



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 01:12 PM JST

PDB ID : 5ZCW
Title : Structure of the Methanosarcina mazei class II CPD-photolyase in complex with intact, phosphodiester linked, CPD-lesion
Authors : Maestre-Reyna, M.; Bessho, Y.
Deposited on : 2018-02-21
Resolution : 2.70 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
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

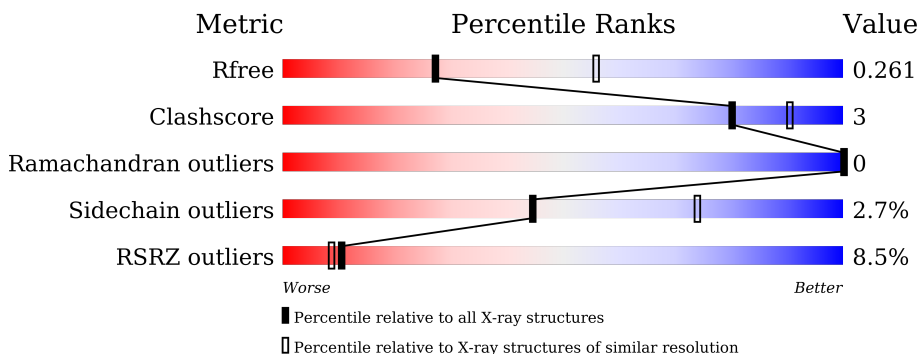
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	
1	B	482	
2	C	14	
2	E	14	
3	D	14	
3	F	14	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8319 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 photolyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	459	3612	2330	610	658	14	0	2	0
1	B	429	3274	2091	558	612	13	0	2	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	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
B	-17	MET	-	expression tag	UNP A0A0F8I5V2
B	-16	GLY	-	expression tag	UNP A0A0F8I5V2
B	-15	SER	-	expression tag	UNP A0A0F8I5V2
B	-14	SER	-	expression tag	UNP A0A0F8I5V2

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is a DNA chain called 5'-D(*AP*TP*CP*GP*GP*CP*(TTD)P*CP*GP*CP*GP*CP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	13	282	135	51	83	13	0	0	0
2	E	9	203	96	36	61	10	0	0	0

- Molecule 3 is a DNA chain called 5'-D(*TP*GP*CP*GP*CP*GP*AP*AP*GP*CP*CP*GP*AP*T)-3'.

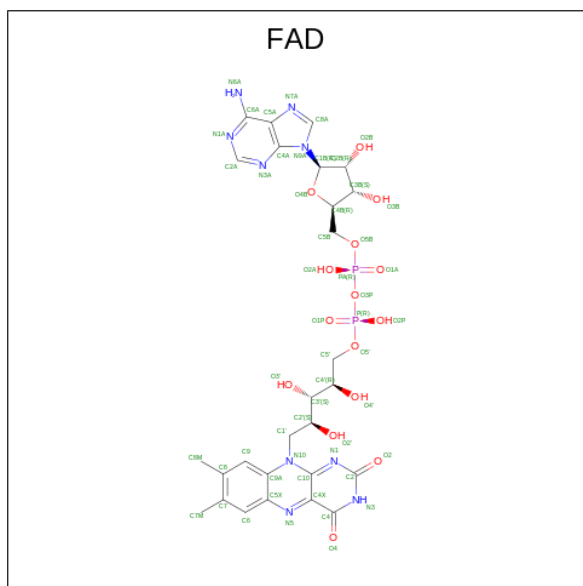
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	14	286	136	56	81	13	0	0	0
3	F	11	208	97	41	60	10	0	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



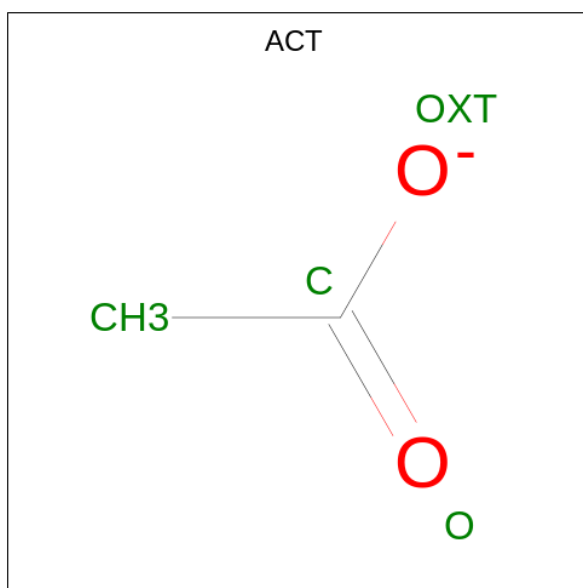
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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 ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

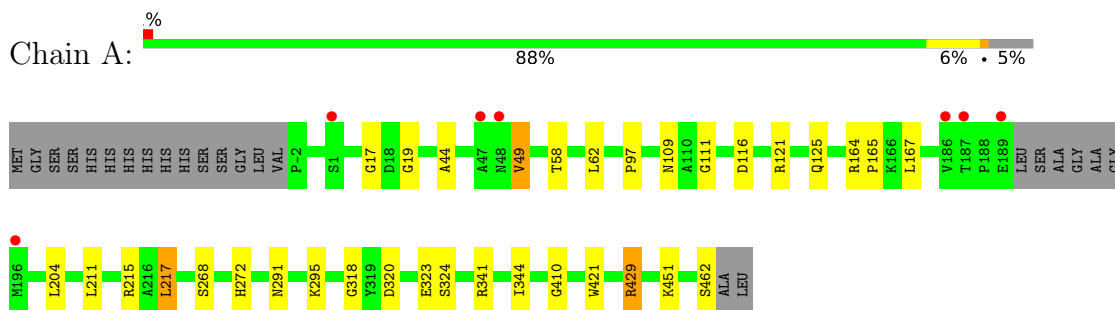
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	212	Total	O	0	1
			213	213		
7	B	85	Total	O	0	0
			85	85		
7	C	14	Total	O	0	0
			14	14		
7	D	11	Total	O	0	0
			11	11		
7	E	7	Total	O	0	0
			7	7		
7	F	9	Total	O	0	0
			9	9		

