



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:10 am BST

PDB ID : 2OOS
Title : Crystal structure of plasmodium falciparum enoyl ACP reductase with triclosan reductase
Authors : Tsai, H.
Deposited on : 2007-01-26
Resolution : 2.10 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.

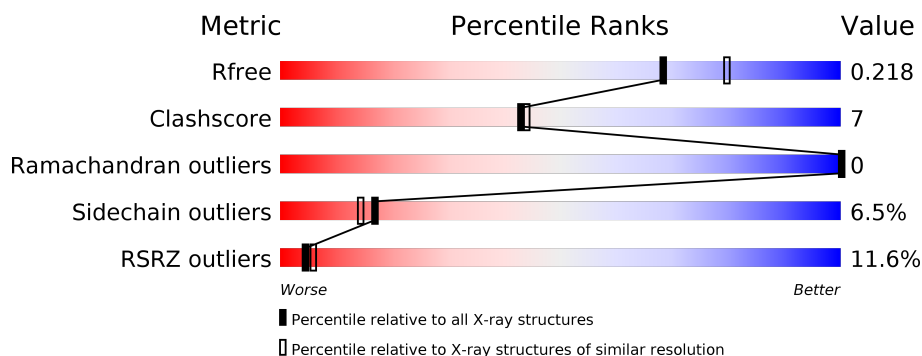
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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

i

X-RAY DIFFRACTION

A.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

Mol	Chain	Length	Quality of chain
1	A	338	<div> <div>9%</div> <div> <div></div> <div>71%</div> <div>12%</div> <div>•</div> <div>15%</div> </div> </div>
1	B	338	<div> <div>11%</div> <div> <div></div> <div>69%</div> <div>12%</div> <div>•</div> <div>16%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4805 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 Enoyl-acyl carrier reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2259	1439	379	430	11			
1	B	283	Total	C	N	O	S	0	0	0
			2233	1423	375	424	11			

There are 16 discrepancies between the modelled and reference sequences:

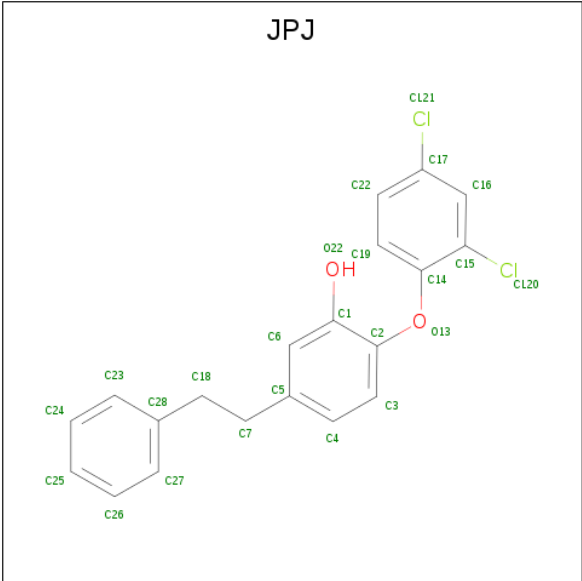
Chain	Residue	Modelled	Actual	Comment	Reference
A	88	MET	-	CLONING ARTIFACT	UNP Q9BH77
A	89	VAL	-	CLONING ARTIFACT	UNP Q9BH77
A	90	HIS	-	EXPRESSION TAG	UNP Q9BH77
A	91	HIS	-	EXPRESSION TAG	UNP Q9BH77
A	92	HIS	-	EXPRESSION TAG	UNP Q9BH77
A	93	HIS	-	EXPRESSION TAG	UNP Q9BH77
A	94	HIS	-	EXPRESSION TAG	UNP Q9BH77
A	95	HIS	-	EXPRESSION TAG	UNP Q9BH77
B	88	MET	-	CLONING ARTIFACT	UNP Q9BH77
B	89	VAL	-	CLONING ARTIFACT	UNP Q9BH77
B	90	HIS	-	EXPRESSION TAG	UNP Q9BH77
B	91	HIS	-	EXPRESSION TAG	UNP Q9BH77
B	92	HIS	-	EXPRESSION TAG	UNP Q9BH77
B	93	HIS	-	EXPRESSION TAG	UNP Q9BH77
B	94	HIS	-	EXPRESSION TAG	UNP Q9BH77
B	95	HIS	-	EXPRESSION TAG	UNP Q9BH77

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 3 is 2-(2,4-DICHLOROPHENOXY)-5-(2-PHENYLETHYL)PHENOL (three-letter code: JPJ) (formula: C₂₀H₁₆Cl₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	O	0	0
			24	20	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	Cl	O	0	0
			24	20	2	2		

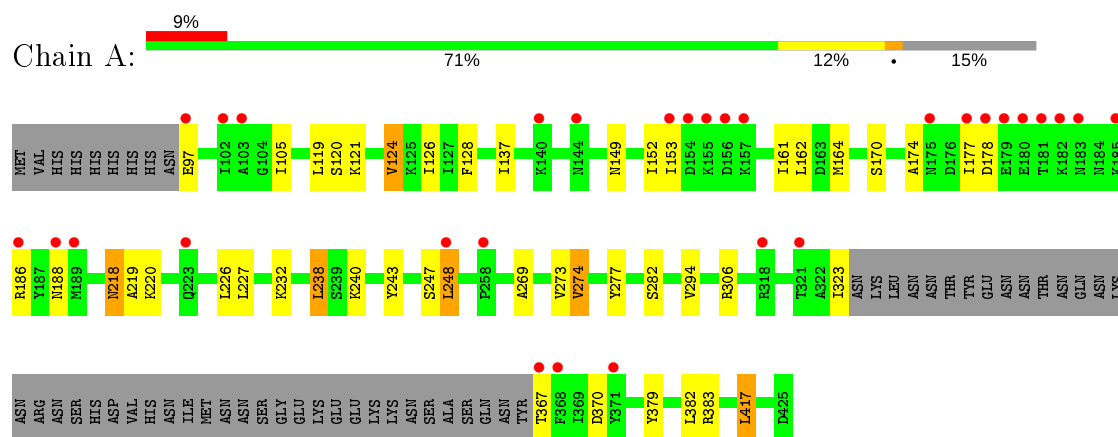
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	86	Total	O	0	0
			86	86		
4	B	91	Total	O	0	0
			91	91		

