Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 03:58 AM JST

PDB ID	:	7YD6
Title	:	TR-SFX MmCPDII-DNA complex: 650 ps snapshot. Includes 650ps, dark, and extrapolated structure factors
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	:	2022-07-04
Resolution	:	2.15 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:

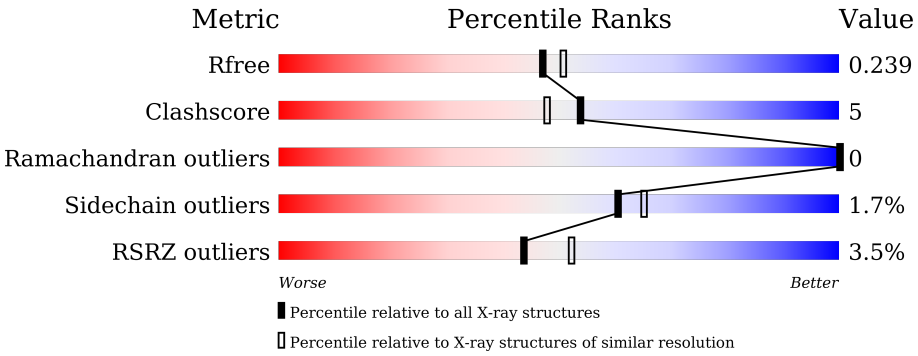
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	4% 82% 12% 5%

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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
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

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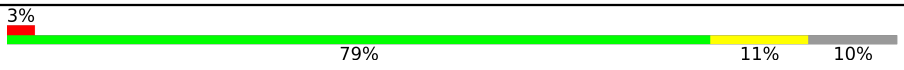
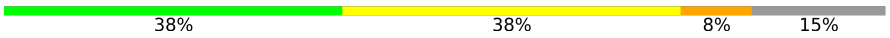
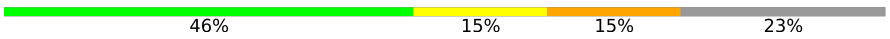
Mol	Chain	Length	Quality of chain
1	B	482	
2	C	13	
2	E	13	
3	D	14	
3	F	14	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8502 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	456	Total	C	N	O	S	0	5	0
			3638	2344	601	679	14			
1	B	434	Total	C	N	O	S	0	6	0
			3459	2222	584	640	13			

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

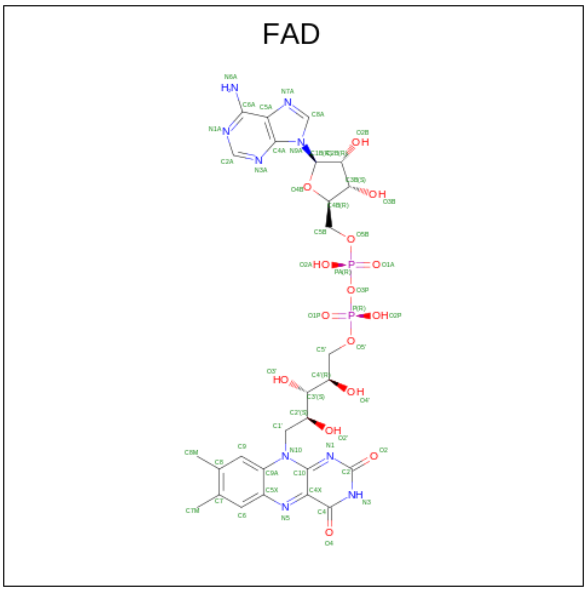
- Molecule 2 is a DNA chain called CPD photolesion containing DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	P	0	0	0
			244	115	44	73	12			
2	E	10	Total	C	N	O	P	0	0	0
			225	106	41	67	11			

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

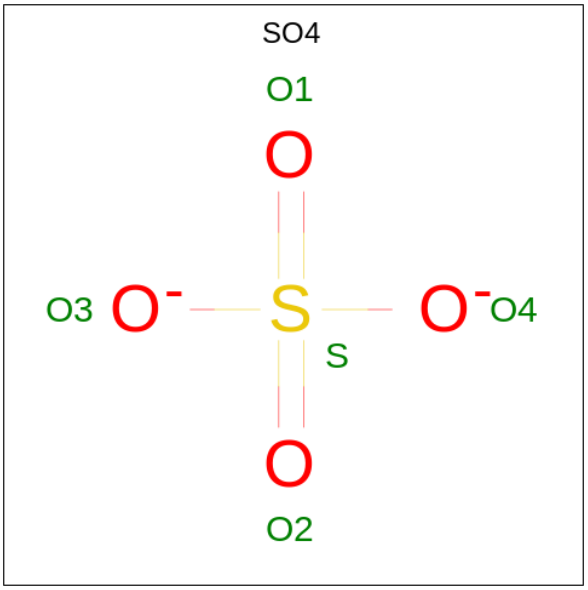
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	14	Total	C	N	O	P	0	0	0
			286	136	56	81	13			
3	F	13	Total	C	N	O	P	0	0	0
			266	126	54	74	12			

- Molecule 4 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
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is SULFATE ION (three-letter code: 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.