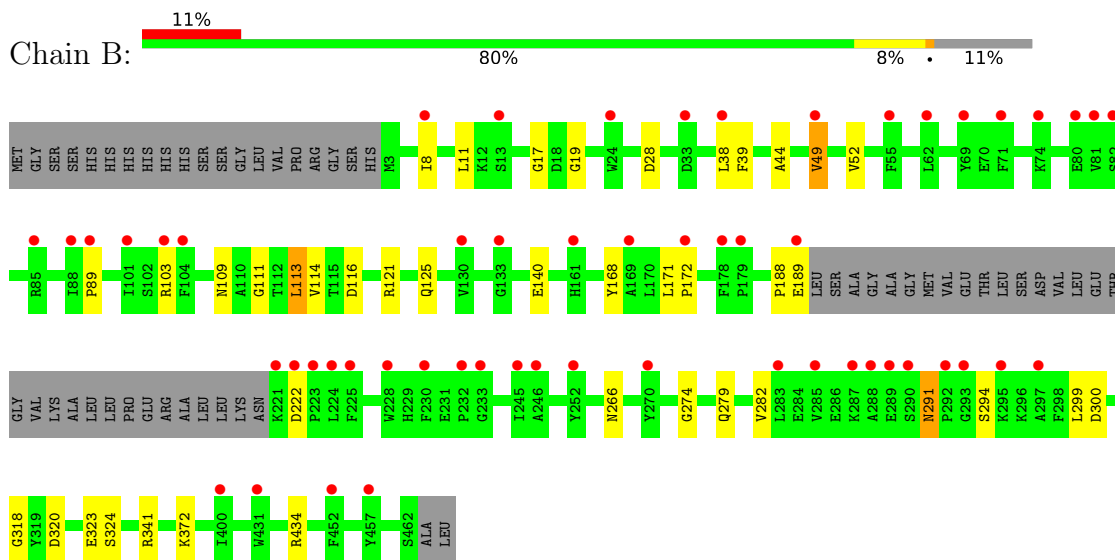
3 Residue-property plots [i](#)

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.

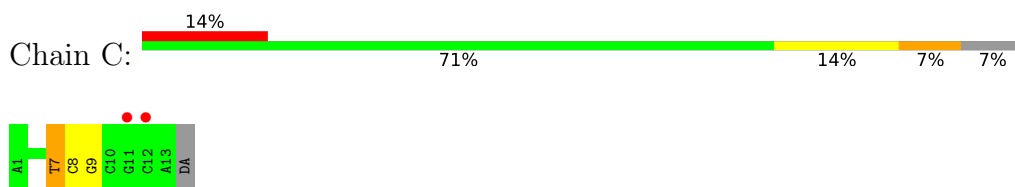
- Molecule 1: Deoxyribodipyrimidine photolyase



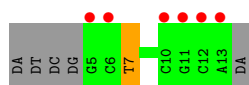
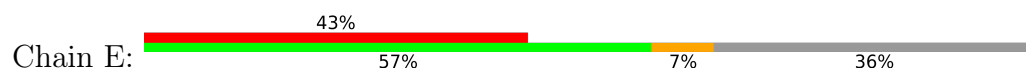
- Molecule 1: Deoxyribodipyrimidine photolyase



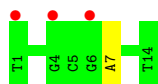
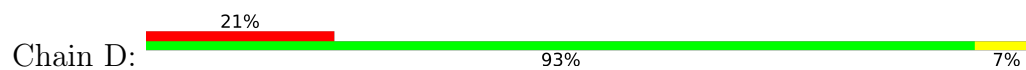
- Molecule 2: 5'-D(*AP*TP*CP*GP*GP*CP*(TTD)P*CP*GP*CP*GP*CP*AP*A)-3'



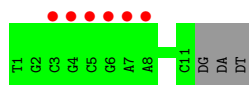
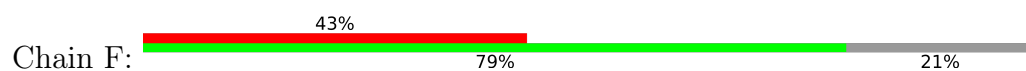
- Molecule 2: 5'-D(*AP*TP*CP*GP*GP*CP*(TTD)P*CP*GP*CP*GP*CP*AP*A)-3'



- Molecule 3: 5'-D(*TP*GP*CP*GP*CP*GP*AP*AP*GP*CP*CP*GP*AP*T)-3'