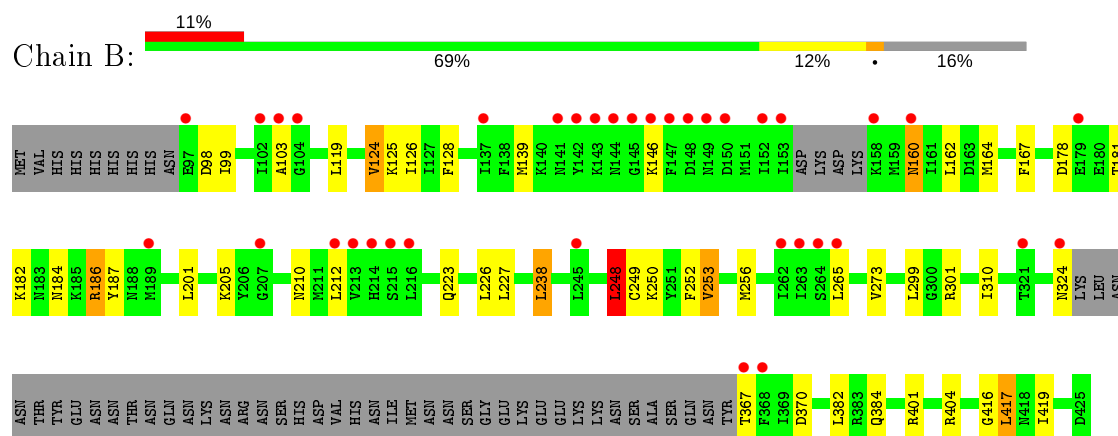
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Enoyl-acyl carrier reductase



• Molecule 1: Enoyl-acyl carrier reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	131.22Å 131.22Å 83.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.85 – 2.10 28.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (92.85-2.10) 99.8 (28.99-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.94 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.227 0.184 , 0.218	Depositor DCC
R_{free} test set	2160 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4805	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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: JPJ, 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	0.85	0/2300	0.85	6/3101 (0.2%)
1	B	0.82	0/2273	0.83	5/3065 (0.2%)
All	All	0.84	0/4573	0.84	11/6166 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	LEU	CA-CB-CG	-8.23	96.38	115.30
1	B	238	LEU	CA-CB-CG	-7.72	97.54	115.30
1	A	248	LEU	CB-CG-CD2	7.12	123.11	111.00
1	A	273	VAL	CG1-CB-CG2	6.34	121.05	110.90
1	B	248	LEU	CA-CB-CG	6.05	129.22	115.30
1	A	417	LEU	CB-CG-CD2	5.71	120.71	111.00
1	A	306	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	248	LEU	CA-CB-CG	5.57	128.12	115.30
1	B	404	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	417	LEU	CB-CG-CD2	5.22	119.87	111.00
1	B	238	LEU	CB-CG-CD1	5.11	119.69	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2259	0	2269	30	0
1	B	2233	0	2240	36	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
3	A	24	0	16	2	0
3	B	24	0	16	0	0
4	A	86	0	0	3	0
4	B	91	0	0	2	0
All	All	4805	0	4593	63	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 7.

