



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:46 PM UTC

PDB ID : 5JCN / pdb_00005jcn
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 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

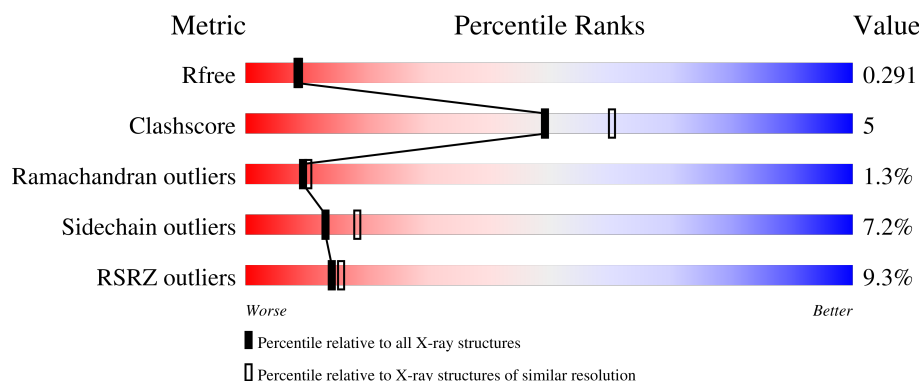
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	451	8% 79% 15% • 5%
1	B	451	10% 78% 14% • 6%

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:

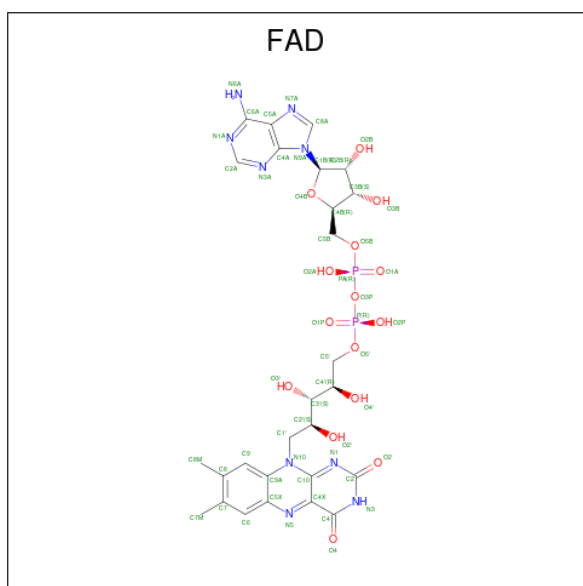
Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP Q652L6
A	-14	HIS	-	expression tag	UNP Q652L6
A	-13	HIS	-	expression tag	UNP Q652L6
A	-12	HIS	-	expression tag	UNP Q652L6
A	-11	HIS	-	expression tag	UNP Q652L6
A	-10	HIS	-	expression tag	UNP Q652L6
A	-9	ALA	-	expression tag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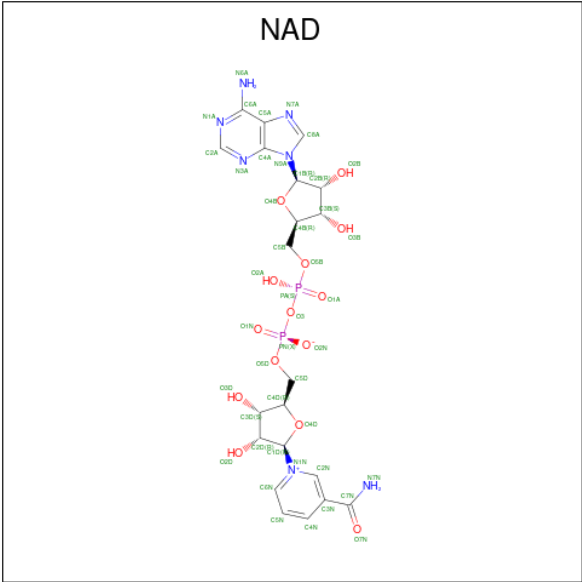
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	GLU	-	expression tag	UNP Q652L6
B	-6	ASN	-	expression tag	UNP Q652L6
B	-5	LEU	-	expression tag	UNP Q652L6
B	-4	TYR	-	expression tag	UNP Q652L6
B	-3	PHE	-	expression tag	UNP Q652L6
B	-2	GLN	-	expression tag	UNP Q652L6
B	-1	GLY	-	expression tag	UNP Q652L6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

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



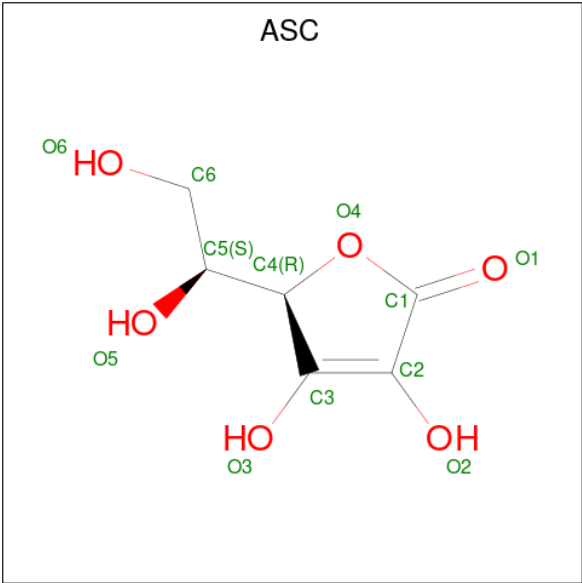
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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 (CCD ID: 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:

8% 79% 15% 5%

HIS HIS HIS HIS HIS HIS HIS SER SER ASN LEU TYR PHE GLN GLY MET MET ALA ALA E4 K5 H6 F7 G19 G29 V30 K31 P32 K40 V43 V49 K53 G54 Y55 R63 V69 G72 R77 L78 L79 P80 I91 I96 T105 V110 T113 F114 T115 Y116 T123 G124 V127 H141 H142 I143 L144 Y145 L146 Y156 Q160 A161 K162 G172 G173 Y174 I175 L179 I186 D189 F194 M200 F204 Y215 K222 G238 N247 G246 S249 D254 V257 L268 T282 D283 F287 T288 S289 V290 P291 Y294 G297 D298 N304 N308 E314 H315 Y316 D317 H318 A319 V327 I330 E337 S338 Y342 D343 Y344 L345 P346 Y347 F348 L355 D372 S373 T376 S377 A378 D403 E404 A407 K413 V418 A421 A422 E423 L424 Y425

Chain B:

10% 78% 14% 6%

Label	Category
L397	Green
N405	Red
A409	Red
K413	Red
P416	Red
P417	Red
VAL	Grey
ALA	Grey
ASN	Grey
ILE	Grey
E422	Green
E423	Green
K425	Green
L424	Red
LYS	Grey
GLU	Grey
G428	Red
L429	Green
A432	Green
S433	Green
K434	Green
ILE	Grey
A209	Yellow
E213	Green
K222	Yellow
A229	Green
A234	Red
V240	Yellow
S249	Yellow
E252	Yellow
V257	Green
L285	Yellow
D298	Yellow
F302	Green
P303	Green
M304	Orange
K305	Yellow
N308	Green
R311	Yellow
H315	Red
A319	Yellow
K331	Yellow
E334	Red
S335	Yellow
G336	Green
E337	Green
S338	Green
V339	Green
V340	Orange
E341	Yellow
Y342	Green
I343	Green
I344	Green
L345	Green
I368	Yellow
L369	Yellow
D372	Red
S373	Orange
F382	Yellow
I387	Green
V388	Green
E85	Yellow
E89	Green
L90	Yellow
T94	Red
K104	Yellow
T105	Green
T107	Yellow
S108	Yellow
A109	Green
V110	Yellow
T113	Red
F114	Green
T115	Red
Y116	Yellow
L119	Yellow
V127	Orange
D132	Yellow
F133	Green
G134	Red
G137	Yellow
S140	Yellow
N141	Green
N142	Yellow
I143	Red
L144	Yellow
Y145	Yellow
D150	Green
K154	Yellow
A167	Green
V168	Green
I169	Red
Y174	Yellow
K184	Yellow
I185	Yellow
F188	Red
V193	Orange
C199	Green
M200	Orange
P201	Yellow
R202	Yellow
W83	Green
Y84	Green
HIS	Grey
HIS	Grey
HIS	Grey
HIS	Grey
HIS	Grey
ALA	Grey
SER	Grey
GLU	Grey
ASN	Grey
LEU	Grey
TYR	Grey
PHE	Grey
GLN	Grey
GLY	Grey
MET	Grey
ALA	Grey
ALA	Grey
SER	Grey
E4	Green
K5	Red
H6	Red
F7	Yellow
V10	Green
I11	Red
L12	Green
G13	Red
A26	Red
K27	Red
V30	Yellow
K30	Orange
E34	Yellow
L35	Green
A36	Red
I37	Yellow
I38	Green
S39	Red
K40	Yellow
P49	Yellow
Y55	Yellow
R63	Yellow
V69	Yellow
C70	Green
V71	Yellow
R77	Red
L78	Green
L79	Red
W82	Red
Y83	Green

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 50.00 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.29) 99.2 (50.00-2.29)	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 (Not available) , 0.291	Depositor DCC
R_{free} test set	1936 reflections (4.67%)	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)	0.36 , 61.7	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: NAD, FAD, ASC

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	1.06	3/3317 (0.1%)	1.14	8/4487 (0.2%)
1	B	1.04	1/3283 (0.0%)	1.14	12/4440 (0.3%)
All	All	1.05	4/6600 (0.1%)	1.14	20/8927 (0.2%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	LYS	CA-C	7.36	1.55	1.52
1	A	43	VAL	CA-C	-5.29	1.47	1.52
1	B	11	ILE	CA-C	-5.28	1.46	1.52
1	A	114	PHE	N-CA	5.13	1.52	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	ASP	N-CA-C	-10.15	100.65	113.43
1	B	372	ASP	CA-C-N	7.98	136.06	121.70
1	B	372	ASP	C-N-CA	7.98	136.06	121.70
1	A	372	ASP	CA-C-N	7.72	135.60	121.70
1	A	372	ASP	C-N-CA	7.72	135.60	121.70
1	B	334	GLU	CA-C-N	6.46	133.32	121.70
1	B	334	GLU	C-N-CA	6.46	133.32	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	GLU	N-CA-C	-6.01	101.59	110.48
1	B	337	GLU	N-CA-C	6.01	118.05	110.24
1	B	69	VAL	CA-C-O	-5.69	116.39	121.97
1	A	315	HIS	N-CA-C	5.67	118.69	109.06
1	A	403	ASP	N-CA-C	-5.63	105.05	111.07
1	A	317	ASP	N-CA-C	-5.57	105.11	111.07
1	A	143	ILE	N-CA-C	-5.51	99.22	107.37
1	B	200	MET	CA-C-N	5.44	125.26	119.28
1	B	200	MET	C-N-CA	5.44	125.26	119.28
1	A	63	ARG	NE-CZ-NH2	-5.32	114.41	119.20
1	A	194	PHE	N-CA-C	5.29	114.93	108.11
1	B	208	ILE	N-CA-C	-5.25	105.38	110.42
1	B	193	VAL	CB-CA-C	-5.03	103.13	110.62

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	38	0
1	B	3215	0	3209	31	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	71	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 (71) 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
1:B:304:MET:HE3	1:B:311:ARG:HD2	1.72	0.71
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
1:A:404:GLU:O	1:A:407:ALA:HB3	2.04	0.57
1:A:174:TYR:CD2	1:A:200:MET:HE1	2.40	0.56
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:55:TYR:O	1:A:63:ARG:NH2	2.44	0.50
1:A:189:ASP:OD1	1:A:222:LYS:NZ	2.36	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
1:A:174:TYR:CG	1:A:200:MET:HE1	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:369:LEU:C	1:B:369:LEU:HD23	2.40	0.46
1:B:37:ILE:HB	1:B:90:LEU:HD23	1.97	0.45
1:A:110:VAL:HG12	1:A:110:VAL:O	2.17	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:247:ASN:OD1	1:A:247:ASN:C	2.62	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
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:A:31:LYS:O	1:A:32:PRO:C	2.61	0.41
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:A:173:GLY:C	1:A:200:MET:HE2	2.46	0.41
1:B:137:GLY:O	1:B:140:SER:OG	2.34	0.41
1:B:265:LEU:HD23	1:B:265:LEU:HA	1.88	0.41
1:B:304:MET:CE	1:B:311:ARG:HD2	2.48	0.40
1:A:304:MET:HE1	1:A:344:TYR:HD2	1.86	0.40
1:B:432:ALA:C	1:B:434:LYS:H	2.29	0.40

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%)	9	9
1	B	419/451 (93%)	387 (92%)	27 (6%)	5 (1%)	10	12
All	All	844/902 (94%)	779 (92%)	54 (6%)	11 (1%)	9	10

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
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%)	317 (95%)	17 (5%)	21	32
1	B	330/353 (94%)	299 (91%)	31 (9%)	8	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	664/706 (94%)	616 (93%)	48 (7%)	13	18

