503	FAD	C5'-C4'-C3'	-2.54	107.42	112.22
3	A	503	FAD	C5A-N7A-C8A	2.37	107.17	103.45
3	A	503	FAD	C4-C4X-N5	-2.30	115.03	118.21
3	A	503	FAD	C3B-C2B-C1B	2.30	105.81	101.46
3	A	503	FAD	O4-C4-C4X	-2.25	120.58	126.53
3	A	503	FAD	C6A-C5A-N7A	2.24	136.41	132.09
3	A	503	FAD	C10-N1-C2	2.23	121.67	116.85
3	A	503	FAD	C2B-C1B-N9A	-2.14	108.00	113.30

There are no chirality outliers.

All (9) torsion outliers are listed below:

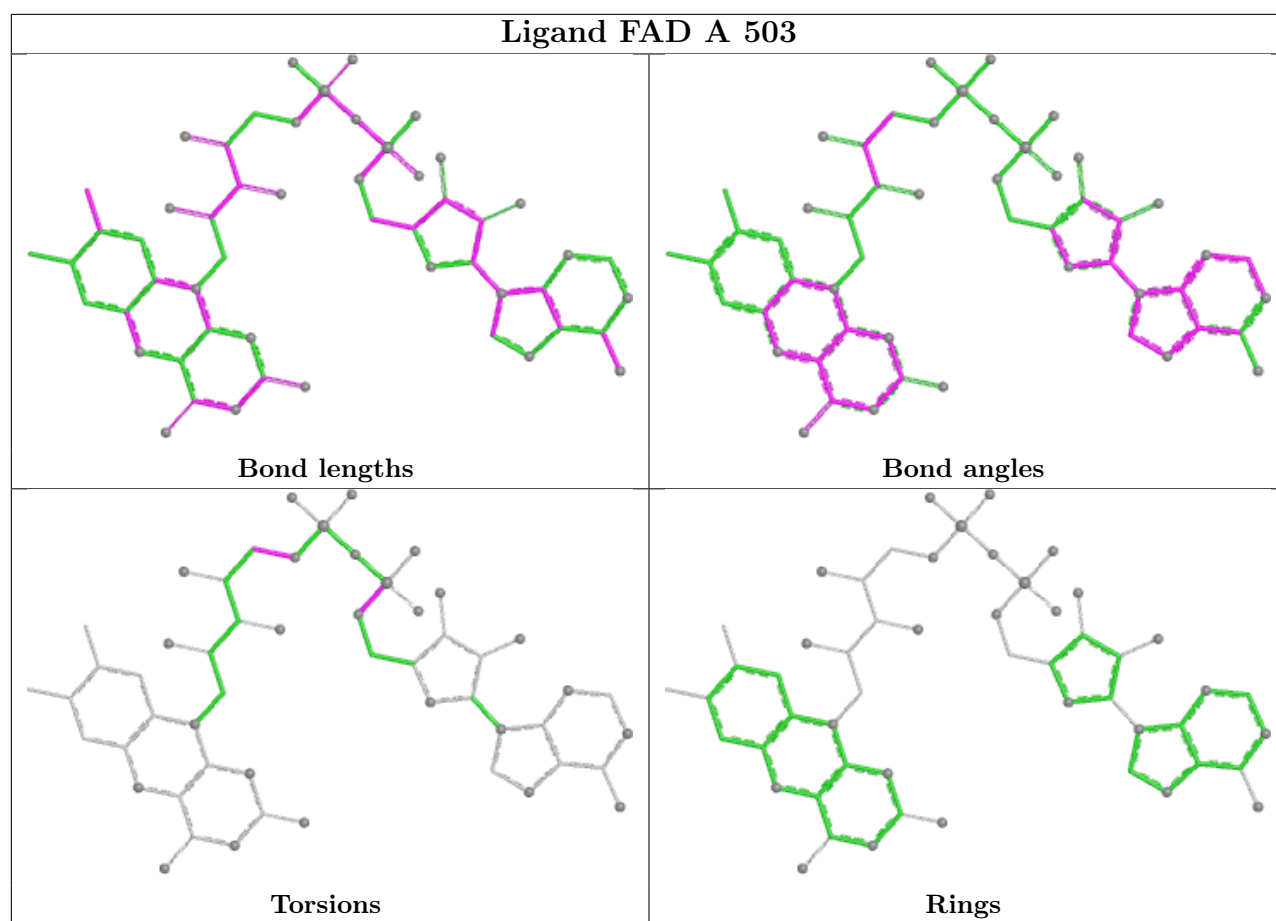
Mol	Chain	Res	Type	Atoms
3	A	503	FAD	C5B-O5B-PA-O1A
3	A	503	FAD	C5B-O5B-PA-O2A
3	A	503	FAD	C5B-O5B-PA-O3P
4	A	505	DTT	C1-C2-C3-O3
4	A	505	DTT	C1-C2-C3-C4
4	A	505	DTT	O2-C2-C3-O3
4	A	505	DTT	O2-C2-C3-C4
4	A	505	DTT	O3-C3-C4-S4
3	A	503	FAD	C4'-C5'-O5'-P