All (63) 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:139:MET:SD	1:B:164:MET:HE2	2.11	0.90
1:B:367:THR:O	1:B:367:THR:HG22	1.73	0.88
1:B:223:GLN:NE2	1:B:324:ASN:HB2	1.90	0.85
1:B:126:ILE:HG21	1:B:128:PHE:HE1	1.45	0.81
1:B:223:GLN:HE21	1:B:324:ASN:H	1.29	0.79
1:B:367:THR:O	1:B:367:THR:CG2	2.35	0.74
1:A:170:SER:HB3	1:A:240:LYS:HD2	1.71	0.73
1:A:277:TYR:HB3	4:A:607:HOH:O	1.90	0.70
1:A:383:ARG:HD3	1:B:301:ARG:HH11	1.56	0.70
1:B:249:CYS:O	1:B:253:VAL:HB	1.97	0.65
1:A:174:ALA:O	1:A:177:ILE:HG12	1.96	0.64
1:A:170:SER:HB3	1:A:240:LYS:CD	2.28	0.64
1:B:367:THR:HG23	1:B:370:ASP:HB2	1.79	0.64
1:B:126:ILE:CG2	1:B:128:PHE:HE1	2.09	0.64
1:B:273:VAL:HG23	4:B:618:HOH:O	1.98	0.63
1:A:220:LYS:HE3	1:A:232:LYS:HE2	1.81	0.62
1:A:218:ASN:HD22	1:A:219:ALA:H	1.44	0.62
1:A:383:ARG:HD3	1:B:301:ARG:NH1	2.15	0.62
1:B:126:ILE:CG2	1:B:128:PHE:CE1	2.83	0.62
1:A:379:TYR:HA	1:B:301:ARG:HH22	1.66	0.61
1:B:184:ASN:ND2	1:B:186:ARG:H	1.97	0.61
1:B:119:LEU:O	1:B:124:VAL:HG13	2.01	0.60
1:B:126:ILE:HG21	1:B:128:PHE:CE1	2.34	0.60
1:A:149:ASN:O	1:A:152:ILE:HG12	2.01	0.59
1:B:99:ILE:HD13	1:B:125:LYS:HB2	1.84	0.59
1:B:178:ASP:OD1	1:B:181:THR:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:SER:CB	1:A:240:LYS:HE2	2.32	0.59
1:B:367:THR:CG2	1:B:370:ASP:HB2	2.34	0.58
1:A:119:LEU:O	1:A:124:VAL:HG13	2.04	0.58
1:A:294:VAL:HG11	4:A:605:HOH:O	2.05	0.56
1:A:269:ALA:HB2	1:A:274:VAL:HG13	1.88	0.55
1:B:253:VAL:HG21	1:B:299:LEU:HD22	1.89	0.55
1:A:170:SER:HB3	1:A:240:LYS:CE	2.38	0.53
1:A:170:SER:HB2	1:A:240:LYS:HE2	1.91	0.52
1:A:170:SER:HB3	1:A:240:LYS:HE2	1.91	0.51
1:B:212:LEU:HD21	1:B:248:LEU:HD13	1.92	0.51
1:B:223:GLN:NE2	1:B:324:ASN:CB	2.68	0.51
1:A:126:ILE:HG21	1:A:128:PHE:CE1	2.46	0.51
1:B:201:LEU:HD11	1:B:205:LYS:HE3	1.92	0.50
1:A:120:SER:HB3	1:A:153:ILE:HD11	1.96	0.48
1:A:367:THR:HB	1:A:370:ASP:OD2	2.13	0.47
1:B:265:LEU:HD23	1:B:310:ILE:HB	1.96	0.47
1:B:126:ILE:HG22	1:B:128:PHE:CE1	2.49	0.47
1:B:252:PHE:O	1:B:256:MET:HG3	2.15	0.47
1:B:103:ALA:HB1	1:B:167:PHE:CE2	2.50	0.46
1:A:121:LYS:HG2	1:A:153:ILE:CG2	2.45	0.46
1:B:253:VAL:HG21	1:B:299:LEU:CD2	2.45	0.46
1:A:161:ILE:HD13	1:A:164:MET:CE	2.45	0.46
1:B:160:ASN:HD22	1:B:160:ASN:C	2.20	0.45
1:B:273:VAL:HA	4:B:516:HOH:O	2.15	0.45
1:A:269:ALA:CB	1:A:274:VAL:HG13	2.46	0.45
1:B:178:ASP:CG	1:B:181:THR:HG23	2.38	0.44
1:A:121:LYS:HG2	1:A:153:ILE:HG21	1.99	0.44
1:B:103:ALA:HB1	1:B:167:PHE:HE2	1.83	0.44
1:A:282:SER:HB3	4:A:607:HOH:O	2.18	0.43
1:A:186:ARG:HA	1:A:186:ARG:NE	2.34	0.43
1:A:120:SER:HB3	1:A:153:ILE:CD1	2.50	0.41
1:A:323:ILE:HD12	3:A:500:JPJ:C24	2.50	0.41
1:B:416:GLY:O	1:B:419:ILE:HG12	2.21	0.41
1:A:243:TYR:CE2	1:A:247:SER:HB2	2.56	0.41
1:B:181:THR:O	1:B:187:TYR:HB2	2.21	0.41
1:A:323:ILE:HD11	3:A:500:JPJ:C19	2.51	0.40
1:B:98:ASP:HB2	1:B:124:VAL:HB	2.03	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	282/338 (83%)	272 (96%)	10 (4%)	0	100	100
1	B	277/338 (82%)	263 (95%)	14 (5%)	0	100	100
All	All	559/676 (83%)	535 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	247/297 (83%)	232 (94%)	15 (6%)	18	16
1	B	244/297 (82%)	227 (93%)	17 (7%)	15	12
All	All	491/594 (83%)	459 (94%)	32 (6%)	17	14

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	GLU
1	A	105	ILE
1	A	124	VAL
1	A	137	ILE
1	A	162	LEU
1	A	178	ASP
1	A	188	ASN
1	A	218	ASN

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Mol	Chain	Res	Type
1	A	226	LEU
1	A	227	LEU
1	A	238	LEU
1	A	248	LEU
1	A	274	VAL
1	A	382	LEU
1	A	417	LEU
1	B	124	VAL
1	B	146	LYS
1	B	160	ASN
1	B	162	LEU
1	B	182	LYS
1	B	186	ARG
1	B	210	ASN
1	B	226	LEU
1	B	227	LEU
1	B	238	LEU
1	B	248	LEU
1	B	250	LYS
1	B	253	VAL
1	B	382	LEU
1	B	384	GLN
1	B	401	ARG
1	B	417	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	ASN
1	A	200	ASN
1	A	218	ASN
1	A	254	ASN
1	A	384	GLN
1	B	160	ASN
1	B	184	ASN
1	B	200	ASN
1	B	223	GLN
1	B	259	GLN
1	B	384	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	JPJ	A	500	-	26,26,26	0.97	2 (7%)	35,35,35	0.86	1 (2%)
3	JPJ	B	500	-	26,26,26	0.91	0	35,35,35	0.94	1 (2%)
2	NAD	B	450	-	42,48,48	0.90	1 (2%)	50,73,73	1.56	11 (22%)
2	NAD	A	450	-	42,48,48	1.01	3 (7%)	50,73,73	1.39	3 (6%)

