



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:57 am BST

PDB ID : 6KG2  
Title : Human MTHFD2 in complex with Compound 18  
Authors : Suzuki, M.; Matsui, Y.; Ota, M.; Kawai, J.  
Deposited on : 2019-07-10  
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](mailto: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.

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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 : 2.11  
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) : 2.11

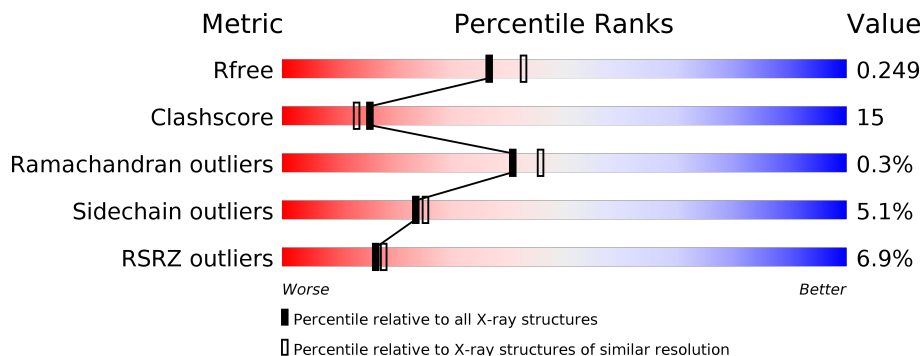
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	323	 7% 66% 23% • 9%
1	B	323	 6% 63% 25% • 10%

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 4601 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 Bifunctional methylenetetrahydrofolate dehydrogenase/cyclohydrolase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	293	Total	C	N	O	S	0	1	0
			2175	1371	388	405	11			
1	B	290	Total	C	N	O	S	0	1	0
			2151	1359	379	402	11			

There are 40 discrepancies between the modelled and reference sequences:

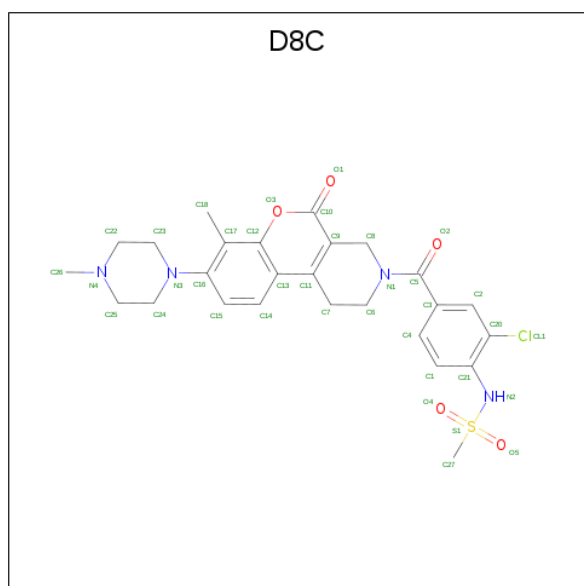
Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	expression tag	UNP P13995
A	17	GLY	-	expression tag	UNP P13995
A	18	SER	-	expression tag	UNP P13995
A	19	SER	-	expression tag	UNP P13995
A	20	HIS	-	expression tag	UNP P13995
A	21	HIS	-	expression tag	UNP P13995
A	22	HIS	-	expression tag	UNP P13995
A	23	HIS	-	expression tag	UNP P13995
A	24	HIS	-	expression tag	UNP P13995
A	25	HIS	-	expression tag	UNP P13995
A	26	SER	-	expression tag	UNP P13995
A	27	SER	-	expression tag	UNP P13995
A	28	GLY	-	expression tag	UNP P13995
A	29	GLU	-	expression tag	UNP P13995
A	30	ASN	-	expression tag	UNP P13995
A	31	LEU	-	expression tag	UNP P13995
A	32	TYR	-	expression tag	UNP P13995
A	33	PHE	-	expression tag	UNP P13995
A	34	GLN	-	expression tag	UNP P13995
A	35	GLY	-	expression tag	UNP P13995
B	16	MET	-	expression tag	UNP P13995
B	17	GLY	-	expression tag	UNP P13995
B	18	SER	-	expression tag	UNP P13995
B	19	SER	-	expression tag	UNP P13995

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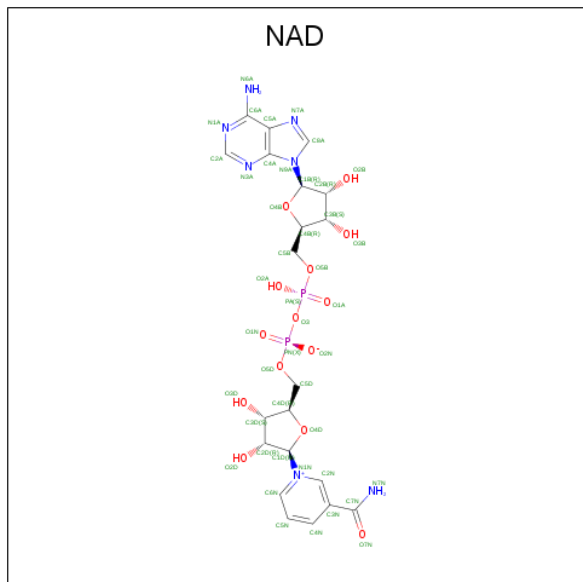
Chain	Residue	Modelled	Actual	Comment	Reference
B	20	HIS	-	expression tag	UNP P13995
B	21	HIS	-	expression tag	UNP P13995
B	22	HIS	-	expression tag	UNP P13995
B	23	HIS	-	expression tag	UNP P13995
B	24	HIS	-	expression tag	UNP P13995
B	25	HIS	-	expression tag	UNP P13995
B	26	SER	-	expression tag	UNP P13995
B	27	SER	-	expression tag	UNP P13995
B	28	GLY	-	expression tag	UNP P13995
B	29	GLU	-	expression tag	UNP P13995
B	30	ASN	-	expression tag	UNP P13995
B	31	LEU	-	expression tag	UNP P13995
B	32	TYR	-	expression tag	UNP P13995
B	33	PHE	-	expression tag	UNP P13995
B	34	GLN	-	expression tag	UNP P13995
B	35	GLY	-	expression tag	UNP P13995

- Molecule 2 is N-[2-chloranyl-4-[[7-methyl-8-(4-methylpiperazin-1-yl)-5-oxidanylidene-2,4-dihydro-1H-chromeno[3,4-c]pyridin-3-yl]carbonyl]phenyl]methanesulfonamide (three-letter code: D8C) (formula: C<sub>26</sub>H<sub>29</sub>ClN<sub>4</sub>O<sub>5</sub>S) (labeled as "Ligand of Interest" by author).