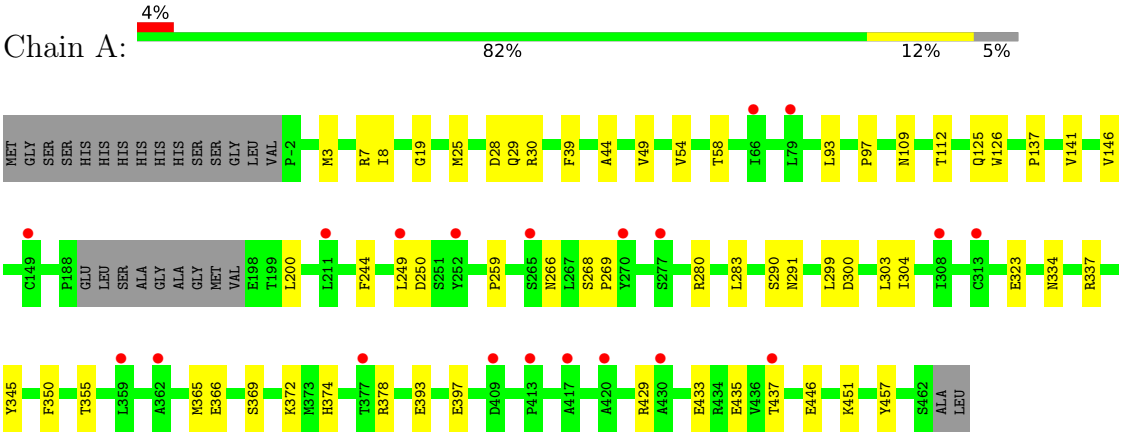
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	150	Total O 150 150	0	0
6	B	104	Total O 104 104	0	0
6	C	6	Total O 6 6	0	0
6	D	7	Total O 7 7	0	0
6	E	2	Total O 2 2	0	0
6	F	4	Total O 4 4	0	0

3 Residue-property plots (i)

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

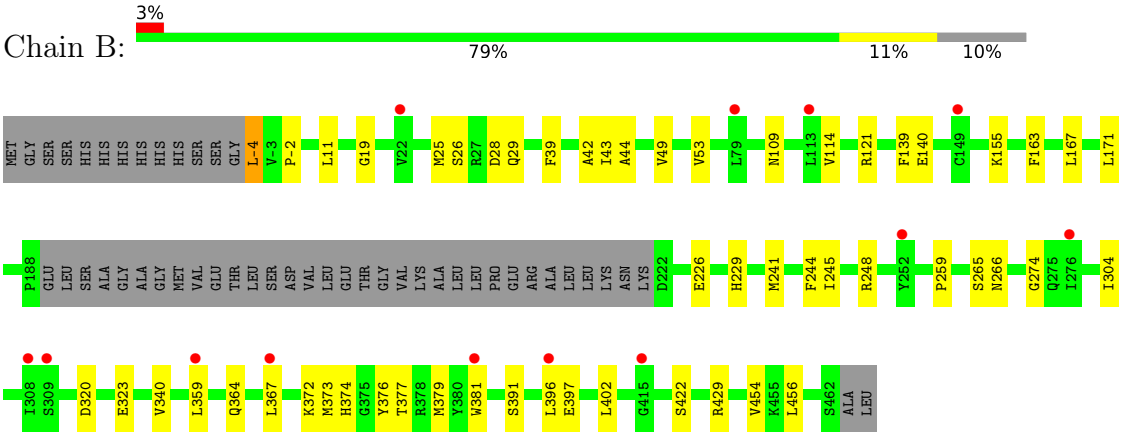
• Molecule 1: Deoxyribodipyrimidine photo-lyase

Chain A:



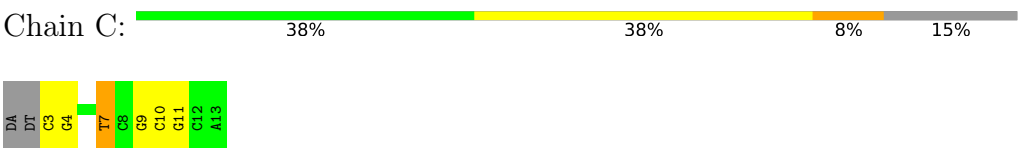
• Molecule 1: Deoxyribodipyrimidine photo-lyase

Chain B:



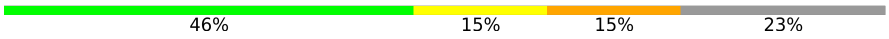
• Molecule 2: CPD photolesion containing DNA

Chain C:



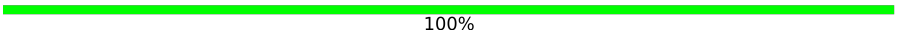
• Molecule 2: CPD photolesion containing DNA

Chain E:



• Molecule 3: complementary oligonucleotide to the CPD containing DNA

Chain D:



There are no outlier residues recorded for this chain.

