Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 03:52 AM JST

PDB ID	:	7YD7
Title	:	TR-SFX MmCPDII-DNA complex: 1 ns snapshot. Includes 1 ns, 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	:	2.25 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 (i) 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 (i)) were used in the production of this report:

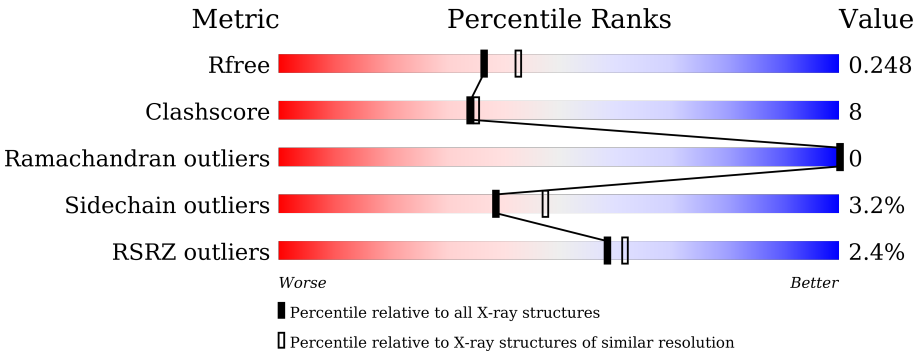
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13

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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	3% 76% 18% • 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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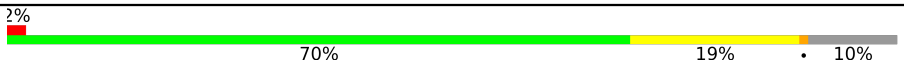
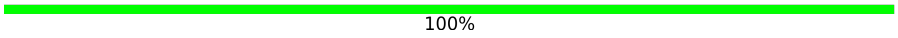
Mol	Chain	Length	Quality of chain
1	B	482	
2	C	13	
2	E	13	
3	D	14	
3	F	14	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8704 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	14	0
			3691	2386	605	686	14			
1	B	434	Total	C	N	O	S	0	9	0
			3486	2248	583	639	16			

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

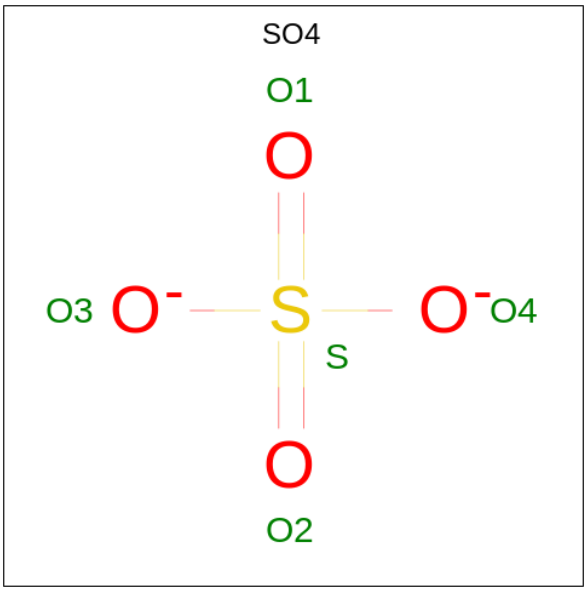
- Molecule 2 is a DNA chain called CPD photolesion containing DNA.

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.

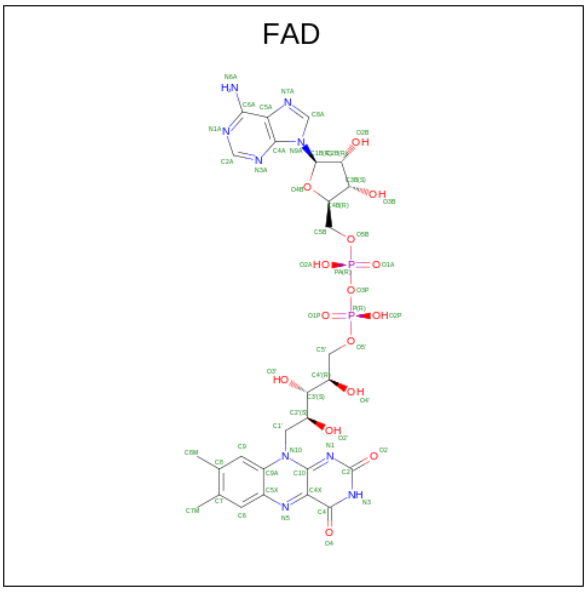
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	14	Total	C	N	O	P	0	0	0
			286	136	56	81	13			
3	F	13	Total	C	N	O	P	0	0	0
			266	126	54	74	12			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 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
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is water.