- Molecule 3: 5'-D(*TP*GP*CP*GP*CP*GP*AP*AP*GP*CP*CP*GP*AP*T)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.10Å 114.42Å 166.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.29 – 2.70 48.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (94.29-2.70) 100.0 (48.88-2.70)	Depositor EDS
R_{merge}	0.54	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.214 , 0.257 0.222 , 0.261	Depositor DCC
R_{free} test set	1883 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtrriage
Anisotropy	0.287	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8319	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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, ACT, 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	0.67	0/3716	0.76	0/5044
1	B	0.66	0/3375	0.76	0/4601
2	C	0.42	0/270	0.76	0/412
2	E	0.37	0/181	0.85	0/274
3	D	0.42	0/321	0.87	0/494
3	F	0.27	0/233	0.72	0/359
All	All	0.64	0/8096	0.77	0/11184

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	3612	0	3400	17	0
1	B	3274	0	2913	23	0
2	C	282	0	159	4	0
2	E	203	0	113	1	0
3	D	286	0	158	1	0
3	F	208	0	112	0	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	53	0	31	1	0
5	B	53	0	31	0	0
6	A	4	0	3	0	0
7	A	213	0	0	0	0
7	B	85	0	0	0	0
7	C	14	0	0	0	0
7	D	11	0	0	0	0
7	E	7	0	0	0	0
7	F	9	0	0	0	0
All	All	8319	0	6920	40	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 3.

All (40) 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:B:19:GLY:HA3	1:B:109:ASN:O	1.66	0.94
1:A:19:GLY:HA3	1:A:109:ASN:O	1.86	0.76
1:B:282:VAL:HG23	1:B:299:LEU:HD22	1.71	0.71
1:B:8:ILE:HD11	1:B:39:PHE:CD1	2.27	0.69
1:B:188:PRO:O	1:B:189:GLU:CB	2.49	0.60
1:A:125:GLN:OE1	1:B:341:ARG:N	2.28	0.57
1:B:168:TYR:OH	1:B:300:ASP:OD1	2.22	0.57
1:A:268:SER:HB3	5:A:502:FAD:H5'2	1.89	0.55
1:A:451:LYS:NZ	2:C:8:DC:OP1	2.40	0.53
1:A:344:ILE:HD12	1:B:125:GLN:HG2	1.93	0.51
1:A:429:ARG:NH1	3:D:7:DA:N1	2.58	0.51
1:B:44:ALA:HB1	1:B:49:VAL:O	2.11	0.51
1:B:279:GLN:O	1:B:282:VAL:HG12	2.11	0.50
1:A:44:ALA:HB1	1:A:49:VAL:O	2.13	0.49
1:B:52:VAL:HG12	1:B:89:PRO:HG2	1.96	0.47
1:B:171:LEU:N	1:B:172:PRO:HD2	2.29	0.47
1:A:215:ARG:O	1:A:217:LEU:HD22	2.14	0.46
1:A:17:GLY:HA3	1:A:111:GLY:HA2	1.98	0.45
1:A:121:ARG:NH2	1:A:320:ASP:OD1	2.49	0.45
1:B:11:LEU:HD21	1:B:140:GLU:HB2	1.97	0.45
2:C:8:DC:H2'	2:C:9:DG:C8	2.52	0.45
1:B:291:ASN:OD1	1:B:294:SER:N	2.44	0.44
1:A:272:HIS:CE1	1:A:410:GLY:O	2.71	0.44
1:A:62:LEU:HA	1:A:211:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:GLY:HA3	1:B:111:GLY:HA2	1.99	0.43
1:B:266:ASN:HA	1:B:372:LYS:HE3	2.00	0.43
1:B:121:ARG:NH2	1:B:320:ASP:OD1	2.52	0.43
1:A:164:ARG:HB3	1:A:165:PRO:HD3	1.99	0.43
2:E:7:TTD:H2R1	2:E:7:TTD:H6T	1.92	0.43
1:A:341:ARG:N	1:B:125:GLN:OE1	2.51	0.42
1:A:421:TRP:CE2	2:C:7:TTD:H72	2.55	0.42
1:B:8:ILE:HD11	1:B:39:PHE:CG	2.54	0.42
1:A:58:THR:HG22	1:A:97:PRO:HD3	2.01	0.41
1:B:28:ASP:HA	1:B:274:GLY:HA3	2.03	0.41
1:B:282:VAL:HG23	1:B:299:LEU:CD2	2.44	0.41
1:A:318:GLY:O	1:A:324:SER:HB3	2.21	0.40
1:B:113:LEU:HD22	1:B:114:VAL:N	2.37	0.40
2:C:7:TTD:H2"	2:C:7:TTD:H6	1.98	0.40
1:B:318:GLY:O	1:B:324:SER:HB3	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	457/482 (95%)	446 (98%)	11 (2%)	0	100	100
1	B	427/482 (89%)	419 (98%)	8 (2%)	0	100	100
All	All	884/964 (92%)	865 (98%)	19 (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	358/416 (86%)	348 (97%)	10 (3%)	43	73
1	B	308/416 (74%)	300 (97%)	8 (3%)	46	75
All	All	666/832 (80%)	648 (97%)	18 (3%)	44	74

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	VAL
1	A	116	ASP
1	A	167	LEU
1	A	204	LEU
1	A	217	LEU
1	A	291	ASN
1	A	295	LYS
1	A	323	GLU
1	A	429	ARG
1	A	462	SER
1	B	49	VAL
1	B	103	ARG
1	B	113	LEU
1	B	116	ASP
1	B	222	ASP
1	B	291	ASN
1	B	323	GLU
1	B	434	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	291	ASN
1	B	16	GLN

5.3.3 RNA [i](#)

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	1.34	5 (11%)	62,74,77	2.00	13 (20%)
2	TTD	C	7	2	42,45,46	1.38	7 (16%)	62,74,77	2.11	15 (24%)