• Molecule 3: complementary oligonucleotide to the CPD containing DNA

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.47Å 115.93Å 169.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.78 – 2.15 16.78 – 2.09	Depositor EDS
% Data completeness (in resolution range)	100.0 (16.78-2.15) 99.9 (16.78-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.34 (at 2.09Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.216 , 0.239 0.216 , 0.239	Depositor DCC
R_{free} test set	4187 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8502	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: TTD, FAD, SO4

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	0.24	0/3754	0.44	0/5092
1	B	0.24	0/3574	0.44	0/4851
2	C	0.52	0/227	0.71	0/345
2	E	0.68	0/206	0.88	1/313 (0.3%)
3	D	0.47	0/321	0.81	0/494
3	F	0.48	0/299	0.75	0/460
All	All	0.29	0/8381	0.50	1/11555 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	8	DC	OP1-P-OP2	-5.98	110.62	119.60

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	3638	0	3446	34	1
1	B	3459	0	3227	33	0
2	C	244	0	135	12	0
2	E	225	0	124	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	286	0	158	0	0
3	F	266	0	146	3	0
4	A	53	0	31	0	0
4	B	53	0	31	1	0
5	A	5	0	0	0	0
6	A	150	0	0	2	0
6	B	104	0	0	3	1
6	C	6	0	0	0	0
6	D	7	0	0	0	0
6	E	2	0	0	0	0
6	F	4	0	0	0	0
All	All	8502	0	7298	82	1

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 5.

All (82) 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:C:7:TTD:C6T	2:C:7:TTD:C6	1.81	1.59
2:C:7:TTD:C5	2:C:7:TTD:C5T	2.27	1.12
2:C:7:TTD:C6	2:C:7:TTD:C5T	2.51	0.86
2:C:7:TTD:C6T	2:C:7:TTD:C5	2.54	0.82
1:A:451:LYS:NZ	2:C:9:DG:OP2	2.17	0.77
1:B:265:SER:OG	4:B:501:FAD:O1A	2.02	0.76
2:C:7:TTD:C6	2:C:7:TTD:N1T	2.50	0.75
1:A:8:ILE:HG13	1:A:141:VAL:HG22	1.82	0.62
1:B:379:MET:HE1	2:E:7:TTD:H2R2	1.82	0.60
2:C:7:TTD:N1T	2:C:7:TTD:N1	2.49	0.60
1:A:290:SER:OG	1:A:291:ASN:N	2.36	0.59
1:B:323:GLU:OE2	6:B:601:HOH:O	2.16	0.59
1:A:378:ARG:NH1	6:A:615:HOH:O	2.37	0.58
2:C:10:DC:H2"	2:C:11:DG:C8	2.40	0.56
2:C:7:TTD:C6T	2:C:7:TTD:N1	2.64	0.56
2:E:7:TTD:O5R	2:E:7:TTD:H2'	2.05	0.56
1:B:167:LEU:HD23	1:B:304:ILE:HD13	1.88	0.56
1:B:-2:PRO:HG2	1:B:42:ALA:HB1	1.88	0.55
1:B:359:LEU:HD13	1:B:454:VAL:HG13	1.86	0.55
1:A:7:ARG:NH1	1:A:146:VAL:O	2.39	0.55
1:A:334:ASN:ND2	6:B:601:HOH:O	2.39	0.55
1:B:25:MET:SD	1:B:29:GLN:HA	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:GLU:OE1	1:A:457:TYR:OH	2.22	0.54
1:B:114:VAL:HG22	1:B:139:PHE:HB2	1.91	0.52