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	JPJ	A	500	-	-	2/9/9/9	0/3/3/3
3	JPJ	B	500	-	-	2/9/9/9	0/3/3/3
2	NAD	B	450	-	-	5/26/62/62	0/5/5/5
2	NAD	A	450	-	-	5/26/62/62	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	450	NAD	O4B-C1B	2.66	1.44	1.41
2	B	450	NAD	O4B-C1B	2.62	1.44	1.41
2	A	450	NAD	C2A-N3A	2.45	1.36	1.32
3	A	500	JPJ	C15-CL20	2.34	1.79	1.73
2	A	450	NAD	O7N-C7N	-2.23	1.19	1.24
3	A	500	JPJ	C6-C1	2.08	1.41	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	450	NAD	N3A-C2A-N1A	-5.60	119.93	128.68
2	A	450	NAD	N3A-C2A-N1A	-4.50	121.65	128.68
2	B	450	NAD	C3N-C7N-N7N	3.89	122.42	117.75
2	A	450	NAD	C3N-C7N-N7N	3.51	121.97	117.75
2	B	450	NAD	O7N-C7N-N7N	-2.70	118.74	122.58
2	B	450	NAD	O3B-C3B-C4B	-2.59	103.55	111.05
2	A	450	NAD	O4D-C1D-C2D	-2.50	103.28	106.93
3	A	500	JPJ	O13-C2-C1	2.32	120.55	116.22
2	B	450	NAD	C1B-N9A-C4A	-2.31	122.58	126.64
2	B	450	NAD	O4D-C1D-C2D	-2.31	103.55	106.93
2	B	450	NAD	O2A-PA-O1A	2.22	123.20	112.24
2	B	450	NAD	C2A-N1A-C6A	2.20	122.52	118.75
2	B	450	NAD	C2B-C3B-C4B	2.15	106.83	102.64
3	B	500	JPJ	C7-C18-C28	2.14	120.78	113.28
2	B	450	NAD	O5B-C5B-C4B	-2.11	101.74	108.99
2	B	450	NAD	C3N-C2N-N1N	-2.10	118.38	120.43

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	450	NAD	C5D-O5D-PN-O1N
2	B	450	NAD	O4D-C1D-N1N-C2N
2	A	450	NAD	C5D-O5D-PN-O1N
2	A	450	NAD	C5D-O5D-PN-O2N
2	A	450	NAD	O4D-C1D-N1N-C2N
2	B	450	NAD	C5D-O5D-PN-O3
2	B	450	NAD	C5D-O5D-PN-O2N
3	A	500	JPJ	C4-C5-C7-C18
3	B	500	JPJ	C7-C18-C28-C23
3	A	500	JPJ	C6-C5-C7-C18

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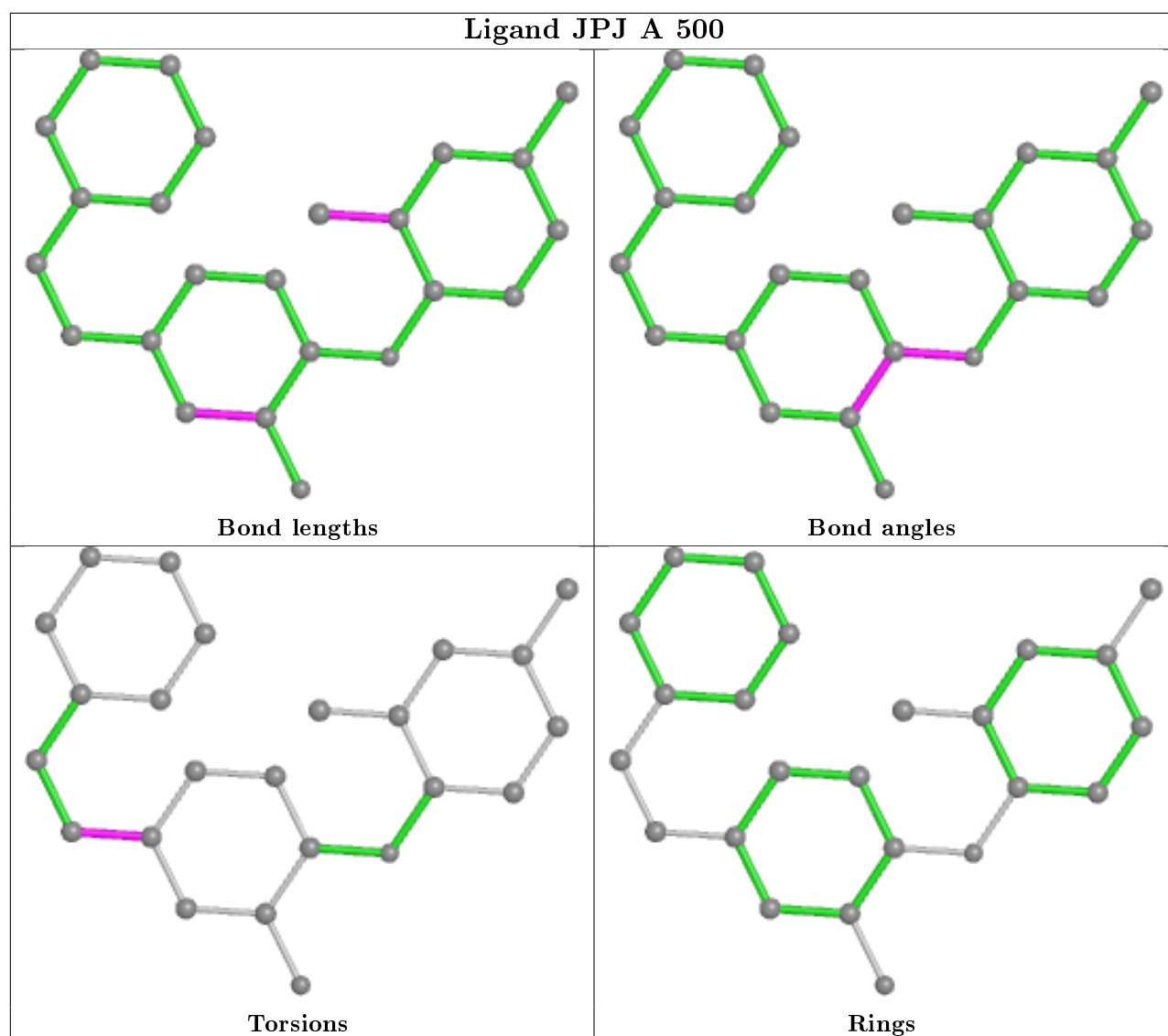
Mol	Chain	Res	Type	Atoms
3	B	500	JPJ	C7-C18-C28-C27
2	A	450	NAD	C5D-O5D-PN-O3
2	A	450	NAD	O4B-C4B-C5B-O5B
2	B	450	NAD	O4B-C4B-C5B-O5B

