



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:48 PM UTC

PDB ID : 7YE0 / pdb_00007ye0
Title : DF-SFX MmCPDII-DNA complex: steady state oxidized complex
Authors : Maestre-Reyna, M.; Wang, P.-H.; Nango, E.; Hosokawa, Y.; Saft, M.; Furrer, A.; Yang, C.-H.; Ngura Putu, E.P.G.; Wu, W.-J.; Emmerich, H.-J.; Engilberge, S.; Caramello, N.; Wranik, M.; Glover, H.L.; Franz-Badur, S.; Wu, H.-Y.; Lee, C.-C.; Huang, W.-C.; Huang, K.-F.; Chang, Y.-K.; Liao, J.-H.; Weng, J.-H.; Gad, W.; Chang, C.-W.; Pang, A.H.; Gashi, D.; Beale, E.; Ozerov, D.; Milne, C.; Cirelli, C.; Bacellar, C.; Sugahara, M.; Owada, S.; Joti, Y.; Yamashita, A.; Tanaka, R.; Tanaka, T.; Luo, F.J.; Tono, K.; Kiontke, S.; Spadaccini, R.; Royant, A.; Yamamoto, J.; Iwata, S.; Standfuss, J.; Essen, L.-O.; Bessho, Y.; Tsai, M.-D.
Deposited on : 2022-07-05
Resolution : 2.75 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

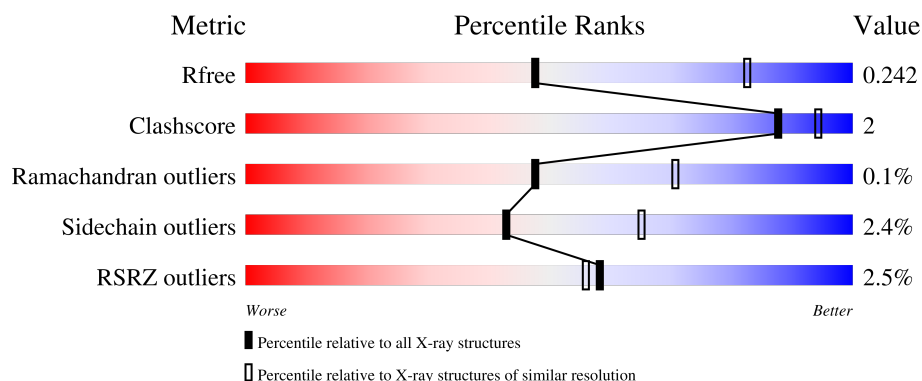
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

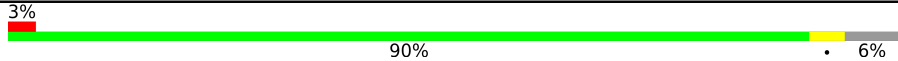
The reported resolution of this entry is 2.75 Å.

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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	

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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

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Mol	Chain	Length	Quality of chain
1	B	482	2% 85% 11%
2	C	13	62% 31% 8%
2	E	13	54% 31% 8% 8%
3	D	14	100%
3	F	14	79% 21%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8298 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 Deoxyribodipyrimidine photo-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	2	0
			3568	2305	597	652	14			
1	B	431	Total	C	N	O	S	0	4	0
			3390	2189	568	619	14			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP A0A0F8I5V2
A	-16	GLY	-	expression tag	UNP A0A0F8I5V2
A	-15	SER	-	expression tag	UNP A0A0F8I5V2
A	-14	SER	-	expression tag	UNP A0A0F8I5V2
A	-13	HIS	-	expression tag	UNP A0A0F8I5V2
A	-12	HIS	-	expression tag	UNP A0A0F8I5V2
A	-11	HIS	-	expression tag	UNP A0A0F8I5V2
A	-10	HIS	-	expression tag	UNP A0A0F8I5V2
A	-9	HIS	-	expression tag	UNP A0A0F8I5V2
A	-8	HIS	-	expression tag	UNP A0A0F8I5V2
A	-7	SER	-	expression tag	UNP A0A0F8I5V2
A	-6	SER	-	expression tag	UNP A0A0F8I5V2
A	-5	GLY	-	expression tag	UNP A0A0F8I5V2
A	-4	LEU	-	expression tag	UNP A0A0F8I5V2
A	-3	VAL	-	expression tag	UNP A0A0F8I5V2
A	-2	PRO	-	expression tag	UNP A0A0F8I5V2
A	-1	ARG	-	expression tag	UNP A0A0F8I5V2
A	0	GLY	-	expression tag	UNP A0A0F8I5V2
A	1	SER	-	expression tag	UNP A0A0F8I5V2
A	2	HIS	-	expression tag	UNP A0A0F8I5V2
A	377	THR	MET	engineered mutation	UNP A0A0F8I5V2
A	463	ALA	-	expression tag	UNP A0A0F8I5V2
A	464	LEU	-	expression tag	UNP A0A0F8I5V2
B	-17	MET	-	initiating methionine	UNP A0A0F8I5V2
B	-16	GLY	-	expression tag	UNP A0A0F8I5V2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	SER	-	expression tag	UNP A0A0F8I5V2
B	-14	SER	-	expression tag	UNP A0A0F8I5V2
B	-13	HIS	-	expression tag	UNP A0A0F8I5V2
B	-12	HIS	-	expression tag	UNP A0A0F8I5V2
B	-11	HIS	-	expression tag	UNP A0A0F8I5V2
B	-10	HIS	-	expression tag	UNP A0A0F8I5V2
B	-9	HIS	-	expression tag	UNP A0A0F8I5V2
B	-8	HIS	-	expression tag	UNP A0A0F8I5V2
B	-7	SER	-	expression tag	UNP A0A0F8I5V2
B	-6	SER	-	expression tag	UNP A0A0F8I5V2
B	-5	GLY	-	expression tag	UNP A0A0F8I5V2
B	-4	LEU	-	expression tag	UNP A0A0F8I5V2
B	-3	VAL	-	expression tag	UNP A0A0F8I5V2
B	-2	PRO	-	expression tag	UNP A0A0F8I5V2
B	-1	ARG	-	expression tag	UNP A0A0F8I5V2
B	0	GLY	-	expression tag	UNP A0A0F8I5V2
B	1	SER	-	expression tag	UNP A0A0F8I5V2
B	2	HIS	-	expression tag	UNP A0A0F8I5V2
B	377	THR	MET	engineered mutation	UNP A0A0F8I5V2
B	463	ALA	-	expression tag	UNP A0A0F8I5V2
B	464	LEU	-	expression tag	UNP A0A0F8I5V2

