



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 13, 2026 – 04:30 pm BST

PDB ID : 28JJ / pdb_000028jj
Title : Crystal structure of rat peroxisomal multifunctional enzyme type-1 complexed with 2E,4E-decadienoyl-CoA, 3R-hydroxy-4E-decenoyl-CoA and NAD
Authors : Kiema, T.-R.; Wierenga, R.K.; Sridhar, S.
Deposited on : 2026-02-03
Resolution : 2.30 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	:	1.8.4, CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

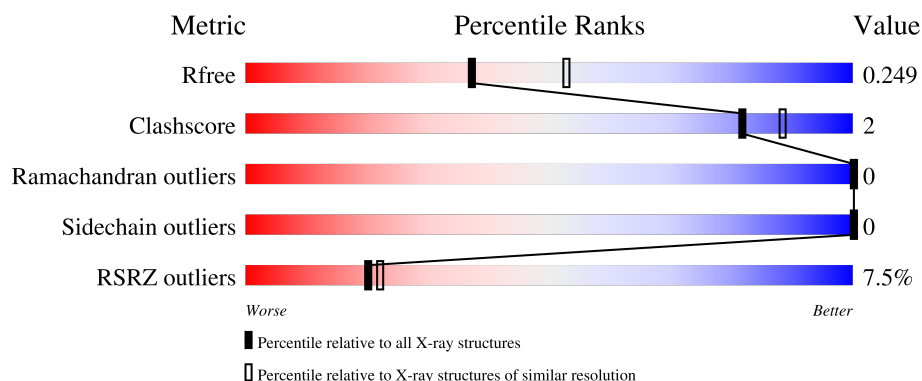
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	742	6% 90% 6% .
1	B	742	8% 89% 6% 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11323 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 Peroxisomal bifunctional enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	714	Total	C	N	O	S	0	1	0
			5489	3511	960	995	23			
1	B	707	Total	C	N	O	S	0	0	0
			5434	3480	945	986	23			

There are 42 discrepancies between the modelled and reference sequences:

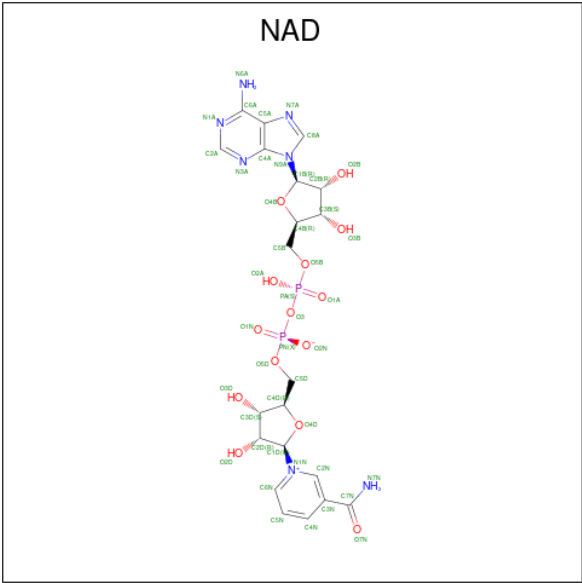
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P07896
A	-18	GLY	-	expression tag	UNP P07896
A	-17	SER	-	expression tag	UNP P07896
A	-16	SER	-	expression tag	UNP P07896
A	-15	HIS	-	expression tag	UNP P07896
A	-14	HIS	-	expression tag	UNP P07896
A	-13	HIS	-	expression tag	UNP P07896
A	-12	HIS	-	expression tag	UNP P07896
A	-11	HIS	-	expression tag	UNP P07896
A	-10	HIS	-	expression tag	UNP P07896
A	-9	SER	-	expression tag	UNP P07896
A	-8	SER	-	expression tag	UNP P07896
A	-7	GLY	-	expression tag	UNP P07896
A	-6	LEU	-	expression tag	UNP P07896
A	-5	VAL	-	expression tag	UNP P07896
A	-4	PRO	-	expression tag	UNP P07896
A	-3	ARG	-	expression tag	UNP P07896
A	-2	GLY	-	expression tag	UNP P07896
A	-1	SER	-	expression tag	UNP P07896
A	0	HIS	-	expression tag	UNP P07896
A	514	ARG	LYS	cloning artifact	UNP P07896
B	-19	MET	-	initiating methionine	UNP P07896
B	-18	GLY	-	expression tag	UNP P07896
B	-17	SER	-	expression tag	UNP P07896
B	-16	SER	-	expression tag	UNP P07896

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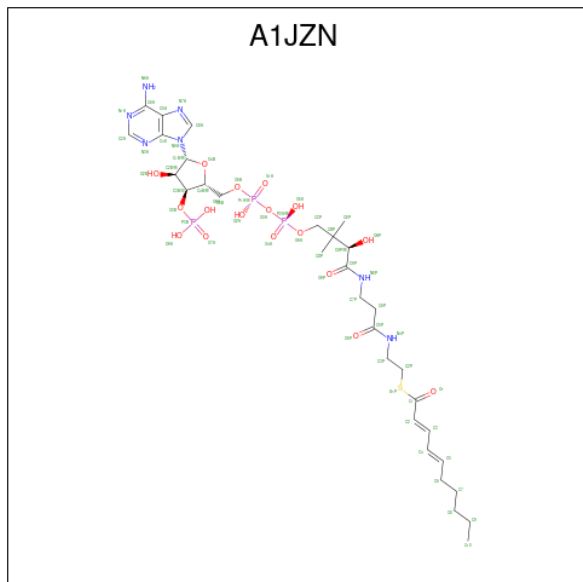
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP P07896
B	-14	HIS	-	expression tag	UNP P07896
B	-13	HIS	-	expression tag	UNP P07896
B	-12	HIS	-	expression tag	UNP P07896
B	-11	HIS	-	expression tag	UNP P07896
B	-10	HIS	-	expression tag	UNP P07896
B	-9	SER	-	expression tag	UNP P07896
B	-8	SER	-	expression tag	UNP P07896
B	-7	GLY	-	expression tag	UNP P07896
B	-6	LEU	-	expression tag	UNP P07896
B	-5	VAL	-	expression tag	UNP P07896
B	-4	PRO	-	expression tag	UNP P07896
B	-3	ARG	-	expression tag	UNP P07896
B	-2	GLY	-	expression tag	UNP P07896
B	-1	SER	-	expression tag	UNP P07896
B	0	HIS	-	expression tag	UNP P07896
B	514	ARG	LYS	cloning artifact	UNP P07896