All (48) 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	144	LEU
1	A	185	ILE
1	A	249	SER
1	A	287	GLU
1	A	314	GLU
1	A	372	ASP
1	A	413	LYS
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
1	B	84	SER
1	B	85	GLU
1	B	89	GLU
1	B	107	THR
1	B	108	SER
1	B	110	VAL
1	B	113	THR
1	B	127	VAL
1	B	144	LEU
1	B	154	LYS
1	B	184	LYS
1	B	185	ILE
1	B	193	VAL
1	B	202	ARG
1	B	222	LYS
1	B	249	SER

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Mol	Chain	Res	Type
1	B	304	MET
1	B	334	GLU
1	B	338	SER
1	B	341	GLU
1	B	368	ILE
1	B	372	ASP
1	B	388	LYS
1	B	422	GLU
1	B	429	LEU
1	B	433	SER
1	B	434	LYS

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

Mol	Chain	Res	Type
1	A	141	ASN
1	A	315	HIS
1	B	186	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 oligosaccharides 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
3	NAD	B	501	-	46,48,48	1.46	6 (13%)	64,73,73	1.84	16 (25%)
2	FAD	A	500	-	58,58,58	1.82	17 (29%)	85,89,89	1.92	24 (28%)
3	NAD	A	501	-	46,48,48	1.39	6 (13%)	64,73,73	1.85	15 (23%)
4	ASC	B	502	-	12,12,12	2.56	1 (8%)	17,17,17	2.83	7 (41%)
2	FAD	B	500	-	58,58,58	2.00	18 (31%)	85,89,89	2.12	25 (29%)
4	ASC	A	502	-	12,12,12	2.37	1 (8%)	17,17,17	3.47	11 (64%)

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
3	NAD	B	501	-	-	6/30/62/62	0/5/5/5
2	FAD	A	500	-	-	9/34/50/50	0/6/6/6
3	NAD	A	501	-	-	4/30/62/62	0/5/5/5
4	ASC	B	502	-	-	4/6/22/22	0/1/1/1
2	FAD	B	500	-	-	10/34/50/50	0/6/6/6
4	ASC	A	502	-	-	3/6/22/22	0/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	ASC	O4-C1	8.46	1.49	1.36
4	A	502	ASC	O4-C1	7.45	1.48	1.36
3	B	501	NAD	C5A-C4A	5.36	1.48	1.39
3	A	501	NAD	C5A-C4A	4.91	1.47	1.39
2	B	500	FAD	C4-N3	-4.42	1.30	1.38
2	A	500	FAD	C9A-C5X	4.40	1.48	1.41
2	B	500	FAD	C5X-N5	-4.29	1.31	1.39
2	B	500	FAD	PA-O3P	-4.21	1.55	1.59
2	A	500	FAD	C5X-N5	-4.14	1.31	1.39
2	A	500	FAD	C4-N3	-4.06	1.31	1.38
2	B	500	FAD	P-O3P	-4.06	1.55	1.59
2	A	500	FAD	C5A-N7A	-4.03	1.31	1.39
2	B	500	FAD	C9A-C5X	3.84	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	FAD	C2-N3	-3.64	1.31	1.39
2	B	500	FAD	C5A-N7A	-3.54	1.32	1.39
2	A	500	FAD	C2-N3	-3.48	1.31	1.39
2	B	500	FAD	C1'-C2'	3.21	1.57	1.52
2	A	500	FAD	P-O3P	-3.19	1.56	1.59
2	B	500	FAD	C4A-N9A	-3.14	1.31	1.37
2	A	500	FAD	C5A-C4A	3.13	1.44	1.39
3	B	501	NAD	O4D-C1D	3.05	1.44	1.40
2	A	500	FAD	PA-O3P	-3.04	1.56	1.59
3	B	501	NAD	C5A-C6A	2.96	1.49	1.41
2	B	500	FAD	C5A-C4A	2.94	1.44	1.39
2	B	500	FAD	C8A-N9A	-2.91	1.32	1.37
3	B	501	NAD	C4A-N9A	-2.80	1.31	1.37
2	A	500	FAD	C4A-N9A	-2.74	1.32	1.37
3	B	501	NAD	C8A-N7A	2.69	1.36	1.31
2	A	500	FAD	C8A-N9A	-2.64	1.33	1.37
2	B	500	FAD	C4'-C3'	-2.64	1.48	1.53
2	B	500	FAD	P-O2P	-2.46	1.43	1.55
3	A	501	NAD	PA-O3	2.45	1.62	1.59
3	A	501	NAD	O4D-C1D	2.41	1.44	1.40
2	A	500	FAD	C2'-C3'	-2.39	1.49	1.53
2	B	500	FAD	C5A-C6A	2.35	1.47	1.41
2	A	500	FAD	PA-O2A	-2.30	1.44	1.55
2	B	500	FAD	PA-O2A	-2.30	1.44	1.55
2	A	500	FAD	C8-C7	2.29	1.46	1.40
3	A	501	NAD	C4A-N9A	-2.28	1.32	1.37
3	A	501	NAD	C5A-C6A	2.26	1.47	1.41
2	A	500	FAD	P-O2P	-2.20	1.45	1.55
3	B	501	NAD	C7N-N7N	2.15	1.36	1.33
2	B	500	FAD	C5'-C4'	2.14	1.54	1.51
2	B	500	FAD	C9-C8	-2.13	1.36	1.39
3	A	501	NAD	C4N-C3N	2.11	1.42	1.39
2	A	500	FAD	C6-C7	-2.07	1.36	1.39
2	B	500	FAD	C2'-C3'	2.07	1.57	1.53
2	A	500	FAD	C6-C5X	-2.06	1.36	1.40
2	A	500	FAD	C5A-C6A	2.04	1.46	1.41