2:C:3:DC:H2"	2:C:4:DG:C8	2.44	0.52
1:A:97:PRO:HG2	1:A:126:TRP:CD2	2.46	0.51
1:A:54:VAL:HG23	1:A:93:LEU:HD23	1.92	0.51
1:A:112:THR:HG23	1:A:137:PRO:HG2	1.92	0.51
3:F:4:DG:H2"	3:F:5:DC:H5"	1.93	0.50
1:B:376:TYR:OH	2:E:8:DC:OP1	2.23	0.50
1:A:334:ASN:OD1	6:A:601:HOH:O	2.20	0.50
3:F:1:DT:H2"	3:F:2:DG:OP1	2.12	0.50
1:A:266:ASN:HA	1:A:372:LYS:HE3	1.94	0.49
1:B:25:MET:HE3	1:B:53:VAL:HG11	1.95	0.48
1:B:-4:LEU:N	6:B:615:HOH:O	2.46	0.48
1:B:379:MET:SD	2:E:7:TTD:H71	2.54	0.48
2:E:4:DG:H4'	2:E:5:DG:OP1	2.14	0.48
1:B:266:ASN:HA	1:B:372:LYS:HE3	1.97	0.47
1:A:25:MET:SD	1:A:29:GLN:HA	2.54	0.47
1:A:244:PHE:CZ	1:A:249:LEU:HD23	2.50	0.47
1:B:121:ARG:NH2	1:B:320:ASP:OD1	2.42	0.47
3:F:1:DT:H2'	3:F:2:DG:C8	2.50	0.47
1:B:364:GLN:HE22	1:B:402:LEU:HD13	1.80	0.46
1:B:11:LEU:HD11	1:B:140:GLU:HB2	1.98	0.46
1:B:44:ALA:HB1	1:B:49:VAL:O	2.17	0.45
1:B:171:LEU:HD23	1:B:171:LEU:HA	1.81	0.45
1:B:28:ASP:HA	1:B:274:GLY:HA3	1.98	0.45
1:B:39:PHE:CZ	1:B:43:ILE:HD11	2.52	0.45
2:E:7:TTD:H6	2:E:7:TTD:H2"	1.51	0.45
1:A:125:GLN:HE22	1:B:340:VAL:HA	1.81	0.45
1:B:259:PRO:HA	1:B:374:HIS:CD2	2.52	0.44
1:A:28:ASP:OD1	1:A:30:ARG:NH1	2.44	0.44
1:A:200:LEU:HD23	1:A:200:LEU:HA	1.85	0.44
2:C:7:TTD:H6	2:C:7:TTD:H2"	1.74	0.44
1:B:19:GLY:HA3	1:B:109:ASN:O	2.17	0.43
1:A:397:GLU:OE2	1:B:397[A]:GLU:HG2	2.18	0.43
1:B:396:LEU:HD23	1:B:396:LEU:HA	1.90	0.43
1:A:244:PHE:O	1:A:249:LEU:N	2.51	0.43
1:A:268:SER:OG	1:A:269:PRO:HD3	2.17	0.43
1:A:446:GLU:OE1	1:A:446:GLU:N	2.45	0.43
1:B:226:GLU:OE1	1:B:229:HIS:NE2	2.50	0.43
1:A:435:GLU:O	1:A:437:THR:N	2.48	0.43
1:B:244:PHE:HD1	1:B:248:ARG:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ARG:HA	1:A:283:LEU:HD12	2.01	0.43
1:A:58:THR:HG21	1:A:126:TRP:CH2	2.54	0.42
1:A:345:TYR:HB2	1:A:350:PHE:CZ	2.54	0.42
1:A:19:GLY:HA3	1:A:109:ASN:O	2.19	0.42
1:B:163:PHE:CE2	1:B:167:LEU:HD22	2.54	0.42
1:A:97:PRO:HG2	1:A:126:TRP:CE2	2.55	0.42
1:A:337:ARG:HH22	1:A:393:GLU:CD	2.22	0.42
1:A:3:MET:HB3	1:A:39:PHE:CZ	2.54	0.42
1:A:259:PRO:HA	1:A:374:HIS:CD2	2.55	0.42
2:C:7:TTD:N1T	2:C:7:TTD:C2	2.83	0.42
1:A:365:MET:O	1:A:369:SER:OG	2.30	0.42
1:B:241:MET:O	1:B:245:ILE:HG13	2.19	0.42
1:B:379:MET:HB3	1:B:379:MET:HE3	1.78	0.42
1:A:300:ASP:HA	1:A:304:ILE:HD12	2.01	0.41
1:B:364:GLN:NE2	1:B:381:TRP:HE1	2.18	0.41
1:B:367:LEU:HB2	1:B:373:MET:HE2	2.02	0.41
1:B:244:PHE:CD1	1:B:248:ARG:HB2	2.56	0.41
1:A:44:ALA:HB1	1:A:49:VAL:O	2.20	0.40
1:A:299:LEU:O	1:A:303:LEU:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:GLU:OE2	6:B:672:HOH:O[4_545]	2.11	0.09