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



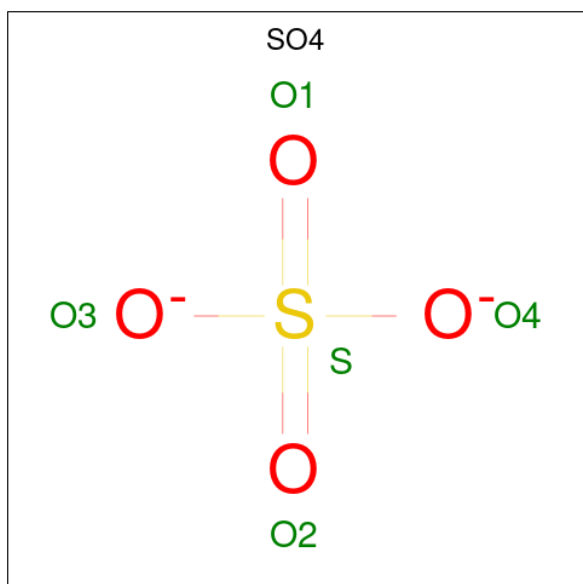
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 3 is 2E,4E-decadienoyl-CoA (CCD ID: A1JZN) (formula: $C_{31}H_{50}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			59	31	7	17	3	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



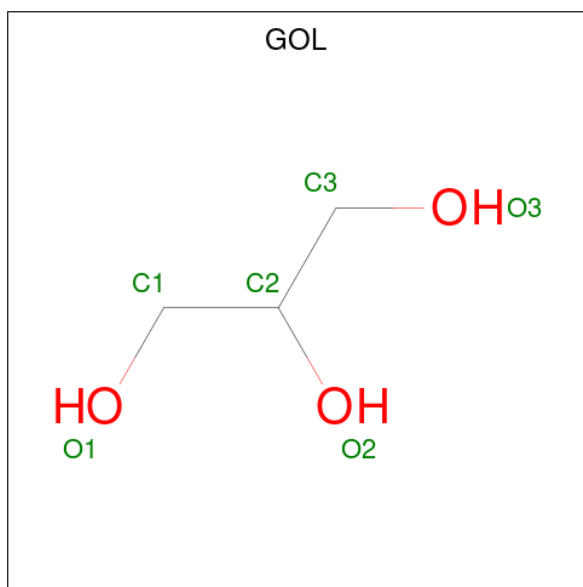
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

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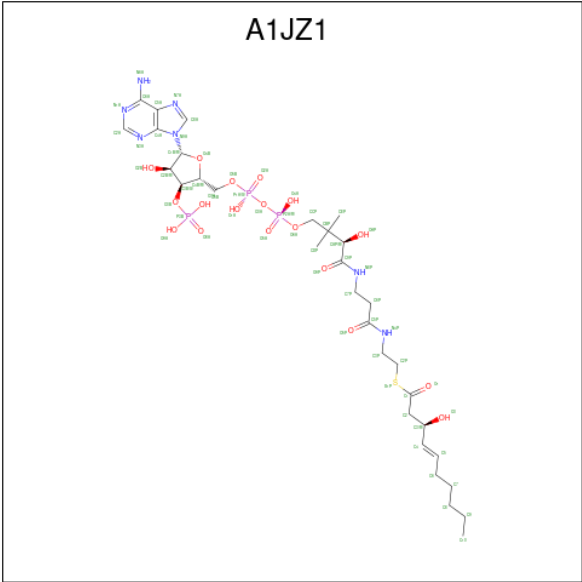
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is (S)-3-HYDROXY-(E)-4-DECENOYL-COA (CCD ID: A1JZ1) (formula: $C_{31}H_{52}N_7O_{18}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	B	1	Total	C	N	O	P	S	0	0
			60	31	7	18	3	1		

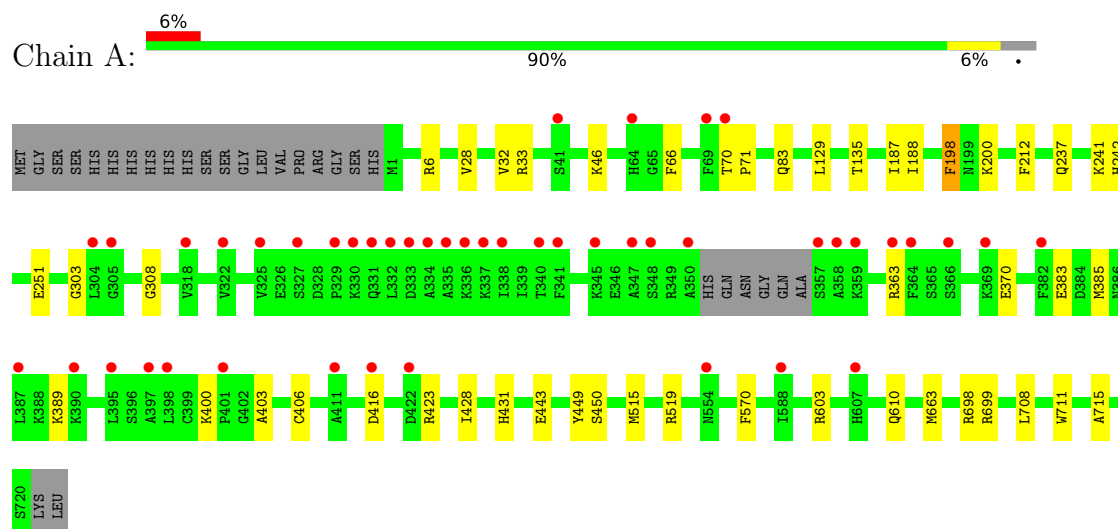
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	134	Total	O	0	0
			134	134		
7	B	37	Total	O	0	1
			38	38		