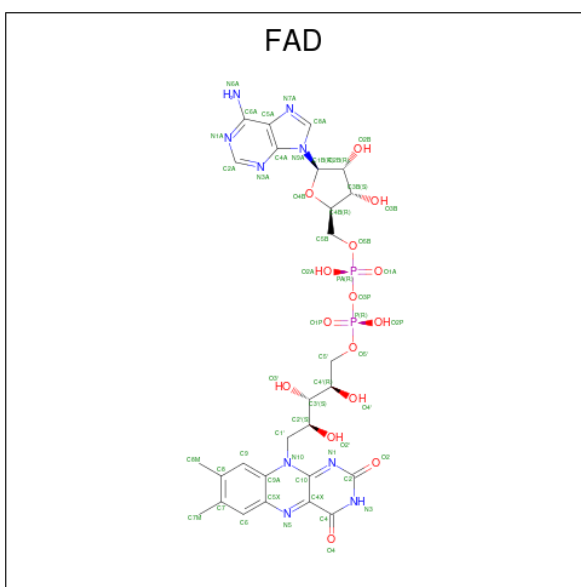
- Molecule 2 is a DNA chain called CPD photolesion containing DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	13	Total	C	N	O	P	0	0	0
			282	135	51	83	13			
2	E	12	Total	C	N	O	P	0	0	0
			264	125	46	80	13			

- Molecule 3 is a DNA chain called complementary oligonucleotide to the CPD containing DNA.

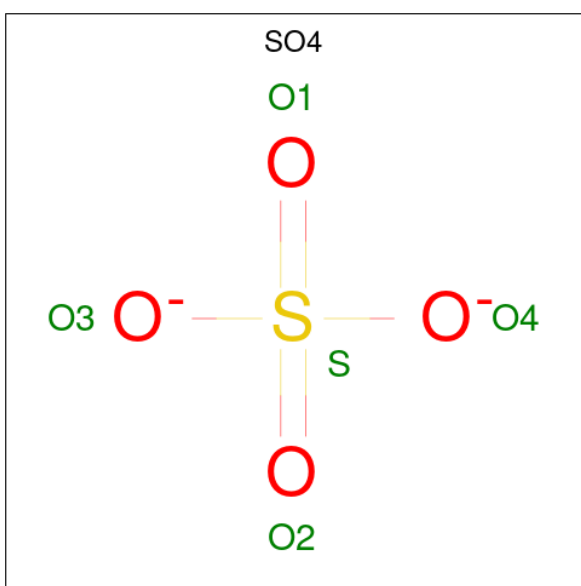
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	14	Total	C	N	O	P	0	0	0
			286	136	56	81	13			
3	F	14	Total	C	N	O	P	0	0	0
			286	136	56	81	13			

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	45	Total 45	O 45	0	0
6	B	58	Total 58	O 58	0	0
6	C	2	Total 2	O 2	0	0
6	D	3	Total 3	O 3	0	0
6	E	2	Total 2	O 2	0	0
6	F	1	Total 1	O 1	0	0

Chain D:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: complementary oligonucleotide to the CPD containing DNA

Chain F:  79% 21%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.58Å 115.87Å 169.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.28 – 2.75 45.28 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.28-2.75) 100.0 (45.28-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.194 , 0.245 0.198 , 0.242	Depositor DCC
R_{free} test set	4223 reflections (4.14%)	wwPDB-VP
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 78.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8298	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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: TTD, 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	0.19	0/3674	0.37	0/4987
1	B	0.17	0/3501	0.35	0/4756
2	C	0.20	0/270	0.49	0/412
2	E	0.30	0/249	0.56	0/379
3	D	0.19	0/321	0.41	0/494
3	F	0.20	0/321	0.42	0/494
All	All	0.19	0/8336	0.38	0/11522