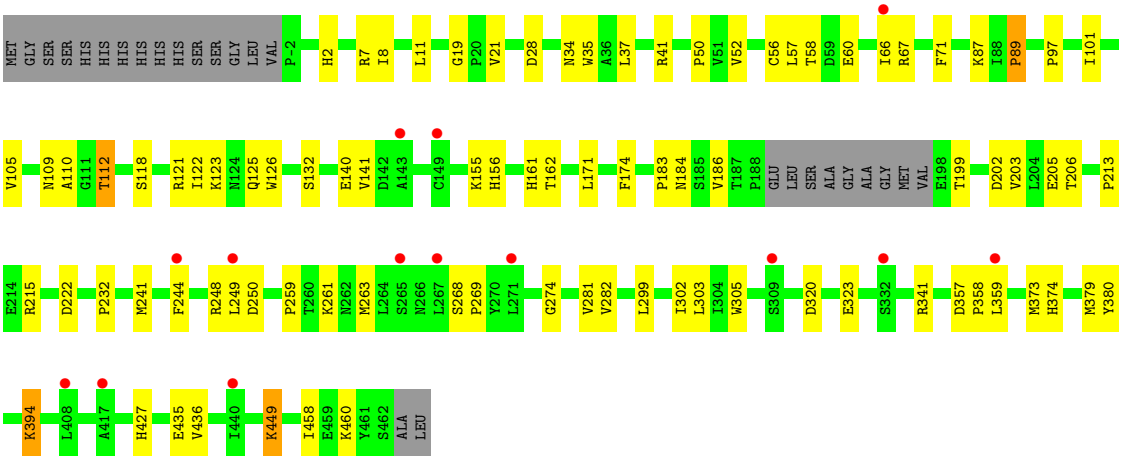
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	197	Total O 197 197	0	0
6	B	156	Total O 156 156	0	0
6	C	13	Total O 13 13	0	0
6	D	9	Total O 9 9	0	0
6	E	4	Total O 4 4	0	0
6	F	16	Total O 16 16	0	0

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.

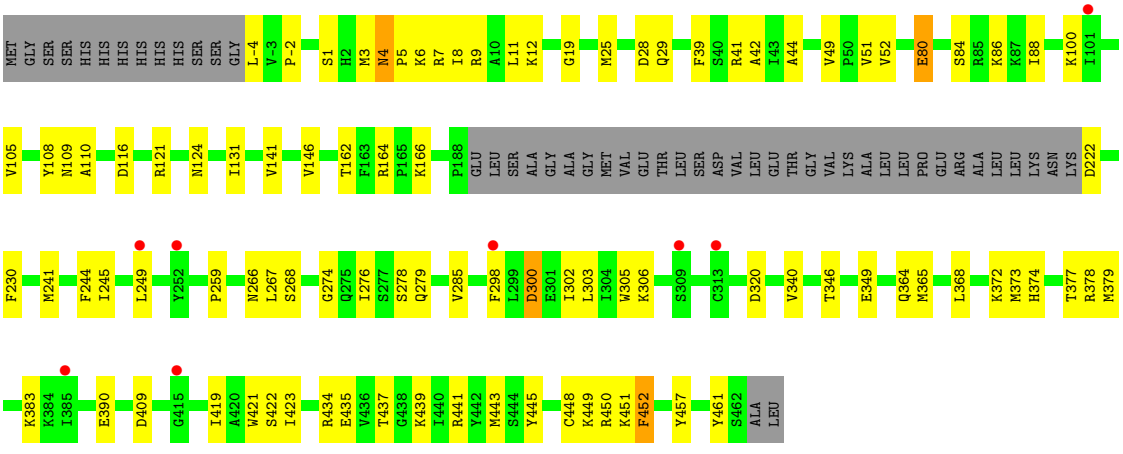
• Molecule 1: Deoxyribodipyrimidine photo-lyase

Chain A:



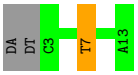
• Molecule 1: Deoxyribodipyrimidine photo-lyase

Chain B:



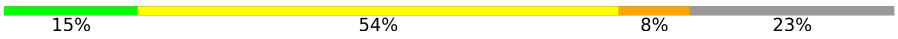
• Molecule 2: CPD photolesion containing DNA

Chain C:



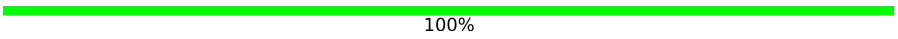
• Molecule 2: CPD photolesion containing DNA

Chain E:



• Molecule 3: complementary oligonucleotide to the CPD containing DNA

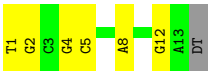
Chain D:



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)	16.76 – 2.25 16.76 – 2.08	Depositor EDS
% Data completeness (in resolution range)	100.0 (16.76-2.25) 99.9 (16.76-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.39 (at 2.09Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.231 , 0.248 0.232 , 0.248	Depositor DCC
R_{free} test set	4248 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	17.9	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8704	wwPDB-VP
Average B, all atoms (Å^2)	23.0	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: SO4, TTD, 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	0.43	4/3834 (0.1%)	0.51	2/5201 (0.0%)
1	B	0.27	1/3614 (0.0%)	0.45	0/4904
2	C	0.45	0/227	0.68	0/345
2	E	0.95	1/206 (0.5%)	0.86	1/313 (0.3%)
3	D	0.47	0/321	0.79	0/494
3	F	0.47	0/299	0.74	0/460
All	All	0.39	6/8501 (0.1%)	0.53	3/11717 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	PRO	N-CD	17.46	1.72	1.47
1	B	80	GLU	CD-OE2	-6.61	1.18	1.25
2	E	6	DC	C3'-O3'	6.61	1.52	1.44
1	A	213	PRO	N-CD	6.34	1.56	1.47
1	A	435[A]	GLU	C-O	5.11	1.33	1.23
1	A	435[B]	GLU	C-O	5.11	1.33	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	213	PRO	CA-N-CD	-10.65	96.58	111.50
1	A	89	PRO	CA-N-CD	-7.85	100.51	111.50
2	E	8	DC	OP1-P-OP2	-6.64	109.64	119.60