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	-	12/22/109/110	0/5/6/6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	7	TTD	C2T-N1T	4.21	1.45	1.36
2	E	7	TTD	C2T-N1T	4.02	1.44	1.36
2	C	7	TTD	C4T-N3T	-3.64	1.31	1.37
2	E	7	TTD	C1R-N1T	3.59	1.50	1.45
2	C	7	TTD	C1'-N1	3.01	1.49	1.45
2	E	7	TTD	C4T-N3T	-2.76	1.33	1.37
2	C	7	TTD	C2T-N3T	-2.72	1.33	1.38
2	E	7	TTD	C1'-N1	2.67	1.49	1.45
2	C	7	TTD	C4-N3	-2.60	1.33	1.37
2	E	7	TTD	C2T-N3T	-2.51	1.33	1.38
2	C	7	TTD	C1R-N1T	2.48	1.49	1.45
2	C	7	TTD	C2-N3	-2.03	1.34	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	7	TTD	N3T-C2T-N1T	7.79	124.78	116.69
2	E	7	TTD	N3T-C2T-N1T	7.13	124.09	116.69
2	C	7	TTD	N3-C2-N1	5.33	122.23	116.69
2	C	7	TTD	O4-C4-C5	-5.27	118.67	122.88
2	E	7	TTD	O4-C4-C5	-5.26	118.68	122.88
2	E	7	TTD	N3-C2-N1	4.75	121.62	116.69
2	E	7	TTD	C5T-C4T-N3T	4.73	120.18	116.06
2	C	7	TTD	C5-C4-N3	4.63	120.09	116.06
2	E	7	TTD	C5-C4-N3	4.54	120.02	116.06
2	E	7	TTD	C2R-C1R-N1T	4.39	121.51	115.59
2	C	7	TTD	C2R-C1R-N1T	4.16	121.21	115.59
2	C	7	TTD	C5T-C4T-N3T	3.90	119.46	116.06
2	E	7	TTD	O4T-C4T-C5T	-3.53	120.06	122.88
2	C	7	TTD	O4T-C4T-C5T	-3.43	120.14	122.88
2	C	7	TTD	O4'-C1'-N1	3.33	112.59	108.65
2	C	7	TTD	O2T-C2T-N3T	-3.10	115.73	121.50
2	E	7	TTD	O2T-C2T-N1T	-2.78	119.18	123.49
2	C	7	TTD	O4R-C1R-N1T	2.76	111.92	108.65
2	C	7	TTD	O4'-C1'-C2'	-2.75	101.05	106.25
2	C	7	TTD	O2T-C2T-N1T	-2.65	119.38	123.49
2	E	7	TTD	O2T-C2T-N3T	-2.60	116.65	121.50
2	C	7	TTD	O2-C2-N1	-2.59	119.47	123.49
2	E	7	TTD	O4'-C1'-N1	2.35	111.43	108.65
2	E	7	TTD	O5R-C5R-C4'	2.28	116.84	108.99
2	E	7	TTD	O4R-C1R-C2R	-2.17	102.16	106.25
2	C	7	TTD	O4R-C1R-C2R	-2.14	102.20	106.25
2	C	7	TTD	C4'-O4R-C1R	-2.13	104.30	109.45
2	E	7	TTD	O2-C2-N1	-2.06	120.29	123.49

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	7	TTD	C5R-O5R-PB-O5P
2	C	7	TTD	C5R-O5R-PB-O4P
2	C	7	TTD	C2'-C1'-N1-C6
2	C	7	TTD	C5R-O5R-PB-O3R
2	C	7	TTD	C2'-C1'-N1-C2
2	E	7	TTD	C2'-C1'-N1-C6
2	E	7	TTD	C2'-C1'-N1-C2
2	E	7	TTD	O4R-C4'-C5R-O5R
2	C	7	TTD	O4'-C1'-N1-C2
2	C	7	TTD	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
2	E	7	TTD	O4'-C1'-N1-C2
2	E	7	TTD	C2R-C1R-N1T-C6T
2	E	7	TTD	O4'-C1'-N1-C6
2	C	7	TTD	C2'-C3R-O3R-PB
2	E	7	TTD	O4'-C4R-C5'-O5'
2	E	7	TTD	C3'-C4'-C5R-O5R
2	E	7	TTD	O4R-C1R-N1T-C6T
2	E	7	TTD	C4R-C5'-O5'-P
2	C	7	TTD	C2R-C1R-N1T-C6T
2	C	7	TTD	O4R-C1R-N1T-C6T
2	C	7	TTD	O4'-C4R-C5'-O5'
2	C	7	TTD	O4R-C4'-C5R-O5R

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	7	TTD	1	0
2	C	7	TTD	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
6	ACT	A	503	-	3,3,3	0.78	0	3,3,3	0.72	0
4	SO4	A	501	-	4,4,4	0.19	0	6,6,6	0.19	0
5	FAD	B	501	-	53,58,58	1.43	9 (16%)	68,89,89	1.44	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FAD	A	502	-	53,58,58	1.34	6 (11%)	68,89,89	1.42	12 (17%)

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	A	502	-	-	4/30/50/50	0/6/6/6
5	FAD	B	501	-	-	4/30/50/50	0/6/6/6