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	ASC	C4-O4-C1	-7.35	101.22	109.27
2	B	500	FAD	C1'-C2'-C3'	7.14	129.02	109.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	ASC	C4-O4-C1	-6.81	101.81	109.27
2	B	500	FAD	C5A-C4A-N3A	-6.18	118.20	126.72
2	A	500	FAD	C5A-C4A-N3A	-5.74	118.81	126.72
4	A	502	ASC	O4-C1-O1	5.57	128.61	121.27
2	A	500	FAD	C5'-C4'-C3'	5.49	122.57	112.22
3	A	501	NAD	N3A-C2A-N1A	-5.17	120.75	128.58
3	B	501	NAD	C4A-N9A-C8A	5.10	111.09	105.74
4	B	502	ASC	O4-C1-O1	4.88	127.70	121.27
4	A	502	ASC	O4-C4-C5	4.65	124.56	110.07
2	B	500	FAD	C4A-C5A-N7A	-4.64	105.27	110.58
3	A	501	NAD	C5A-C4A-N3A	-4.62	120.36	126.72
2	A	500	FAD	N3A-C4A-N9A	4.59	134.98	127.17
4	A	502	ASC	O1-C1-C2	-4.58	122.47	129.33
3	A	501	NAD	N3A-C4A-N9A	4.57	134.94	127.17
3	B	501	NAD	N3A-C2A-N1A	-4.40	121.93	128.58
2	B	500	FAD	C4'-C3'-C2'	4.22	120.59	113.57
3	B	501	NAD	O4B-C1B-N9A	-4.20	100.01	108.09
2	B	500	FAD	N3A-C4A-N9A	4.12	134.18	127.17
4	B	502	ASC	O4-C4-C5	4.12	122.90	110.07
4	A	502	ASC	O5-C5-C4	4.07	118.46	110.74
3	B	501	NAD	C2A-N1A-C6A	4.06	125.41	118.73
4	A	502	ASC	O4-C4-C3	-3.98	99.77	103.76
2	A	500	FAD	O4'-C4'-C5'	-3.88	101.43	109.99
2	B	500	FAD	C2A-N3A-C4A	3.86	121.26	111.83
3	A	501	NAD	C4A-N9A-C8A	3.82	109.75	105.74
3	A	501	NAD	C2A-N1A-C6A	3.81	125.00	118.73
3	A	501	NAD	C2A-N3A-C4A	3.75	121.00	111.83
2	B	500	FAD	O3'-C3'-C2'	3.74	117.43	108.93
4	B	502	ASC	O1-C1-C2	-3.67	123.83	129.33
2	B	500	FAD	C5X-C9A-N10	3.60	121.22	117.97
3	B	501	NAD	C4A-C5A-N7A	-3.59	106.48	110.58
2	A	500	FAD	C1'-N10-C9A	3.57	127.57	120.63
4	A	502	ASC	O3-C3-C2	-3.52	123.38	132.40
2	A	500	FAD	C2'-C1'-N10	3.51	126.81	110.20
3	A	501	NAD	C3N-C7N-N7N	3.44	121.97	117.74
3	B	501	NAD	C5A-C4A-N3A	-3.43	121.99	126.72
2	B	500	FAD	O3'-C3'-C4'	-3.42	101.15	108.93
2	A	500	FAD	C9A-N10-C10	-3.39	115.58	120.75
2	A	500	FAD	C2A-N3A-C4A	3.29	119.87	111.83
2	A	500	FAD	C4X-C10-N10	3.28	121.18	116.48
3	B	501	NAD	N9A-C8A-N7A	-3.26	109.31	113.94
3	B	501	NAD	N3A-C4A-N9A	3.26	132.71	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	FAD	C4A-C5A-N7A	-3.24	106.88	110.58
2	B	500	FAD	C5A-N7A-C8A	3.22	108.52	103.45
2	B	500	FAD	O5'-C5'-C4'	3.22	117.95	109.36
4	B	502	ASC	O4-C4-C3	-3.15	100.60	103.76
2	A	500	FAD	C1'-C2'-C3'	3.15	118.19	109.66
2	B	500	FAD	O4'-C4'-C3'	-3.11	101.97	109.25
2	B	500	FAD	C9A-N10-C10	-3.11	116.02	120.75
3	A	501	NAD	O7N-C7N-N7N	-3.08	118.16	122.62
3	B	501	NAD	C2D-C3D-C4D	3.07	108.55	102.61
2	B	500	FAD	C4X-C10-N1	-2.98	117.29	124.59
2	B	500	FAD	N3A-C2A-N1A	-2.94	124.13	128.58
2	A	500	FAD	C4X-C10-N1	-2.89	117.51	124.59
3	B	501	NAD	C6A-C5A-N7A	2.87	137.62	132.09
3	B	501	NAD	C2A-N3A-C4A	2.87	118.83	111.83
2	A	500	FAD	O2'-C2'-C3'	-2.84	102.59	109.25
3	B	501	NAD	C4A-N9A-C1B	-2.82	120.03	126.63
3	B	501	NAD	C5A-N7A-C8A	2.77	107.80	103.45
2	A	500	FAD	C5A-N7A-C8A	2.72	107.73	103.45
2	A	500	FAD	N3A-C2A-N1A	-2.72	124.47	128.58
3	A	501	NAD	O3-PA-O1A	-2.67	102.66	110.70
2	B	500	FAD	C4X-C10-N10	2.67	120.30	116.48
2	B	500	FAD	C4-N3-C2	-2.65	120.94	125.64
2	B	500	FAD	C6A-C5A-N7A	2.55	137.00	132.09
2	A	500	FAD	O5'-C5'-C4'	-2.51	102.67	109.36
3	B	501	NAD	O4B-C1B-C2B	2.51	111.98	106.62
4	A	502	ASC	O3-C3-C4	2.49	124.32	117.99
2	B	500	FAD	N9A-C8A-N7A	-2.45	110.46	113.94
2	B	500	FAD	C10-N1-C2	2.45	122.15	116.85
2	A	500	FAD	O3'-C3'-C2'	-2.41	103.46	108.93
2	A	500	FAD	C4A-N9A-C8A	2.39	108.24	105.74
4	B	502	ASC	C1-C2-C3	-2.38	104.85	107.77
2	B	500	FAD	C4X-C4-N3	2.37	119.29	113.25
2	B	500	FAD	O4-C4-C4X	-2.37	120.28	126.53
2	A	500	FAD	C10-N1-C2	2.35	121.94	116.85
2	B	500	FAD	C9A-C5X-N5	-2.35	119.96	122.45
3	A	501	NAD	C6N-N1N-C2N	-2.33	119.90	121.88
4	A	502	ASC	C5-C4-C3	-2.31	110.48	114.71
2	A	500	FAD	C4-N3-C2	-2.29	121.57	125.64
2	B	500	FAD	C4A-N9A-C8A	2.28	108.14	105.74
3	A	501	NAD	O2A-PA-O3	2.28	113.43	107.27
2	A	500	FAD	O4-C4-C4X	-2.24	120.61	126.53
4	A	502	ASC	O2-C2-C1	2.23	127.66	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NAD	O2A-PA-O1A	2.21	122.72	112.44
3	A	501	NAD	O4B-C4B-C3B	2.18	109.48	105.15
2	A	500	FAD	C5X-C9A-N10	2.17	119.93	117.97
4	A	502	ASC	C1-C2-C3	-2.17	105.11	107.77
2	A	500	FAD	C4X-C4-N3	2.16	118.75	113.25
4	B	502	ASC	O5-C5-C4	2.16	114.83	110.74
3	A	501	NAD	C4A-C5A-N7A	-2.16	108.12	110.58
2	A	500	FAD	N9A-C8A-N7A	-2.12	110.94	113.94
3	B	501	NAD	O2A-PA-O1A	2.08	122.13	112.44
3	A	501	NAD	N6A-C6A-N1A	2.08	123.00	118.38
3	B	501	NAD	C3N-C7N-N7N	2.03	120.24	117.74
2	B	500	FAD	O2'-C2'-C3'	-2.01	104.54	109.25