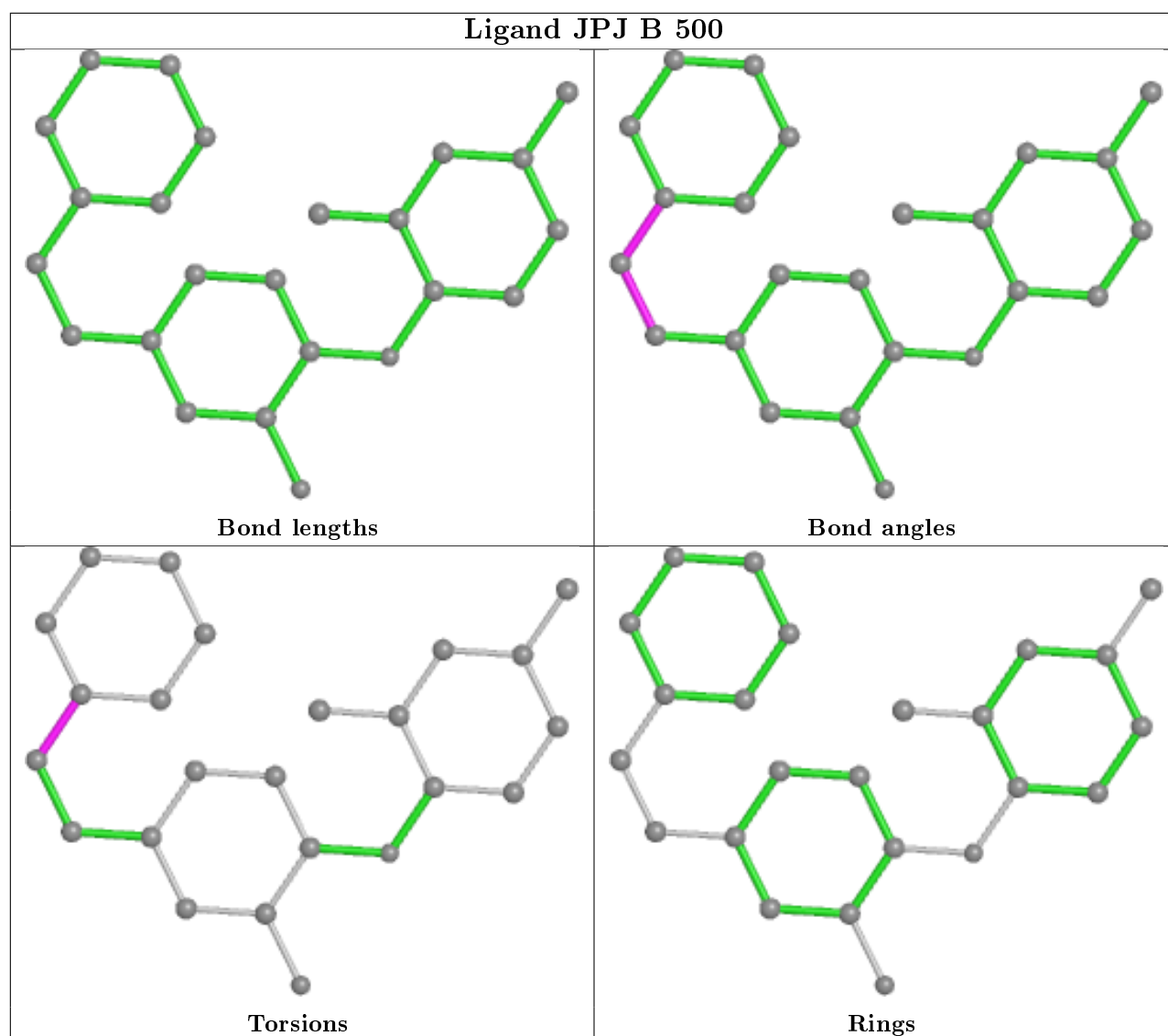
There are no ring outliers.