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 [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	3568	0	3334	10	0
1	B	3390	0	3131	12	0
2	C	282	0	159	5	0
2	E	264	0	147	6	0
3	D	286	0	158	0	0
3	F	286	0	158	2	0
4	A	53	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	53	0	28	1	0
5	A	5	0	0	1	0
6	A	45	0	0	0	0
6	B	58	0	0	1	0
6	C	2	0	0	1	0
6	D	3	0	0	0	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
All	All	8298	0	7143	31	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 (31) 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:168:TYR:HE2	1:A:304:ILE:HD11	1.57	0.69
1:A:450:ARG:NH1	6:C:101:HOH:O	2.32	0.62
1:B:39:PHE:CZ	1:B:43:ILE:HD11	2.36	0.60
1:B:3:MET:HE3	1:B:39:PHE:HB2	1.85	0.58
2:C:7:TTD:O4R	2:C:7:TTD:H1'	2.05	0.56
1:A:300:ASP:HA	1:A:304:ILE:HD12	1.88	0.54
2:C:4:DG:H2''	2:C:5:DG:O5'	2.08	0.52
2:E:8:DC:H2''	2:E:9:DG:H5'	1.93	0.51
1:B:435:GLU:O	1:B:436:VAL:HG22	2.10	0.50
1:B:6:LYS:NZ	6:B:1602:HOH:O	2.44	0.50
1:A:67:ARG:NE	5:A:1502:SO4:O4	2.43	0.49
2:E:4:DG:H4'	2:E:5:DG:OP1	2.11	0.49
2:E:7:TTD:H6T	2:E:7:TTD:H2R1	1.41	0.45
1:B:8:ILE:HD13	1:B:39:PHE:CE1	2.51	0.45
1:B:305:TRP:CZ2	2:E:7:TTD:H5A2	2.53	0.44
1:B:461:TYR:O	1:B:462:SER:C	2.60	0.44
1:A:305:TRP:HA	1:A:308:ILE:HG22	1.99	0.44
2:E:8:DC:H2'	2:E:9:DG:C8	2.52	0.44
1:A:58:THR:HG22	1:A:97:PRO:HD3	2.01	0.43
1:B:415:GLY:HA2	4:B:1501:FAD:N5	2.34	0.43
2:C:9:DG:C4	2:C:10:DC:C5	3.08	0.42
1:A:389[A]:SER:OG	1:A:395:ALA:HB2	2.19	0.42
1:A:411:ARG:HB2	1:A:411:ARG:NH1	2.35	0.42
1:B:435:GLU:C	1:B:437:THR:H	2.28	0.42
1:B:421:TRP:CE2	2:E:7:TTD:H72	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:4:DG:H2''	3:F:5:DC:H5''	2.02	0.41
1:A:421:TRP:CE2	2:C:7:TTD:H72	2.56	0.41
1:A:258:ASP:OD1	1:A:260:THR:OG1	2.37	0.41
1:B:450:ARG:NH1	3:F:2:DG:O6	2.54	0.41
2:C:7:TTD:H2R1	2:C:7:TTD:H6T	1.93	0.40
1:B:389:SER:OG	1:B:395:ALA:HB2	2.21	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	451/482 (94%)	439 (97%)	12 (3%)	0	100	100
1	B	429/482 (89%)	417 (97%)	11 (3%)	1 (0%)	43	64
All	All	880/964 (91%)	856 (97%)	23 (3%)	1 (0%)	48	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	-1	ARG

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	350/416 (84%)	342 (98%)	8 (2%)	44	66
1	B	330/416 (79%)	321 (97%)	9 (3%)	39	62
All	All	680/832 (82%)	663 (98%)	17 (2%)	43	64

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	57	LEU
1	A	103	ARG
1	A	125	GLN
1	A	167	LEU
1	A	300	ASP
1	A	344	ILE
1	A	411	ARG
1	B	3	MET
1	B	57	LEU
1	B	60	GLU
1	B	113	LEU
1	B	125[A]	GLN
1	B	125[B]	GLN
1	B	300	ASP
1	B	396	LEU
1	B	436	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	343	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	TTD	E	7	2	42,45,46	0.76	3 (7%)	61,74,77	0.83	1 (1%)
2	TTD	C	7	2	42,45,46	3.17	18 (42%)	61,74,77	2.88	19 (31%)

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	TTD	E	7	2	-	10/22/109/110	0/5/6/6
2	TTD	C	7	2	-	5/22/109/110	0/5/6/6