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	FAD	C9A-C5X	5.37	1.50	1.41
5	A	502	FAD	C9A-C5X	4.80	1.49	1.41
5	B	501	FAD	C8-C7	3.48	1.49	1.40
5	B	501	FAD	C4-N3	-3.00	1.33	1.38
5	A	502	FAD	C8-C7	2.90	1.48	1.40
5	A	502	FAD	C10-N10	2.57	1.43	1.37
5	A	502	FAD	C4X-N5	2.56	1.35	1.30
5	A	502	FAD	C4-N3	-2.51	1.34	1.38
5	B	501	FAD	C10-N10	2.50	1.42	1.37
5	B	501	FAD	C5A-C4A	2.48	1.47	1.40
5	B	501	FAD	C2-N3	-2.43	1.33	1.39
5	B	501	FAD	C5X-N5	-2.41	1.34	1.39
5	A	502	FAD	C5A-C4A	2.26	1.46	1.40
5	B	501	FAD	C1'-C2'	2.22	1.55	1.52
5	B	501	FAD	C4X-N5	2.00	1.34	1.30

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	FAD	N3A-C2A-N1A	-3.75	122.81	128.68
5	B	501	FAD	C4X-C10-N1	-3.60	116.36	124.73
5	A	502	FAD	C10-N1-C2	3.24	123.38	116.90
5	A	502	FAD	C4X-C10-N1	-3.21	117.29	124.73
5	A	502	FAD	C4-C4X-N5	2.98	122.47	118.23
5	A	502	FAD	N3A-C2A-N1A	-2.82	124.27	128.68
5	B	501	FAD	C4A-C5A-N7A	-2.82	106.46	109.40
5	A	502	FAD	O2P-P-O1P	2.78	125.97	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	FAD	C10-N1-C2	2.70	122.30	116.90
5	A	502	FAD	C4A-C5A-N7A	-2.64	106.64	109.40
5	A	502	FAD	C1B-N9A-C4A	-2.58	122.11	126.64
5	A	502	FAD	C4X-C4-N3	2.54	119.63	113.19
5	A	502	FAD	C5'-C4'-C3'	-2.47	107.42	112.20
5	A	502	FAD	O4-C4-C4X	-2.39	120.25	126.60
5	B	501	FAD	C5'-C4'-C3'	-2.37	107.63	112.20
5	B	501	FAD	C4-N3-C2	-2.33	121.33	125.64
5	B	501	FAD	C4X-C4-N3	2.31	119.07	113.19
5	B	501	FAD	C4X-C10-N10	2.25	119.77	116.48
5	B	501	FAD	C9A-N10-C10	-2.21	117.32	120.77
5	A	502	FAD	C4X-C10-N10	2.19	119.68	116.48
5	B	501	FAD	O4'-C4'-C3'	2.13	114.29	109.10
5	B	501	FAD	C2A-N1A-C6A	2.07	122.30	118.75
5	B	501	FAD	C4-C4X-N5	2.06	121.16	118.23
5	B	501	FAD	N3-C2-N1	2.05	123.42	119.38
5	B	501	FAD	O2P-P-O1P	2.04	122.35	112.24
5	A	502	FAD	C3B-C2B-C1B	2.01	104.00	100.98

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	FAD	C5B-O5B-PA-O1A
5	B	501	FAD	C5B-O5B-PA-O1A
5	A	502	FAD	C4'-C5'-O5'-P
5	B	501	FAD	C4'-C5'-O5'-P
5	A	502	FAD	C5B-O5B-PA-O3P
5	B	501	FAD	C5B-O5B-PA-O3P
5	A	502	FAD	C5B-O5B-PA-O2A
5	B	501	FAD	C5B-O5B-PA-O2A

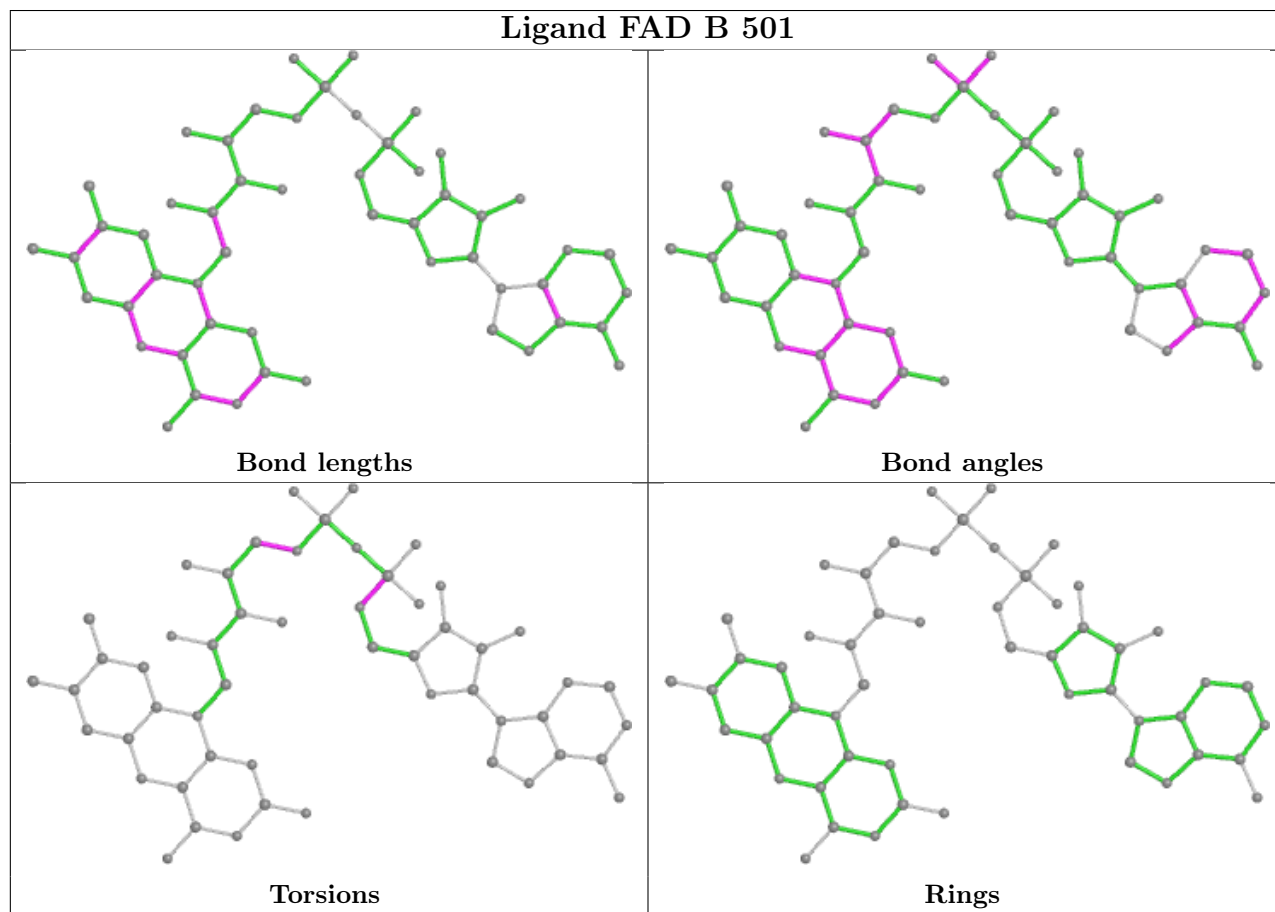
There are no ring outliers.