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	3691	0	3547	57	0
1	B	3486	0	3309	66	0
2	C	244	0	135	7	0
2	E	225	0	124	8	0
3	D	286	0	158	0	0
3	F	266	0	146	5	0
4	A	5	0	0	0	0
5	A	53	0	31	0	0
5	B	53	0	31	3	0
6	A	197	0	0	4	0
6	B	156	0	0	5	0
6	C	13	0	0	0	0
6	D	9	0	0	0	0
6	E	4	0	0	0	0
6	F	16	0	0	0	0
All	All	8704	0	7481	132	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 (132) 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:89:PRO:N	1:A:89:PRO:CD	1.72	1.34
2:C:7:TTD:C6T	2:C:7:TTD:C6	2.30	1.09
1:B:146:VAL:HG13	1:B:279:GLN:HG3	1.49	0.94
1:A:101:ILE:O	1:A:105:VAL:HG23	1.83	0.77
1:B:86:LYS:HB2	1:B:88:ILE:HD12	1.65	0.77
1:B:390:GLU:OE2	6:B:601:HOH:O	2.02	0.76
1:B:451:LYS:NZ	2:E:9:DG:OP2	2.19	0.76
1:A:52:VAL:HA	1:A:89:PRO:HD2	1.70	0.72
1:A:105:VAL:HG13	1:A:110:ALA:HB3	1.72	0.72
1:A:248:ARG:HG2	1:A:263:MET:HA	1.73	0.71
1:A:8:ILE:HG13	1:A:141:VAL:HG22	1.71	0.71
1:B:146:VAL:HG13	1:B:279:GLN:CG	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:7:TTD:C5	2:C:7:TTD:C5T	2.74	0.65
1:A:58:THR:HG21	1:A:126:TRP:CH2	2.32	0.65
1:B:278:SER:HB2	1:B:302:ILE:HD11	1.80	0.62
1:A:11[B]:LEU:HD11	1:A:140:GLU:HB2	1.81	0.62
1:B:249:LEU:HD21	1:B:285:VAL:HG23	1.80	0.62
1:A:21:VAL:HG23	1:A:112:THR:HB	1.84	0.60
1:A:305:TRP:CE2	2:C:7:TTD:H5A2	2.37	0.60
2:C:7:TTD:C6T	2:C:7:TTD:C5	2.80	0.59
1:A:359:LEU:HD12	1:A:359:LEU:O	2.03	0.59
3:F:1:DT:H2"	3:F:2:DG:OP1	2.01	0.59
1:B:4:ASN:ND2	1:B:6:LYS:H	2.01	0.58
1:B:434:ARG:NH1	6:B:610:HOH:O	2.36	0.58
1:A:202:ASP:HA	1:A:205:GLU:OE1	2.03	0.57
1:B:268:SER:OG	1:B:409:ASP:OD2	2.15	0.56
1:B:298:PHE:O	1:B:302:ILE:HG22	2.05	0.56
1:B:4:ASN:C	1:B:4:ASN:HD22	2.08	0.55
3:F:4:DG:H2"	3:F:5:DC:H5"	1.88	0.55
1:A:305:TRP:HH2	1:A:427:HIS:HB3	1.72	0.54
1:B:379:MET:SD	2:E:7:TTD:H71	2.48	0.53
1:A:60:GLU:OE2	1:A:122:ILE:HD13	2.08	0.53
1:B:4:ASN:HD22	1:B:6:LYS:H	1.56	0.53
1:A:379:MET:HE1	2:C:7:TTD:C2T	2.38	0.53
1:B:378:ARG:NH1	6:B:604:HOH:O	2.41	0.53
1:B:441:ARG:NH2	2:E:7:TTD:O4P	2.39	0.53
1:B:439:LYS:HE2	3:F:8:DA:H5"	1.91	0.52
1:A:71:PHE:HA	1:A:232:PRO:HG3	1.92	0.52
1:B:28:ASP:HA	1:B:274:GLY:HA3	1.92	0.52
1:A:259:PRO:HA	1:A:374:HIS:CD2	2.45	0.51
1:B:373:MET:O	1:B:378:ARG:NH1	2.42	0.51
1:B:105:VAL:HG13	1:B:110:ALA:HB3	1.92	0.51
1:B:4:ASN:HD22	1:B:5:PRO:N	2.07	0.51
1:A:97:PRO:HD2	1:A:126:TRP:CE2	2.46	0.51
1:B:25:MET:SD	1:B:29:GLN:HA	2.51	0.51
1:A:161:HIS:CE1	1:A:162:THR:HG23	2.47	0.50
1:A:67:ARG:NH1	6:A:629:HOH:O	2.44	0.50
1:A:121[A]:ARG:NH1	1:B:390:GLU:OE1	2.44	0.50
1:B:41:ARG:HD2	1:B:51:VAL:HG21	1.92	0.50
1:B:8:ILE:HG12	1:B:141:VAL:HG22	1.94	0.50
1:B:302:ILE:HG23	1:B:303:LEU:HD12	1.94	0.50
1:B:346:THR:HG23	1:B:349:GLU:OE1	2.12	0.50
1:A:305:TRP:CZ2	2:C:7:TTD:H5A2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:MET:O	6:A:602:HOH:O	2.19	0.50
1:B:259:PRO:HA	1:B:374:HIS:CD2	2.48	0.49
1:B:11:LEU:HD12	1:B:131:ILE:HD11	1.95	0.49
1:B:39:PHE:HB3	6:B:606:HOH:O	2.12	0.49
1:A:52:VAL:HA	1:A:89:PRO:CD	2.42	0.49
1:B:100:LYS:HA	1:B:100:LYS:HD2	1.61	0.48
2:E:4:DG:H4'	2:E:5:DG:OP1	2.12	0.48
1:A:28:ASP:HA	1:A:274:GLY:HA3	1.96	0.48
2:E:10:DC:H2"	2:E:11:DG:C8	2.48	0.48
1:B:245:ILE:HG23	1:B:249:LEU:HD23	1.96	0.48
1:B:-2:PRO:HG2	1:B:42:ALA:HB1	1.96	0.48
1:B:162:THR:HG22	3:F:12:DG:H5'	1.95	0.48
1:B:121:ARG:NH2	1:B:320:ASP:OD1	2.42	0.48