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	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
2	B	500	FAD	C5'-O5'-P-O3P
3	A	501	NAD	C5B-O5B-PA-O1A
3	A	501	NAD	C3B-C4B-C5B-O5B
3	A	501	NAD	O4D-C1D-N1N-C2N
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
4	A	502	ASC	O4-C4-C5-C6
4	B	502	ASC	O4-C4-C5-C6
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	A	500	FAD	O4B-C4B-C5B-O5B

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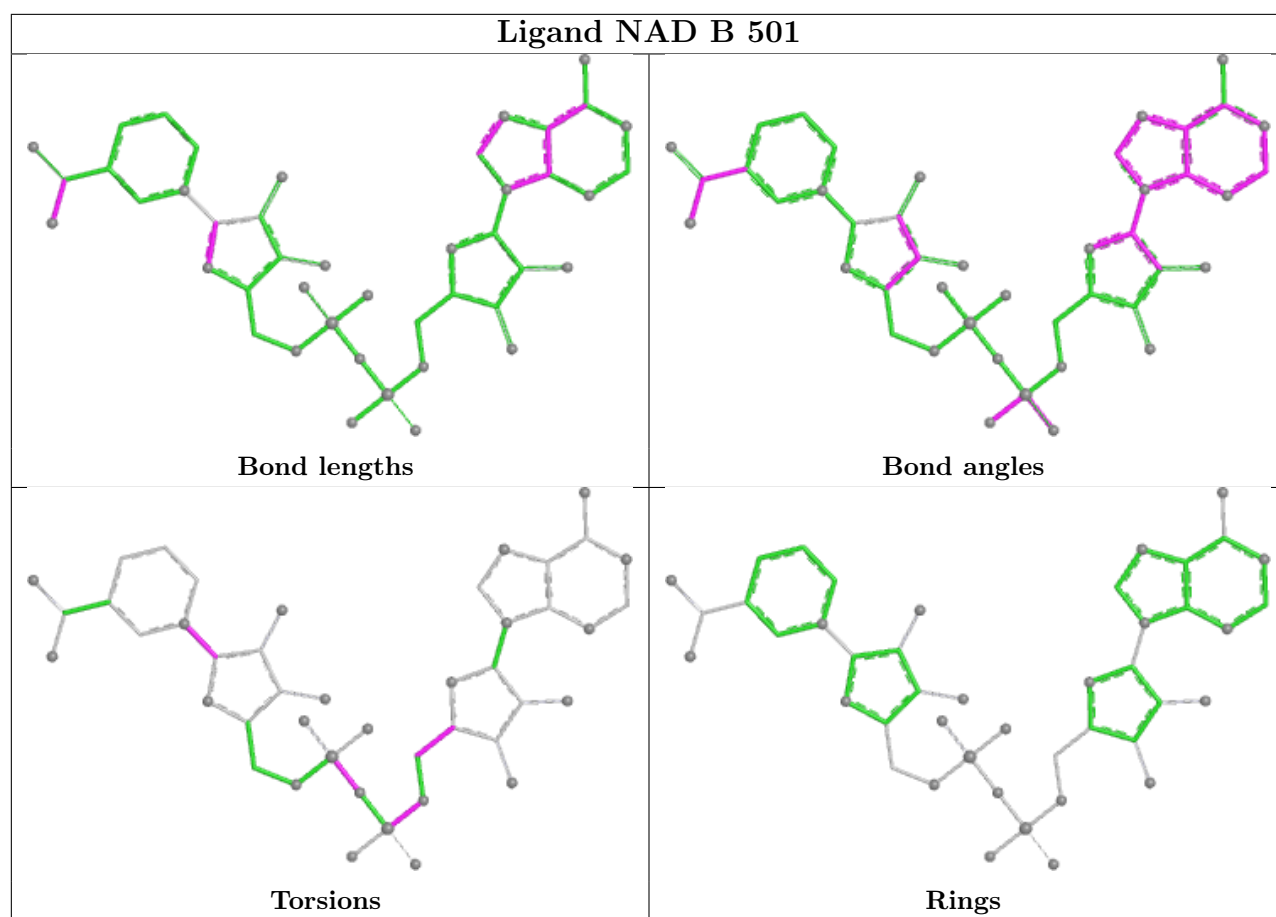
Mol	Chain	Res	Type	Atoms
2	B	500	FAD	C5'-O5'-P-O1P
3	B	501	NAD	C5B-O5B-PA-O3
2	B	500	FAD	O4B-C4B-C5B-O5B
4	B	502	ASC	C4-C5-C6-O6
4	A	502	ASC	C3-C4-C5-O5
2	B	500	FAD	P-O3P-PA-O2A
3	B	501	NAD	PA-O3-PN-O1N
4	A	502	ASC	C3-C4-C5-C6
4	B	502	ASC	C3-C4-C5-C6
2	B	500	FAD	C3B-C4B-C5B-O5B
4	B	502	ASC	O5-C5-C6-O6