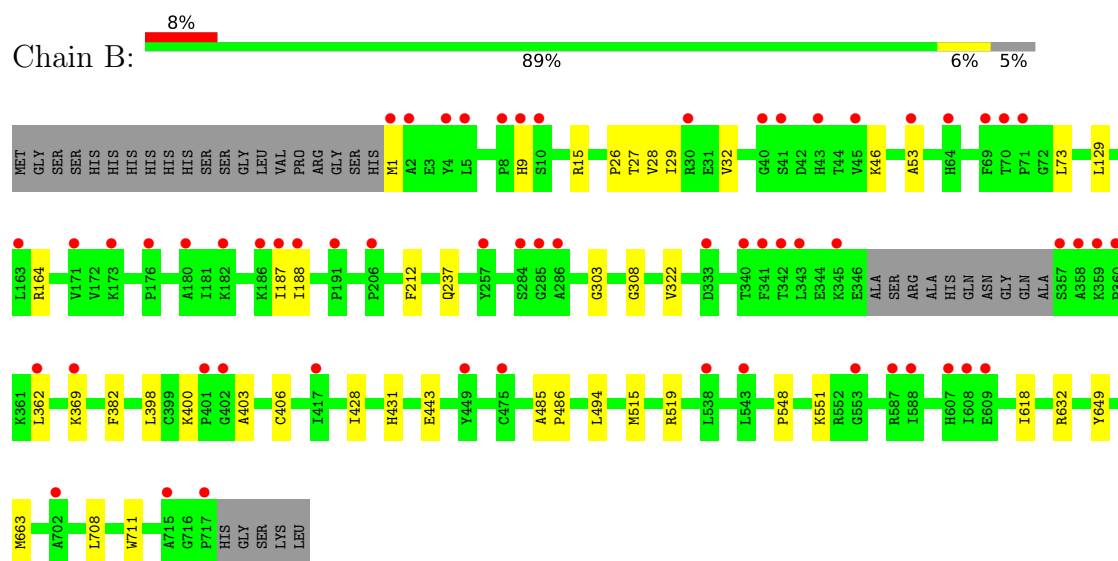
3 Residue-property plots [i](#)

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

• Molecule 1: Peroxisomal bifunctional enzyme



• Molecule 1: Peroxisomal bifunctional enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.48Å 126.72Å 226.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.80 – 2.30 64.80 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (64.80-2.30) 99.8 (64.80-2.30)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.221 , 0.247 0.225 , 0.249	Depositor DCC
R_{free} test set	5540 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11323	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: A1JZN, A1JZ1, SO4, NAD, GOL

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	0.60	0/5617	1.04	4/7608 (0.1%)
1	B	0.54	0/5558	1.00	2/7530 (0.0%)
All	All	0.57	0/11175	1.02	6/15138 (0.0%)

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	3
1	B	0	2
All	All	0	5

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	LYS	CB-CA-C	7.37	118.25	109.85
1	A	198	PHE	CA-CB-CG	6.12	119.92	113.80
1	A	570	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	70	THR	O-C-N	-5.33	118.12	121.85
1	B	9	HIS	CB-CA-C	5.19	118.69	111.63
1	B	649	TYR	CA-CB-CG	-5.01	104.88	113.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	33	ARG	Sidechain
1	A	423	ARG	Sidechain
1	A	6	ARG	Sidechain
1	B	164	ARG	Sidechain
1	B	632	ARG	Sidechain

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	5489	0	5607	26	0
1	B	5434	0	5551	28	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
3	A	59	0	0	2	0
4	A	15	0	0	0	0
5	B	6	0	8	0	0
6	B	60	0	0	0	0
7	A	134	0	0	2	0
7	B	38	0	0	0	0
All	All	11323	0	11218	56	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 2.

All (56) 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:1:MET:HE3	1:B:27:THR:HB	1.67	0.74
1:B:322:VAL:HB	1:B:362:LEU:HD13	1.71	0.73
1:B:1:MET:CE	1:B:27:THR:HB	2.23	0.68
3:A:802:A1JZN:C4	7:A:915:HOH:O	2.46	0.63
1:A:698[A]:ARG:HG2	1:A:698[A]:ARG:HH11	1.64	0.63
1:B:46:LYS:HB2	1:B:188:ILE:HD11	1.82	0.62
3:A:802:A1JZN:C5	7:A:915:HOH:O	2.49	0.60
1:B:663:MET:HA	1:B:663:MET:HE2	1.85	0.58
1:B:548:PRO:HG2	1:B:551:LYS:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:MET:HA	1:A:663:MET:HE2	1.86	0.57
1:B:129:LEU:HD12	1:B:129:LEU:C	2.30	0.56
1:B:382:PHE:CZ	2:B:801:NAD:H2B	2.40	0.56
1:A:129:LEU:C	1:A:129:LEU:HD12	2.31	0.54
1:B:322:VAL:CB	1:B:362:LEU:HD13	2.38	0.54
1:B:322:VAL:CG1	1:B:362:LEU:CD1	2.86	0.53
1:B:322:VAL:CG1	1:B:362:LEU:HD13	2.39	0.53
1:B:322:VAL:HG12	1:B:362:LEU:CD1	2.40	0.51
1:B:29:ILE:HD12	1:B:73:LEU:HD22	1.94	0.49
1:A:515:MET:HE3	1:A:519:ARG:HB3	1.94	0.49
1:A:400:LYS:HG3	1:A:403:ALA:HB2	1.94	0.48
1:B:515:MET:HE3	1:B:519:ARG:HB3	1.94	0.48
1:B:708:LEU:HA	1:B:711:TRP:CE2	2.48	0.48
1:A:66:PHE:CD1	1:A:71:PRO:HD3	2.49	0.48
1:B:303:GLY:O	1:B:308:GLY:HA3	2.14	0.48
1:A:363:ARG:HH22	1:A:370:GLU:CD	2.20	0.48
1:A:708:LEU:HA	1:A:711:TRP:CE2	2.49	0.47
1:B:369:LYS:HA	1:B:398:LEU:HD13	1.97	0.47
1:A:241:LYS:HD2	1:A:242:HIS:NE2	2.29	0.47
1:A:431:HIS:HB3	1:A:443:GLU:HB2	1.97	0.47
1:A:406:CYS:HA	1:A:428:ILE:O	2.15	0.46
1:A:83:GLN:HB2	1:A:198:PHE:HE2	1.80	0.46
1:A:303:GLY:O	1:A:308:GLY:HA3	2.16	0.45
1:A:698[A]:ARG:HG2	1:A:698[A]:ARG:NH1	2.29	0.45
1:A:135:THR:OG1	1:A:251:GLU:OE1	2.32	0.45
1:B:212:PHE:CZ	1:B:237:GLN:HA	2.52	0.45
1:B:400:LYS:HG3	1:B:403:ALA:HB2	1.98	0.45
1:A:385:MET:HE2	1:A:416:ASP:HB3	2.00	0.44
1:A:212:PHE:CZ	1:A:237:GLN:HA	2.53	0.44
1:B:26:PRO:HD3	1:B:73:LEU:HD21	2.00	0.44
1:B:187:ILE:C	1:B:187:ILE:HD12	2.43	0.43
1:A:187:ILE:C	1:A:187:ILE:HD12	2.44	0.43
1:B:485:ALA:HB3	1:B:486:PRO:HD3	2.01	0.42
1:B:322:VAL:HB	1:B:362:LEU:CD1	2.43	0.42
1:A:383:GLU:HG2	2:A:801:NAD:O2D	2.20	0.41
1:A:449:TYR:O	1:A:450:SER:C	2.63	0.41
1:B:406:CYS:HA	1:B:428:ILE:O	2.19	0.41
1:A:83:GLN:CD	1:A:198:PHE:HD2	2.28	0.41
1:A:699:ARG:HH12	1:A:715:ALA:HA	1.85	0.41
1:A:46:LYS:C	1:A:188:ILE:HD11	2.46	0.41
1:B:15:ARG:HD3	1:B:53:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:VAL:O	1:A:32:VAL:HG23	2.21	0.41
1:B:494:LEU:HD13	1:B:618:ILE:HG12	2.02	0.40
1:A:385:MET:O	1:A:389:LYS:HG3	2.21	0.40
1:A:603:ARG:HD3	1:A:610:GLN:OE1	2.21	0.40
1:B:431:HIS:HB3	1:B:443:GLU:HB2	2.03	0.40
1:B:28:VAL:O	1:B:32:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	711/742 (96%)	691 (97%)	20 (3%)	0	100	100
1	B	703/742 (95%)	684 (97%)	19 (3%)	0	100	100
All	All	1414/1484 (95%)	1375 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	587/609 (96%)	587 (100%)	0	100	100
1	B	582/609 (96%)	582 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1169/1218 (96%)	1169 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	B	554	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	A1JZ1	B	803	-	56,62,62	1.56	10 (17%)	75,89,89	1.92	16 (21%)
3	A1JZN	A	802	-	54,61,61	1.75	10 (18%)	74,87,87	2.00	20 (27%)
4	SO4	A	804	-	4,4,4	0.36	0	6,6,6	0.07	0
5	GOL	B	802	-	5,5,5	0.12	0	5,5,5	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	B	801	-	45,48,48	0.62	1 (2%)	63,73,73	0.70	1 (1%)
2	NAD	A	801	-	45,48,48	0.63	1 (2%)	63,73,73	0.75	1 (1%)
4	SO4	A	805	-	4,4,4	0.32	0	6,6,6	0.06	0
4	SO4	A	803	-	4,4,4	0.26	0	6,6,6	0.24	0

