



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 04:33 PM BST

PDB ID : 5JCN
Title : Structure and catalytic mechanism of monodehydroascorbate reductase, MD-HAR, from *Oryza sativa* L. japonica
Authors : Park, A.K.; Kim, H.W.
Deposited on : 2016-04-15
Resolution : 2.29 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 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 : 2.13.1
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) : 2.13.1

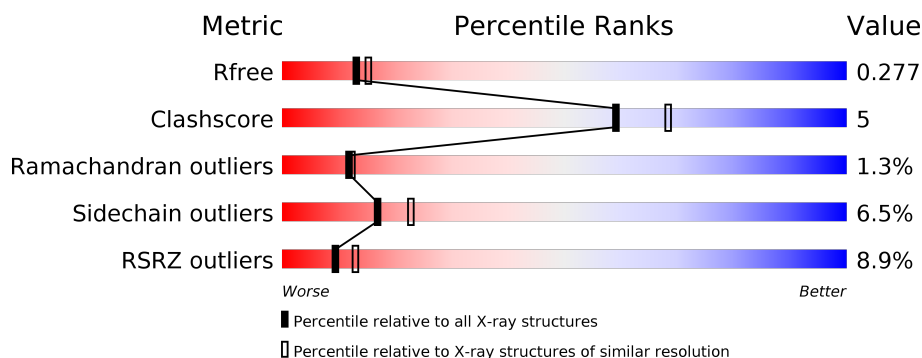
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 ≥ 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	451	<div> <div>9%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	B	451	<div> <div>8%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>•• 6%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6790 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 Os09g0567300 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3248	2095	531	616	6			
1	B	425	Total	C	N	O	S	0	0	0
			3215	2073	526	610	6			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP Q652L6
A	-14	HIS	-	expression tag	UNP Q652L6
A	-13	HIS	-	expression tag	UNP Q652L6
A	-12	HIS	-	expression tag	UNP Q652L6
A	-11	HIS	-	expression tag	UNP Q652L6
A	-10	HIS	-	expression tag	UNP Q652L6
A	-9	ALA	-	expression tag	UNP Q652L6
A	-8	SER	-	expression tag	UNP Q652L6
A	-7	GLU	-	expression tag	UNP Q652L6
A	-6	ASN	-	expression tag	UNP Q652L6
A	-5	LEU	-	expression tag	UNP Q652L6
A	-4	TYR	-	expression tag	UNP Q652L6
A	-3	PHE	-	expression tag	UNP Q652L6
A	-2	GLN	-	expression tag	UNP Q652L6
A	-1	GLY	-	expression tag	UNP Q652L6
A	0	ALA	-	expression tag	UNP Q652L6
A	349	PHE	TYR	engineered mutation	UNP Q652L6
B	-15	HIS	-	expression tag	UNP Q652L6
B	-14	HIS	-	expression tag	UNP Q652L6
B	-13	HIS	-	expression tag	UNP Q652L6
B	-12	HIS	-	expression tag	UNP Q652L6
B	-11	HIS	-	expression tag	UNP Q652L6
B	-10	HIS	-	expression tag	UNP Q652L6
B	-9	ALA	-	expression tag	UNP Q652L6
B	-8	SER	-	expression tag	UNP Q652L6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	GLU	-	expression tag	UNP Q652L6
B	-6	ASN	-	expression tag	UNP Q652L6
B	-5	LEU	-	expression tag	UNP Q652L6
B	-4	TYR	-	expression tag	UNP Q652L6
B	-3	PHE	-	expression tag	UNP Q652L6
B	-2	GLN	-	expression tag	UNP Q652L6
B	-1	GLY	-	expression tag	UNP Q652L6
B	0	ALA	-	expression tag	UNP Q652L6
B	349	PHE	TYR	engineered mutation	UNP Q652L6

- # FAD

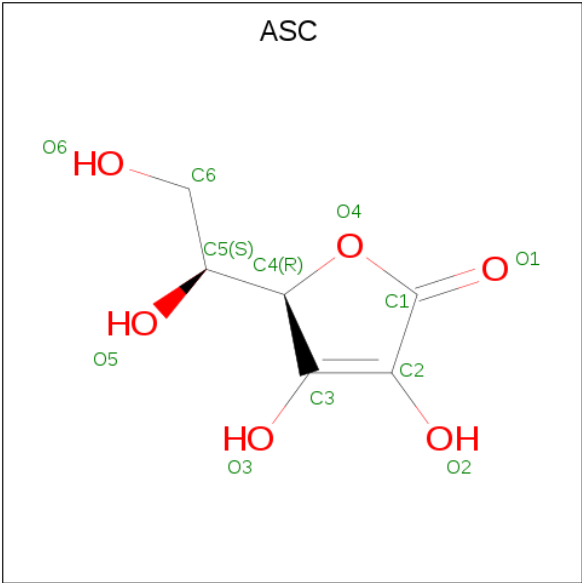
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

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

- Molecule 4 is ASCORBIC ACID (three-letter code: ASC) (formula: C₆H₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		
4	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	58	Total 58	O 58	0	0
5	B	51	Total 51	O 51	0	0

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.

- Chain A:
-
- 9%
- 82%
- 12%
- 5%

- Chain B:
-
- | Amino Acid | Count |
|------------|-------|
| HIS | 1 |
| HIS | 1 |
| HIS | 1 |
| HIS | 1 |
| HIS | 1 |
| HIS | 1 |
| ALA | 1 |
| SER | 1 |
| GLU | 1 |
| ASN | 1 |
| LEU | 1 |
| TTR | 1 |
| PHE | 1 |
| GLN | 1 |
| GLY | 1 |
| ALA | 1 |
| MET | 1 |
| ALA | 1 |
| SER | 1 |
| E4 | 1 |
| K5 | 1 |
| H6 | 1 |
| F7 | 1 |
| V30 | 1 |
| K31 | 1 |
| E34 | 1 |
| I37 | 1 |
| I38 | 1 |
| S39 | 1 |
| K40 | 1 |
| P49 | 1 |
| Y55 | 1 |
| R63 | 1 |
| V71 | 1 |
| R77 | 1 |
| S84 | 1 |
| E85 | 1 |
| K86 | 1 |
| E89 | 1 |
| L90 | 1 |
| V97 | 1 |
| A102 | 1 |
| S103 | 1 |
| K104 | 1 |
| I105 | 1 |
| L106 | 1 |
| T107 | 1 |
| S108 | 1 |
| A109 | 1 |
| V110 | 1 |
| T113 | 1 |
| F114 | 1 |
| T115 | 1 |
| Y116 | 1 |
| L119 | 1 |
| V127 | 1 |
| D132 | 1 |
| N142 | 1 |
| I143 | 1 |
| L144 | 1 |
| Y145 | 1 |
| K154 | 1 |
| K154 | 1 |
| Y174 | 1 |
| K184 | 1 |
| F188 | 1 |
| M192 | 1 |
| M200 | 1 |
| P201 | 1 |
| R202 | 1 |
| A209 | 1 |
| E213 | 1 |
| K222 | 1 |
| I223 | 1 |
| V224 | 1 |
| A229 | 1 |
| V240 | 1 |
| S249 | 1 |
| V257 | 1 |
| V260 | 1 |
| L265 | 1 |
| D298 | 1 |
| M304 | 1 |
| K305 | 1 |
| K306 | 1 |
| Y307 | 1 |
| V308 | 1 |
| R311 | 1 |
| A319 | 1 |
| K331 | 1 |
| E334 | 1 |
| S335 | 1 |
| S338 | 1 |
| V339 | 1 |
| V340 | 1 |
| E341 | 1 |
| Y342 | 1 |
| D343 | 1 |
| Y344 | 1 |
| L345 | 1 |
| D362 | 1 |
| N363 | 1 |
| V364 | 1 |
| L369 | 1 |
| D372 | 1 |
| S373 | 1 |
| F382 | 1 |
| I387 | 1 |
| K388 | 1 |
| V392 | 1 |
| L397 | 1 |
| A409 | 1 |
| F413 | 1 |
| F416 | 1 |
| P417 | 1 |
| VAL | 1 |
| ALA | 1 |
| ASN | 1 |
| I1E | 1 |
| E422 | 1 |
| E423 | 1 |
| L424 | 1 |
| K425 | 1 |
| LYS | 1 |
| GLU | 1 |
| G428 | 1 |
| L429 | 1 |
| Q430 | 1 |
| F431 | 1 |
| A432 | 1 |
| S433 | 1 |
| V434 | 1 |