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	457/482 (95%)	450 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	436/482 (90%)	433 (99%)	3 (1%)	0	100 100
All	All	893/964 (93%)	883 (99%)	10 (1%)	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	372/416 (89%)	367 (99%)	5 (1%)	69 74
1	B	347/416 (83%)	339 (98%)	8 (2%)	50 53
All	All	719/832 (86%)	706 (98%)	13 (2%)	60 63

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	ASP
1	A	323[A]	GLU
1	A	323[B]	GLU
1	A	355	THR
1	A	429	ARG
1	B	-4	LEU
1	B	26	SER
1	B	155	LYS
1	B	377	THR
1	B	391	SER
1	B	422	SER
1	B	429	ARG
1	B	456	LEU

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

Mol	Chain	Res	Type
1	B	364	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	C	7	2	42,45,46	2.09	8 (19%)	62,74,77	2.98	20 (32%)
2	TTD	E	7	2	42,45,46	0.98	3 (7%)	62,74,77	1.35	6 (9%)

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	C	7	2	-	9/22/109/110	0/5/6/6
2	TTD	E	7	2	-	12/22/109/110	0/5/6/6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	7	TTD	C6T-C6	8.49	1.81	1.56
2	C	7	TTD	C5T-C5	7.24	2.27	1.61
2	E	7	TTD	C1R-N1T	3.97	1.50	1.45
2	C	7	TTD	C2T-N1T	3.30	1.43	1.36
2	C	7	TTD	C5T-C6T	-2.78	1.51	1.55
2	C	7	TTD	C1R-N1T	2.77	1.49	1.45
2	E	7	TTD	C2-N3	-2.58	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	7	TTD	C4T-N3T	-2.45	1.33	1.37
2	C	7	TTD	C2T-N3T	-2.25	1.34	1.38
2	E	7	TTD	C1'-N1	2.14	1.48	1.45
2	C	7	TTD	C2-N3	-2.09	1.34	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	7	TTD	C5A-C5-C4	10.27	125.93	108.22
2	C	7	TTD	O4-C4-C5	-7.01	117.28	122.88
2	C	7	TTD	C5T-C5-C6	-6.61	80.15	88.38
2	C	7	TTD	N3T-C2T-N1T	5.99	122.91	116.69
2	C	7	TTD	C5-C6-C6T	5.85	98.88	89.28
2	C	7	TTD	C5-C4-N3	5.62	120.95	116.06
2	C	7	TTD	C5-C5T-C6T	-5.40	81.66	88.38
2	C	7	TTD	C5T-C6T-C6	5.27	97.92	89.28
2	C	7	TTD	C5M-C5T-C6T	5.01	129.55	114.16
2	C	7	TTD	C6-C6T-N1T	-4.78	99.09	118.20
2	E	7	TTD	C2R-C1R-N1T	4.65	121.86	115.59
2	C	7	TTD	O2T-C2T-N1T	-4.26	116.89	123.49
2	E	7	TTD	O3'-C3'-C2R	4.14	125.73	110.90
2	C	7	TTD	O4R-C1R-N1T	4.05	113.45	108.65
2	C	7	TTD	C5M-C5T-C5	-3.91	105.08	116.39
2	C	7	TTD	O4T-C4T-C5T	-3.60	120.00	122.88
2	C	7	TTD	C5A-C5-C5T	-3.46	106.38	116.39
2	C	7	TTD	N3-C2-N1	3.26	120.07	116.69
2	C	7	TTD	C2'-C1'-N1	-3.23	111.22	115.59
2	E	7	TTD	O4'-C1'-N1	-2.93	105.18	108.65
2	C	7	TTD	C6T-C6-N1	-2.81	106.96	118.20
2	C	7	TTD	C5T-C4T-N3T	2.67	118.39	116.06
2	E	7	TTD	O4P-PB-O3R	2.57	116.94	106.78
2	E	7	TTD	O4R-C1R-N1T	2.55	111.67	108.65
2	C	7	TTD	O2-C2-N1	-2.34	119.85	123.49
2	E	7	TTD	C2'-C1'-N1	-2.27	112.52	115.59

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	7	TTD	O4'-C4R-C5'-O5'
2	E	7	TTD	C5R-O5R-PB-O5P
2	C	7	TTD	O4'-C4R-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	C	7	TTD	C3R-C4R-C5'-O5'
2	E	7	TTD	C3R-C4R-C5'-O5'
2	C	7	TTD	C2'-C1'-N1-C6
2	E	7	TTD	C2'-C1'-N1-C6
2	E	7	TTD	C2R-C1R-N1T-C6T
2	C	7	TTD	C2R-C1R-N1T-C6T
2	E	7	TTD	C2'-C1'-N1-C2
2	C	7	TTD	C2'-C1'-N1-C2
2	C	7	TTD	O4R-C1R-N1T-C6T
2	C	7	TTD	O4'-C1'-N1-C6
2	E	7	TTD	C5R-O5R-PB-O4P
2	E	7	TTD	O4'-C1'-N1-C6
2	E	7	TTD	O4R-C1R-N1T-C6T
2	C	7	TTD	C2'-C3R-O3R-PB
2	E	7	TTD	C2'-C3R-O3R-PB
2	C	7	TTD	O4'-C1'-N1-C2
2	E	7	TTD	O4'-C1'-N1-C2
2	E	7	TTD	C5R-O5R-PB-O3R

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	7	TTD	9	0
2	E	7	TTD	4	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	502	-	4,4,4	0.14	0	6,6,6	0.05	0
4	FAD	B	501	-	53,58,58	0.46	0	68,89,89	0.54	2 (2%)
4	FAD	A	501	-	53,58,58	0.61	0	68,89,89	0.78	2 (2%)

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	501	-	-	4/30/50/50	0/6/6/6
4	FAD	A	501	-	-	9/30/50/50	0/6/6/6

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	FAD	P-O3P-PA	-2.86	123.00	132.83
4	B	501	FAD	P-O3P-PA	-2.73	123.46	132.83
4	B	501	FAD	C5A-C6A-N6A	2.29	123.83	120.35
4	A	501	FAD	C5A-C6A-N6A	2.27	123.80	120.35

There are no chirality outliers.

All (13) torsion outliers are listed below:

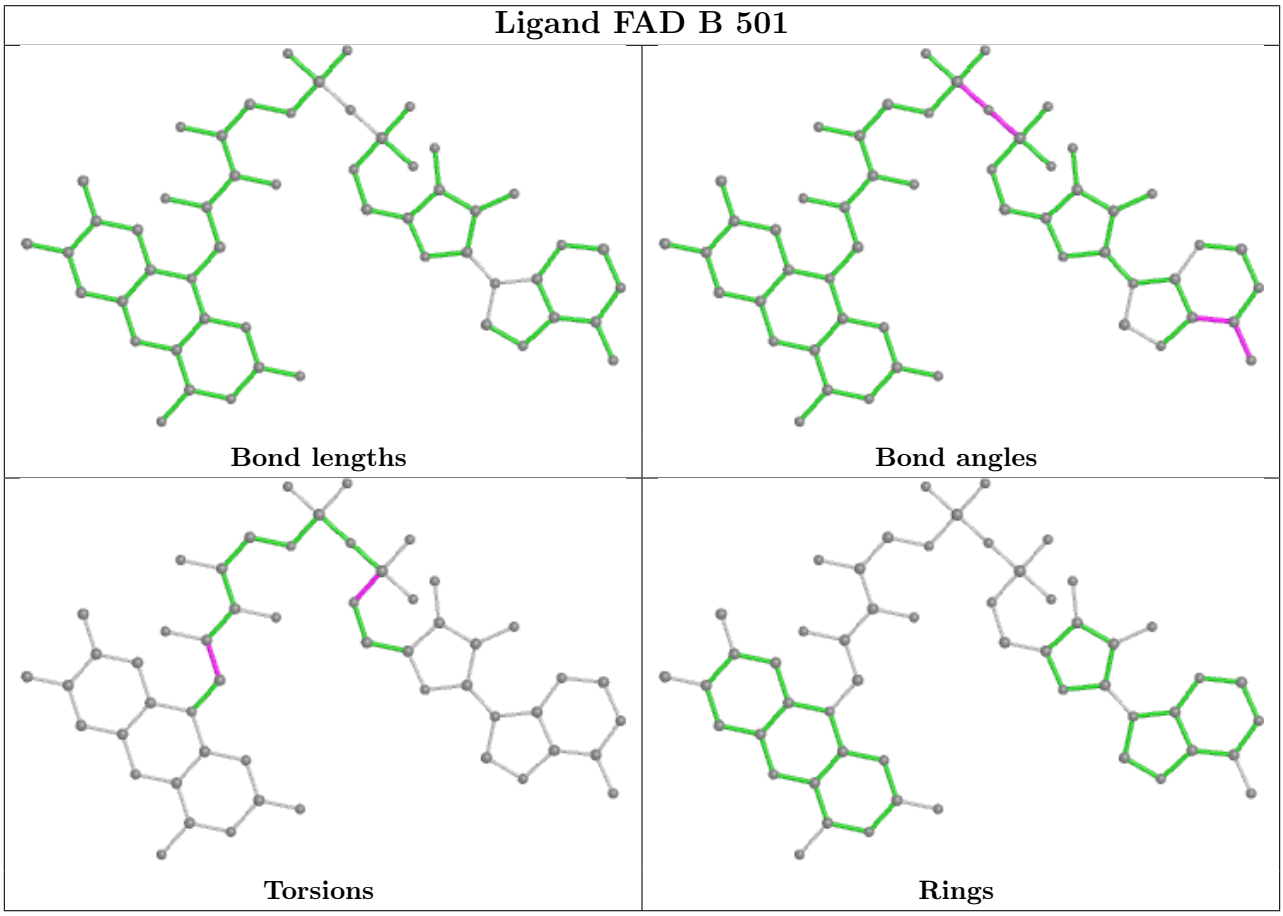
Mol	Chain	Res	Type	Atoms
4	A	501	FAD	C5B-O5B-PA-O2A
4	A	501	FAD	C5B-O5B-PA-O3P
4	A	501	FAD	C5'-O5'-P-O1P
4	B	501	FAD	C5B-O5B-PA-O1A
4	B	501	FAD	C5B-O5B-PA-O2A
4	B	501	FAD	C5B-O5B-PA-O3P
4	B	501	FAD	N10-C1'-C2'-C3'
4	A	501	FAD	O4B-C4B-C5B-O5B
4	A	501	FAD	C5'-O5'-P-O3P
4	A	501	FAD	C3B-C4B-C5B-O5B
4	A	501	FAD	C4'-C5'-O5'-P
4	A	501	FAD	C5'-O5'-P-O2P
4	A	501	FAD	N10-C1'-C2'-C3'

There are no ring outliers.