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	7	TTD	C5-C6	-7.33	1.47	1.55
2	C	7	TTD	C5T-C6T	-7.25	1.47	1.55
2	C	7	TTD	C2T-N1T	6.77	1.49	1.36
2	C	7	TTD	C2-N1	6.29	1.48	1.36
2	C	7	TTD	C2-N3	6.26	1.48	1.38
2	C	7	TTD	C2'-C3R	-6.11	1.39	1.52
2	C	7	TTD	C2T-N3T	5.91	1.48	1.38
2	C	7	TTD	C4-N3	5.30	1.45	1.37
2	C	7	TTD	C4T-N3T	4.38	1.44	1.37
2	C	7	TTD	C1R-N1T	-2.71	1.42	1.45
2	C	7	TTD	O4T-C4T	-2.63	1.18	1.22
2	C	7	TTD	O2T-C2T	-2.61	1.18	1.23
2	C	7	TTD	O4-C4	-2.55	1.18	1.22
2	C	7	TTD	O2-C2	-2.45	1.18	1.23
2	C	7	TTD	C2'-C1'	-2.44	1.45	1.52
2	E	7	TTD	C1'-N1	2.31	1.48	1.45
2	C	7	TTD	C3'-C4'	-2.25	1.47	1.53
2	C	7	TTD	C6T-C6	2.18	1.62	1.56
2	C	7	TTD	PB-O3R	2.18	1.65	1.59
2	E	7	TTD	C2T-N3T	-2.12	1.34	1.38
2	E	7	TTD	C2-N3	-2.10	1.34	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	7	TTD	O4R-C1R-N1T	12.96	124.01	108.65
2	C	7	TTD	C2R-C1R-N1T	-6.11	107.33	115.59
2	C	7	TTD	C4T-N3T-C2T	-5.81	117.90	126.67
2	C	7	TTD	C5-C4-N3	5.00	120.28	116.09
2	C	7	TTD	N3T-C2T-N1T	4.89	121.90	116.78
2	C	7	TTD	C4-N3-C2	-4.88	119.31	126.67
2	C	7	TTD	C5T-C4T-N3T	4.87	120.18	116.09
2	C	7	TTD	O4'-C1'-N1	-4.13	103.76	108.65
2	C	7	TTD	N3-C2-N1	3.87	120.84	116.78
2	C	7	TTD	C4'-O4R-C1R	-3.57	101.02	109.51
2	C	7	TTD	C6T-C5T-C4T	3.38	123.39	114.34
2	C	7	TTD	O4R-C1R-C2R	-3.32	100.04	106.25
2	C	7	TTD	C5-C6-N1	3.12	119.78	115.65
2	C	7	TTD	C5T-C5-C6	2.75	91.57	88.36
2	C	7	TTD	O4T-C4T-C5T	-2.67	120.23	122.71
2	C	7	TTD	O4P-PB-O3R	2.65	117.48	106.70
2	C	7	TTD	O2-C2-N1	-2.46	119.75	123.44
2	C	7	TTD	O2T-C2T-N1T	-2.42	119.81	123.44
2	E	7	TTD	C5T-C6T-N1T	-2.16	112.79	115.65
2	C	7	TTD	O4P-PB-O5R	2.01	116.67	107.57

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	7	TTD	O4R-C4'-C5R-O5R
2	E	7	TTD	C3'-C4'-C5R-O5R
2	E	7	TTD	C2'-C1'-N1-C6
2	E	7	TTD	C2'-C1'-N1-C2
2	C	7	TTD	C2'-C1'-N1-C6
2	C	7	TTD	C2'-C1'-N1-C2
2	E	7	TTD	C2R-C1R-N1T-C6T
2	C	7	TTD	O4'-C1'-N1-C2
2	C	7	TTD	O4'-C1'-N1-C6
2	E	7	TTD	O4'-C1'-N1-C6
2	E	7	TTD	O4'-C1'-N1-C2
2	E	7	TTD	O4R-C1R-N1T-C6T
2	E	7	TTD	C4R-C5'-O5'-P
2	C	7	TTD	O4'-C4R-C5'-O5'
2	E	7	TTD	O4'-C4R-C5'-O5'

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	7	TTD	3	0
2	C	7	TTD	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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$
5	SO4	A	1502	-	4,4,4	0.22	0	6,6,6	0.09	0
4	FAD	B	1501	-	58,58,58	3.46	29 (50%)	85,89,89	1.97	22 (25%)
4	FAD	A	1501	-	58,58,58	3.43	28 (48%)	85,89,89	1.96	22 (25%)

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	FAD	B	1501	-	-	4/34/50/50	0/6/6/6
4	FAD	A	1501	-	-	5/34/50/50	0/6/6/6