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.64Å 85.11Å 133.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.29 43.84 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.29) 99.3 (43.84-2.29)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.205 , 0.264 0.231 , 0.277	Depositor DCC
R_{free} test set	1936 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6790	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ASC, FAD, 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	0.78	0/3317	0.93	6/4487 (0.1%)
1	B	0.74	0/3283	0.91	6/4440 (0.1%)
All	All	0.76	0/6600	0.92	12/8927 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	63	ARG	NE-CZ-NH2	-11.78	114.41	120.30
1	A	63	ARG	NE-CZ-NH1	11.44	126.02	120.30
1	B	63	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	B	132	ASP	CB-CG-OD1	6.31	123.98	118.30
1	B	63	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	B	372	ASP	C-N-CA	5.74	136.06	121.70
1	A	372	ASP	C-N-CA	5.56	135.60	121.70
1	B	373	SER	N-CA-CB	5.30	118.46	110.50
1	A	147	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	373	SER	N-CA-CB	5.08	118.12	110.50
1	B	362	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	377	SER	CB-CA-C	5.00	119.61	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	376	THR	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3248	0	3249	32	0
1	B	3215	0	3209	28	0
2	A	53	0	31	1	0
2	B	53	0	31	3	0
3	A	44	0	26	1	0
3	B	44	0	26	3	0
4	A	12	0	6	1	0
4	B	12	0	6	1	0
5	A	58	0	0	1	0
5	B	51	0	0	0	0
All	All	6790	0	6584	62	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 5.

All (62) 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:175:ILE:HG23	1:A:179:LEU:HD12	1.48	0.95
1:B:331:LYS:O	1:B:335:SER:OG	2.00	0.78
1:A:287:GLU:OE2	1:A:291:PRO:HA	1.86	0.76
3:A:501:NAD:N1A	5:A:602:HOH:O	2.23	0.71
1:B:331:LYS:O	1:B:335:SER:CB	2.41	0.68
1:A:377:SER:HB3	1:A:378:ALA:HB2	1.83	0.61
1:A:200:MET:HB2	1:A:204:PHE:CD2	2.37	0.60
1:A:418:VAL:HG11	1:A:422:GLU:HB2	1.84	0.59
1:B:319:ALA:HB2	2:B:500:FAD:H5'2	1.85	0.58
1:A:175:ILE:HG23	1:A:179:LEU:CD1	2.29	0.58
1:B:372:ASP:HA	1:B:373:SER:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:GLU:O	1:A:407:ALA:HB3	2.04	0.57
1:A:344:TYR:CE2	1:A:346:PRO:HA	2.41	0.56
1:B:127:VAL:HG21	1:B:145:TYR:HB3	1.88	0.56
1:A:179:LEU:HD13	1:A:257:VAL:HG11	1.89	0.53
1:B:104:LYS:HD2	1:B:116:TYR:O	2.10	0.52
1:B:7:PHE:O	1:B:116:TYR:HA	2.11	0.51
1:B:331:LYS:O	1:B:335:SER:HB2	2.11	0.50
1:A:189:ASP:OD1	1:A:222:LYS:NZ	2.36	0.50
1:A:55:TYR:O	1:A:63:ARG:NH2	2.44	0.50
1:A:377:SER:HB3	1:A:378:ALA:CB	2.41	0.49
1:A:342:TYR:CE2	1:A:344:TYR:HB2	2.48	0.49
1:A:7:PHE:O	1:A:116:TYR:HA	2.12	0.49
1:A:123:THR:O	2:A:500:FAD:H8A	2.13	0.49
1:B:49:PRO:HB2	4:B:502:ASC:H5	1.93	0.49
1:A:4:GLU:HG3	1:A:113:THR:HG23	1.94	0.48
1:B:342:TYR:CE2	1:B:344:TYR:HB2	2.48	0.48
1:A:79:LEU:HB3	1:A:80:PRO:HD2	1.95	0.48
1:B:71:VAL:CG1	1:B:77:ARG:HG3	2.43	0.48
2:B:500:FAD:C4	3:B:501:NAD:C7N	2.92	0.48
1:A:19:GLY:HA3	1:A:69:VAL:HG21	1.95	0.48
1:B:142:ASN:HB2	1:B:240:VAL:HG12	1.96	0.48
1:A:377:SER:CB	1:A:378:ALA:HB2	2.45	0.47
1:B:31:LYS:HB2	1:B:34:GLU:OE1	2.14	0.47
1:B:372:ASP:HA	1:B:373:SER:CB	2.45	0.47
1:A:422:GLU:O	1:A:424:LEU:N	2.49	0.46
1:A:372:ASP:HA	1:A:373:SER:CB	2.46	0.46
1:A:377:SER:HB3	1:A:378:ALA:CA	2.46	0.46
1:A:175:ILE:CG2	1:A:179:LEU:HD12	2.35	0.46
1:B:37:ILE:HB	1:B:90:LEU:HD23	1.97	0.45
1:A:110:VAL:O	1:A:110:VAL:HG12	2.17	0.44
1:B:304:MET:CE	1:B:311:ARG:HD2	2.48	0.44
1:A:49:PRO:HB2	4:A:502:ASC:H5	1.98	0.44
1:A:162:LYS:HD2	1:A:254:ASP:HB3	1.99	0.44
1:B:174:TYR:HB3	3:B:501:NAD:C4N	2.47	0.44
1:B:340:VAL:HG12	1:B:341:GLU:O	2.17	0.44
1:B:334:GLU:CB	1:B:335:SER:HB2	2.48	0.44
1:A:304:MET:CE	1:A:344:TYR:HD2	2.30	0.43
1:A:377:SER:HB3	1:A:378:ALA:HA	2.00	0.43
1:B:55:TYR:O	1:B:63:ARG:NH2	2.51	0.43
1:A:215:TYR:CD1	1:A:355:LEU:HD11	2.54	0.43
1:B:209:ALA:O	1:B:213:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:TYR:CD2	3:B:501:NAD:C7N	3.02	0.42
1:A:418:VAL:HG11	1:A:422:GLU:CB	2.49	0.42
1:B:369:LEU:HD23	1:B:369:LEU:C	2.40	0.42
1:B:200:MET:N	1:B:201:PRO:CD	2.83	0.41
1:B:382:PHE:O	1:B:397:LEU:HD12	2.21	0.41
1:A:372:ASP:HA	1:A:373:SER:HB2	2.01	0.41
1:B:298:ASP:OD1	2:B:500:FAD:H5'1	2.20	0.41
1:A:287:GLU:HG3	1:A:294:TYR:CZ	2.56	0.41
1:B:106:LEU:HD11	1:B:119:LEU:HD13	2.02	0.41
1:B:265:LEU:HD23	1:B:265:LEU:HA	1.88	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	425/451 (94%)	392 (92%)	27 (6%)	6 (1%)	11	11
1	B	419/451 (93%)	387 (92%)	27 (6%)	5 (1%)	13	14
All	All	844/902 (94%)	779 (92%)	54 (6%)	11 (1%)	12	12