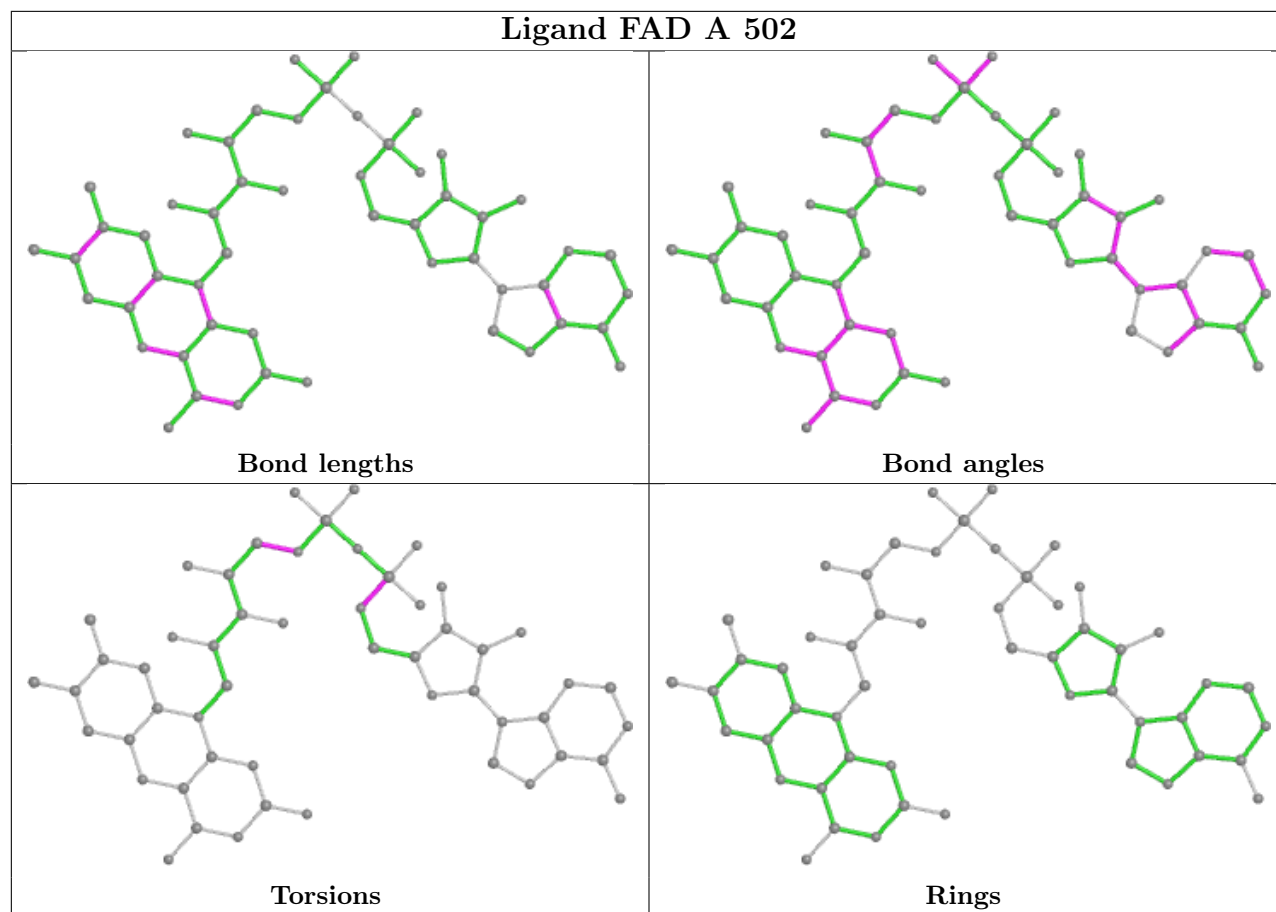
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	502	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	459/482 (95%)	0.03	7 (1%) 73 76	33, 55, 87, 111	6 (1%)
1	B	429/482 (89%)	0.83	55 (12%) 3 3	54, 94, 122, 141	2 (0%)
2	C	12/14 (85%)	1.06	2 (16%) 1 1	53, 85, 106, 118	0
2	E	8/14 (57%)	2.56	6 (75%) 0 0	85, 94, 133, 151	0
3	D	14/14 (100%)	0.89	3 (21%) 0 0	63, 77, 117, 117	0
3	F	11/14 (78%)	2.63	6 (54%) 0 0	109, 125, 144, 147	0
All	All	933/1020 (91%)	0.48	79 (8%) 10 9	33, 71, 118, 151	8 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	PHE	7.0
3	F	5	DC	5.5
2	E	5	DG	5.3
1	B	222	ASP	5.2
3	F	4	DG	4.7
1	B	13[A]	SER	4.6
1	B	246	ALA	4.6
3	F	7	DA	4.5
1	B	221	LYS	4.4
1	B	283	LEU	4.2
1	B	81	VAL	4.2
1	B	292	PRO	4.1
1	B	89	PRO	4.0
3	F	8	DA	3.9
1	B	288	ALA	3.8
1	B	169	ALA	3.7
1	B	245	ILE	3.6
1	B	223	PRO	3.4
1	B	225	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
2	E	11	DG	3.3
2	E	13	DA	3.3
1	B	80	GLU	3.2
1	B	88	ILE	3.2
1	B	252	TYR	3.1
1	B	82	SER	3.0
1	B	130	VAL	3.0
1	A	196	MET	3.0
1	B	224	LEU	3.0
1	B	293	GLY	3.0
1	A	189	GLU	2.8
2	E	6	DC	2.8
1	A	187	THR	2.8
3	F	3	DC	2.8
1	B	69	TYR	2.7
1	A	48	ASN	2.7
1	B	287	LYS	2.7
3	F	6	DG	2.7
1	B	8	ILE	2.6
2	C	11	DG	2.6
3	D	4	DG	2.6
1	B	49	VAL	2.6
1	B	33	ASP	2.6
1	B	230	PHE	2.6
1	B	55	PHE	2.5
1	B	297	ALA	2.5
1	A	1	SER	2.4
1	B	285	VAL	2.4
1	B	270	TYR	2.4
1	B	457	TYR	2.3
1	B	452	PHE	2.3
2	E	12	DC	2.3
1	B	24	TRP	2.3
1	B	103	ARG	2.3
1	B	290	SER	2.3
1	B	295	LYS	2.3
1	B	228	TRP	2.3
1	B	161	HIS	2.3
1	A	47	ALA	2.3
1	B	189	GLU	2.3
2	E	10	DC	2.3
1	B	71	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	85	ARG	2.2
3	D	6	DG	2.2
1	B	232	PRO	2.2
1	B	74	LYS	2.2
2	C	12	DC	2.2
1	B	178	PHE	2.1
1	B	172	PRO	2.1
1	B	400	ILE	2.1
1	B	289	GLU	2.1
1	B	62	LEU	2.1
3	D	1	DT	2.1
1	B	38	LEU	2.1
1	B	101	ILE	2.1
1	B	133	GLY	2.1
1	B	431	TRP	2.1
1	A	186	VAL	2.0
1	B	179	PRO	2.0
1	B	233	GLY	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	E	7	40/41	0.93	0.17	88,101,113,114	0
2	TTD	C	7	40/41	0.98	0.14	48,51,55,56	0