2:C:7:TTD:H6T	2:C:7:TTD:H2R1	1.55	0.47
1:A:41:ARG:NH2	1:A:183:PRO:O	2.48	0.47
1:A:248:ARG:HG3	1:A:263:MET:SD	2.55	0.47
1:A:66:ILE:HD12	1:A:215:ARG:HG3	1.96	0.47
1:A:123:LYS:NZ	6:A:604:HOH:O	2.26	0.47
1:B:448:CYS:O	1:B:452:PHE:CE2	2.68	0.47
1:B:244:PHE:CZ	1:B:249:LEU:HD13	2.49	0.47
1:B:245:ILE:HA	1:B:249:LEU:HB2	1.95	0.46
1:B:372[B]:LYS:HB3	1:B:372[B]:LYS:HE3	1.49	0.46
1:B:44:ALA:HB1	1:B:49:VAL:O	2.16	0.46
1:B:12:LYS:HD2	1:B:131:ILE:HG23	1.97	0.46
1:B:230:PHE:HE1	1:B:266:ASN:HB3	1.80	0.46
1:A:121[A]:ARG:NH2	1:A:320:ASP:OD1	2.43	0.46
5:B:501:FAD:H8A	5:B:501:FAD:O5B	2.15	0.46
1:B:364:GLN:HE21	1:B:368:LEU:HD21	1.81	0.46
1:A:358:PRO:HB2	1:A:458[A]:ILE:HD13	1.97	0.45
1:B:452:PHE:N	1:B:452:PHE:CD2	2.84	0.45
1:B:383:LYS:HE2	1:B:422:SER:HA	1.99	0.45
1:A:199:THR:HG22	1:A:202:ASP:H	1.80	0.45
1:A:105:VAL:CG1	1:A:110:ALA:HB3	2.45	0.45
1:B:306:LYS:HB2	5:B:501:FAD:H1B	1.98	0.45
1:A:394:LYS:HZ2	1:A:394:LYS:HG3	1.71	0.44
1:A:56:CYS:HB3	1:A:97:PRO:HG3	1.98	0.44
1:A:244:PHE:O	1:A:249:LEU:N	2.50	0.44
1:A:394:LYS:HA	1:A:394:LYS:HZ3	1.82	0.44
2:E:7:TTD:H2"	2:E:7:TTD:H6	1.72	0.44
1:A:155:LYS:HG2	1:A:156:HIS:N	2.32	0.44
1:A:87:LYS:HB2	1:A:184:ASN:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LYS:NZ	6:A:645:HOH:O	2.51	0.44
1:B:365:MET:HB3	1:B:461:TYR:HB3	2.00	0.43
1:A:118:SER:HB3	1:A:123:LYS:HZ3	1.84	0.43
1:A:241:MET:SD	1:A:281:VAL:HG22	2.59	0.43
1:A:268:SER:OG	1:A:269:PRO:HD3	2.19	0.43
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.84	0.43
1:A:357:ASP:OD2	1:A:380:TYR:OH	2.24	0.43
1:B:305:TRP:HZ2	2:E:7:TTD:H5"	1.84	0.43
1:A:449[B]:LYS:HB3	1:A:449[B]:LYS:HE2	1.62	0.43
1:B:124[B]:ASN:ND2	6:B:624:HOH:O	2.51	0.43
1:B:379:MET:HG2	1:B:421:TRP:HZ3	1.84	0.43
1:A:282:VAL:HG23	1:A:302[B]:ILE:HD11	2.00	0.42
1:B:419:ILE:HG23	1:B:423:ILE:HD12	2.00	0.42
1:B:445:TYR:O	1:B:449:LYS:HD3	2.19	0.42
1:A:299:LEU:O	1:A:303:LEU:HB2	2.18	0.42
1:B:378:ARG:NH1	5:B:501:FAD:O4'	2.52	0.42
1:B:443[B]:MET:HE3	1:B:443[B]:MET:H	1.85	0.42
1:B:19:GLY:HA3	1:B:109:ASN:O	2.19	0.42
1:A:19:GLY:HA3	1:A:109:ASN:O	2.20	0.42
1:B:435:GLU:O	1:B:437:THR:N	2.49	0.42
1:B:241:MET:O	1:B:245:ILE:HD12	2.19	0.42
1:A:57:LEU:HD13	1:A:203:VAL:HG21	2.01	0.42
1:B:52:VAL:HG11	1:B:108[B]:TYR:HE2	1.85	0.42
2:E:7:TTD:H6T	2:E:7:TTD:H2R1	1.46	0.42
1:A:125:GLN:HE22	1:B:340:VAL:HA	1.83	0.41
1:A:101:ILE:N	1:A:101:ILE:HD13	2.35	0.41
1:B:450:ARG:HD3	3:F:1:DT:H71	2.01	0.41
1:B:244:PHE:CE2	1:B:249:LEU:HD13	2.56	0.41
1:A:341:ARG:CZ	1:A:436:VAL:HG13	2.50	0.41
1:B:164:ARG:NH2	1:B:300:ASP:OD2	2.52	0.41
1:B:267:LEU:HD12	1:B:276:ILE:HG21	2.01	0.41
1:B:-4:LEU:HD23	1:B:-4:LEU:HA	1.88	0.41
1:A:34:ASN:HB3	1:A:37:LEU:HB3	2.03	0.40
1:B:266:ASN:HA	1:B:372[A]:LYS:HE3	2.02	0.40
1:A:35:TRP:HA	1:A:35:TRP:CE3	2.56	0.40
1:A:7:ARG:NH2	1:A:174:PHE:O	2.40	0.40
1:A:50:PRO:HB3	1:A:186:VAL:O	2.22	0.40
1:B:377:THR:HG21	1:B:457:TYR:CZ	2.56	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	466/482 (97%)	454 (97%)	12 (3%)	0	100	100
1	B	439/482 (91%)	436 (99%)	3 (1%)	0	100	100
All	All	905/964 (94%)	890 (98%)	15 (2%)	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	385/416 (92%)	370 (96%)	15 (4%)	32	38
1	B	358/416 (86%)	345 (96%)	13 (4%)	35	42
All	All	743/832 (89%)	715 (96%)	28 (4%)	39	39