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	335	SER
1	A	289	SER
1	A	337	GLU
1	A	373	SER
1	B	373	SER
1	A	308	ASN
1	B	433	SER
1	A	268	LEU

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Mol	Chain	Res	Type
1	B	334	GLU
1	A	423	GLU
1	B	305	LYS

5.3.2 Protein sidechains ⓘ

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	334/353 (95%)	318 (95%)	16 (5%)	25	36
1	B	330/353 (94%)	303 (92%)	27 (8%)	11	14
All	All	664/706 (94%)	621 (94%)	43 (6%)	17	23

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	40	LYS
1	A	77	ARG
1	A	78	LEU
1	A	105	THR
1	A	127	VAL
1	A	136	GLN
1	A	144	LEU
1	A	185	ILE
1	A	249	SER
1	A	372	ASP
1	A	373	SER
1	A	422	GLU
1	A	424	LEU
1	A	426	LYS
1	A	429	LEU
1	B	6	HIS
1	B	30	VAL
1	B	31	LYS
1	B	40	LYS

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Mol	Chain	Res	Type
1	B	84	SER
1	B	85	GLU
1	B	86	LYS
1	B	89	GLU
1	B	107	THR
1	B	108	SER
1	B	113	THR
1	B	144	LEU
1	B	154	LYS
1	B	184	LYS
1	B	192	MET
1	B	202	ARG
1	B	222	LYS
1	B	249	SER
1	B	304	MET
1	B	334	GLU
1	B	338	SER
1	B	341	GLU
1	B	372	ASP
1	B	388	LYS
1	B	429	LEU
1	B	433	SER
1	B	434	LYS

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

Mol	Chain	Res	Type
1	A	318	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	FAD	B	500	-	51,58,58	1.78	14 (27%)	60,89,89	2.47	19 (31%)
3	NAD	A	501	-	42,48,48	1.16	3 (7%)	50,73,73	1.57	11 (22%)
4	ASC	B	502	-	12,12,12	2.73	1 (8%)	17,17,17	2.81	7 (41%)
4	ASC	A	502	-	12,12,12	2.53	1 (8%)	17,17,17	3.43	11 (64%)
3	NAD	B	501	-	42,48,48	1.23	5 (11%)	50,73,73	1.59	9 (18%)
2	FAD	A	500	-	51,58,58	1.77	13 (25%)	60,89,89	2.63	19 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	500	-	-	10/30/50/50	0/6/6/6
3	NAD	A	501	-	-	4/26/62/62	0/5/5/5
4	ASC	B	502	-	-	4/6/22/22	0/1/1/1
4	ASC	A	502	-	-	3/6/22/22	0/1/1/1
3	NAD	B	501	-	-	6/26/62/62	0/5/5/5
2	FAD	A	500	-	-	9/30/50/50	0/6/6/6

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	ASC	O4-C1	9.08	1.49	1.36
4	A	502	ASC	O4-C1	7.99	1.48	1.36
2	A	500	FAD	C4X-C10	6.65	1.45	1.38
2	B	500	FAD	C4X-C10	6.15	1.45	1.38
3	A	501	NAD	O4B-C1B	3.69	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	FAD	C2-N3	-3.63	1.31	1.38
2	A	500	FAD	C2-N3	-3.45	1.31	1.38
2	A	500	FAD	C6-C5X	-3.21	1.36	1.41
2	A	500	FAD	C2B-C1B	-2.99	1.49	1.53
2	B	500	FAD	C6-C5X	-2.93	1.37	1.41
3	B	501	NAD	C5A-C4A	2.92	1.48	1.40
2	A	500	FAD	C9A-C5X	2.84	1.48	1.42
3	B	501	NAD	O4D-C1D	2.74	1.44	1.41
2	B	500	FAD	C4-C4X	2.62	1.45	1.41
3	A	501	NAD	C5A-C4A	2.61	1.47	1.40
2	B	500	FAD	C2B-C1B	-2.49	1.50	1.53
2	A	500	FAD	C2-N1	-2.49	1.33	1.38
2	B	500	FAD	C4'-C3'	-2.47	1.48	1.53
2	B	500	FAD	C2-N1	-2.47	1.33	1.38
2	A	500	FAD	C4-C4X	2.44	1.45	1.41
2	B	500	FAD	P-O2P	-2.42	1.43	1.55
2	B	500	FAD	C9A-C5X	2.40	1.47	1.42
2	B	500	FAD	C5X-N5	-2.28	1.31	1.35
2	A	500	FAD	PA-O2A	-2.27	1.44	1.55
2	B	500	FAD	PA-O2A	-2.26	1.44	1.55
2	A	500	FAD	C2'-C3'	-2.24	1.49	1.53
2	A	500	FAD	C8-C7	2.23	1.46	1.40
2	A	500	FAD	C5A-N7A	-2.20	1.31	1.39
3	B	501	NAD	C2D-C1D	-2.20	1.50	1.53
2	B	500	FAD	C4A-N3A	-2.18	1.32	1.35
2	A	500	FAD	P-O2P	-2.16	1.45	1.55
3	B	501	NAD	O4B-C1B	2.16	1.44	1.41
3	A	501	NAD	O4D-C1D	2.13	1.44	1.41
2	A	500	FAD	C5X-N5	-2.12	1.31	1.35
2	B	500	FAD	C5'-C4'	2.07	1.54	1.51
3	B	501	NAD	C7N-N7N	2.07	1.36	1.33
2	B	500	FAD	C9-C9A	-2.00	1.36	1.40