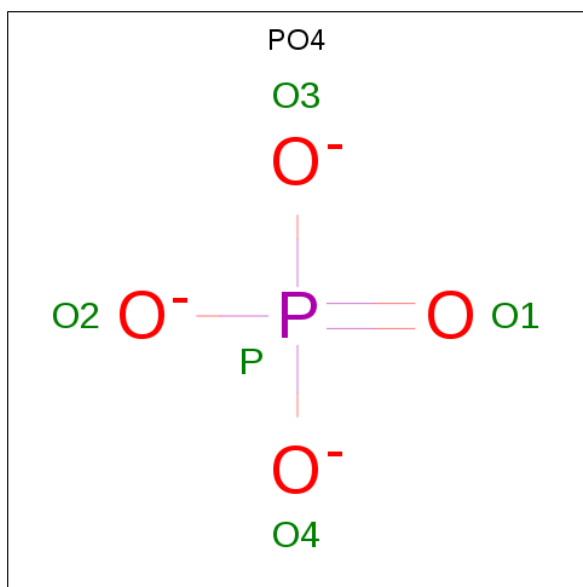
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			S
2	A	1	37	26	1	4	5	1	0	0
2	B	1	37	26	1	4	5	1	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	A	1	44	21	7	14	2	0	0
3	B	1	44	21	7	14	2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	52	Total O 52 52	0	0
5	B	51	Total O 51 51	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.99Å 116.99Å 112.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.25 24.71 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (25.00-2.25) 99.8 (24.71-2.25)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 2.26Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.193 , 0.250 0.192 , 0.249	Depositor DCC
$R_{free}$ test set	2136 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.7	Xtrriage
Anisotropy	0.013	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.045 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4601	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PO4, D8C, NAD

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	0.40	0/2216	0.82	1/3017 (0.0%)
1	B	0.41	0/2192	0.82	1/2985 (0.0%)
All	All	0.40	0/4408	0.82	2/6002 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	TYR	CB-CA-C	-6.09	98.22	110.40
1	B	287	PRO	CA-N-CD	-5.27	104.12	111.50

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	2175	0	2186	62	0
1	B	2151	0	2175	69	0
2	A	37	0	0	3	0
2	B	37	0	0	1	0
3	A	44	0	26	4	0
3	B	44	0	26	2	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	5	0	0	0	0
5	A	52	0	0	3	0
5	B	51	0	0	6	0
All	All	4601	0	4413	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 15.