6.3 Carbohydrates [i](#)

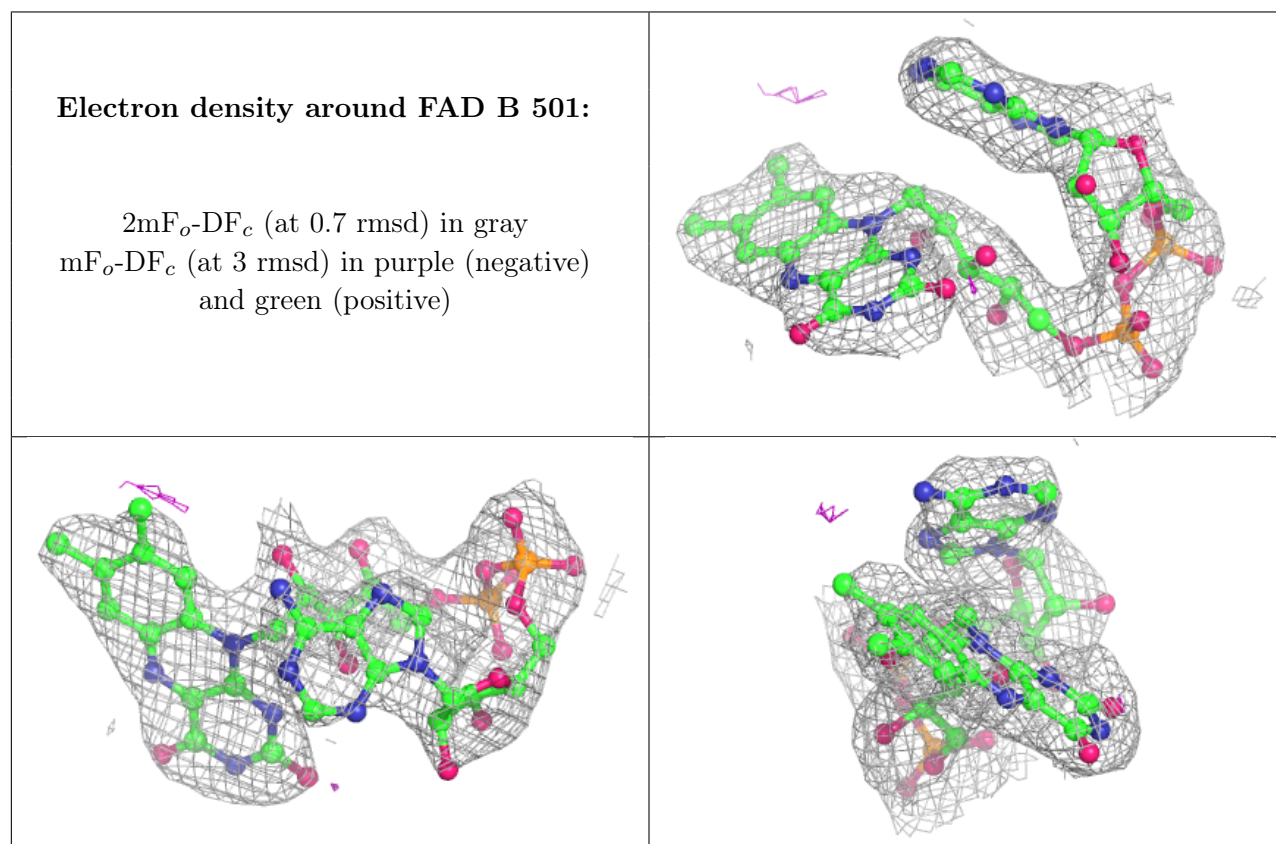
There are no monosaccharides in this entry.