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
6	A1JZ1	B	803	-	-	15/62/78/78	0/3/3/3
3	A1JZN	A	802	-	-	3/60/76/76	0/3/3/3
5	GOL	B	802	-	-	3/4/4/4	-
2	NAD	B	801	-	-	10/30/62/62	0/5/5/5
2	NAD	A	801	-	-	8/30/62/62	0/5/5/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	A1JZN	C3-C2	6.22	1.50	1.34
6	B	803	A1JZ1	C4-C5	4.93	1.52	1.31
3	A	802	A1JZN	C4-C5	4.57	1.49	1.33
6	B	803	A1JZ1	C1-S1P	4.42	1.86	1.76
6	B	803	A1JZ1	C2A-N1A	3.73	1.40	1.33
3	A	802	A1JZN	C5A-N7A	-3.57	1.32	1.39
3	A	802	A1JZN	C2A-N1A	3.54	1.40	1.33
2	A	801	NAD	C2N-N1N	3.03	1.38	1.35
2	B	801	NAD	C2N-N1N	3.03	1.38	1.35
3	A	802	A1JZN	C2A-N3A	3.00	1.39	1.33
3	A	802	A1JZN	C8A-N9A	-2.95	1.32	1.37
6	B	803	A1JZ1	C2A-N3A	2.93	1.39	1.33
6	B	803	A1JZ1	C5A-N7A	-2.81	1.33	1.39
6	B	803	A1JZ1	C5A-C4A	-2.81	1.33	1.39
3	A	802	A1JZN	C3-C4	2.74	1.52	1.44
3	A	802	A1JZN	C5A-C6A	-2.73	1.33	1.41
6	B	803	A1JZ1	C8A-N9A	-2.67	1.32	1.37
3	A	802	A1JZN	C5A-C4A	-2.63	1.34	1.39
6	B	803	A1JZ1	C5A-C6A	-2.63	1.33	1.41
3	A	802	A1JZN	C4A-N9A	-2.43	1.32	1.37
6	B	803	A1JZ1	C4A-N9A	-2.25	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	803	A1JZ1	O3-C3	2.06	1.47	1.43