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:B:258:ASN:ND2	1:B:294:ASP:HB2	1.56	1.19
1:B:258:ASN:HD21	1:B:294:ASP:HB2	1.35	0.85
1:B:258:ASN:HD22	1:B:294:ASP:HB2	1.39	0.85
1:A:118:ASN:O	1:A:122:ASN:ND2	2.13	0.78
1:A:37:ALA:HB2	1:A:302:ALA:O	1.86	0.74
1:B:130:LEU:C	1:B:130:LEU:HD12	2.08	0.74
1:B:248:ASP:N	1:B:248:ASP:OD1	2.21	0.71
1:B:37:ALA:HB3	1:B:299:ARG:O	1.91	0.71
1:B:37:ALA:CB	1:B:299:ARG:O	2.40	0.69
1:A:256:ILE:HG22	1:A:259:LEU:HB2	1.75	0.69
1:A:86:LEU:HD21	1:A:90:ARG:HH21	1.57	0.69
1:B:260:ILE:CG2	1:B:265:ILE:HD11	2.23	0.68
1:B:322:LYS:HE3	5:B:640:HOH:O	1.93	0.68
1:A:192:LEU:HD23	1:A:192:LEU:C	2.14	0.68
3:A:501:NAD:H5N	5:A:639:HOH:O	1.93	0.67
3:B:501:NAD:H5N	5:B:642:HOH:O	1.95	0.67
1:A:56:GLU:HG2	1:A:325:ILE:HG12	1.77	0.66
1:A:295:PHE:O	1:A:299:ARG:HG2	1.97	0.65
1:A:138:HIS:CD2	1:A:138:HIS:H	2.16	0.62
1:A:297:GLY:O	1:A:300:GLN:HG2	2.00	0.61
1:B:114:LEU:HD21	1:B:144:ILE:HD13	1.83	0.61
1:B:294:ASP:OD2	1:B:297:GLY:HA3	2.01	0.60
1:A:86:LEU:HD21	1:A:90:ARG:NH2	2.17	0.59
1:B:265:ILE:HG22	1:B:266:LYS:N	2.17	0.59
1:A:112:GLU:O	1:A:115:ASN:HB2	2.03	0.59
1:B:258:ASN:ND2	1:B:294:ASP:CB	2.49	0.59
1:A:243:HIS:HE1	1:B:195:ASN:ND2	2.02	0.58
1:A:130:LEU:HD12	1:A:130:LEU:C	2.24	0.58
1:B:287:PRO:O	1:B:288:LYS:HB2	2.05	0.57
1:A:310:GLY:N	2:A:500:D8C:O4	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HG23	1:A:322:LYS:HD2	1.87	0.56
1:A:77:GLU:O	1:A:78:ASN:C	2.44	0.55
1:B:192:LEU:C	1:B:192:LEU:HD23	2.26	0.55
1:B:138:HIS:CD2	1:B:138:HIS:H	2.22	0.55
1:A:236:PRO:HB2	1:A:239:GLN:HG2	1.87	0.55
1:A:288:LYS:O	1:A:289:LEU:HD12	2.06	0.55
1:A:280:HIS:CE1	1:A:287:PRO:HB3	2.42	0.55
1:B:142:ARG:NH1	1:B:146:ASN:OD1	2.40	0.54
1:B:176:THR:HB	1:B:177:PRO:HD3	1.90	0.54
1:A:256:ILE:CG2	1:A:259:LEU:HB2	2.37	0.53
1:B:207:MET:HB3	1:B:208:PRO:HD3	1.90	0.53
1:A:238:GLU:O	1:A:242:LYS:HG3	2.08	0.53
1:B:260:ILE:HG21	1:B:265:ILE:HD11	1.91	0.53
1:B:293:VAL:HG13	1:B:298:VAL:HG21	1.91	0.52
1:A:260:ILE:CG2	1:A:265:ILE:HD11	2.40	0.52
1:A:232:HIS:HA	3:A:501:NAD:N3A	2.25	0.52
1:A:53:VAL:O	1:A:57:VAL:HG23	2.11	0.51
1:A:130:LEU:HD12	1:A:130:LEU:O	2.11	0.50
1:B:108:ILE:O	1:B:138:HIS:HE1	1.94	0.50
1:B:236:PRO:HD2	1:B:239:GLN:CG	2.41	0.50
1:B:37:ALA:HB2	1:B:299:ARG:O	2.11	0.50
1:A:47:GLN:HG3	1:A:50:LYS:HE3	1.93	0.50
1:A:258:ASN:HD22	1:A:294:ASP:HB2	1.77	0.49
1:B:295:PHE:HD1	1:B:305:ILE:HD13	1.77	0.49
1:A:41:SER:HB3	1:A:44:LYS:HB2	1.95	0.49
1:B:275:GLY:O	1:B:276:ILE:HG13	2.12	0.49
1:B:45:LEU:O	1:B:49:ILE:HD12	2.12	0.49
1:B:79:PRO:C	5:B:608:HOH:O	2.51	0.49
1:A:242:LYS:O	1:A:246:LEU:HD12	2.13	0.49
1:B:80:ALA:N	5:B:608:HOH:O	2.46	0.49
1:A:165:MET:HA	5:A:616:HOH:O	2.13	0.49
1:A:242:LYS:O	1:A:246:LEU:CD1	2.61	0.49
1:B:295:PHE:CD1	1:B:305:ILE:HD13	2.47	0.48
1:A:108:ILE:HG12	1:A:109:SER:N	2.28	0.48
1:A:256:ILE:O	1:A:292:ASP:HA	2.13	0.48
1:A:296:GLU:HA	1:A:296:GLU:OE1	2.13	0.47
1:B:105:PRO:O	1:B:108:ILE:HG22	2.15	0.47
1:B:240:LEU:HD12	1:B:244:THR:HG23	1.95	0.47
1:B:84:TYR:HA	1:B:87:ASN:HD22	1.79	0.47
1:A:57:VAL:HG22	1:A:325:ILE:HD13	1.95	0.47
1:B:110:GLU:O	1:B:114:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HD21	1:A:82:HIS:NE2	2.30	0.47
1:B:313:GLY:N	1:B:314:PRO:HD2	2.30	0.46
1:A:176:THR:HB	1:A:177:PRO:HD3	1.98	0.46
1:B:310:GLY:N	2:B:500:D8C:O4	2.34	0.46
1:A:185:LYS:HA	1:A:185:LYS:HD2	1.80	0.45
1:B:48:GLN:NE2	1:B:186:ARG:HH11	2.13	0.45
1:B:273:ASP:OD2	1:B:291:GLY:HA3	2.17	0.45
1:B:258:ASN:HD22	1:B:294:ASP:CB	2.21	0.45
1:A:187:THR:HG22	1:A:187:THR:O	2.16	0.45
1:A:194:LYS:HD2	1:A:248:ASP:OD2	2.17	0.45
1:B:274:VAL:O	3:B:501:NAD:H2N	2.17	0.44
1:B:301:LYS:CB	5:B:604:HOH:O	2.66	0.44
2:A:500:D8C:C6	2:A:500:D8C:C4	2.96	0.44
1:B:174:PRO:HB2	1:B:177:PRO:HD2	1.99	0.44
1:B:70:LEU:O	1:B:99:SER:HA	2.18	0.44
1:B:216:ASP:HB3	1:B:219:HIS:CE1	2.53	0.44
1:B:235:THR:HA	1:B:236:PRO:HD3	1.87	0.44
1:A:144:ILE:O	1:A:147:ALA:HB3	2.18	0.44
1:A:114:LEU:HD21	1:A:144:ILE:HD13	2.00	0.43
1:A:100:GLU:O	1:A:100:GLU:HG3	2.19	0.43
1:A:200:GLY:HA2	3:A:501:NAD:H1B	2.00	0.43
1:B:265:ILE:CG2	1:B:266:LYS:N	2.81	0.43
1:B:259:LEU:HD23	1:B:260:ILE:HD11	2.00	0.43
1:A:196:VAL:HG22	1:A:249:ILE:HB	2.01	0.43
1:B:265:ILE:HG22	1:B:266:LYS:H	1.83	0.43
1:A:48:GLN:O	1:A:51:GLN:HB3	2.18	0.43
1:A:74:LEU:HD21	1:A:82:HIS:CE1	2.52	0.43
1:A:74:LEU:HD13	1:A:85:VAL:HG21	2.00	0.43
1:A:181:TRP:CH2	1:A:185:LYS:HE2	2.54	0.43
1:B:189:ILE:HA	1:B:190:PRO:HD3	1.88	0.43
1:B:48:GLN:HE21	1:B:186:ARG:NH1	2.17	0.43
1:A:104:LYS:HA	1:A:104:LYS:HD2	1.74	0.42
1:A:274:VAL:O	3:A:501:NAD:H2N	2.18	0.42
1:B:112:GLU:O	1:B:115:ASN:HB2	2.19	0.42
1:B:233:ARG:CB	1:B:233:ARG:HH11	2.32	0.42
1:A:309:PRO:HB3	2:A:500:D8C:C27	2.49	0.42
1:A:243:HIS:CE1	1:B:195:ASN:ND2	2.84	0.42
1:B:181:TRP:CZ2	1:B:185:LYS:HE3	2.54	0.42
1:B:54:ARG:HD2	5:B:633:HOH:O	2.19	0.42
1:B:185:LYS:HA	1:B:185:LYS:HD3	1.77	0.42
1:B:89:THR:HG22	1:B:99:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ILE:O	1:A:307:PRO:HD2	2.20	0.42
1:B:130:LEU:O	1:B:130:LEU:HD12	2.20	0.42
1:B:216:ASP:HB3	1:B:219:HIS:ND1	2.35	0.41
1:B:67:ARG:NH1	1:B:96:GLY:O	2.45	0.41
1:A:181:TRP:CZ2	1:A:185:LYS:HE2	2.56	0.41
1:B:144:ILE:O	1:B:145:CYS:C	2.57	0.41
1:A:47:GLN:HG2	5:A:646:HOH:O	2.21	0.41
1:A:90:ARG:O	1:A:94:VAL:HG13	2.20	0.41
1:A:136:PRO:HB2	1:A:138:HIS:NE2	2.35	0.41
1:A:192:LEU:O	1:A:192:LEU:HD23	2.21	0.41
1:B:129:LEU:HD12	1:B:130:LEU:N	2.35	0.41
1:B:130:LEU:C	1:B:130:LEU:CD1	2.81	0.41
1:B:88:LYS:NZ	1:B:132:GLN:OE1	2.44	0.41
1:B:241:LYS:O	1:B:245:ILE:HG23	2.22	0.40
1:A:243:HIS:HA	1:A:246:LEU:HD12	2.03	0.40
1:B:332:LEU:HG	1:B:332:LEU:H	1.63	0.40
1:A:74:LEU:HD21	1:A:82:HIS:CD2	2.56	0.40
1:A:37:ALA:CB	1:A:302:ALA:O	2.64	0.40
1:B:192:LEU:HD23	1:B:193:GLY:N	2.36	0.40
1:B:153:ASP:O	1:B:172:MET:HG2	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	290/323 (90%)	271 (93%)	19 (7%)	0	100	100
1	B	287/323 (89%)	275 (96%)	10 (4%)	2 (1%)	22	21
All	All	577/646 (89%)	546 (95%)	29 (5%)	2 (0%)	41	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	288	LYS
1	B	106	ALA