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1501	FAD	PA-O3P	7.95	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1501	FAD	PA-O3P	7.55	1.67	1.59
4	A	1501	FAD	O2'-C2'	-7.30	1.28	1.43
4	B	1501	FAD	P-O3P	7.28	1.67	1.59
4	B	1501	FAD	O2'-C2'	-7.19	1.28	1.43
4	B	1501	FAD	O4'-C4'	-6.91	1.28	1.43
4	A	1501	FAD	O4'-C4'	-6.90	1.28	1.43
4	B	1501	FAD	C3B-C4B	-6.86	1.35	1.53
4	A	1501	FAD	C3B-C4B	-6.77	1.35	1.53
4	A	1501	FAD	P-O3P	6.75	1.66	1.59
4	A	1501	FAD	C4'-C3'	-6.60	1.41	1.53
4	B	1501	FAD	C4'-C3'	-6.38	1.42	1.53
4	A	1501	FAD	O4-C4	5.89	1.34	1.23
4	B	1501	FAD	O4-C4	5.89	1.34	1.23
4	A	1501	FAD	C2B-C1B	-5.75	1.35	1.53
4	B	1501	FAD	C2B-C1B	-5.72	1.35	1.53
4	A	1501	FAD	C2B-C3B	-5.65	1.38	1.53
4	B	1501	FAD	C2'-C3'	-5.64	1.43	1.53
4	B	1501	FAD	C2B-C3B	-5.60	1.38	1.53
4	A	1501	FAD	C2'-C3'	-5.60	1.43	1.53
4	B	1501	FAD	C9A-N10	-5.53	1.31	1.41
4	B	1501	FAD	O2-C2	5.46	1.35	1.24
4	A	1501	FAD	C9A-N10	-5.44	1.31	1.41
4	A	1501	FAD	O2-C2	5.38	1.35	1.24
4	A	1501	FAD	C8A-N9A	-5.04	1.29	1.37
4	B	1501	FAD	C8A-N9A	-5.00	1.29	1.37
4	A	1501	FAD	C6A-N6A	4.52	1.45	1.34
4	B	1501	FAD	C6A-N6A	4.41	1.45	1.34
4	A	1501	FAD	C4-N3	-4.41	1.30	1.38
4	B	1501	FAD	C4-N3	-4.37	1.30	1.38
4	B	1501	FAD	O3'-C3'	-3.52	1.34	1.43
4	A	1501	FAD	C4A-N9A	-3.52	1.30	1.37
4	B	1501	FAD	C4A-N9A	-3.50	1.30	1.37
4	A	1501	FAD	O3'-C3'	-3.49	1.34	1.43
4	A	1501	FAD	C1B-N9A	-3.18	1.37	1.46
4	B	1501	FAD	C1B-N9A	-3.17	1.37	1.46
4	A	1501	FAD	C2-N3	-2.96	1.32	1.39
4	B	1501	FAD	C5B-C4B	-2.95	1.42	1.51
4	B	1501	FAD	P-O5'	2.94	1.70	1.59
4	A	1501	FAD	C5B-C4B	-2.88	1.42	1.51
4	A	1501	FAD	P-O5'	2.88	1.70	1.59
4	B	1501	FAD	C2-N3	-2.82	1.32	1.39
4	B	1501	FAD	C5X-N5	-2.66	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1501	FAD	PA-O2A	2.55	1.67	1.55
4	A	1501	FAD	PA-O2A	2.53	1.67	1.55
4	A	1501	FAD	C5X-N5	-2.53	1.34	1.39
4	A	1501	FAD	PA-O5B	2.52	1.69	1.59
4	B	1501	FAD	PA-O5B	2.48	1.69	1.59
4	A	1501	FAD	C8M-C8	2.48	1.55	1.51
4	B	1501	FAD	C8M-C8	2.48	1.55	1.51
4	B	1501	FAD	P-O2P	2.31	1.66	1.55
4	A	1501	FAD	P-O2P	2.30	1.66	1.55
4	A	1501	FAD	C10-N10	-2.30	1.32	1.37
4	B	1501	FAD	C10-N10	-2.20	1.32	1.37
4	A	1501	FAD	C5A-C4A	2.19	1.43	1.39
4	B	1501	FAD	C5A-C4A	2.13	1.42	1.39
4	B	1501	FAD	C7M-C7	2.03	1.54	1.51

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1501	FAD	C4A-N9A-C8A	7.45	113.56	105.74
4	B	1501	FAD	C4A-N9A-C8A	7.44	113.55	105.74
4	B	1501	FAD	C5A-C4A-N3A	-5.77	118.78	126.72
4	A	1501	FAD	C5A-C4A-N3A	-5.75	118.79	126.72
4	A	1501	FAD	N3A-C4A-N9A	5.31	136.19	127.17
4	B	1501	FAD	N3A-C4A-N9A	5.29	136.16	127.17
4	B	1501	FAD	C4A-C5A-N7A	-4.64	105.28	110.58
4	A	1501	FAD	C4A-C5A-N7A	-4.62	105.30	110.58
4	B	1501	FAD	N3A-C2A-N1A	-4.21	122.21	128.58
4	A	1501	FAD	N3A-C2A-N1A	-4.13	122.33	128.58
4	B	1501	FAD	N9A-C8A-N7A	-3.72	108.65	113.94
4	A	1501	FAD	N9A-C8A-N7A	-3.70	108.68	113.94
4	B	1501	FAD	C4X-C10-N1	-3.51	115.98	124.59
4	B	1501	FAD	C2A-N3A-C4A	3.49	120.34	111.83
4	A	1501	FAD	C4X-C10-N1	-3.46	116.10	124.59
4	A	1501	FAD	C2A-N3A-C4A	3.42	120.18	111.83
4	A	1501	FAD	C4X-C10-N10	2.99	120.76	116.48
4	B	1501	FAD	C4X-C10-N10	2.91	120.64	116.48
4	B	1501	FAD	C5'-C4'-C3'	-2.85	106.84	112.22
4	B	1501	FAD	C4B-O4B-C1B	-2.79	103.31	109.47
4	B	1501	FAD	C6-C5X-C9A	2.72	122.78	119.05
4	A	1501	FAD	C6-C5X-C9A	2.66	122.71	119.05
4	A	1501	FAD	C5'-C4'-C3'	-2.65	107.22	112.22
4	A	1501	FAD	C4B-O4B-C1B	-2.61	103.70	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1501	FAD	C4-C4X-C10	2.59	121.37	116.93
4	B	1501	FAD	C5A-N7A-C8A	2.55	107.45	103.45
4	B	1501	FAD	C3B-C2B-C1B	2.55	106.28	101.46
4	A	1501	FAD	C3B-C2B-C1B	2.54	106.28	101.46
4	A	1501	FAD	C5A-N7A-C8A	2.54	107.44	103.45
4	B	1501	FAD	C6A-C5A-N7A	2.54	136.98	132.09
4	A	1501	FAD	C9-C9A-C5X	-2.50	115.61	120.03
4	B	1501	FAD	C9-C9A-C5X	-2.46	115.67	120.03
4	A	1501	FAD	C6A-C5A-N7A	2.45	136.82	132.09
4	A	1501	FAD	C4-C4X-C10	2.43	121.10	116.93
4	A	1501	FAD	O4B-C1B-N9A	2.36	112.63	108.09
4	A	1501	FAD	C4X-C4-N3	2.34	119.22	113.25
4	B	1501	FAD	C5X-C9A-N10	2.26	120.02	117.97
4	B	1501	FAD	C4X-C4-N3	2.26	119.00	113.25
4	B	1501	FAD	O4B-C1B-N9A	2.22	112.34	108.09
4	B	1501	FAD	C10-N1-C2	2.15	121.51	116.85
4	A	1501	FAD	C10-N1-C2	2.14	121.48	116.85
4	B	1501	FAD	O4-C4-C4X	-2.12	120.93	126.53
4	A	1501	FAD	C5X-C9A-N10	2.11	119.88	117.97
4	A	1501	FAD	O4-C4-C4X	-2.05	121.12	126.53