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	112	THR
1	A	132[A]	SER
1	A	132[B]	SER
1	A	206	THR
1	A	222[A]	ASP
1	A	222[B]	ASP
1	A	250	ASP

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Mol	Chain	Res	Type
1	A	261	LYS
1	A	323[A]	GLU
1	A	323[B]	GLU
1	A	394	LYS
1	A	449[A]	LYS
1	A	449[B]	LYS
1	A	460	LYS
1	B	1	SER
1	B	3[A]	MET
1	B	3[B]	MET
1	B	4	ASN
1	B	7	ARG
1	B	9	ARG
1	B	80	GLU
1	B	84	SER
1	B	116	ASP
1	B	166	LYS
1	B	222	ASP
1	B	300	ASP
1	B	452	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	403	ASN
1	B	4	ASN

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	4.58	8 (19%)	62,74,77	3.04	18 (29%)
2	TTD	E	7	2	42,45,46	1.05	3 (7%)	62,74,77	1.22	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	-	10/22/109/110	0/5/6/6
2	TTD	E	7	2	-	8/22/109/110	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	25.80	2.30	1.56
2	C	7	TTD	C5T-C5	12.39	2.74	1.61
2	E	7	TTD	C1R-N1T	3.94	1.50	1.45
2	C	7	TTD	C2T-N1T	3.20	1.42	1.36
2	C	7	TTD	C5T-C6T	-2.94	1.51	1.55
2	E	7	TTD	C1'-N1	2.72	1.49	1.45
2	C	7	TTD	C1'-N1	-2.65	1.42	1.45
2	C	7	TTD	C4T-N3T	-2.60	1.33	1.37
2	C	7	TTD	C2-N3	-2.18	1.34	1.38
2	C	7	TTD	C2T-N3T	-2.12	1.34	1.38
2	E	7	TTD	O3R-C3R	-2.01	1.42	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	7	TTD	C5A-C5-C4	10.45	126.24	108.22
2	C	7	TTD	C5-C5T-C6T	-9.83	76.14	88.38
2	C	7	TTD	C5T-C6T-C6	8.91	103.90	89.28
2	C	7	TTD	O4-C4-C5	-6.81	117.44	122.88
2	C	7	TTD	N3T-C2T-N1T	6.01	122.93	116.69
2	C	7	TTD	C6-C6T-N1T	-5.60	95.80	118.20
2	C	7	TTD	C5-C4-N3	5.49	120.84	116.06
2	C	7	TTD	C5A-C5-C6	-4.83	99.32	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	7	TTD	O2T-C2T-N1T	-4.24	116.90	123.49
2	C	7	TTD	O4T-C4T-C5T	-3.75	119.88	122.88
2	C	7	TTD	C2'-C1'-N1	-3.60	110.73	115.59
2	C	7	TTD	N3-C2-N1	3.12	119.93	116.69
2	C	7	TTD	C5M-C5T-C4T	2.87	113.16	108.22
2	C	7	TTD	C5T-C4T-N3T	2.80	118.50	116.06
2	E	7	TTD	O4R-C1R-N1T	2.71	111.87	108.65
2	E	7	TTD	N3T-C2T-N1T	2.61	119.40	116.69
2	E	7	TTD	C2'-C1'-N1	-2.48	112.24	115.59
2	C	7	TTD	O2-C2-N1	-2.40	119.77	123.49
2	C	7	TTD	O4R-C1R-N1T	2.29	111.37	108.65
2	E	7	TTD	O3'-C3'-C2R	2.26	119.00	110.90
2	C	7	TTD	O4'-C1'-N1	2.25	111.31	108.65
2	E	7	TTD	O2-C2-N1	-2.07	120.27	123.49
2	E	7	TTD	O4-C4-C5	-2.02	121.26	122.88
2	C	7	TTD	C5T-C5-C6	-2.00	85.88	88.38