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	803	A1JZ1	N3A-C2A-N1A	-7.10	117.49	128.60
3	A	802	A1JZN	N1A-C2A-N3A	-6.57	118.33	128.60
3	A	802	A1JZN	C7P-C6P-C5P	-5.86	102.61	112.36
6	B	803	A1JZ1	C7P-C6P-C5P	-5.43	103.32	112.36
3	A	802	A1JZN	N9A-C8A-N7A	-4.51	107.74	113.91
6	B	803	A1JZ1	N9A-C8A-N7A	-4.31	108.01	113.91
3	A	802	A1JZN	C2P-C3P-N4P	-4.09	103.83	112.42
3	A	802	A1JZN	C4-C3-C2	-3.94	114.83	124.67
6	B	803	A1JZ1	C2-C1-S1P	3.84	118.38	113.63
6	B	803	A1JZ1	C5A-C4A-N3A	-3.59	122.07	126.75
3	A	802	A1JZN	C5A-C4A-N3A	-3.54	122.13	126.75
3	A	802	A1JZN	C5A-N7A-C8A	3.49	108.47	103.51
6	B	803	A1JZ1	C6P-C7P-N8P	-3.30	105.24	111.90
6	B	803	A1JZ1	C2A-N3A-C4A	3.22	119.35	111.75
6	B	803	A1JZ1	P2A-O3A-P1A	-3.21	121.81	132.83
6	B	803	A1JZ1	C5A-N7A-C8A	3.08	107.88	103.51
6	B	803	A1JZ1	C5A-C6A-N6A	-2.94	117.04	123.43
3	A	802	A1JZN	O4B-C1B-N9A	2.84	113.66	108.06
3	A	802	A1JZN	C4A-N9A-C8A	2.82	108.78	105.73
3	A	802	A1JZN	C6P-C7P-N8P	-2.80	106.24	111.90
6	B	803	A1JZ1	C4A-N9A-C8A	2.80	108.76	105.73
6	B	803	A1JZ1	O6A-CCP-CBP	-2.78	106.08	110.55
3	A	802	A1JZN	C2A-N3A-C4A	2.70	118.14	111.75
6	B	803	A1JZ1	C7P-N8P-C9P	2.66	127.33	122.59
3	A	802	A1JZN	C6A-C5A-C4A	2.66	120.76	117.18
3	A	802	A1JZN	C5A-C6A-N6A	-2.58	117.81	123.43
2	A	801	NAD	C6N-N1N-C2N	-2.50	119.70	121.97
3	A	802	A1JZN	C4A-C5A-N7A	-2.37	107.73	110.62
3	A	802	A1JZN	C7-C6-C5	-2.36	98.88	112.43
3	A	802	A1JZN	C2P-S1P-C1	-2.35	96.84	99.80
2	B	801	NAD	C6N-N1N-C2N	-2.31	119.87	121.97
6	B	803	A1JZ1	C4A-C5A-N7A	-2.16	107.99	110.62
3	A	802	A1JZN	C3P-N4P-C5P	2.16	126.84	122.84
3	A	802	A1JZN	N3A-C4A-N9A	2.14	130.60	127.08
6	B	803	A1JZ1	N3A-C4A-N9A	2.12	130.57	127.08
3	A	802	A1JZN	O5B-P1A-O1A	2.11	117.31	109.07
6	B	803	A1JZ1	C6A-C5A-C4A	2.09	119.99	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	A1JZN	O9A-P3B-O3B	-2.04	96.86	105.99

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAD	C5D-O5D-PN-O1N
2	A	801	NAD	O4D-C1D-N1N-C2N
2	A	801	NAD	O4D-C1D-N1N-C6N
2	A	801	NAD	C2D-C1D-N1N-C2N
2	A	801	NAD	C2D-C1D-N1N-C6N
2	B	801	NAD	C5D-O5D-PN-O1N
2	B	801	NAD	O4D-C1D-N1N-C2N
2	B	801	NAD	O4D-C1D-N1N-C6N
2	B	801	NAD	C2D-C1D-N1N-C2N
2	B	801	NAD	C2D-C1D-N1N-C6N
3	A	802	A1JZN	O1-C1-S1P-C2P
6	B	803	A1JZ1	S1P-C1-C2-C3
6	B	803	A1JZ1	C1-C2-C3-O3
6	B	803	A1JZ1	O3-C3-C4-C5
6	B	803	A1JZ1	C3P-C2P-S1P-C1
6	B	803	A1JZ1	CCP-O6A-P2A-O4A
6	B	803	A1JZ1	CCP-O6A-P2A-O5A
6	B	803	A1JZ1	CAP-CBP-CCP-O6A
6	B	803	A1JZ1	CDP-CBP-CCP-O6A
6	B	803	A1JZ1	CEP-CBP-CCP-O6A
5	B	802	GOL	C1-C2-C3-O3
6	B	803	A1JZ1	C6-C7-C8-C9
6	B	803	A1JZ1	C5-C6-C7-C8
3	A	802	A1JZN	C2-C1-S1P-C2P
2	A	801	NAD	C5D-O5D-PN-O3
2	B	801	NAD	C5D-O5D-PN-O3
2	A	801	NAD	C5D-O5D-PN-O2N
2	B	801	NAD	C5D-O5D-PN-O2N
2	B	801	NAD	O4D-C4D-C5D-O5D
6	B	803	A1JZ1	C2-C3-C4-C5
2	B	801	NAD	O4B-C4B-C5B-O5B
5	B	802	GOL	O1-C1-C2-C3
3	A	802	A1JZN	P1A-O3A-P2A-O6A
5	B	802	GOL	O2-C2-C3-O3
6	B	803	A1JZ1	C1-C2-C3-C4
6	B	803	A1JZ1	CCP-O6A-P2A-O3A

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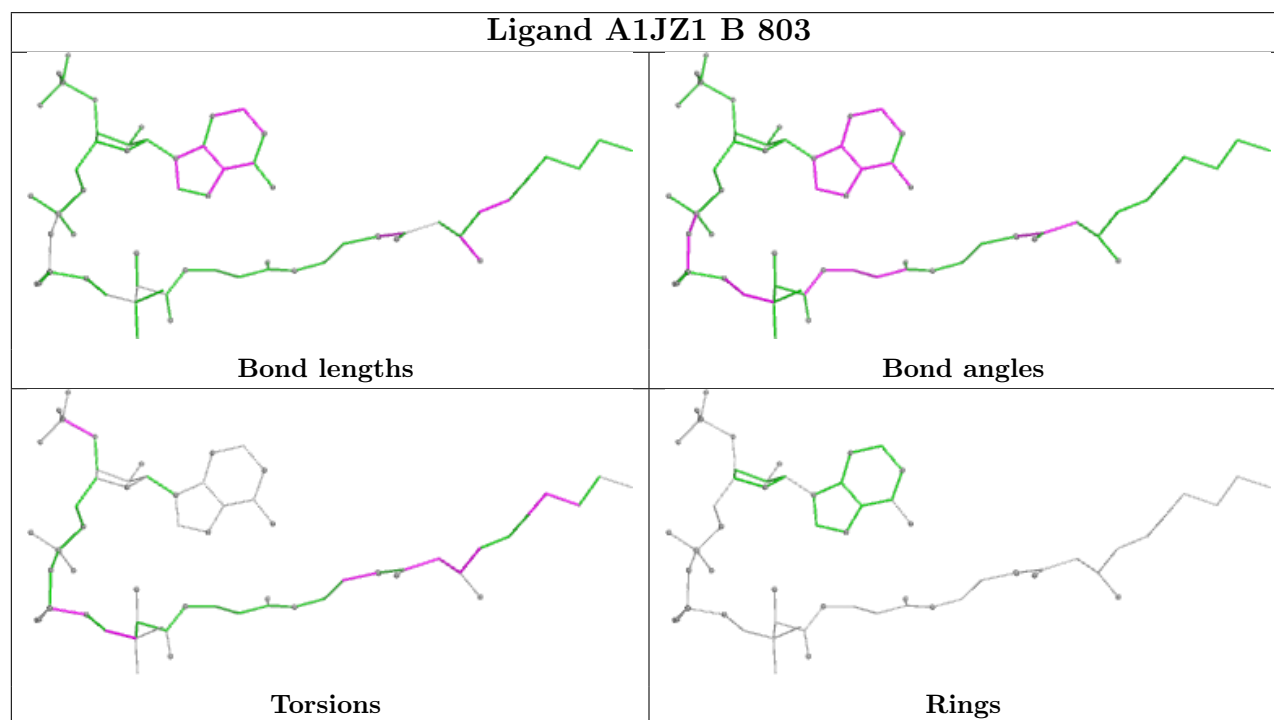
Mol	Chain	Res	Type	Atoms
6	B	803	A1JZ1	C3B-O3B-P3B-O9A
2	A	801	NAD	O4B-C4B-C5B-O5B
2	B	801	NAD	C3D-C4D-C5D-O5D