There are no chirality outliers.

All (9) torsion outliers are listed below:

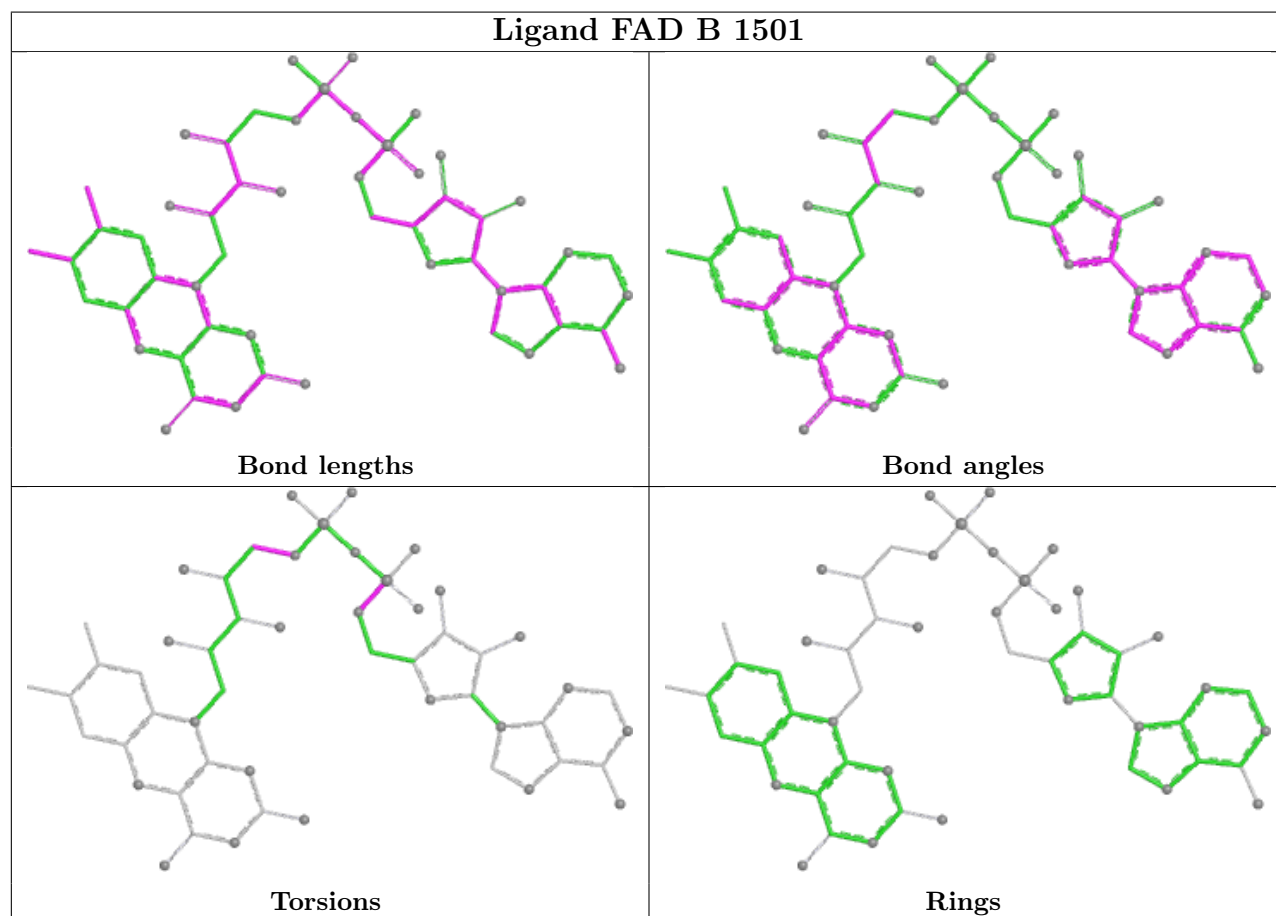
Mol	Chain	Res	Type	Atoms
4	A	1501	FAD	C5B-O5B-PA-O2A
4	A	1501	FAD	C5B-O5B-PA-O3P
4	B	1501	FAD	C5B-O5B-PA-O2A
4	B	1501	FAD	C5B-O5B-PA-O3P
4	A	1501	FAD	C5B-O5B-PA-O1A
4	B	1501	FAD	C5B-O5B-PA-O1A
4	A	1501	FAD	C4'-C5'-O5'-P
4	B	1501	FAD	C4'-C5'-O5'-P
4	A	1501	FAD	N10-C1'-C2'-C3'