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	FAD	C1'-N10-C9A	11.79	127.57	118.29
2	A	500	FAD	C4-N3-C2	7.61	121.57	115.14
4	A	502	ASC	C4-O4-C1	-7.12	101.22	109.25
2	B	500	FAD	C1'-C2'-C3'	6.88	129.02	109.79
2	B	500	FAD	C4-N3-C2	6.87	120.94	115.14
4	B	502	ASC	C4-O4-C1	-6.59	101.81	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	ASC	O4-C1-O1	6.23	128.61	121.25
4	B	502	ASC	O4-C1-O1	5.46	127.70	121.25
2	A	500	FAD	C5'-C4'-C3'	5.37	122.57	112.20
3	A	501	NAD	N3A-C2A-N1A	-5.07	120.75	128.68
2	B	500	FAD	C5X-C9A-N10	4.84	121.22	117.72
2	A	500	FAD	C9A-N10-C10	-4.83	115.58	121.91
2	B	500	FAD	C4-C4X-C10	-4.71	116.83	119.95
2	B	500	FAD	C1'-N10-C9A	4.51	121.84	118.29
2	B	500	FAD	C9A-N10-C10	-4.50	116.02	121.91
4	A	502	ASC	O4-C4-C5	4.44	124.56	110.04
2	A	500	FAD	C4-C4X-C10	-4.44	117.01	119.95
4	A	502	ASC	O1-C1-C2	-4.40	122.47	129.37
3	B	501	NAD	N3A-C2A-N1A	-4.32	121.93	128.68
2	B	500	FAD	P-O3P-PA	-3.99	119.15	132.83
2	B	500	FAD	C4A-C5A-N7A	-3.96	105.27	109.40
4	B	502	ASC	O4-C4-C5	3.94	122.90	110.04
4	A	502	ASC	O5-C5-C4	3.90	118.46	110.77
3	B	501	NAD	C2A-N1A-C6A	3.89	125.41	118.75
2	B	500	FAD	C1'-N10-C10	3.84	121.85	118.41
4	A	502	ASC	O4-C4-C3	-3.82	99.77	103.71
2	A	500	FAD	O4'-C4'-C5'	-3.77	101.43	109.92
3	B	501	NAD	C1B-N9A-C4A	-3.76	120.03	126.64
3	A	501	NAD	C2A-N1A-C6A	3.65	125.00	118.75
2	B	500	FAD	O3'-C3'-C2'	3.57	117.43	108.81
4	B	502	ASC	O1-C1-C2	-3.53	123.83	129.37
3	A	501	NAD	C3N-C7N-N7N	3.52	121.97	117.75
2	B	500	FAD	C4X-N5-C5X	3.49	120.26	116.77
2	B	500	FAD	C4'-C3'-C2'	3.48	120.59	113.36
3	B	501	NAD	O4B-C1B-C2B	3.46	111.98	106.93
2	A	500	FAD	C4X-C4-N3	-3.42	118.75	123.43
4	A	502	ASC	O3-C3-C2	-3.39	123.38	132.29
2	B	500	FAD	O5'-C5'-C4'	3.22	117.95	109.36
2	B	500	FAD	O3'-C3'-C4'	-3.17	101.15	108.81
3	A	501	NAD	O7N-C7N-N7N	-3.11	118.16	122.58
2	A	500	FAD	C5X-C9A-N10	3.05	119.93	117.72
3	B	501	NAD	C2D-C3D-C4D	3.04	108.55	102.64
2	B	500	FAD	C4X-C4-N3	-3.03	119.29	123.43
4	B	502	ASC	O4-C4-C3	-3.02	100.60	103.71
2	A	500	FAD	C1'-C2'-C3'	3.01	118.19	109.79
2	B	500	FAD	O4'-C4'-C3'	-2.93	101.97	109.10
2	B	500	FAD	N3A-C2A-N1A	-2.91	124.13	128.68
2	A	500	FAD	P-O3P-PA	-2.91	122.85	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	NAD	C4A-C5A-N7A	-2.80	106.48	109.40
2	A	500	FAD	N3A-C2A-N1A	-2.69	124.47	128.68
2	A	500	FAD	O2'-C2'-C3'	-2.68	102.59	109.10
2	A	500	FAD	O5'-C5'-C4'	-2.51	102.67	109.36
2	A	500	FAD	C4A-C5A-N7A	-2.42	106.88	109.40
4	A	502	ASC	O3-C3-C4	2.39	124.32	118.08
3	A	501	NAD	PN-O3-PA	-2.38	124.64	132.83
2	A	500	FAD	C6-C5X-N5	-2.33	116.48	119.05
4	B	502	ASC	C1-C2-C3	-2.32	104.85	107.80
3	A	501	NAD	O4B-C1B-C2B	2.31	110.31	106.93
3	A	501	NAD	C6N-N1N-C2N	-2.28	119.90	121.97
4	A	502	ASC	C5-C4-C3	-2.27	110.48	114.78
2	B	500	FAD	O4B-C1B-C2B	-2.24	103.65	106.93
3	B	501	NAD	PN-O3-PA	-2.24	125.15	132.83
2	A	500	FAD	O3'-C3'-C2'	-2.22	103.46	108.81
3	A	501	NAD	O4B-C4B-C3B	2.21	109.48	105.11
2	A	500	FAD	C4X-N5-C5X	2.20	118.97	116.77
2	A	500	FAD	O4B-C1B-C2B	-2.20	103.71	106.93
3	A	501	NAD	N6A-C6A-N1A	2.13	123.00	118.57
3	A	501	NAD	O2A-PA-O1A	2.12	122.72	112.24
4	A	502	ASC	C1-C2-C3	-2.11	105.11	107.80
3	B	501	NAD	C3N-C7N-N7N	2.07	120.24	117.75
4	A	502	ASC	O2-C2-C1	2.07	127.66	122.37
2	B	500	FAD	C4-C4X-N5	2.06	120.95	118.60
4	B	502	ASC	O5-C5-C4	2.06	114.83	110.77
2	A	500	FAD	C6-C5X-C9A	2.05	121.73	119.05
3	A	501	NAD	C3B-C2B-C1B	2.03	104.04	100.98
3	B	501	NAD	O2A-PA-O1A	2.00	122.13	112.24