### 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	228/271 (84%)	219 (96%)	9 (4%)	32	38
1	B	229/271 (84%)	215 (94%)	14 (6%)	18	18
All	All	457/542 (84%)	434 (95%)	23 (5%)	24	26

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	47	GLN
1	A	83	SER
1	A	86	LEU
1	A	94	VAL
1	A	104	LYS
1	A	138	HIS
1	A	248	ASP
1	A	331	VAL
1	B	36	GLU
1	B	40	ILE
1	B	83	SER
1	B	100	GLU
1	B	102	ILE
1	B	108	ILE
1	B	109	SER
1	B	111	GLU
1	B	130	LEU
1	B	233	ARG
1	B	240	LEU
1	B	248	ASP
1	B	287	PRO

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Mol	Chain	Res	Type
1	B	332	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	243	HIS
1	A	258	ASN
1	B	48	GLN
1	B	87	ASN
1	B	138	HIS
1	B	195	ASN
1	B	243	HIS
1	B	258	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

6 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
2	D8C	B	500	-	38,41,41	1.71	7 (18%)	54,62,62	2.58	12 (22%)
3	NAD	A	501	-	42,48,48	0.62	0	50,73,73	0.86	2 (4%)
2	D8C	A	500	-	38,41,41	1.61	9 (23%)	54,62,62	2.49	14 (25%)
4	PO4	B	502	-	4,4,4	1.32	0	6,6,6	0.71	0
4	PO4	A	502	-	4,4,4	0.63	0	6,6,6	0.70	0
3	NAD	B	501	-	42,48,48	0.81	1 (2%)	50,73,73	0.99	4 (8%)

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	D8C	A	500	-	-	0/17/36/36	0/5/5/5
2	D8C	B	500	-	-	0/17/36/36	0/5/5/5
3	NAD	B	501	-	-	6/26/62/62	0/5/5/5
3	NAD	A	501	-	-	7/26/62/62	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	D8C	C11-C13	4.02	1.49	1.43
2	A	500	D8C	S1-N2	3.95	1.68	1.63
2	B	500	D8C	S1-N2	3.58	1.68	1.63
2	A	500	D8C	C27-S1	3.42	1.83	1.75
2	B	500	D8C	C16-C17	3.21	1.44	1.40
2	A	500	D8C	O5-S1	3.05	1.48	1.43
2	B	500	D8C	C14-C15	2.92	1.42	1.36
2	B	500	D8C	C21-N2	-2.83	1.38	1.42
2	B	500	D8C	C27-S1	2.82	1.82	1.75
2	B	500	D8C	O5-S1	2.78	1.48	1.43
2	A	500	D8C	C21-N2	-2.76	1.38	1.42
2	A	500	D8C	C11-C13	2.70	1.47	1.43
2	A	500	D8C	C14-C15	2.68	1.42	1.36
2	A	500	D8C	C16-C17	2.66	1.43	1.40
2	A	500	D8C	O4-S1	2.42	1.47	1.43
2	A	500	D8C	C10-C9	2.39	1.48	1.40
3	B	501	NAD	C2N-N1N	2.22	1.37	1.35