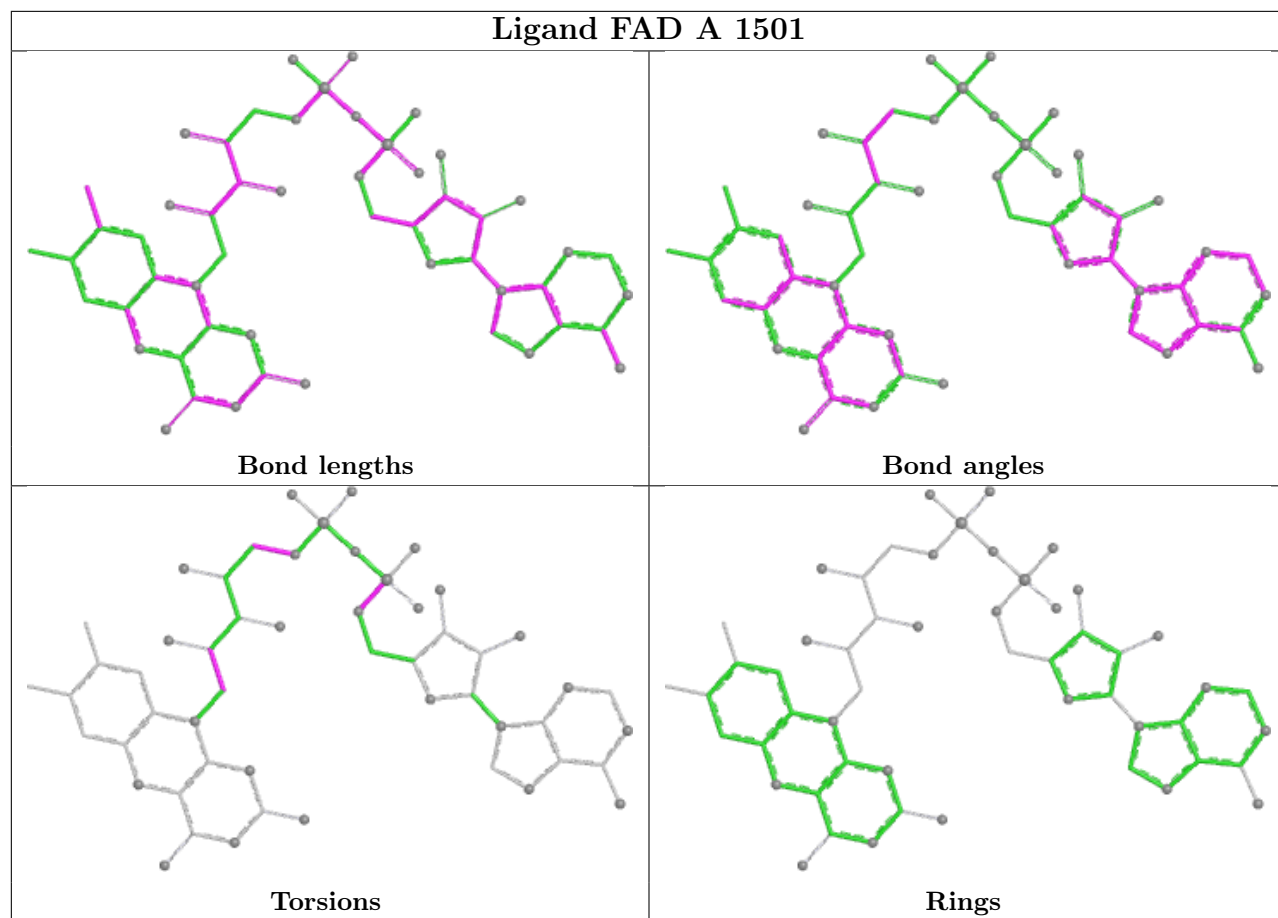
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1502	SO4	1	0
4	B	1501	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 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	455/482 (94%)	0.03	13 (2%)	53	52	36, 59, 100, 136	3 (0%)
1	B	431/482 (89%)	0.13	10 (2%)	61	59	37, 66, 97, 142	5 (1%)
2	C	12/13 (92%)	0.16	0	100	100	58, 92, 165, 177	0
2	E	11/13 (84%)	0.26	0	100	100	63, 96, 156, 165	0
3	D	14/14 (100%)	0.21	0	100	100	68, 90, 138, 164	0
3	F	14/14 (100%)	0.39	0	100	100	75, 114, 158, 161	0
All	All	937/1018 (92%)	0.09	23 (2%)	58	56	36, 64, 104, 177	8 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0	GLY	3.8
1	A	-1	ARG	3.5
1	A	222	ASP	3.2
1	A	187	THR	3.2
1	B	1	SER	3.1
1	A	59	ASP	2.8
1	B	435	GLU	2.8
1	A	213	PRO	2.8
1	B	62	LEU	2.7
1	B	2	HIS	2.7
1	B	12	LYS	2.4
1	A	216	ALA	2.4
1	A	57	LEU	2.3
1	A	1	SER	2.3
1	B	462	SER	2.3
1	B	69	TYR	2.2
1	B	161[A]	HIS	2.2
1	A	199	THR	2.2
1	A	-3	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	135	SER	2.0
1	A	62	LEU	2.0
1	A	450	ARG	2.0
1	B	-1	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	TTD	C	7	40/41	0.94	0.10	48,54,60,61	0
2	TTD	E	7	40/41	0.94	0.09	57,65,76,80	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