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	FAD	C1'-C2'-C3'-O3'
2	B	500	FAD	C1'-C2'-C3'-C4'
2	B	500	FAD	O2'-C2'-C3'-O3'
2	B	500	FAD	C5'-O5'-P-O2P
3	A	501	NAD	C5B-O5B-PA-O1A
3	A	501	NAD	C3B-C4B-C5B-O5B
3	A	501	NAD	O4D-C1D-N1N-C2N
4	B	502	ASC	O4-C4-C5-C6
4	A	502	ASC	O4-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	B	501	NAD	C5B-O5B-PA-O1A
3	B	501	NAD	O4B-C4B-C5B-O5B
3	B	501	NAD	C3B-C4B-C5B-O5B
3	B	501	NAD	O4D-C1D-N1N-C6N
2	A	500	FAD	C2'-C1'-N10-C10
2	A	500	FAD	N10-C1'-C2'-O2'
2	A	500	FAD	N10-C1'-C2'-C3'
2	A	500	FAD	C2'-C3'-C4'-O4'
2	A	500	FAD	C2'-C3'-C4'-C5'
2	A	500	FAD	O3'-C3'-C4'-O4'
2	A	500	FAD	O4B-C4B-C5B-O5B
2	B	500	FAD	O2'-C2'-C3'-C4'
2	A	500	FAD	O3'-C3'-C4'-C5'
3	A	501	NAD	O4B-C4B-C5B-O5B
2	A	500	FAD	C3B-C4B-C5B-O5B
2	B	500	FAD	C5'-O5'-P-O3P
3	B	501	NAD	C5B-O5B-PA-O3
2	B	500	FAD	C5'-O5'-P-O1P
2	B	500	FAD	O4B-C4B-C5B-O5B
2	B	500	FAD	C3B-C4B-C5B-O5B
4	B	502	ASC	C4-C5-C6-O6
2	B	500	FAD	P-O3P-PA-O2A
3	B	501	NAD	PA-O3-PN-O1N
4	A	502	ASC	C3-C4-C5-O5
4	B	502	ASC	C3-C4-C5-C6
4	A	502	ASC	C3-C4-C5-C6
4	B	502	ASC	O5-C5-C6-O6

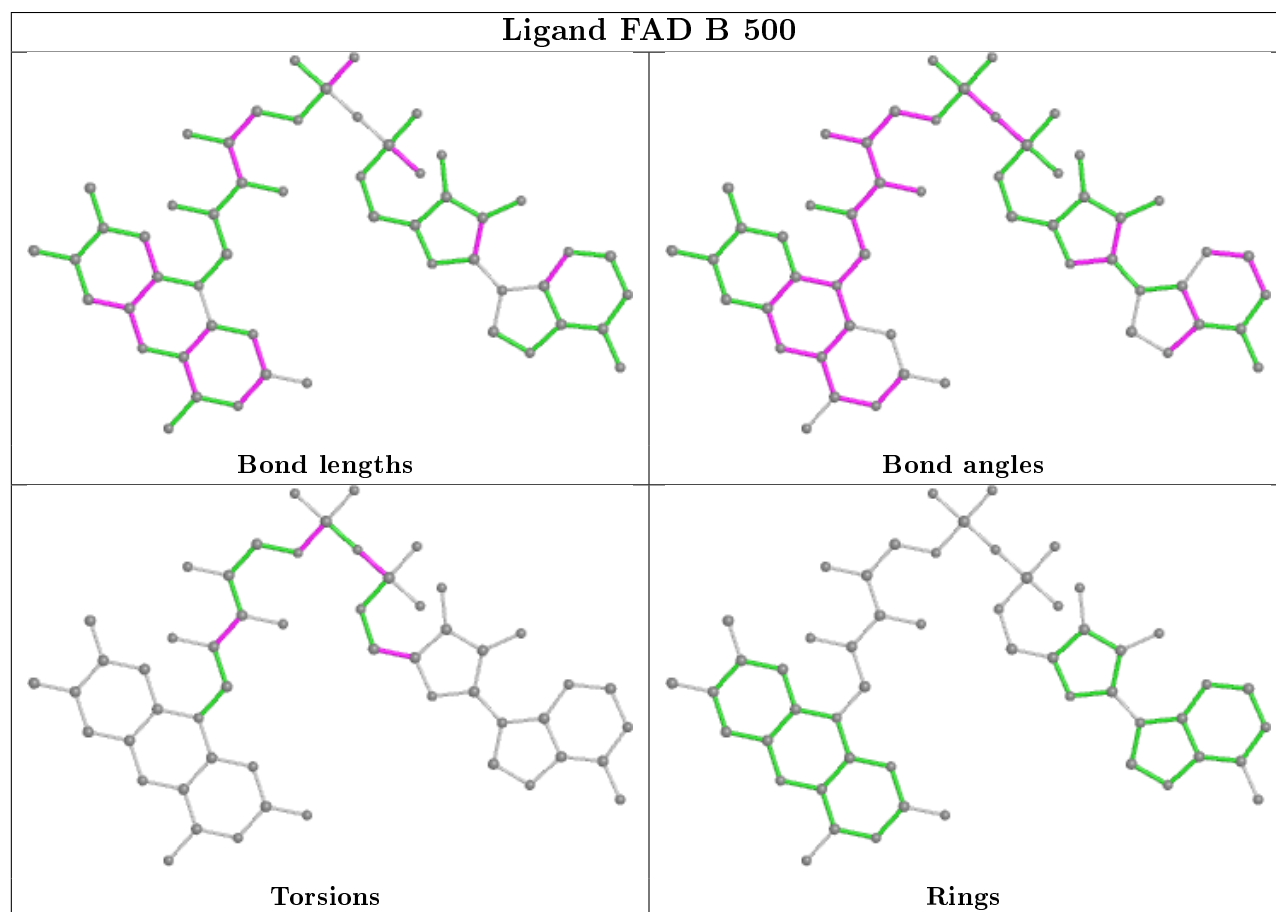
There are no ring outliers.