There are no ring outliers.

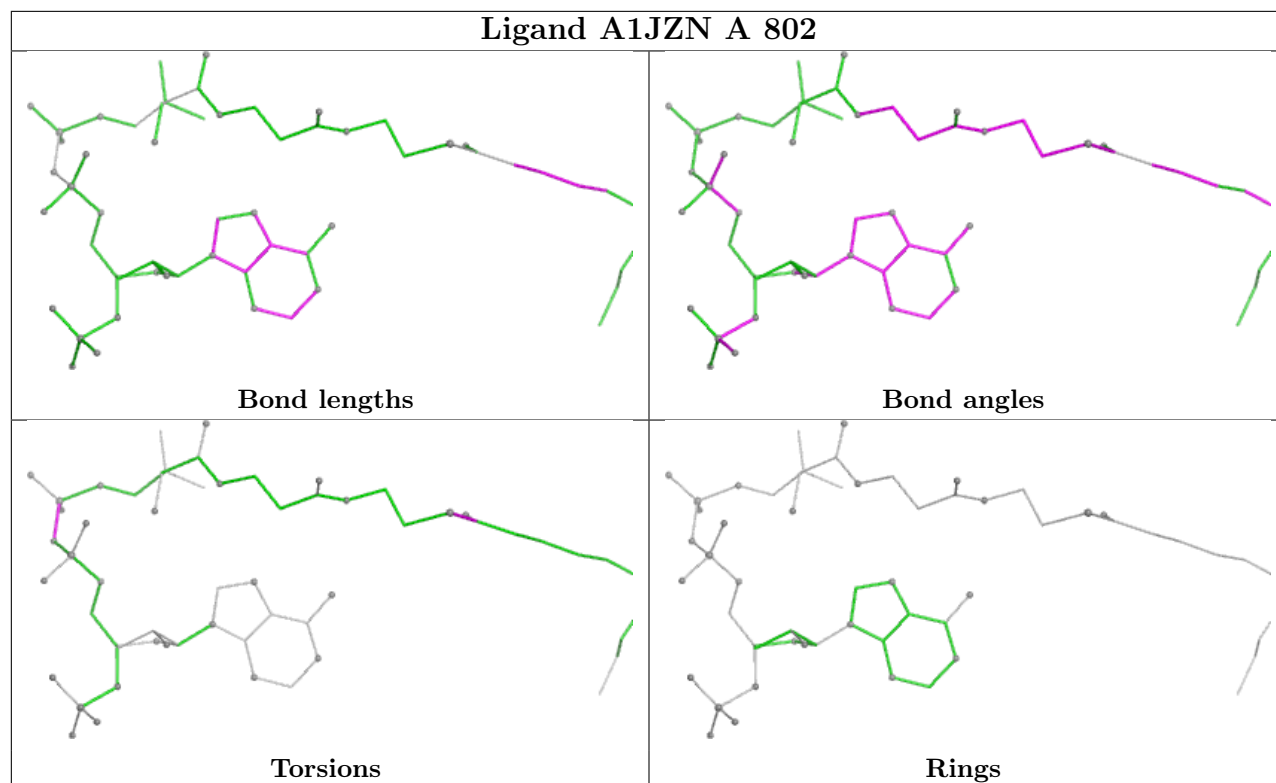
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	A1JZN	2	0
2	B	801	NAD	1	0
2	A	801	NAD	1	0

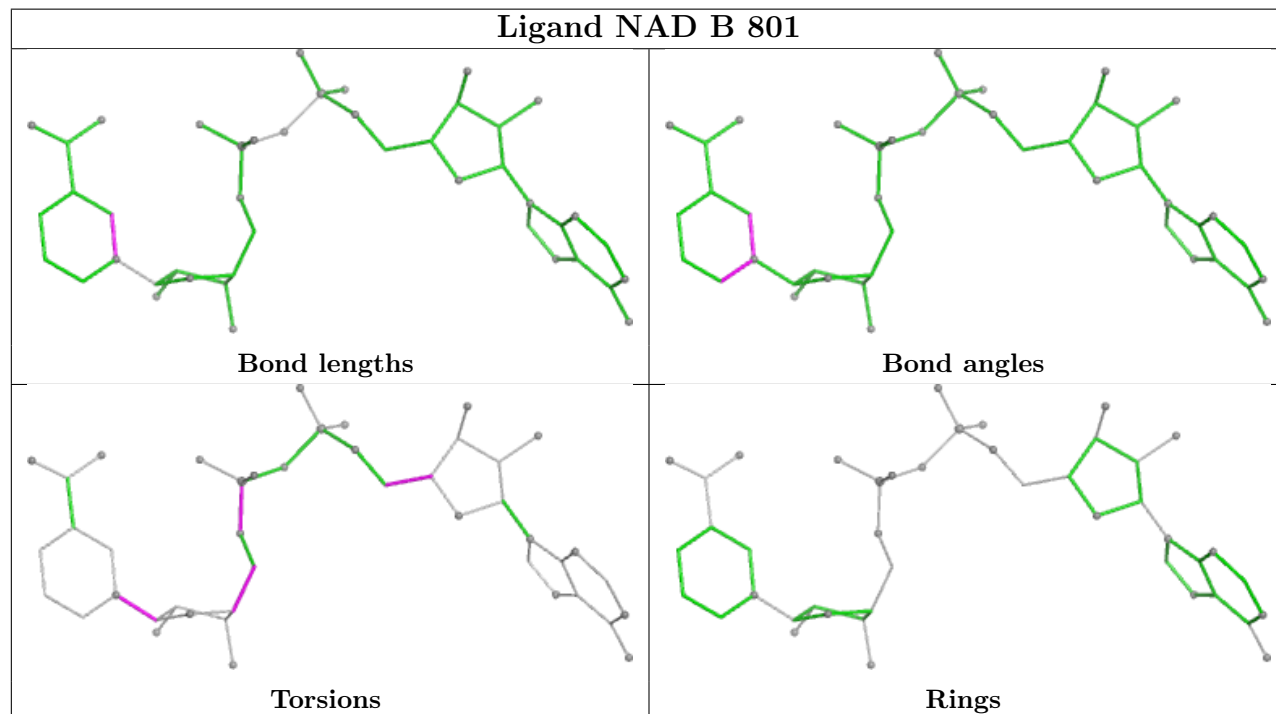
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