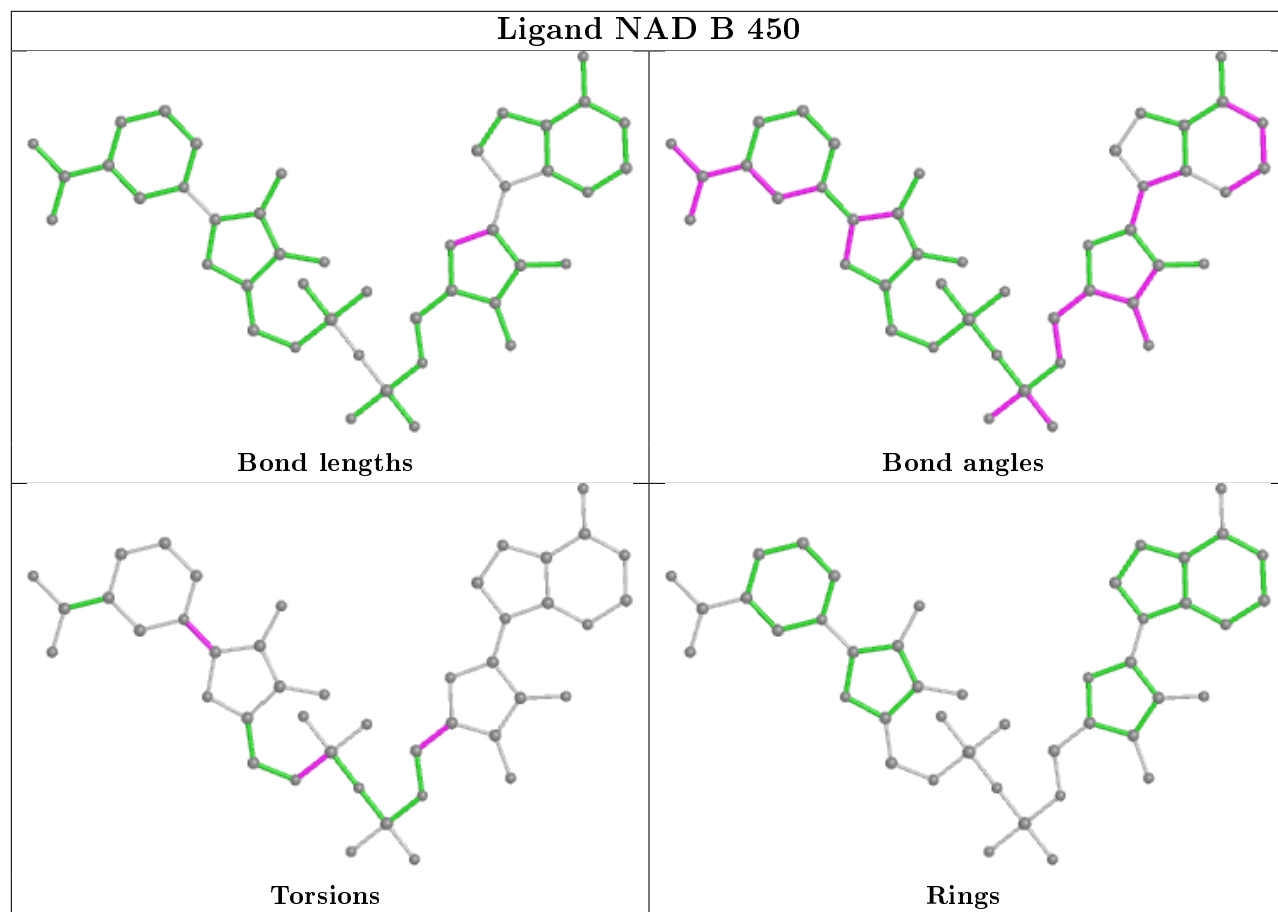
1 monomer is involved in 2 short contacts:

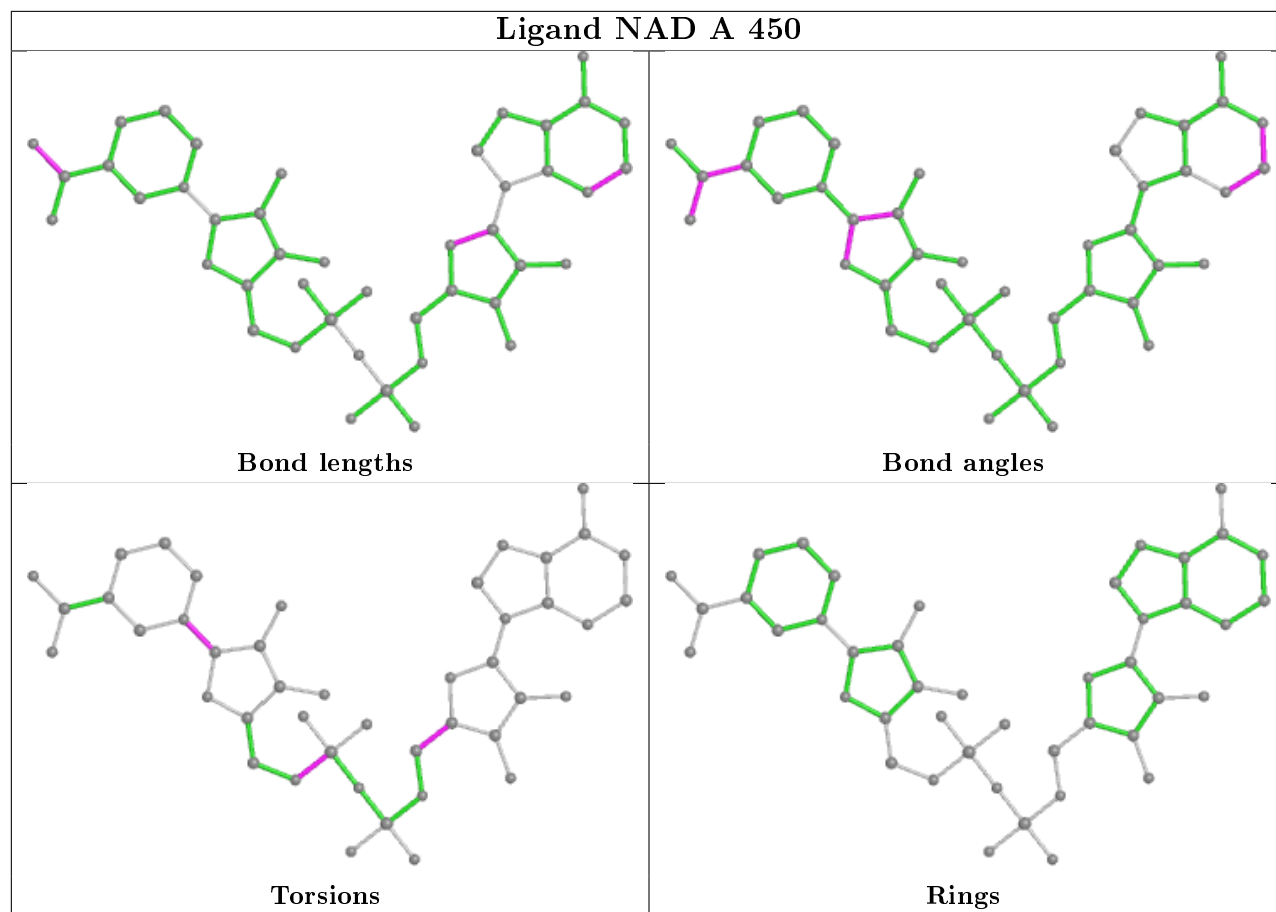
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	JPJ	2	0