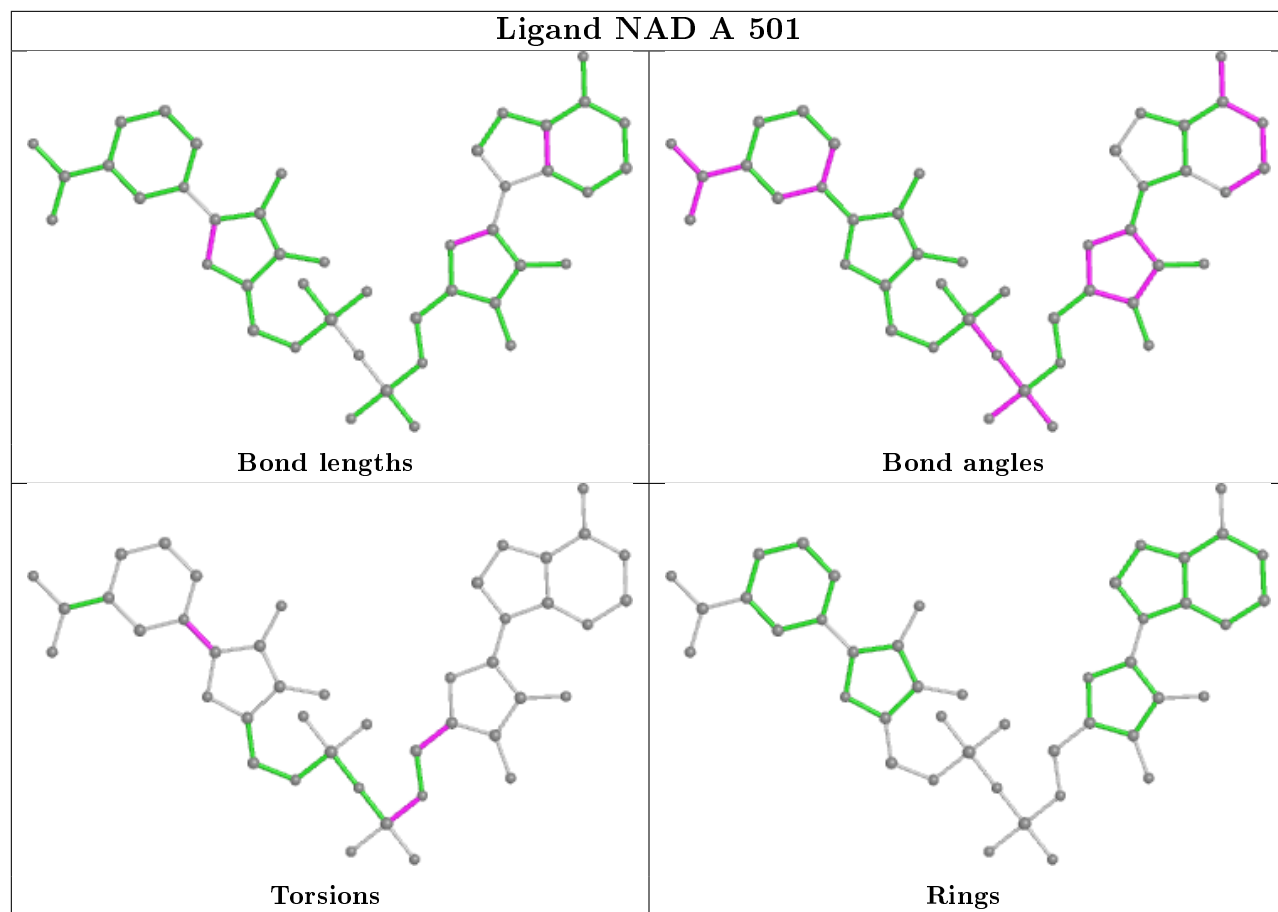
6 monomers are involved in 9 short contacts:

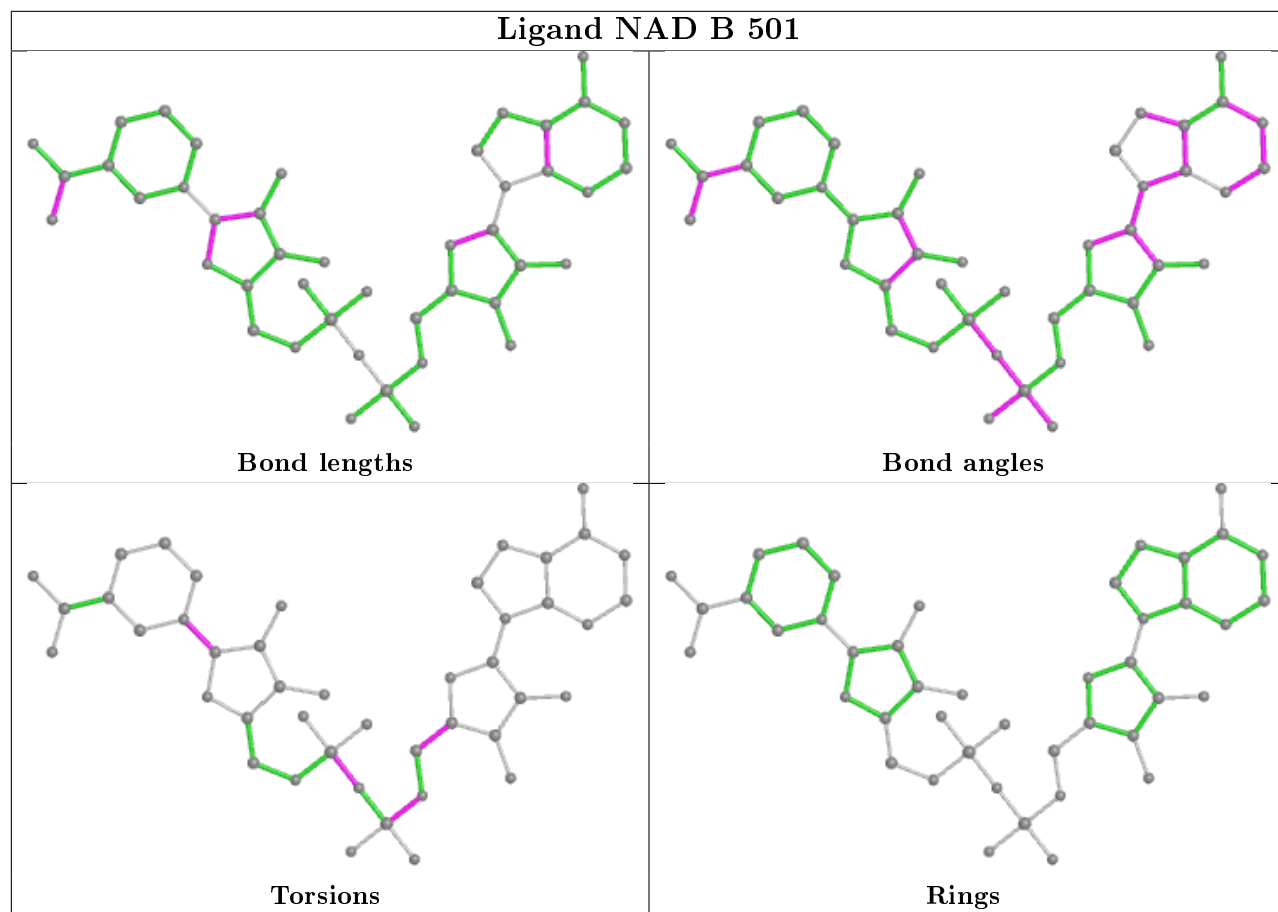
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	FAD	3	0
3	A	501	NAD	1	0
4	B	502	ASC	1	0
4	A	502	ASC	1	0
3	B	501	NAD	3	0
2	A	500	FAD	1	0