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	7	TTD	O4'-C4R-C5'-O5'
2	C	7	TTD	C3R-C4R-C5'-O5'
2	E	7	TTD	O4'-C4R-C5'-O5'
2	E	7	TTD	C3R-C4R-C5'-O5'
2	E	7	TTD	O4'-C1'-N1-C2
2	E	7	TTD	C2'-C1'-N1-C6
2	C	7	TTD	C2R-C1R-N1T-C6T
2	C	7	TTD	O4R-C4'-C5R-O5R
2	E	7	TTD	O4'-C1'-N1-C6
2	C	7	TTD	C3'-C4'-C5R-O5R
2	C	7	TTD	C2'-C1'-N1-C6
2	C	7	TTD	O4R-C1R-N1T-C6T
2	E	7	TTD	C2'-C1'-N1-C2
2	C	7	TTD	O4'-C1'-N1-C6
2	C	7	TTD	C2'-C1'-N1-C2
2	E	7	TTD	O4R-C1R-N1T-C6T
2	C	7	TTD	O4'-C1'-N1-C2
2	E	7	TTD	C2R-C1R-N1T-C6T

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	7	TTD	7	0
2	E	7	TTD	5	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	FAD	B	501	-	53,58,58	0.45	0	68,89,89	0.54	2 (2%)
5	FAD	A	502	-	53,58,58	0.64	0	68,89,89	0.86	4 (5%)
4	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.06	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
5	FAD	B	501	-	-	6/30/50/50	0/6/6/6
5	FAD	A	502	-	-	5/30/50/50	0/6/6/6

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	502	FAD	P-O3P-PA	-2.78	123.29	132.83
5	B	501	FAD	P-O3P-PA	-2.76	123.34	132.83
5	A	502	FAD	C4-C4X-N5	2.50	121.78	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	502	FAD	C5A-C6A-N6A	2.31	123.87	120.35
5	B	501	FAD	C5A-C6A-N6A	2.26	123.78	120.35
5	A	502	FAD	C4-N3-C2	-2.11	121.73	125.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	FAD	C5B-O5B-PA-O1A
5	A	502	FAD	N10-C1'-C2'-C3'
5	B	501	FAD	C5B-O5B-PA-O2A
5	B	501	FAD	C5B-O5B-PA-O3P
5	B	501	FAD	N10-C1'-C2'-O2'
5	B	501	FAD	N10-C1'-C2'-C3'
5	B	501	FAD	C4'-C5'-O5'-P
5	A	502	FAD	C5B-O5B-PA-O2A
5	B	501	FAD	C2'-C3'-C4'-O4'
5	A	502	FAD	C4'-C5'-O5'-P
5	A	502	FAD	C5B-O5B-PA-O3P

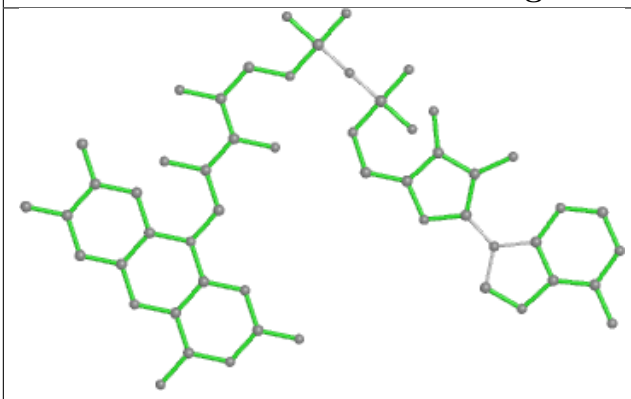
There are no ring outliers.

1 monomer is involved in 3 short contacts:

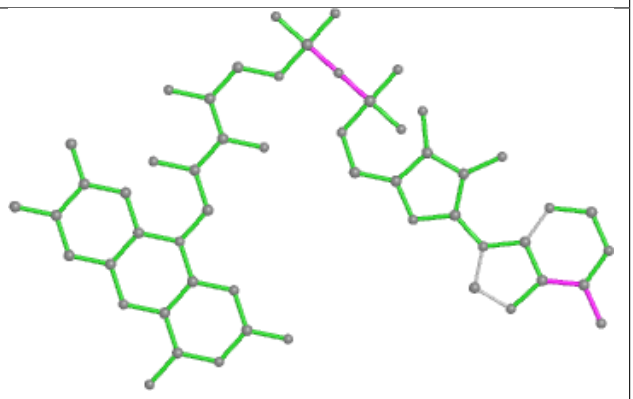
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	FAD	3	0

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.