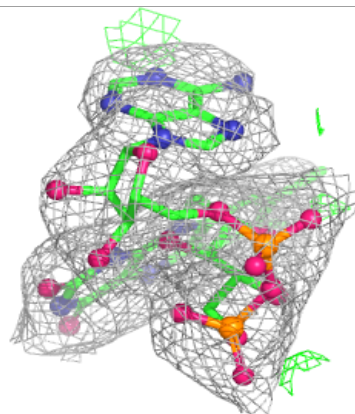
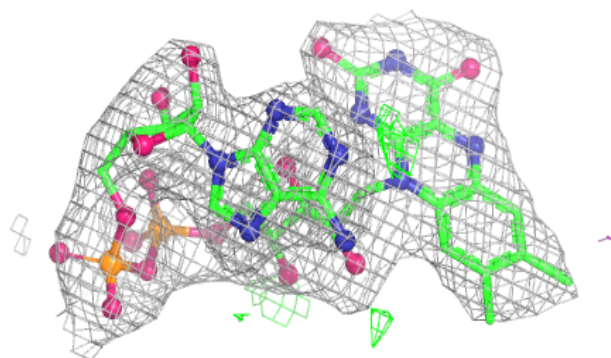
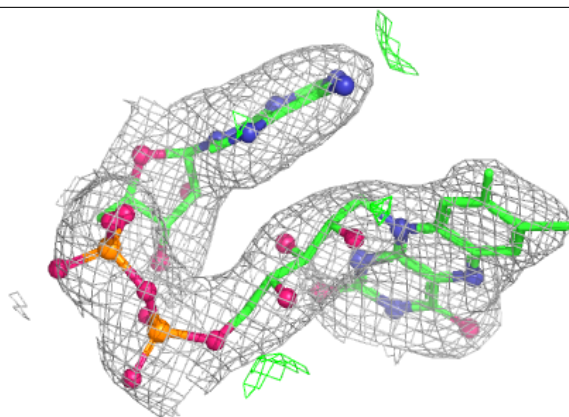
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	A	1502	5/5	0.96	0.07	63,68,70,71	0
4	FAD	B	1501	53/53	0.97	0.07	50,56,63,69	0
4	FAD	A	1501	53/53	0.97	0.07	39,47,51,56	0

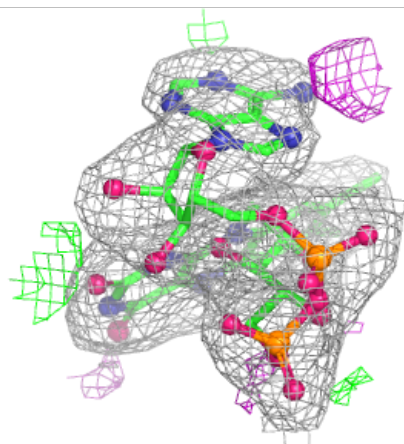
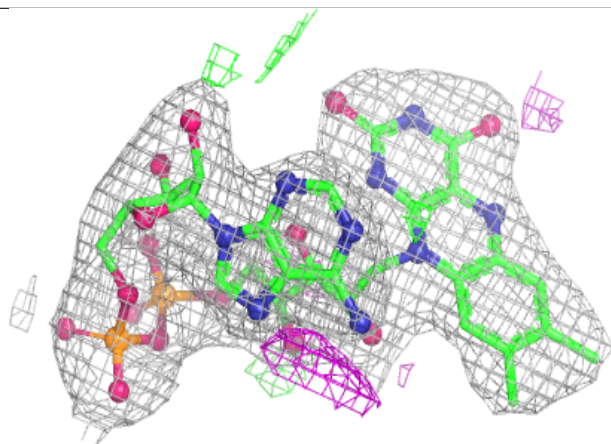
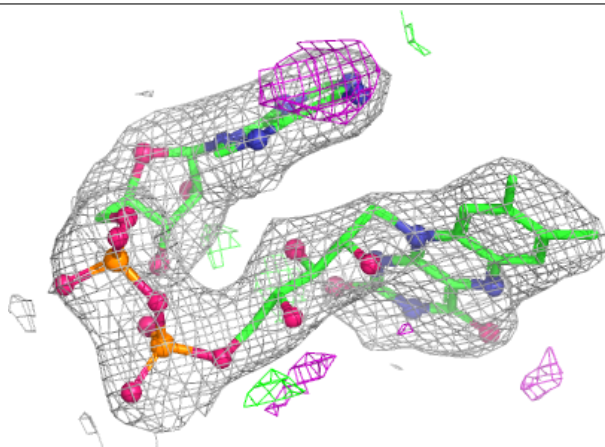
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 1501:

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

**Electron density around FAD A 1501:**

$2mF_o-DF_c$ (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.