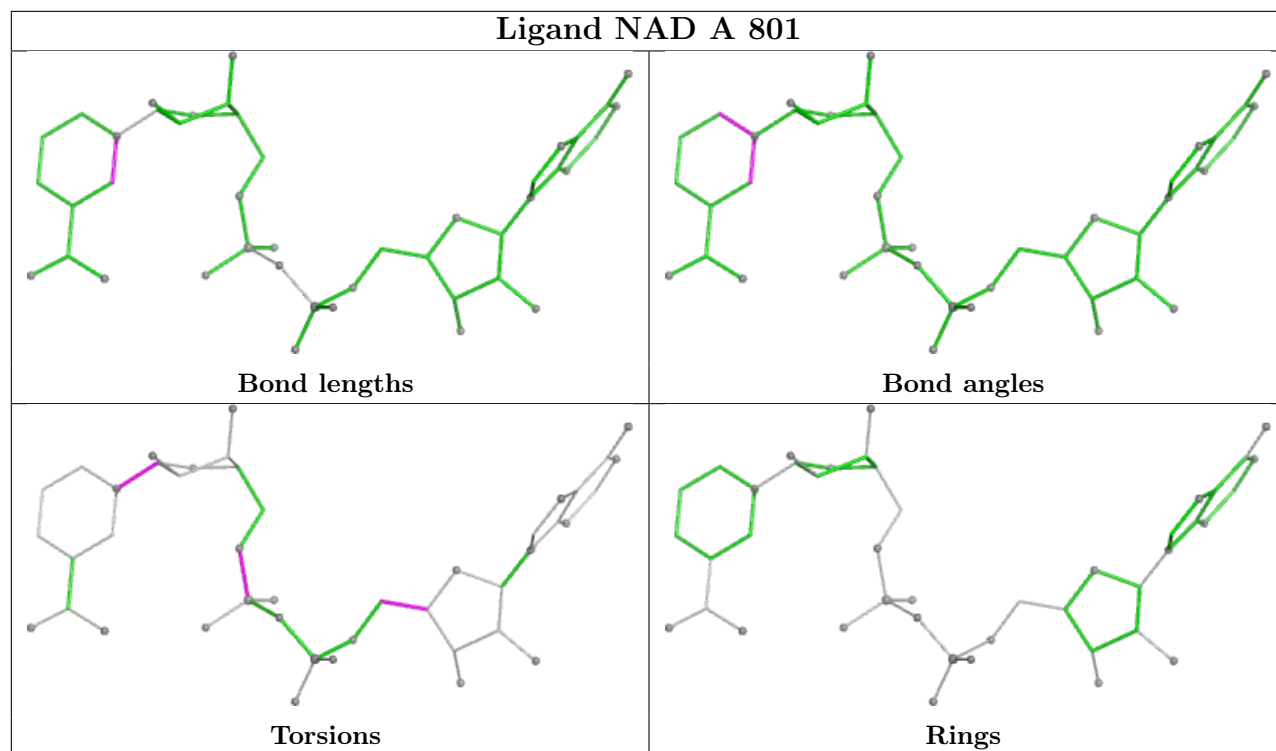


Ligand A1JZN A 802



Ligand NAD B 801





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	714/742 (96%)	0.23	46 (6%)	25 27	9, 31, 91, 119	1 (0%)
1	B	707/742 (95%)	0.68	60 (8%)	16 18	20, 52, 90, 117	0
All	All	1421/1484 (95%)	0.45	106 (7%)	20 22	9, 42, 90, 119	1 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	ALA	6.9
1	B	449	TYR	4.5
1	B	53	ALA	4.1
1	B	475	CYS	4.1
1	B	341	PHE	3.8
1	B	182	LYS	3.5
1	B	717	PRO	3.5
1	A	329	PRO	3.4
1	B	64	HIS	3.3
1	A	341	PHE	3.3
1	B	176	PRO	3.3
1	B	360	PRO	3.3
1	A	366	SER	3.3
1	B	357	SER	3.3
1	B	553	GLY	3.2
1	B	8	PRO	3.2
1	A	330	LYS	3.2
1	B	343	LEU	3.2
1	B	401	PRO	3.2
1	A	333	ASP	3.1
1	B	43	HIS	3.1
1	A	348	SER	3.1
1	B	180	ALA	3.1
1	A	554	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	359	LYS	3.0
1	B	2	ALA	2.9
1	B	369	LYS	2.9
1	A	69	PHE	2.9
1	A	358	ALA	2.9
1	B	1	MET	2.9
1	A	334	ALA	2.8
1	A	41	SER	2.8
1	B	402	GLY	2.8
1	B	45	VAL	2.8
1	A	347	ALA	2.7
1	B	41	SER	2.7
1	A	304	LEU	2.7
1	A	70	THR	2.7
1	A	327	SER	2.7
1	B	9	HIS	2.6
1	A	359	LYS	2.6
1	A	382	PHE	2.6
1	B	186	LYS	2.6
1	B	607	HIS	2.6
1	A	390	LYS	2.6
1	A	387	LEU	2.5
1	A	335	ALA	2.5
1	B	188	ILE	2.5
1	B	588	ILE	2.5
1	B	333	ASP	2.5
1	A	397	ALA	2.5
1	B	715	ALA	2.5
1	B	206	PRO	2.4
1	B	358	ALA	2.4
1	A	325	VAL	2.4
1	A	337	LYS	2.4
1	B	609	GLU	2.4
1	A	338	ILE	2.4
1	B	5	LEU	2.4
1	B	362	LEU	2.4
1	A	363	ARG	2.4
1	A	422	ASP	2.3
1	B	284	SER	2.3
1	A	332	LEU	2.3
1	B	71	PRO	2.3
1	B	163	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	369	LYS	2.3