All (32) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	D8C	C17-C16-N3	12.03	125.29	118.55
2	A	500	D8C	C17-C16-N3	10.44	124.40	118.55
2	B	500	D8C	C27-S1-N2	-7.75	97.79	106.63
2	A	500	D8C	C27-S1-N2	-6.83	98.84	106.63
2	A	500	D8C	C20-C21-N2	-5.19	115.92	120.74
2	B	500	D8C	O4-S1-C27	5.08	116.44	108.28
2	A	500	D8C	C9-C8-N1	-4.29	108.24	112.72
2	A	500	D8C	O4-S1-C27	4.16	114.96	108.28
2	B	500	D8C	C20-C21-N2	-3.98	117.04	120.74
2	A	500	D8C	C15-C16-N3	-3.72	116.36	122.30
2	B	500	D8C	C2-C20-C21	-3.71	118.68	121.72
2	B	500	D8C	C15-C16-N3	-3.35	116.96	122.30
2	B	500	D8C	C24-N3-C16	-3.24	108.59	116.27
2	A	500	D8C	C14-C13-C12	3.22	120.23	116.50
2	A	500	D8C	C24-N3-C16	-3.10	108.92	116.27
2	B	500	D8C	C15-C16-C17	-2.94	117.71	121.35
3	B	501	NAD	C6N-N1N-C2N	-2.93	119.30	121.97
2	A	500	D8C	C18-C17-C12	-2.85	116.12	119.39
2	A	500	D8C	C18-C17-C16	2.84	124.86	121.43
2	A	500	D8C	C26-N4-C25	-2.73	106.58	110.66
2	A	500	D8C	C7-C6-N1	2.65	113.16	110.04
2	B	500	D8C	C8-C9-C10	-2.53	110.49	119.96
2	B	500	D8C	C1-C21-C20	2.41	121.34	117.94
2	B	500	D8C	C26-N4-C25	-2.33	107.18	110.66
2	A	500	D8C	O4-S1-N2	-2.30	102.40	107.10
3	A	501	NAD	C6N-N1N-C2N	-2.28	119.90	121.97
3	B	501	NAD	O4D-C1D-C2D	-2.26	103.62	106.93
3	B	501	NAD	C4N-C3N-C7N	2.20	126.92	121.04
2	A	500	D8C	C8-C9-C10	-2.17	111.84	119.96
2	B	500	D8C	C10-O3-C12	2.10	123.16	119.19
3	A	501	NAD	C5A-C6A-N6A	2.06	123.48	120.35
3	B	501	NAD	C5A-C6A-N6A	2.02	123.42	120.35

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	NAD	O4D-C1D-N1N-C2N
3	A	501	NAD	O4D-C1D-N1N-C6N
3	A	501	NAD	C2D-C1D-N1N-C2N
3	B	501	NAD	O4B-C4B-C5B-O5B
3	B	501	NAD	O4D-C1D-N1N-C2N
3	B	501	NAD	O4D-C1D-N1N-C6N

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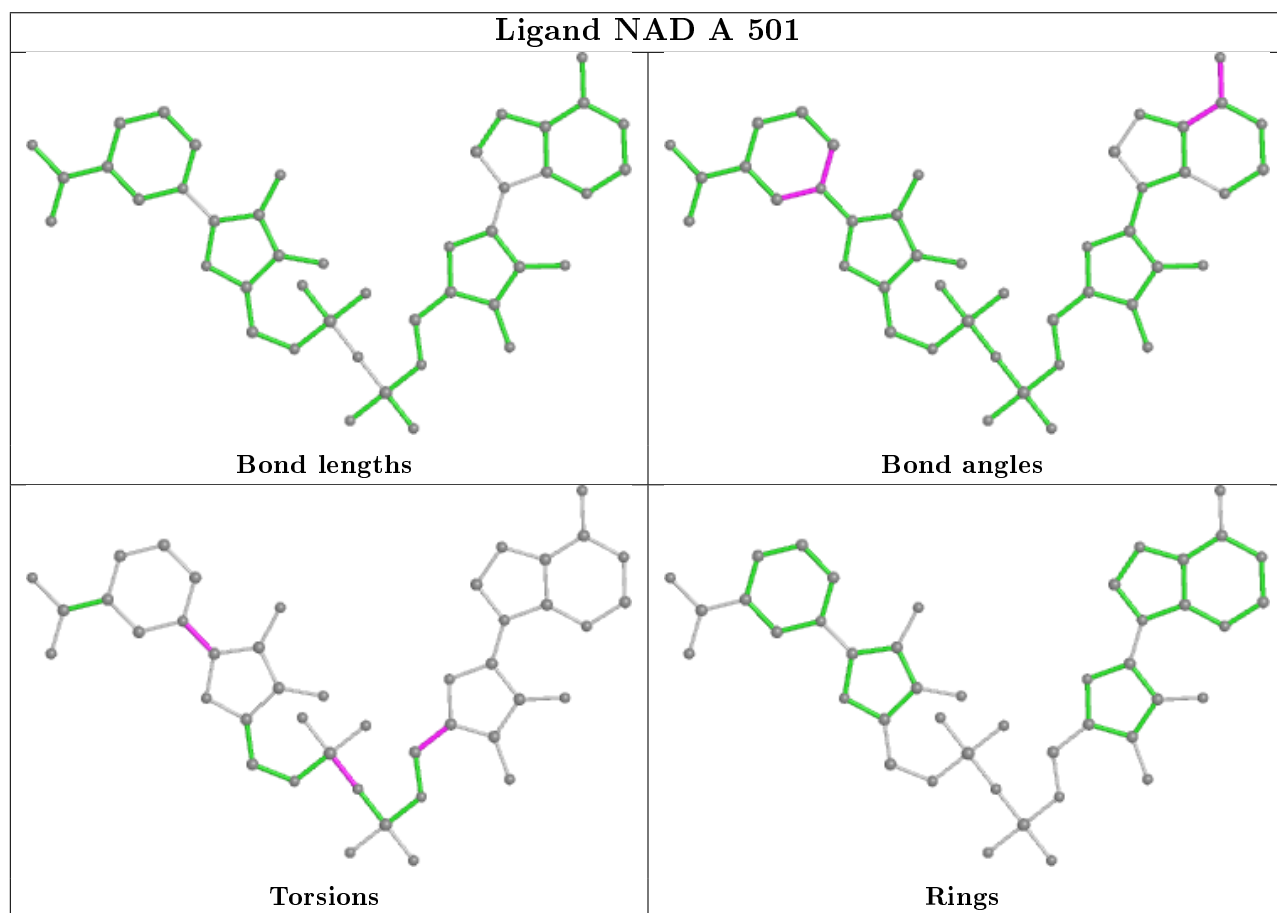
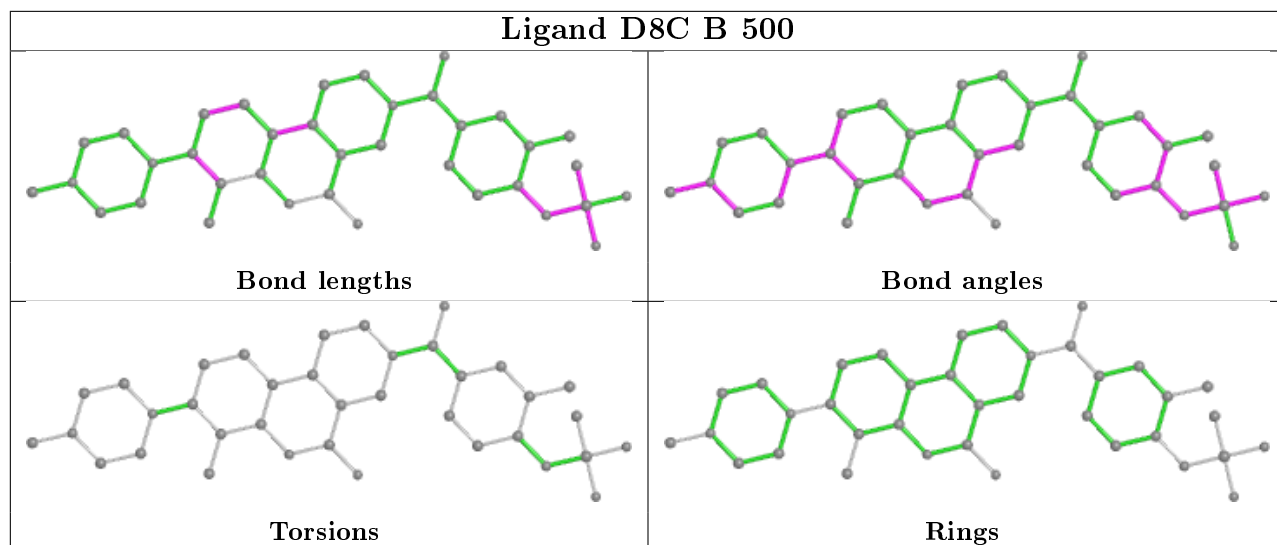
Mol	Chain	Res	Type	Atoms
3	B	501	NAD	C2D-C1D-N1N-C2N
3	B	501	NAD	C2D-C1D-N1N-C6N
3	A	501	NAD	O4B-C4B-C5B-O5B
3	A	501	NAD	PA-O3-PN-O1N
3	B	501	NAD	C3B-C4B-C5B-O5B
3	A	501	NAD	C2D-C1D-N1N-C6N
3	A	501	NAD	PA-O3-PN-O2N