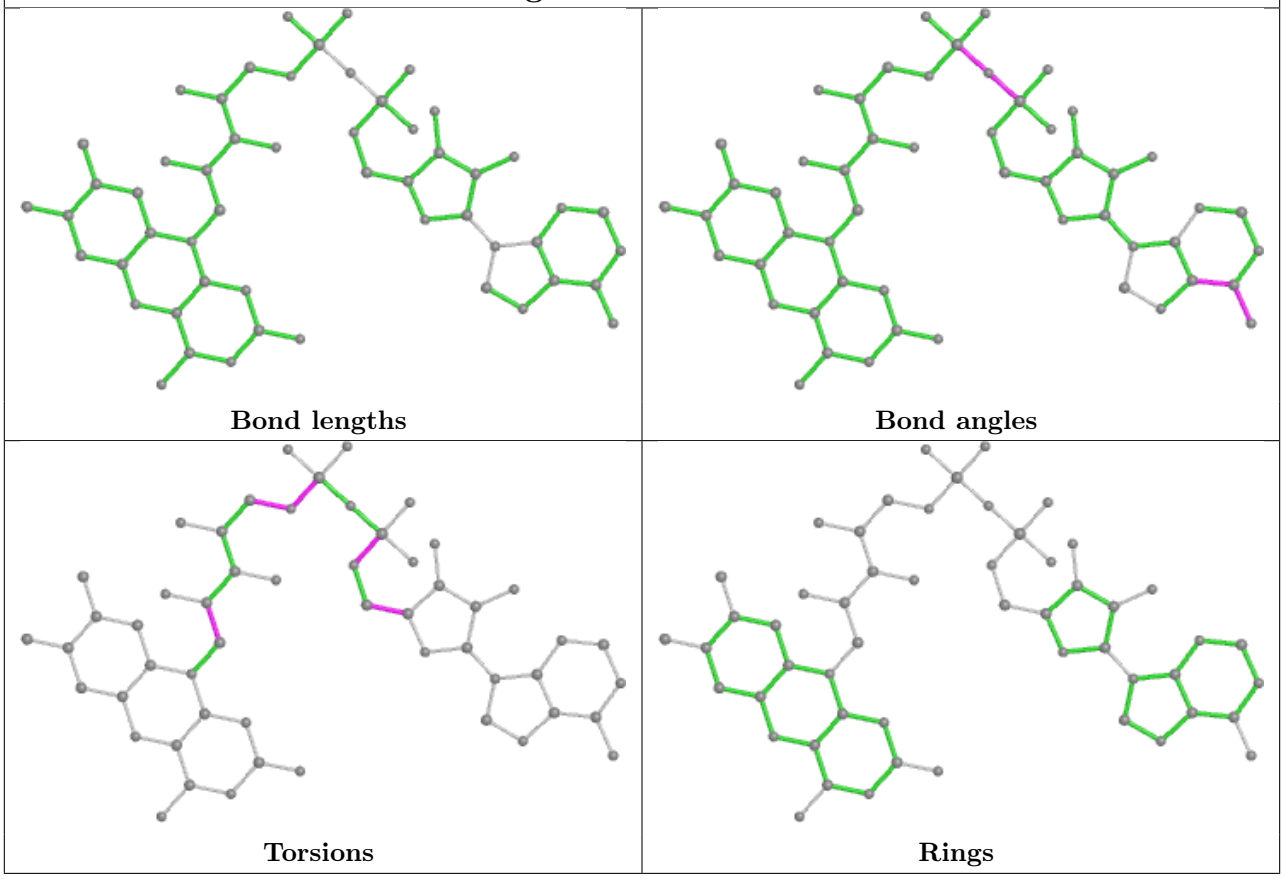
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	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 501



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, 95^{th} 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	456/482 (94%)	0.65	20 (4%) 34 43	14, 23, 48, 71	0
1	B	434/482 (90%)	0.50	13 (2%) 50 59	15, 29, 48, 62	0
2	C	10/13 (76%)	-0.19	0 100 100	22, 57, 72, 73	0
2	E	9/13 (69%)	0.07	0 100 100	44, 61, 72, 81	0
3	D	14/14 (100%)	-0.13	0 100 100	34, 58, 70, 77	0
3	F	13/14 (92%)	-0.12	0 100 100	46, 67, 75, 77	0
All	All	936/1018 (91%)	0.54	33 (3%) 44 52	14, 27, 56, 81	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	LEU	3.1
1	B	381	TRP	3.0
1	A	308	ILE	2.9
1	A	265	SER	2.9
1	B	308	ILE	2.8
1	A	149	CYS	2.7
1	A	437	THR	2.7
1	A	377	THR	2.6
1	B	252	TYR	2.5
1	B	79	LEU	2.4
1	A	313	CYS	2.3
1	B	22	VAL	2.3
1	B	359	LEU	2.3
1	B	309	SER	2.3
1	B	415	GLY	2.3
1	A	359	LEU	2.2
1	A	413	PRO	2.2
1	B	149	CYS	2.2
1	A	211	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	417	ALA	2.2
1	B	276	ILE	2.1
1	A	252	TYR	2.1
1	A	270	TYR	2.1
1	B	113	LEU	2.1
1	B	396	LEU	2.1
1	A	430	ALA	2.1
1	A	249	LEU	2.1
1	A	277	SER	2.0
1	A	409	ASP	2.0
1	A	420	ALA	2.0
1	A	66	ILE	2.0
1	A	362	ALA	2.0
1	B	367	LEU	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, 95^{th} 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	0.86	0.16	16,20,39,41	0
2	TTD	E	7	40/41	0.89	0.13	27,33,45,49	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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
4	FAD	A	501	53/53	0.87	0.17	14,15,18,20	0
4	FAD	B	501	53/53	0.88	0.17	16,21,24,27	0