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	FAD	5	0
2	A	501	SO4	1	0
4	A	505	DTT	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 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	453/482 (93%)	2.00	201 (44%) 0 1	17, 39, 57, 85	13 (2%)

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	VAL	7.6
1	A	218[A]	LEU	6.1
1	A	39	PHE	6.0
1	A	186	VAL	5.9
1	A	233	GLY	5.9
1	A	50	PRO	4.9
1	A	49	VAL	4.9
1	A	462	SER	4.8
1	A	419	ILE	4.8
1	A	362	ALA	4.6
1	A	251	SER	4.4
1	A	423	ILE	4.4
1	A	219	LYS	4.3
1	A	161[A]	HIS	4.3
1	A	198	GLU	4.2
1	A	350	PHE	4.2
1	A	202	ASP	4.1
1	A	208	VAL	4.1
1	A	222	ASP	4.1
1	A	16	GLN	4.1
1	A	204	LEU	4.0
1	A	212	LEU	4.0
1	A	343	HIS	4.0
1	A	158	TYR	4.0
1	A	344	ILE	4.0
1	A	220	ASN	3.9
1	A	84	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	189	GLU	3.9
1	A	437	THR	3.9
1	A	43	ILE	3.9
1	A	205	GLU	3.8
1	A	102	SER	3.8
1	A	342	SER	3.7
1	A	134	ILE	3.7
1	A	291	ASN	3.7
1	A	221	LYS	3.7
1	A	199	THR	3.6
1	A	432	GLY	3.6
1	A	132	SER	3.6
1	A	345	TYR	3.5
1	A	54	VAL	3.5
1	A	203	VAL	3.4
1	A	62	LEU	3.4
1	A	20	PRO	3.4
1	A	81	VAL	3.4
1	A	31	ALA	3.4
1	A	170	LEU	3.4
1	A	108	TYR	3.3
1	A	356	HIS	3.3
1	A	410	GLY	3.3
1	A	18	ASP	3.3
1	A	431	TRP	3.2
1	A	83	LEU	3.2
1	A	61	PHE	3.2
1	A	77	GLN	3.2
1	A	57	LEU	3.2
1	A	136	ILE	3.2
1	A	450	ARG	3.2
1	A	13	SER	3.2
1	A	53	VAL	3.1
1	A	138	PHE	3.1
1	A	292	PRO	3.1
1	A	262	ASN	3.1
1	A	130	VAL	3.1
1	A	92	PHE	3.1
1	A	22	VAL	3.1
1	A	454	VAL	3.1
1	A	175	LEU	3.1
1	A	3	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	290	SER	3.1
1	A	421	TRP	3.0
1	A	45	LYS	3.0
1	A	237	ALA	3.0
1	A	267	LEU	3.0
1	A	440	ILE	3.0
1	A	346[A]	THR	3.0
1	A	340	VAL	3.0
1	A	381	TRP	3.0
1	A	38	LEU	2.9
1	A	359	LEU	2.9
1	A	426	VAL	2.9
1	A	185	SER	2.9
1	A	458	ILE	2.9
1	A	187	THR	2.9
1	A	174	PHE	2.9
1	A	137	PRO	2.9
1	A	46	GLU	2.9
1	A	40	SER	2.9
1	A	104	PHE	2.8
1	A	442	TYR	2.8
1	A	445	TYR	2.8
1	A	460	LYS	2.8
1	A	95	GLY	2.8
1	A	167	LEU	2.8
1	A	264	LEU	2.8
1	A	44	ALA	2.7
1	A	86	LYS	2.7
1	A	456	LEU	2.7
1	A	116	ASP	2.7
1	A	215	ARG	2.7
1	A	283	LEU	2.7
1	A	8	ILE	2.7
1	A	201	SER	2.7
1	A	19	GLY	2.7
1	A	25	MET	2.7
1	A	21	VAL	2.7
1	A	293	GLY	2.7
1	A	365[A]	MET	2.6
1	A	52	VAL	2.6
1	A	368	LEU	2.6
1	A	17	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	162	THR	2.6
1	A	216	ALA	2.6
1	A	250[A]	ASP	2.6
1	A	88	ILE	2.6
1	A	266	ASN	2.6
1	A	430	ALA	2.6
1	A	107	ASP	2.6
1	A	73[A]	LEU	2.6
1	A	211	LEU	2.6
1	A	249	LEU	2.6
1	A	388	TRP	2.6
1	A	87	LYS	2.5
1	A	303	LEU	2.5
1	A	133	GLY	2.5
1	A	457	TYR	2.5
1	A	96	ASP	2.5
1	A	213	PRO	2.5
1	A	184	ASN	2.5
1	A	42	ALA	2.5
1	A	223	PRO	2.5
1	A	181	LEU	2.5
1	A	168	TYR	2.4
1	A	265	SER	2.4
1	A	373	MET	2.4
1	A	200	LEU	2.4
1	A	384	LYS	2.4
1	A	207	GLY	2.4
1	A	228	TRP	2.4
1	A	232	PRO	2.4
1	A	55	PHE	2.4
1	A	349	GLU	2.4
1	A	327	SER	2.4
1	A	389	SER	2.4
1	A	56[A]	CYS	2.4
1	A	452	PHE	2.4
1	A	285	VAL	2.4
1	A	305	TRP	2.3
1	A	11	LEU	2.3
1	A	59	ASP	2.3
1	A	357	ASP	2.3
1	A	82	SER	2.3
1	A	188	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	335	ALA	2.3
1	A	23	TYR	2.3
1	A	451	LYS	2.3
1	A	105	VAL	2.3
1	A	269	PRO	2.3
1	A	85	ARG	2.3
1	A	6	LYS	2.3
1	A	339	ASP	2.3
1	A	453	ASP	2.3
1	A	79	LEU	2.3
1	A	113	LEU	2.3
1	A	443	MET	2.3
1	A	322	PHE	2.2
1	A	89	PRO	2.2
1	A	171	LEU	2.2
1	A	299	LEU	2.2
1	A	126[A]	TRP	2.2
1	A	298	PHE	2.2
1	A	127	ILE	2.2
1	A	183	PRO	2.2
1	A	206	THR	2.2
1	A	254	ALA	2.2
1	A	448	CYS	2.2
1	A	129	LYS	2.2
1	A	101	ILE	2.2
1	A	131	ILE	2.2
1	A	99	GLU	2.2
1	A	274	GLY	2.2
1	A	15	LYS	2.2
1	A	51	VAL	2.1
1	A	37	LEU	2.1
1	A	224	LEU	2.1
1	A	241	MET	2.1
1	A	416	TYR	2.1
1	A	289	GLU	2.1
1	A	58	THR	2.1
1	A	355	THR	2.1
1	A	273	PHE	2.1
1	A	240	VAL	2.1
1	A	9	ARG	2.1
1	A	210	ALA	2.1
1	A	297	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	91	PHE	2.1
1	A	32	GLU	2.1
1	A	69	TYR	2.1
1	A	351	GLU	2.0
1	A	397	GLU	2.0
1	A	66	ILE	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](#)