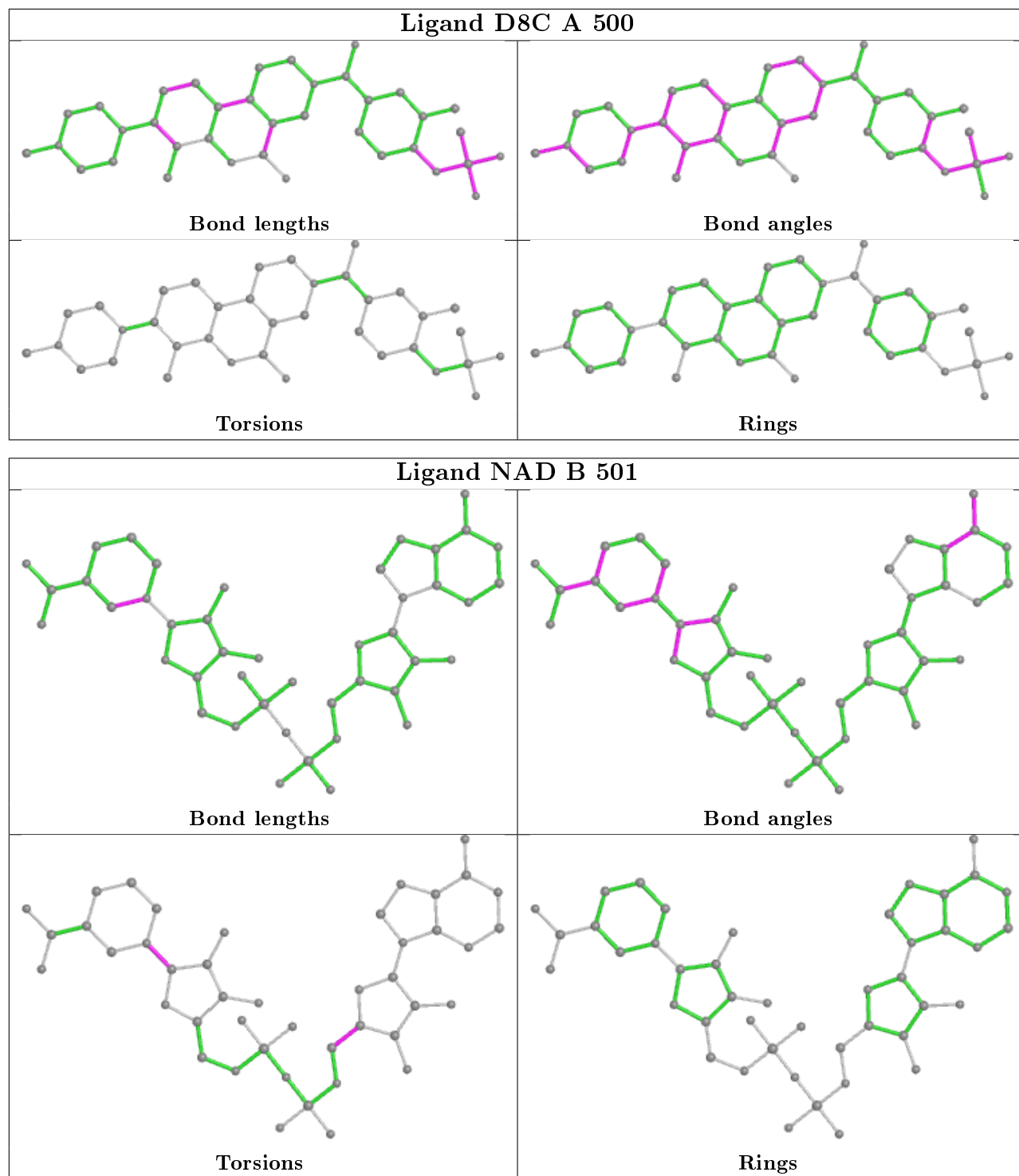
There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	D8C	1	0
3	A	501	NAD	4	0
2	A	500	D8C	3	0
3	B	501	NAD	2	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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	293/323 (90%)	0.16	21 (7%) 15 16	39, 56, 86, 118	0
1	B	290/323 (89%)	0.27	19 (6%) 18 20	39, 58, 90, 123	0
All	All	583/646 (90%)	0.21	40 (6%) 16 18	39, 57, 88, 123	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	287	PRO	5.1
1	A	332	LEU	4.7
1	A	279	VAL	4.5
1	A	280	HIS	4.1
1	A	287	PRO	4.1
1	B	251	ILE	4.0
1	A	197	VAL	3.8
1	B	197	VAL	3.8
1	B	230	ILE	3.8
1	B	229	THR	3.7
1	A	230	ILE	3.7
1	A	331	VAL	3.6
1	B	279	VAL	3.6
1	A	228	VAL	3.3
1	A	251	ILE	3.2
1	A	288	LYS	3.2
1	A	229	THR	3.2
1	A	196	VAL	3.1
1	B	289	LEU	3.1
1	B	198	VAL	3.0
1	A	130	LEU	3.0
1	B	196	VAL	2.8
1	B	288	LYS	2.8
1	A	198	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	271	VAL	2.7
1	B	250	VAL	2.6
1	A	272	ILE	2.5
1	B	228	VAL	2.4
1	A	250	VAL	2.3
1	B	177	PRO	2.3
1	B	136	PRO	2.3
1	B	188	GLY	2.3
1	B	62	ALA	2.2
1	A	170	TYR	2.2
1	A	209	ILE	2.2
1	B	272	ILE	2.1
1	A	101	THR	2.1
1	A	333	ARG	2.1
1	B	199	ALA	2.1
1	A	79	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