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 [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	286/338 (84%)	0.47	30 (10%) 6 8	24, 35, 64, 81	0
1	B	283/338 (83%)	0.49	36 (12%) 3 5	24, 37, 67, 81	0
All	All	569/676 (84%)	0.48	66 (11%) 4 6	24, 36, 67, 81	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	153	ILE	6.2
1	B	152	ILE	6.0
1	A	156	ASP	5.9
1	A	181	THR	5.7
1	A	177	ILE	5.6
1	B	149	ASN	5.3
1	B	213	VAL	4.7
1	B	142	TYR	4.6
1	A	155	LYS	4.5
1	A	154	ASP	4.5
1	A	368	PHE	4.5
1	B	148	ASP	4.4
1	B	143	LYS	4.2
1	A	183	ASN	4.1
1	A	186	ARG	4.1
1	B	368	PHE	4.0
1	A	180	GLU	4.0
1	B	145	GLY	4.0
1	B	97	GLU	4.0
1	B	144	ASN	3.9
1	A	153	ILE	3.9
1	B	146	LYS	3.9
1	B	216	LEU	3.6
1	B	102	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	321	THR	3.5
1	B	150	ASP	3.4
1	A	178	ASP	3.4
1	B	179	GLU	3.4
1	B	103	ALA	3.3
1	B	137	ILE	3.3
1	B	212	LEU	3.3
1	A	157	LYS	3.1
1	A	318	ARG	3.0
1	A	179	GLU	3.0
1	A	103	ALA	2.9
1	B	263	ILE	2.9
1	A	185	LYS	2.9
1	A	189	MET	2.9
1	A	102	ILE	2.7
1	B	189	MET	2.7
1	A	248	LEU	2.7
1	A	223	GLN	2.7
1	B	158	LYS	2.7
1	A	175	ASN	2.6
1	A	188	ASN	2.6
1	A	367	THR	2.6
1	B	141	ASN	2.6
1	B	104	GLY	2.6
1	B	207	GLY	2.6
1	B	262	ILE	2.5
1	B	324	ASN	2.4
1	A	144	ASN	2.3
1	A	371	TYR	2.2
1	B	265	LEU	2.2
1	B	214	HIS	2.2
1	A	140	LYS	2.2
1	B	264	SER	2.2
1	B	160	ASN	2.2
1	A	182	LYS	2.2
1	B	215	SER	2.2
1	B	367	THR	2.1
1	B	321	THR	2.1
1	A	97	GLU	2.1
1	B	147	PHE	2.1
1	A	258	PRO	2.0
1	B	245	LEU	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](#)

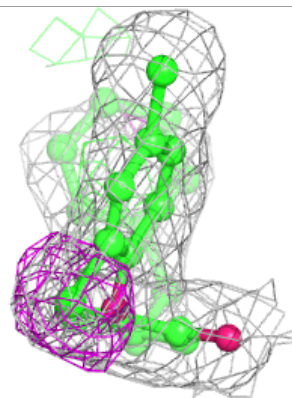
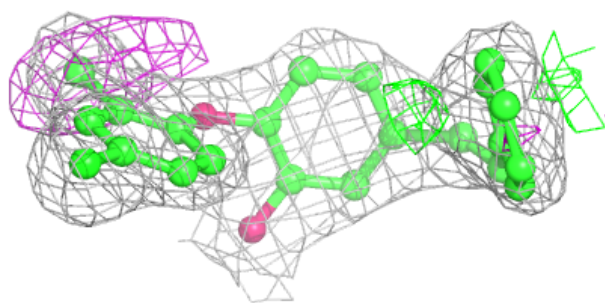
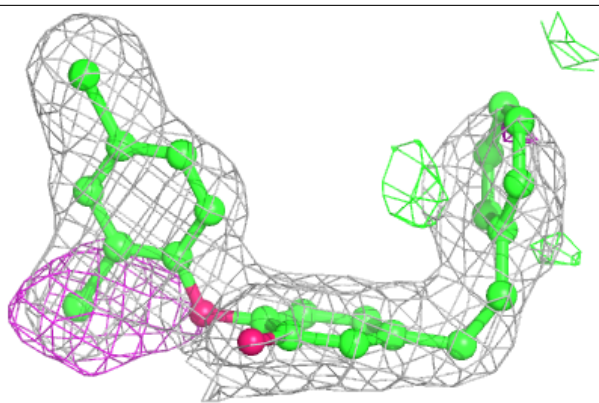
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	JPJ	B	500	24/24	0.95	0.11	31,35,51,52	0
3	JPJ	A	500	24/24	0.97	0.12	32,36,47,50	0
2	NAD	B	450	44/44	0.97	0.13	27,33,41,44	0
2	NAD	A	450	44/44	0.97	0.10	28,37,42,44	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.