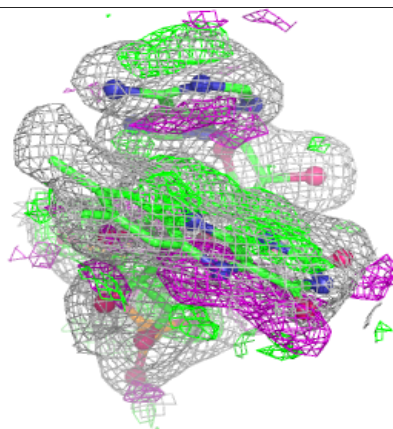
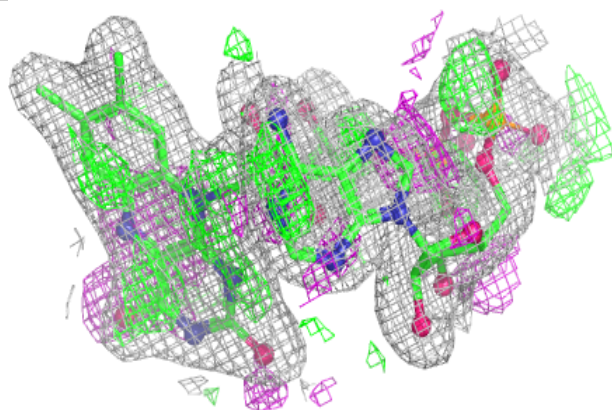
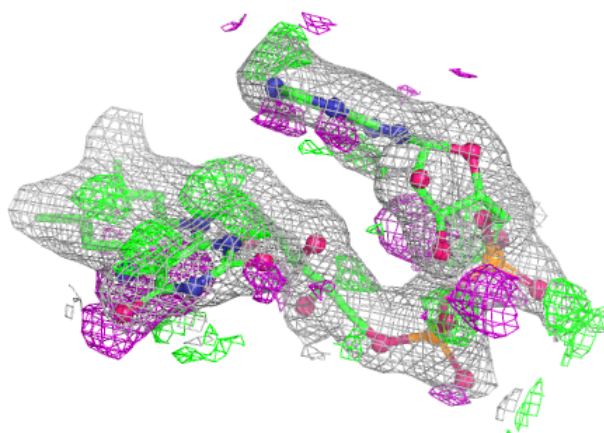
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	SO4	A	504	5/5	0.47	0.16	69,73,77,87	5
2	SO4	A	502	5/5	0.68	0.15	56,57,69,69	0
4	DTT	A	505	8/8	0.68	0.27	23,35,71,91	8
3	FAD	A	503	53/53	0.84	0.16	20,21,30,44	0
2	SO4	A	501	5/5	0.93	0.14	25,37,45,45	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:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.