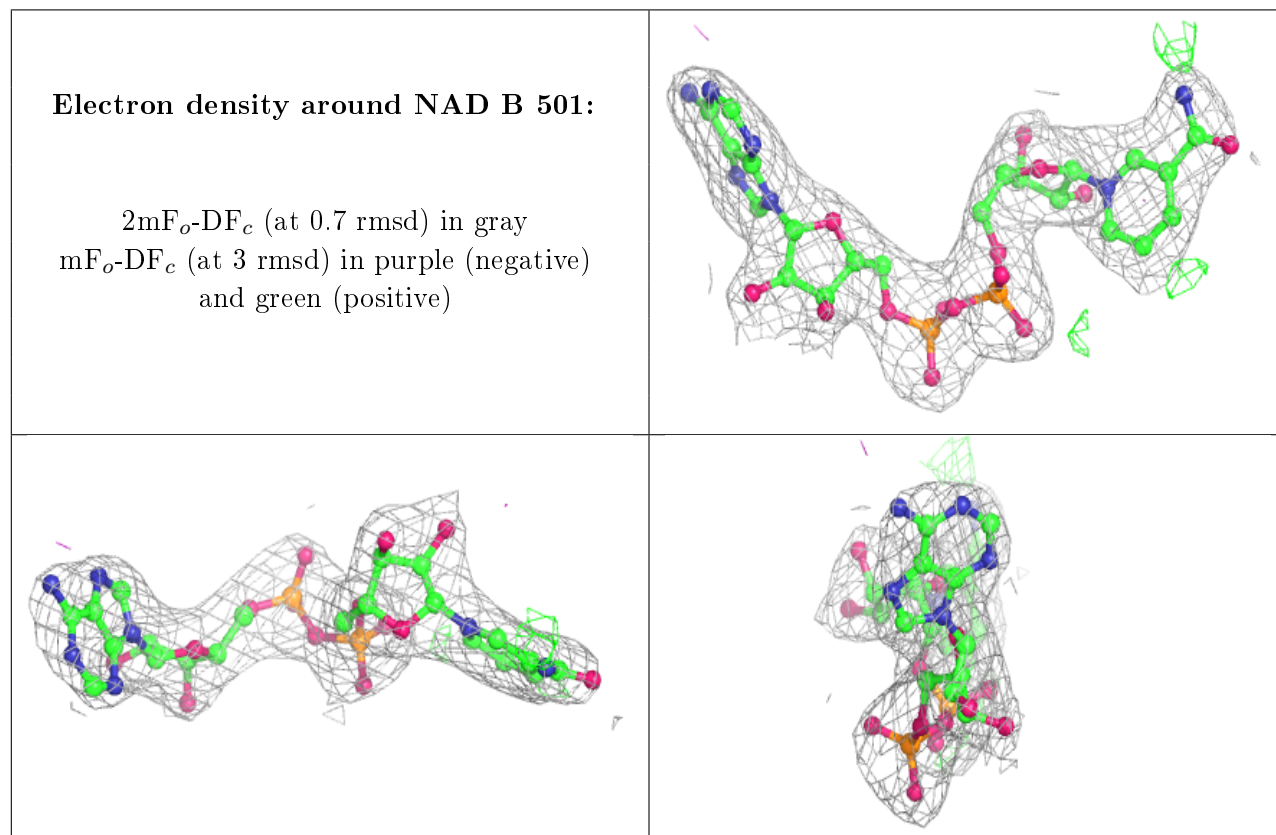
There are no carbohydrates in this entry.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAD	B	501	44/44	0.95	0.10	50,66,85,91	0
3	NAD	A	501	44/44	0.96	0.10	48,63,73,80	0
2	D8C	A	500	37/37	0.96	0.11	42,61,89,96	0
2	D8C	B	500	37/37	0.96	0.12	46,64,91,106	0
4	PO4	A	502	5/5	0.99	0.09	40,52,56,60	0
4	PO4	B	502	5/5	0.99	0.12	51,53,55,59	0