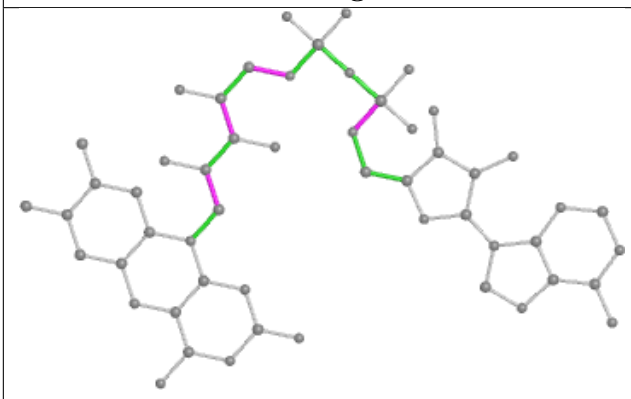
Ligand FAD B 501



Bond lengths



Bond angles



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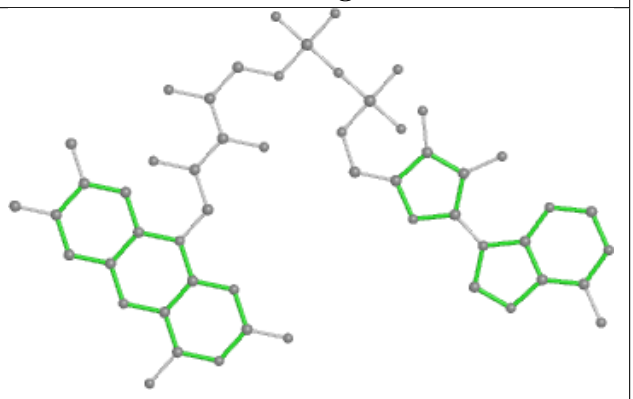
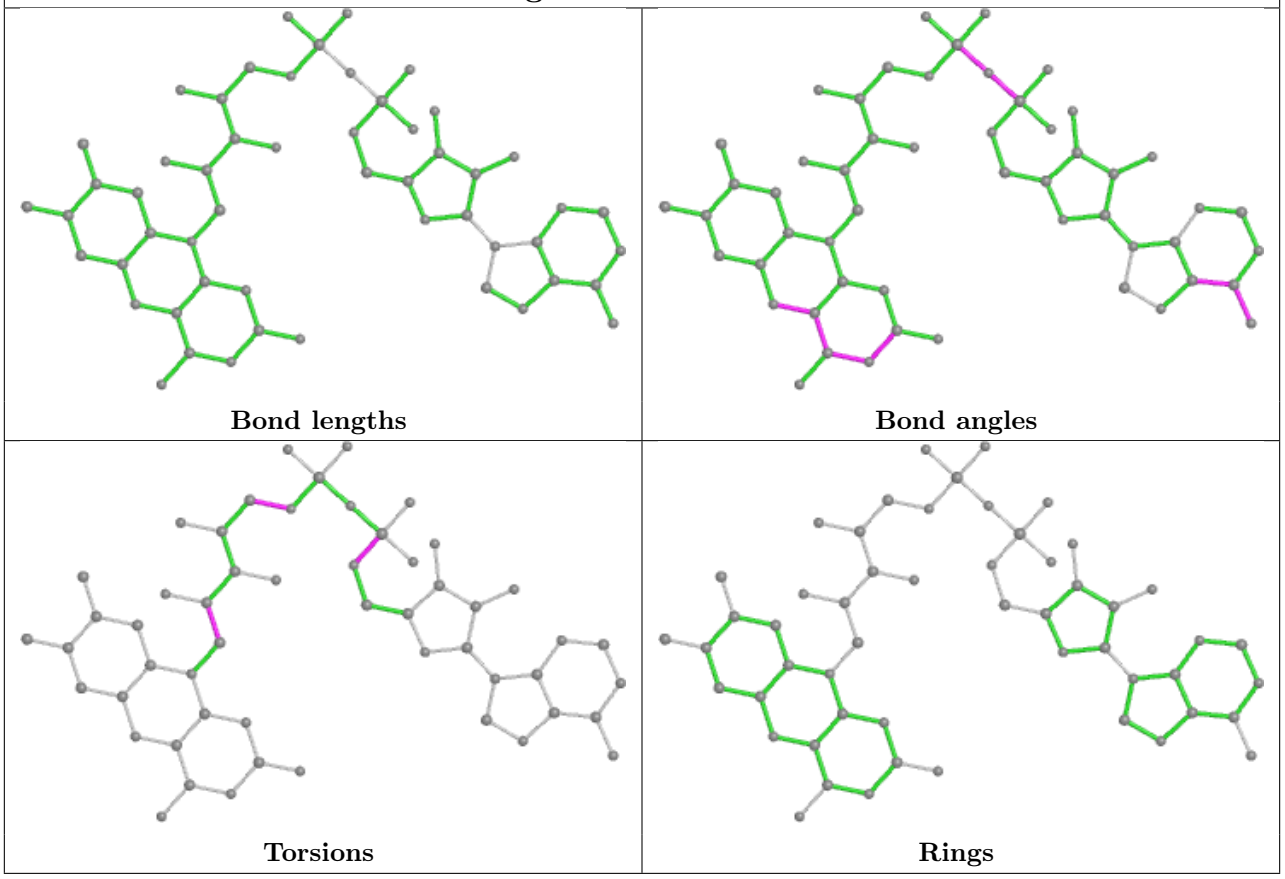