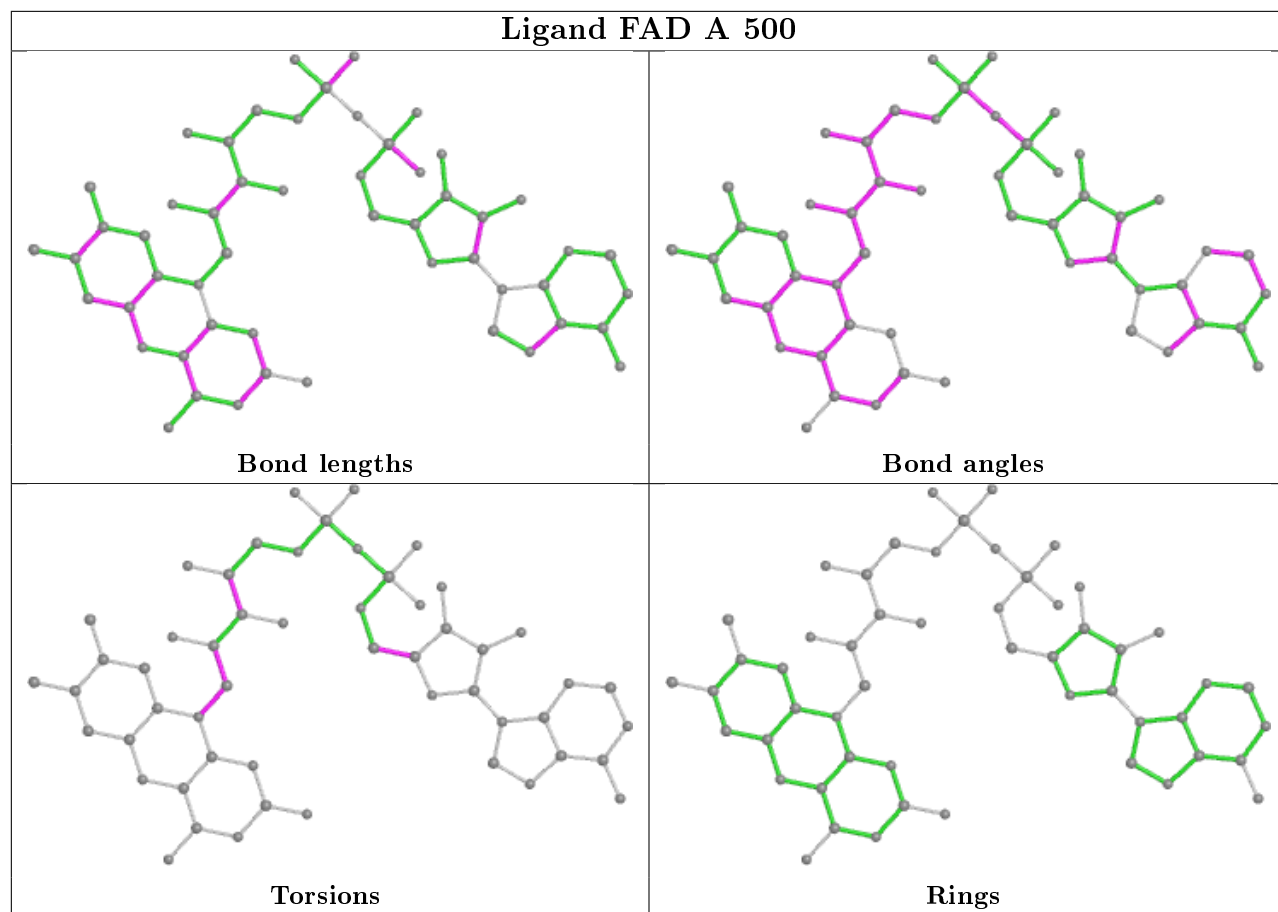
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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	429/451 (95%)	0.66	42 (9%) 7 10	51, 72, 113, 135	0
1	B	425/451 (94%)	0.55	34 (8%) 12 16	49, 70, 100, 138	0
All	All	854/902 (94%)	0.60	76 (8%) 9 13	49, 71, 107, 138	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	308	ASN	6.8
1	B	6	HIS	5.9
1	A	340	VAL	5.2
1	A	96	ILE	5.1
1	A	114	PHE	5.0
1	A	424	LEU	5.0
1	B	425	LYS	4.9
1	B	306	MET	4.9
1	A	283	ASP	4.9
1	B	392	VAL	4.8
1	A	430	GLN	4.6
1	B	434	LYS	4.6
1	A	97	VAL	4.4
1	A	413	LYS	4.1
1	A	423	GLU	4.1
1	A	427	GLU	4.0
1	B	338	SER	4.0
1	B	417	PRO	3.9
1	A	433	SER	3.4
1	A	273	VAL	3.4
1	A	422	GLU	3.3
1	A	432	ALA	3.2
1	B	432	ALA	3.2
1	A	285	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	428	GLY	3.1
1	A	315	HIS	3.0
1	A	160	GLN	3.0
1	B	115	THR	3.0
1	B	416	PRO	2.9
1	A	297	GLY	2.9
1	A	310	LEU	2.8
1	B	77	ARG	2.7
1	B	307	TYR	2.7
1	B	229	ALA	2.6
1	A	271	GLY	2.6
1	B	424	LEU	2.6
1	A	223	ILE	2.6
1	B	387	ILE	2.6
1	B	388	LYS	2.5
1	B	345	LEU	2.5
1	B	110	VAL	2.5
1	A	282	THR	2.5
1	B	257	VAL	2.5
1	A	146	LEU	2.5
1	A	341	GLU	2.4
1	B	97	VAL	2.4
1	A	378	ALA	2.4
1	A	6	HIS	2.4
1	A	113	THR	2.4
1	B	433	SER	2.3
1	B	430	GLN	2.3
1	A	238	GLY	2.3
1	B	39	SER	2.3
1	B	224	VAL	2.3
1	B	105	THR	2.2
1	B	409	ALA	2.2
1	A	390	GLY	2.2
1	B	260	VAL	2.2
1	A	333	LYS	2.2
1	B	364	VAL	2.2
1	A	286	PHE	2.2
1	B	102	ALA	2.1
1	A	426	LYS	2.1
1	A	329	ALA	2.1
1	A	107	THR	2.1
1	A	115	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	202	ARG	2.1
1	B	304	MET	2.1
1	A	105	THR	2.1
1	A	236	ALA	2.1
1	A	379	LYS	2.1
1	B	188	PHE	2.0
1	A	280	ILE	2.0
1	A	435	ILE	2.0
1	B	413	LYS	2.0
1	A	59	GLN	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 monosaccharides in this entry.