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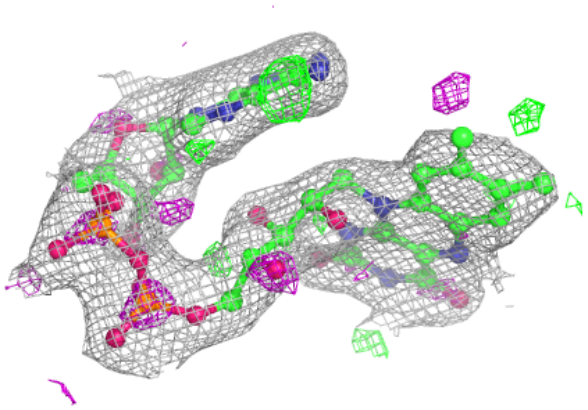
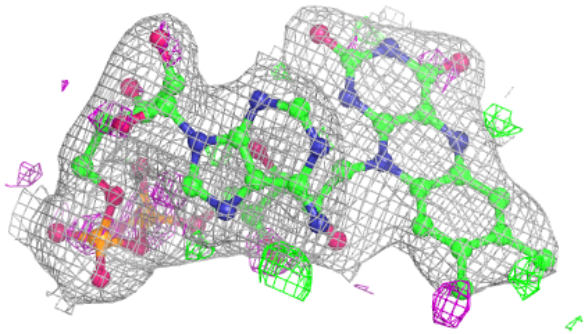
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	A	502	5/5	0.96	0.12	18,23,27,28	0

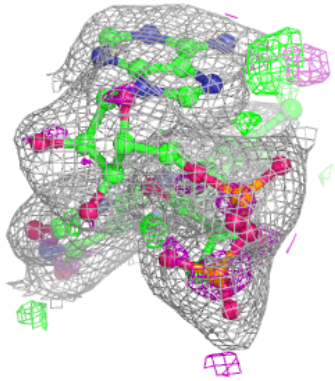
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 501:

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

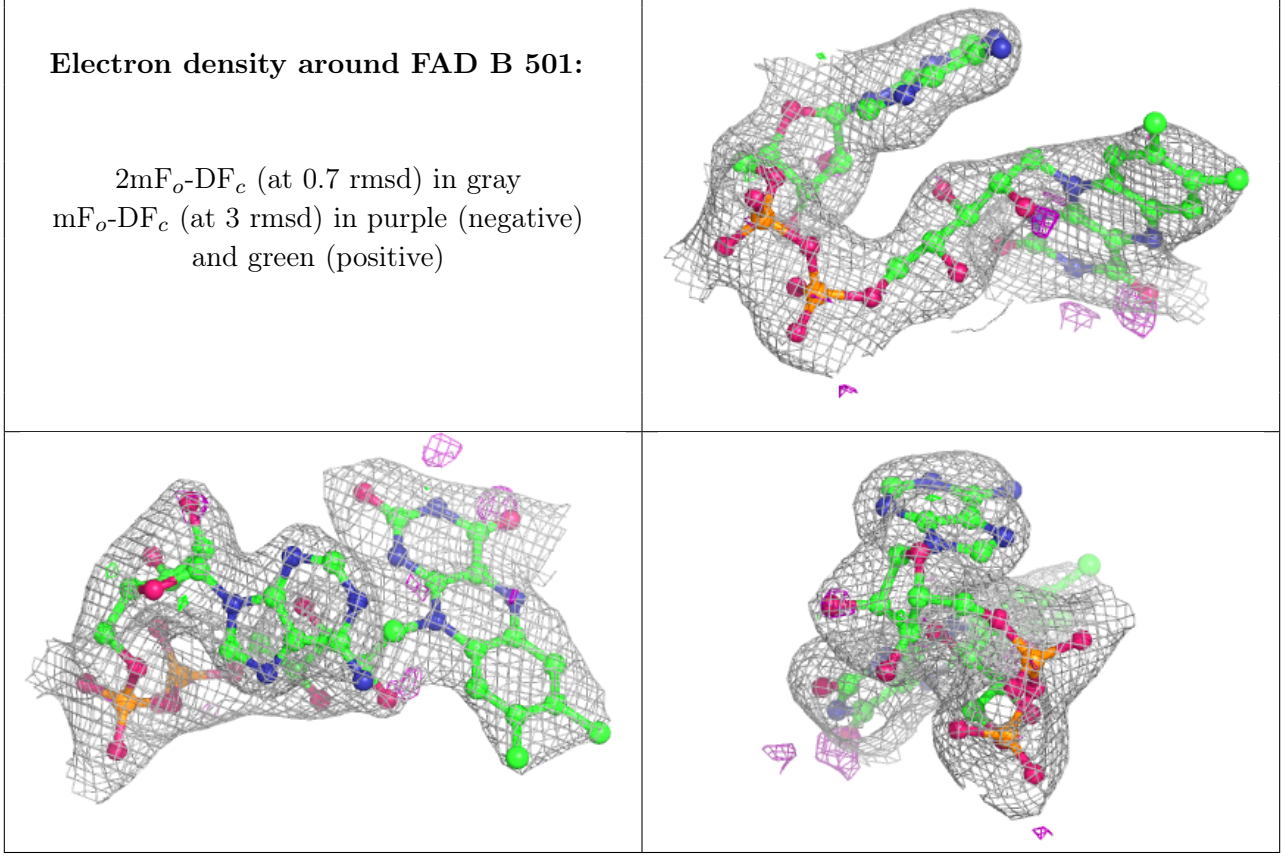






Electron density around FAD B 501:

$2mF_o$-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.