Rings

Ligand FAD A 502



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%)	0.52	14 (3%) 49 52	2, 14, 47, 103	0
1	B	434/482 (90%)	0.41	8 (1%) 68 71	4, 21, 50, 70	0
2	C	10/13 (76%)	-0.10	0 100 100	16, 50, 72, 77	0
2	E	9/13 (69%)	0.12	0 100 100	41, 57, 71, 71	0
3	D	14/14 (100%)	0.10	0 100 100	23, 50, 69, 70	0
3	F	13/14 (92%)	0.19	0 100 100	46, 63, 72, 78	0
All	All	936/1018 (91%)	0.45	22 (2%) 59 62	2, 18, 55, 103	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	252	TYR	4.1
1	A	149	CYS	3.2
1	A	440	ILE	3.1
1	A	309	SER	3.0
1	A	332	SER	3.0
1	A	408[A]	LEU	2.9
1	A	244	PHE	2.9
1	A	265	SER	2.8
1	A	417	ALA	2.6
1	A	143	ALA	2.5
1	A	249	LEU	2.4
1	B	415	GLY	2.3
1	A	359	LEU	2.3
1	A	66	ILE	2.3
1	B	101	ILE	2.3
1	B	313	CYS	2.2
1	B	309	SER	2.1
1	A	271	LEU	2.1
1	B	298	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	385	ILE	2.1
1	B	249	LEU	2.1
1	A	267	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	E	7	40/41	0.85	0.15	20,37,47,63	0
2	TTD	C	7	40/41	0.89	0.14	7,18,34,40	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

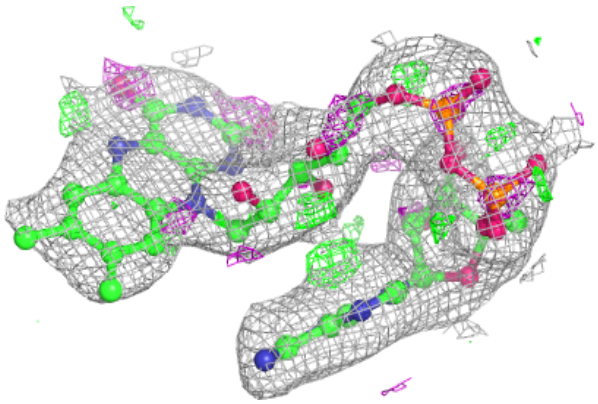
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

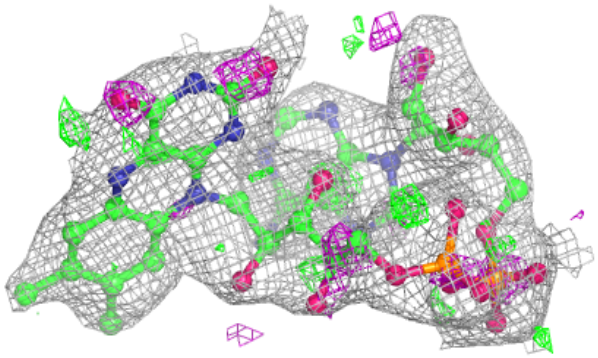
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FAD	A	502	53/53	0.81	0.19	2,3,7,10	0
5	FAD	B	501	53/53	0.84	0.17	6,16,25,31	0
4	SO4	A	501	5/5	0.94	0.14	7,8,17,21	0

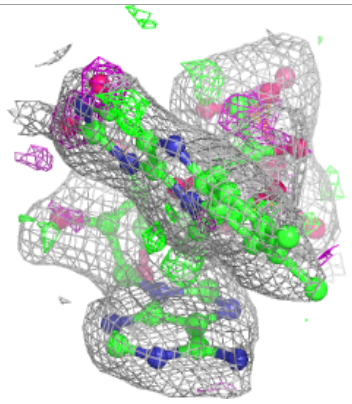
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 502:

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

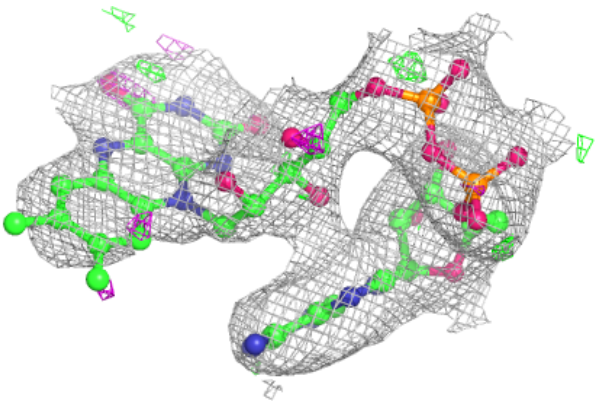


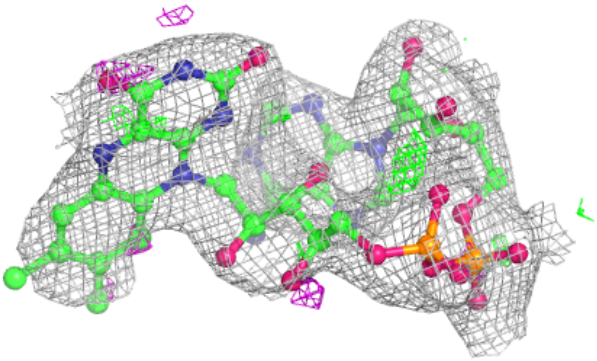


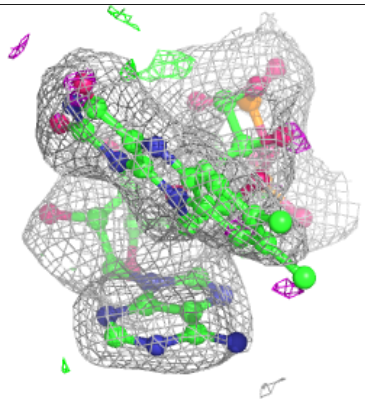


Electron density around FAD B 501:

$2mF_o$-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 (i)

There are no such residues in this entry.