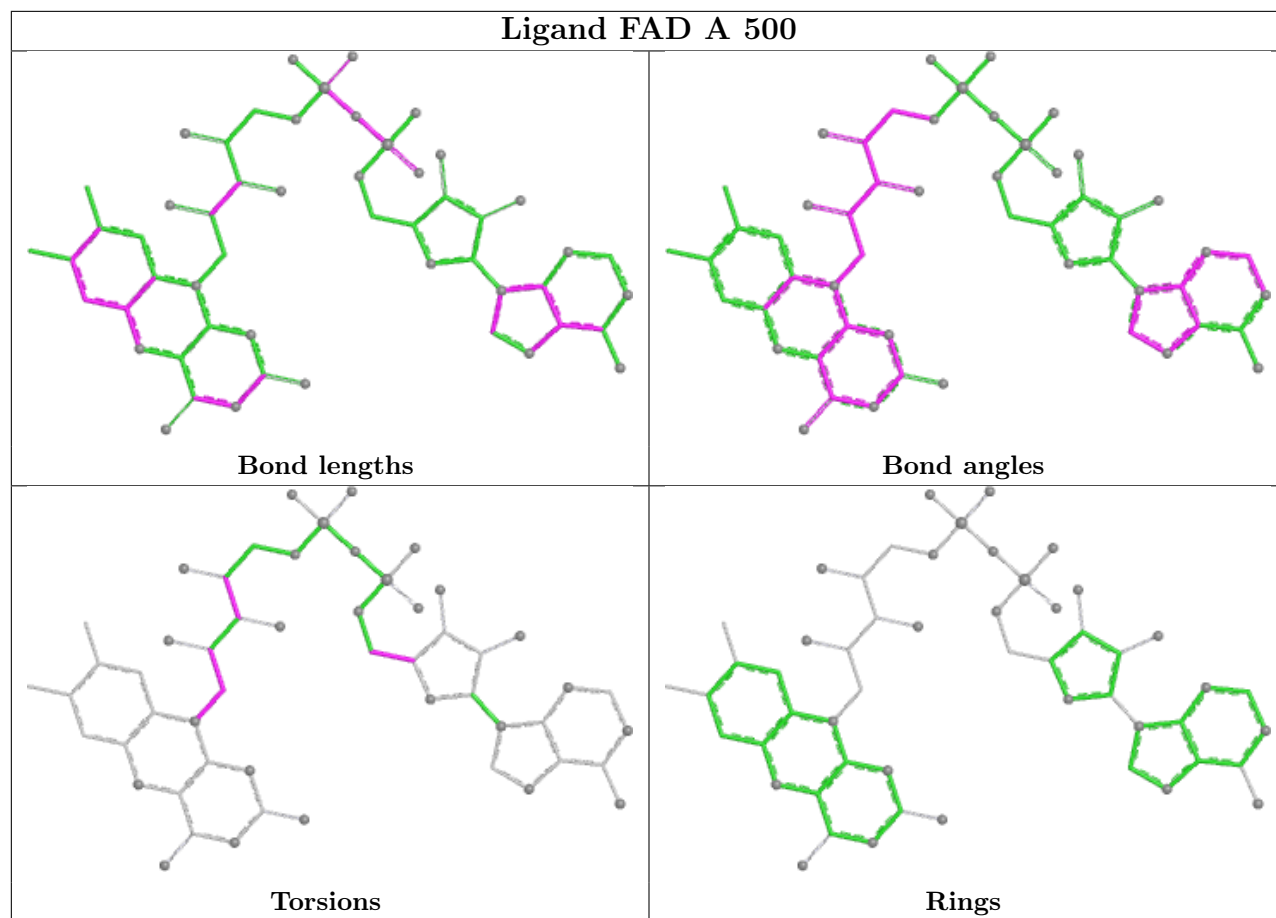
There are no ring outliers.

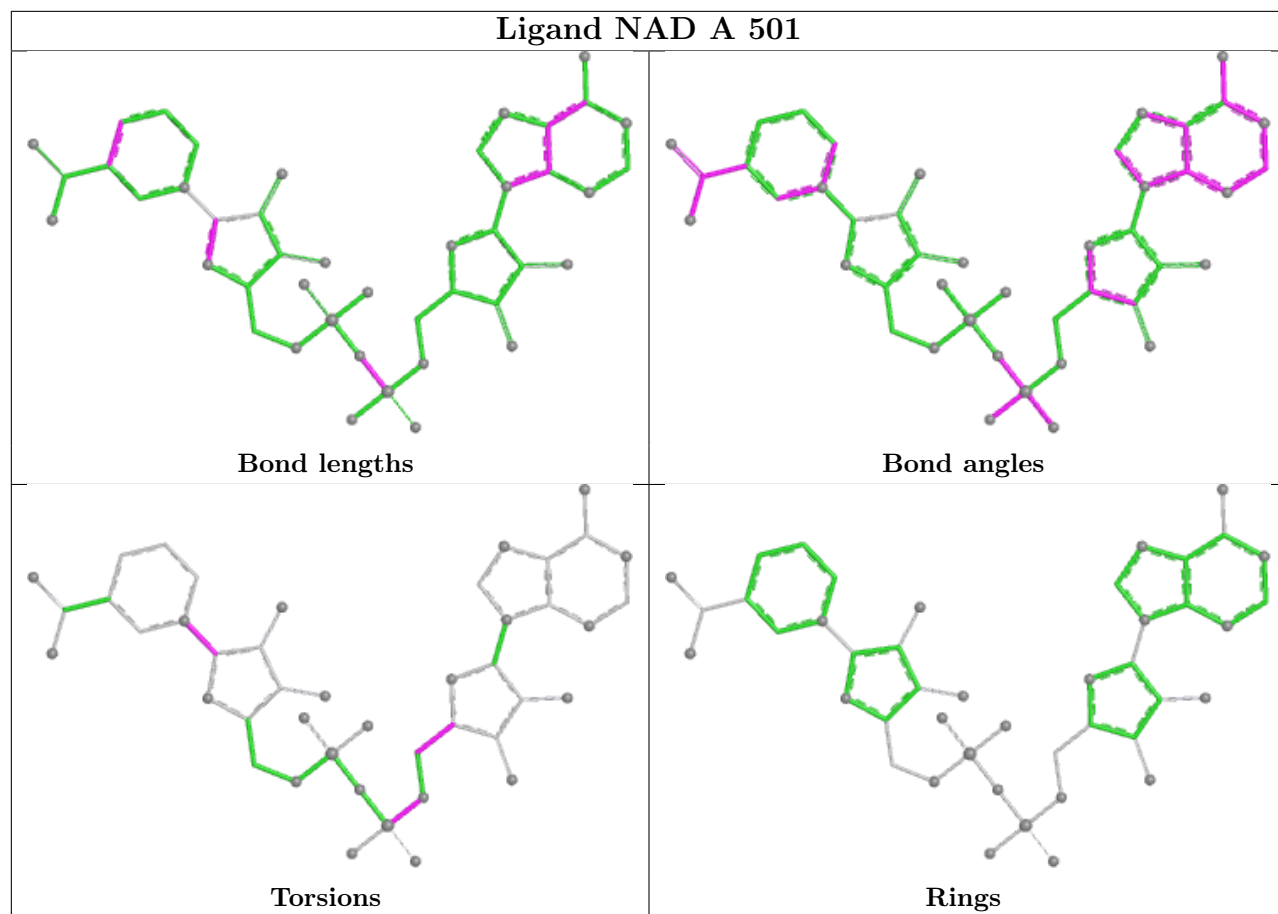
6 monomers are involved in 9 short contacts:

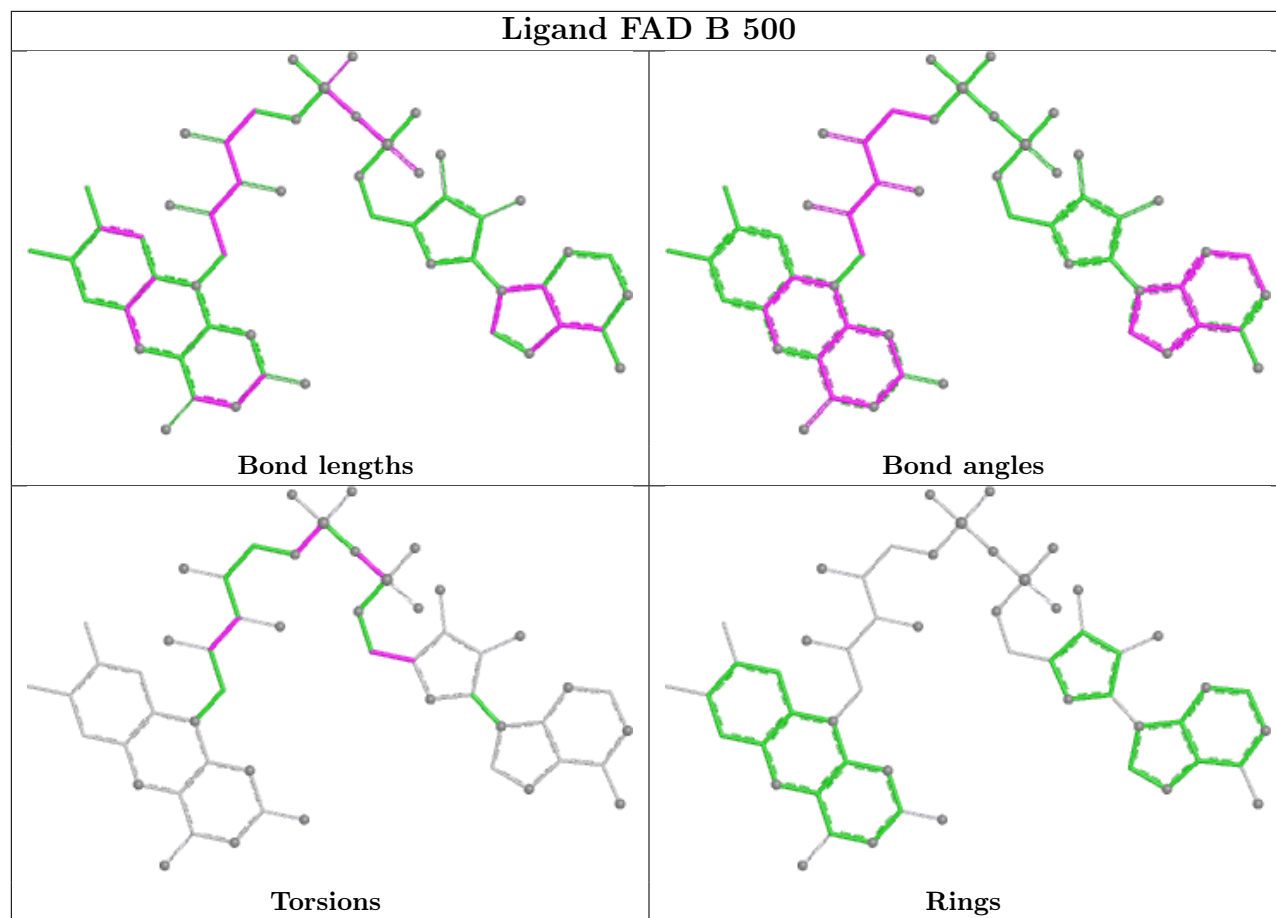
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	NAD	3	0
2	A	500	FAD	1	0
3	A	501	NAD	1	0
4	B	502	ASC	1	0
2	B	500	FAD	3	0
4	A	502	ASC	1	0

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%)	0.75	36 (8%) 17 18	51, 72, 113, 135	0
1	B	425/451 (94%)	0.68	43 (10%) 12 14	49, 70, 100, 138	0
All	All	854/902 (94%)	0.71	79 (9%) 14 16	49, 71, 107, 138	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	115	THR	6.2
1	A	54	GLY	5.3
1	A	114	PHE	4.7
1	B	167	ALA	4.7
1	B	94	THR	4.5
1	B	39	SER	4.5
1	A	283	ASP	4.3
1	B	38	ILE	4.3
1	B	234	ALA	4.1
1	A	298	ASP	4.0
1	A	297	GLY	3.9
1	A	319	ALA	3.8
1	B	6	HIS	3.8
1	B	345	LEU	3.6
1	B	36	ALA	3.3
1	A	315	HIS	3.2
1	A	113	THR	3.2
1	A	173	GLY	3.1
1	A	418	VAL	3.1
1	B	424	LEU	3.1
1	B	302	PHE	3.0
1	A	282	THR	3.0
1	B	413	LYS	3.0
1	B	37	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	257	VAL	2.9
1	A	413	LYS	2.8
1	A	174	TYR	2.8
1	A	268	LEU	2.8
1	A	337	GLU	2.7
1	B	10	VAL	2.7
1	A	79	LEU	2.7
1	A	6	HIS	2.6
1	A	378	ALA	2.6
1	A	348	PHE	2.6
1	B	308	ASN	2.6
1	B	339	VAL	2.6
1	A	96	ILE	2.6
1	B	340	VAL	2.6
1	B	79	LEU	2.5
1	A	115	THR	2.5
1	B	134	GLY	2.4
1	B	428	GLY	2.4
1	B	27	LYS	2.4
1	A	160	GLN	2.4
1	B	82	TRP	2.4
1	A	29	GLY	2.3
1	B	229	ALA	2.3
1	A	124	GLY	2.3
1	A	238	GLY	2.3
1	B	113	THR	2.3
1	A	338	SER	2.3
1	A	146	LEU	2.2
1	A	156	VAL	2.3
1	B	188	PHE	2.2
1	A	141	ASN	2.2
1	B	417	PRO	2.2
1	A	172	GLY	2.2
1	B	143	ILE	2.2
1	A	327	VAL	2.2
1	A	330	ILE	2.2
1	B	11	ILE	2.2
1	B	315	HIS	2.2
1	B	387	ILE	2.2
1	A	316	VAL	2.2
1	B	416	PRO	2.2
1	B	409	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	91	ILE	2.1
1	B	5	LYS	2.1
1	B	169	ILE	2.1
1	B	110	VAL	2.1
1	A	72	GLY	2.1
1	B	174	TYR	2.1
1	B	199	CYS	2.0
1	B	405	ASN	2.0
1	B	77	ARG	2.0
1	B	13	GLY	2.0
1	A	426	LYS	2.0
1	B	26	ALA	2.0
1	B	150	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