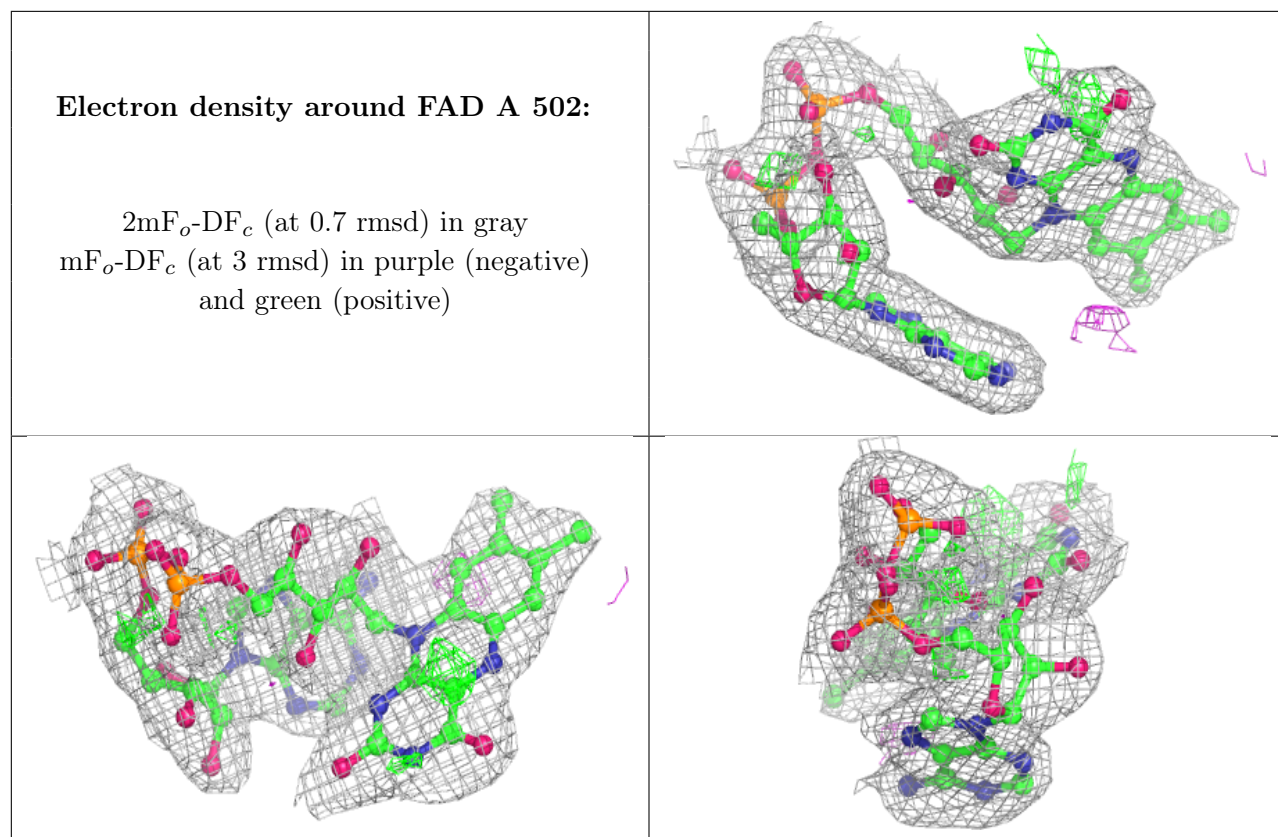
6.4 Ligands [i](#)

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, 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(\AA^2)	Q<0.9
6	ACT	A	503	4/4	0.71	0.26	116,117,118,118	0
5	FAD	B	501	53/53	0.94	0.18	62,77,85,87	0
4	SO4	A	501	5/5	0.98	0.17	42,44,46,47	0
5	FAD	A	502	53/53	0.98	0.17	34,35,37,38	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.