6.4 Ligands [i](#)

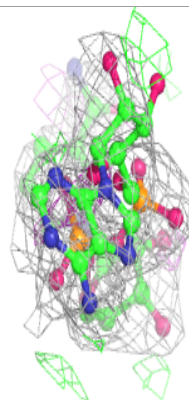
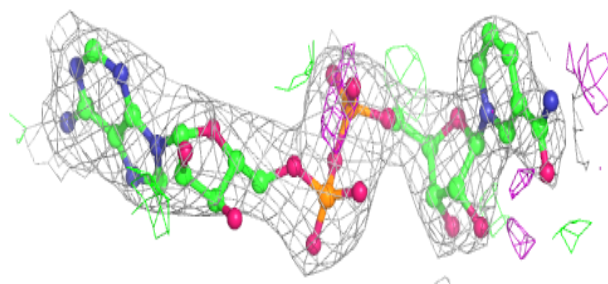
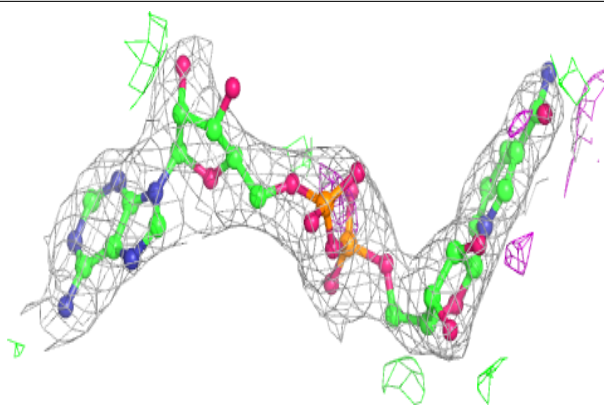
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ASC	B	502	12/12	0.66	0.35	73,86,95,97	0
4	ASC	A	502	12/12	0.84	0.19	71,78,90,90	0
3	NAD	B	501	44/44	0.88	0.19	50,71,102,109	0
3	NAD	A	501	44/44	0.91	0.18	61,71,99,127	0
2	FAD	B	500	53/53	0.94	0.13	17,22,27,30	0
2	FAD	A	500	53/53	0.94	0.13	17,22,27,30	0

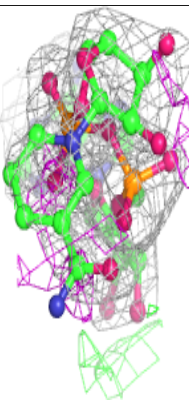
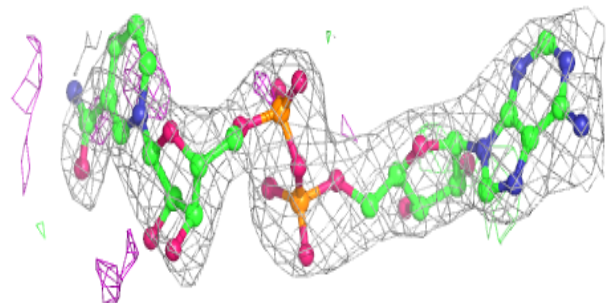
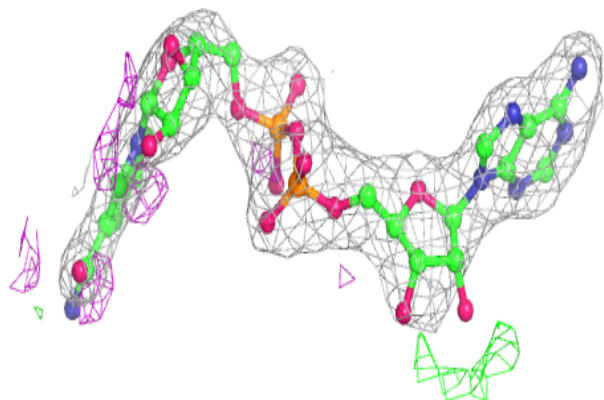
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD 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)

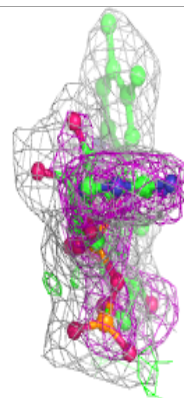
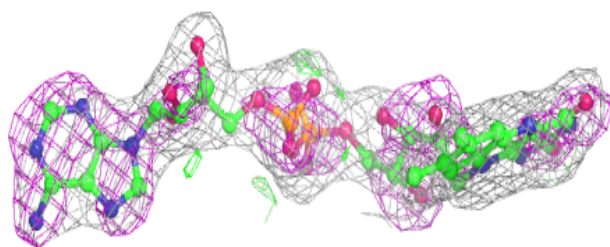
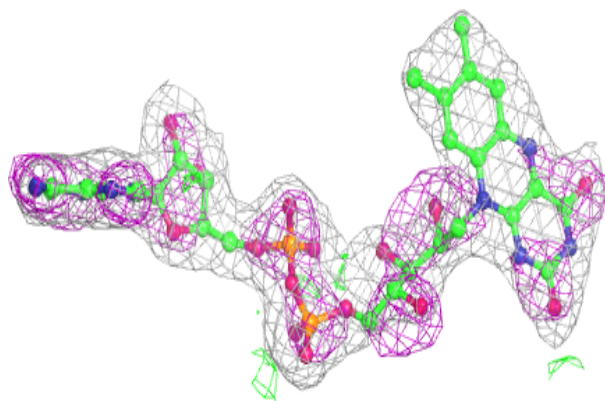
**Electron density around NAD A 501:**

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

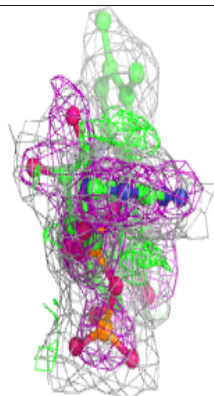
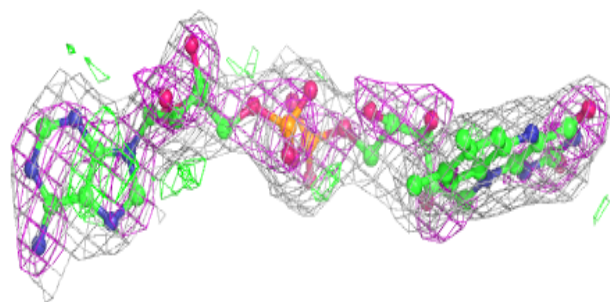
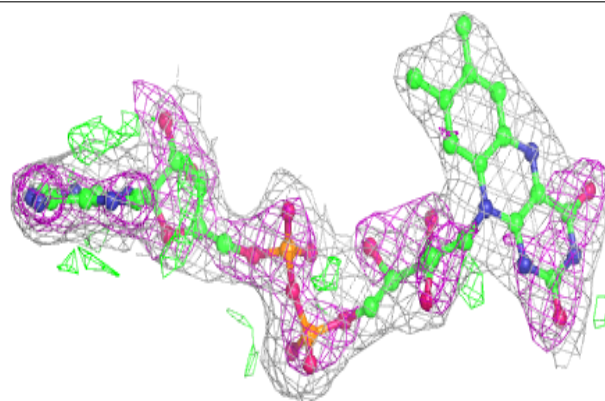


Electron density around FAD B 500:

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

**Electron density around FAD A 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.