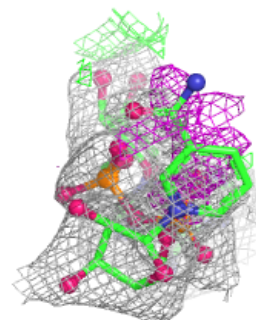
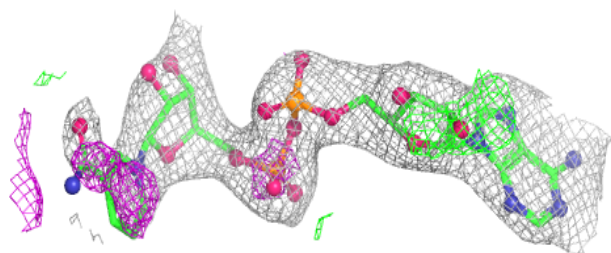
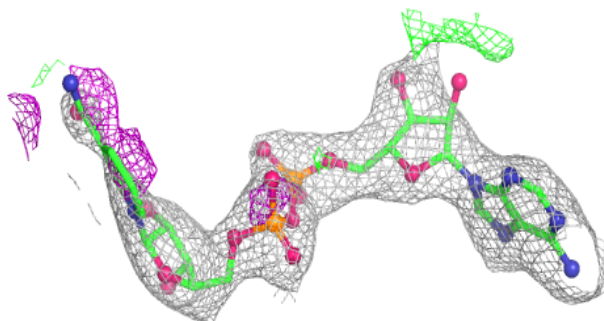
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ASC	B	502	12/12	0.77	0.13	73,86,95,97	0
4	ASC	A	502	12/12	0.82	0.10	71,78,90,90	0
3	NAD	A	501	44/44	0.84	0.14	61,71,99,127	0
3	NAD	B	501	44/44	0.86	0.13	50,71,102,109	0
2	FAD	B	500	53/53	0.89	0.11	17,22,27,30	0
2	FAD	A	500	53/53	0.90	0.11	17,22,27,30	0

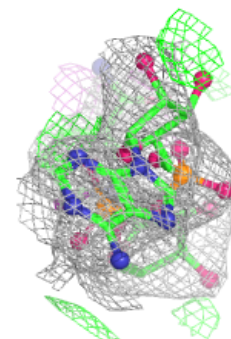
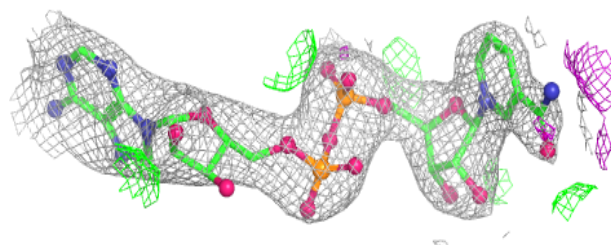
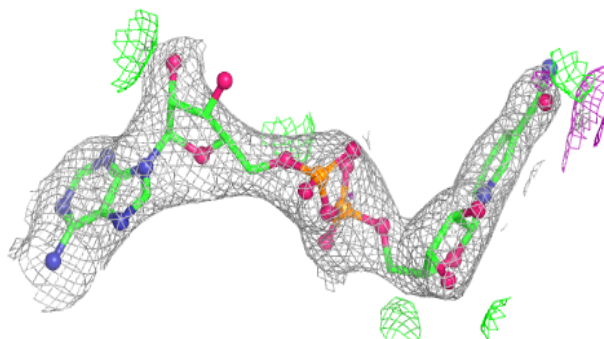
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD 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)

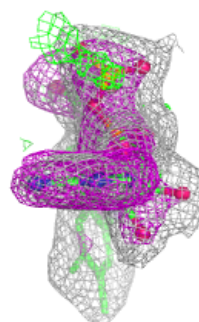
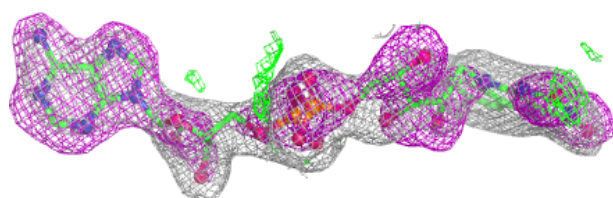
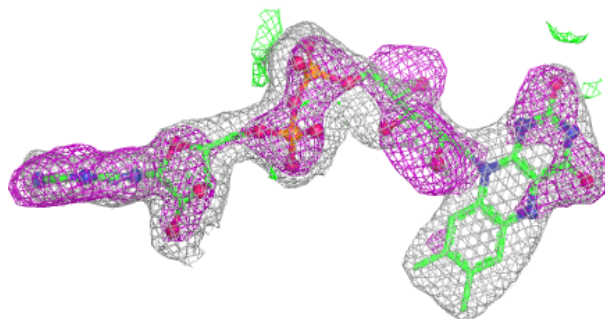
**Electron density around NAD B 501:**

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

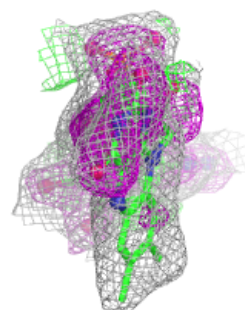
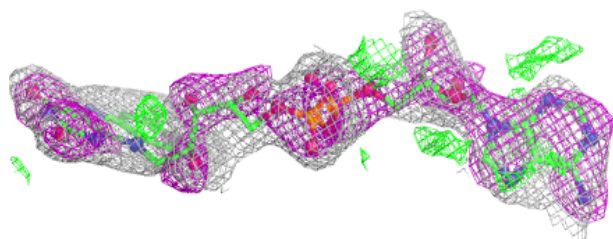
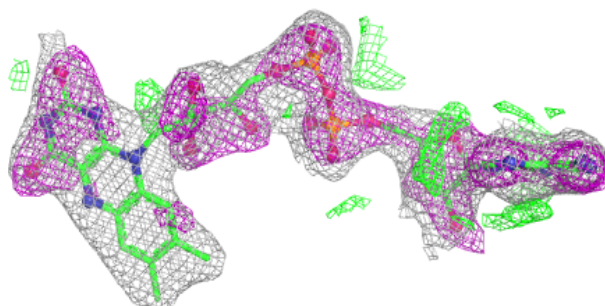


Electron density around FAD B 500:

$2mF_o-DF_c$ (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.