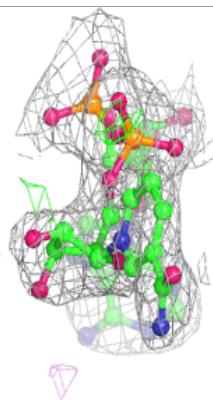
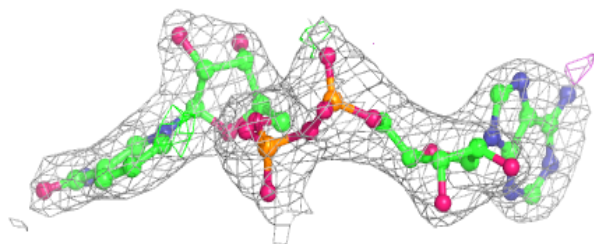
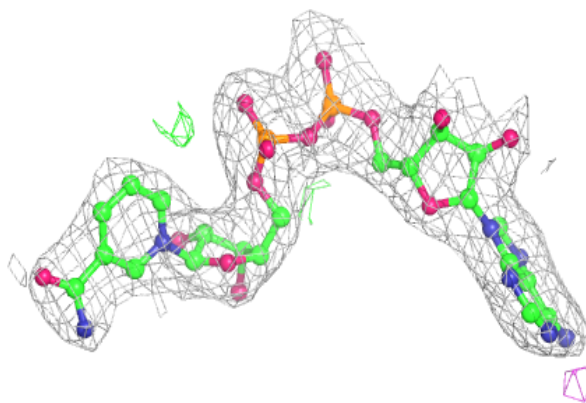
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



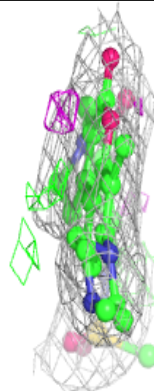
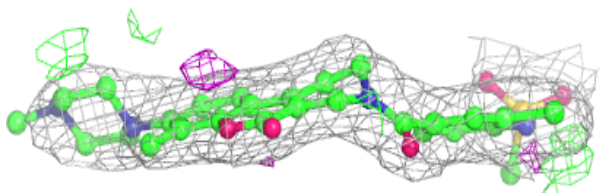
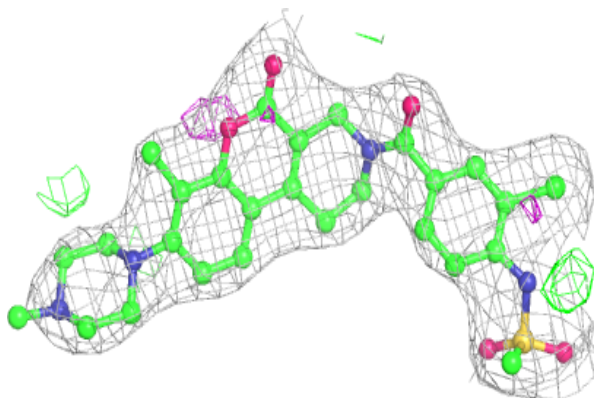


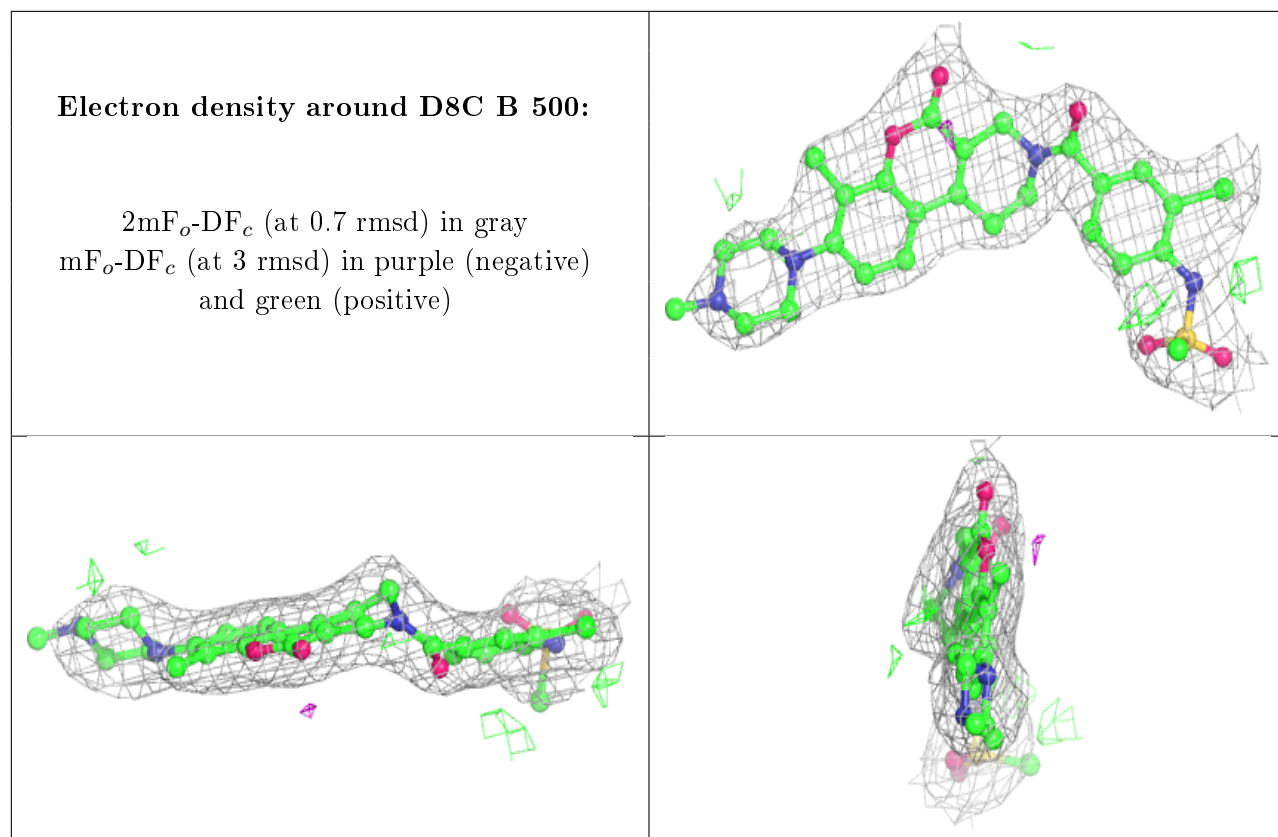
**Electron density around NAD A 501:**

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

**Electron density around D8C A 500:**

$2mF_o-DF_c$  (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.