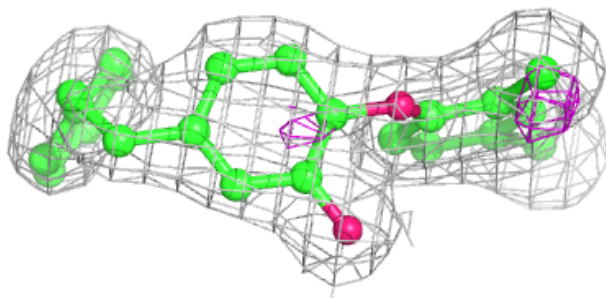
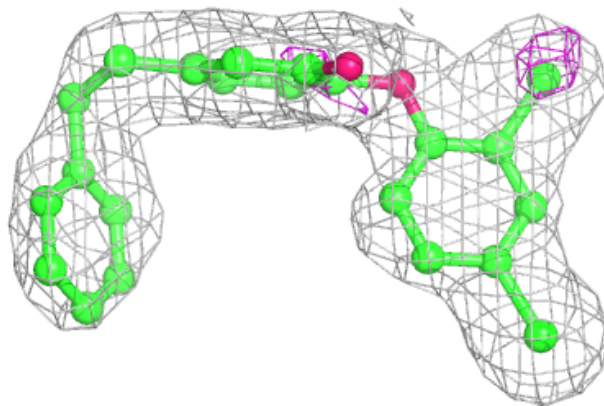
Electron density around JPJ B 500:

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



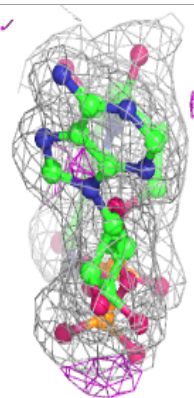
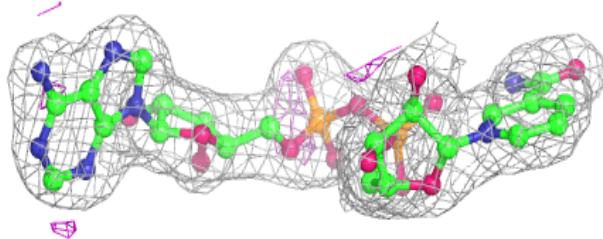
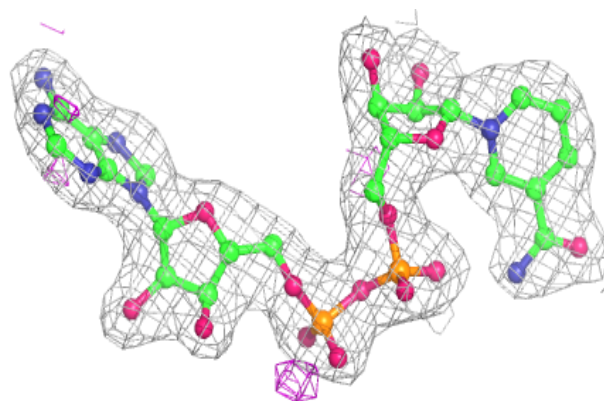
Electron density around JPJ A 500:

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

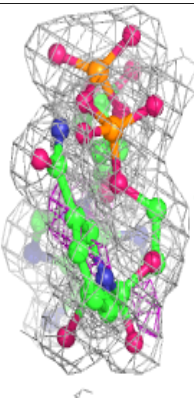
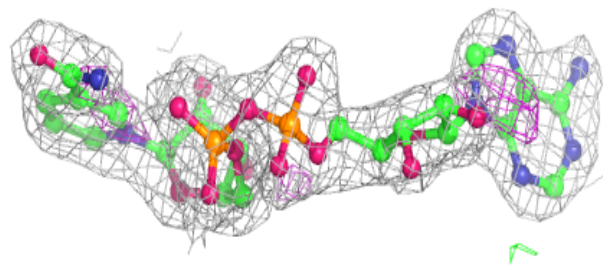
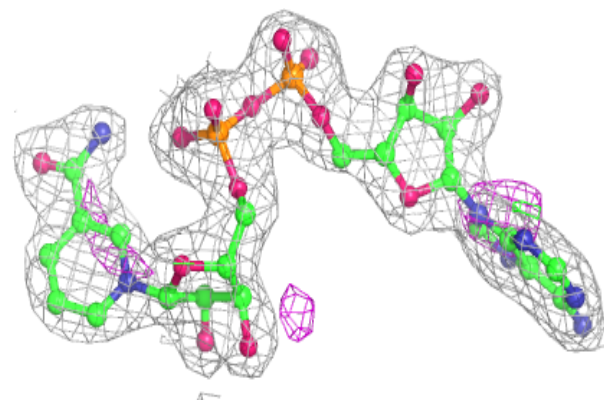


Electron density around NAD B 450:

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

**Electron density around NAD A 450:**

$2mF_o-DF_c$ (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.