1	B	40	GLY	2.3
1	B	285	GLY	2.3
1	B	286	ALA	2.3
1	A	357	SER	2.3
1	B	70	THR	2.3
1	A	318	VAL	2.3
1	B	257	TYR	2.2
1	B	69	PHE	2.2
1	B	10	SER	2.2
1	B	587	ARG	2.2
1	A	398	LEU	2.2
1	A	588	ILE	2.1
1	B	187	ILE	2.1
1	A	411	ALA	2.1
1	B	340	THR	2.1
1	B	4	TYR	2.1
1	B	417	ILE	2.1
1	B	543	LEU	2.1
1	A	305	GLY	2.1
1	A	340	THR	2.1
1	B	538	LEU	2.1
1	A	331	GLN	2.1
1	A	401	PRO	2.1
1	A	364	PHE	2.1
1	B	342	THR	2.1
1	B	191	PRO	2.1
1	B	171	VAL	2.1
1	B	30	ARG	2.1
1	A	336	LYS	2.0
1	B	345	LYS	2.0
1	B	702	ALA	2.0
1	A	607	HIS	2.0
1	A	416	ASP	2.0
1	A	322	VAL	2.0
1	A	345	LYS	2.0
1	B	173	LYS	2.0
1	A	64	HIS	2.0
1	A	395	LEU	2.0
1	B	608	ILE	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](#)

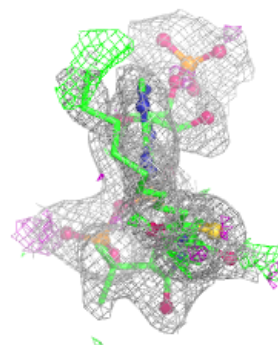
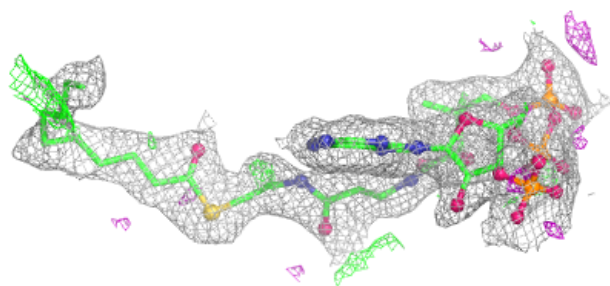
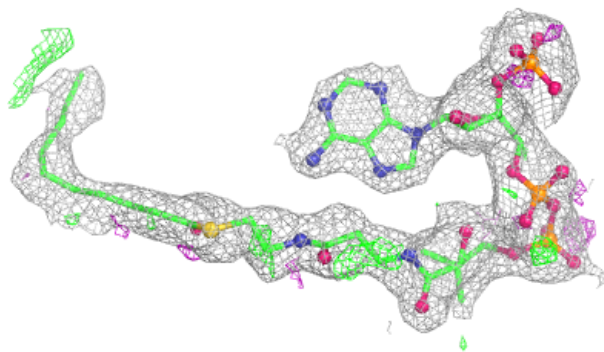
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	A	805	5/5	0.75	0.16	76,78,85,98	0
4	SO4	A	804	5/5	0.77	0.12	75,84,86,89	0
5	GOL	B	802	6/6	0.81	0.16	44,47,48,55	0
3	A1JZN	A	802	59/59	0.88	0.13	33,42,60,64	0
2	NAD	A	801	44/44	0.88	0.13	42,57,70,74	0
6	A1JZ1	B	803	60/60	0.91	0.12	40,55,71,74	0
2	NAD	B	801	44/44	0.93	0.10	42,53,66,67	0
4	SO4	A	803	5/5	0.95	0.12	26,36,39,39	0

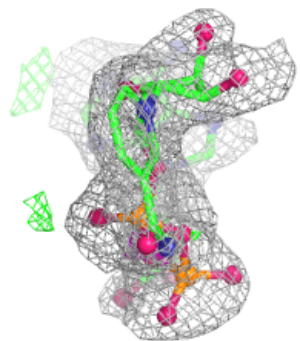
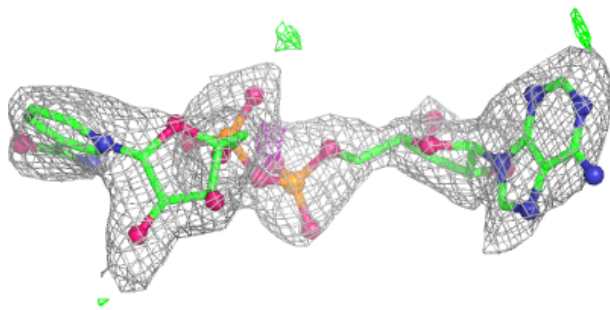
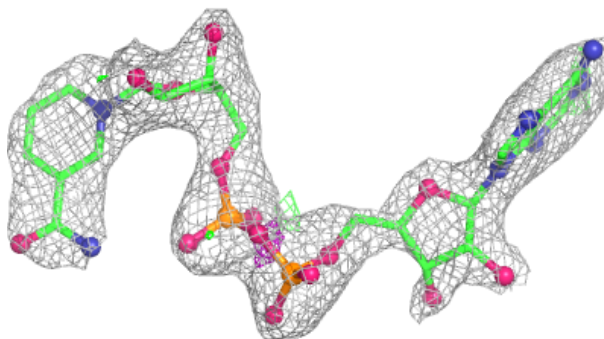
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1JZN A 802:

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

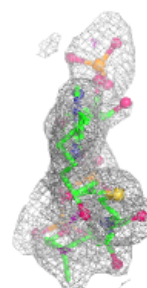
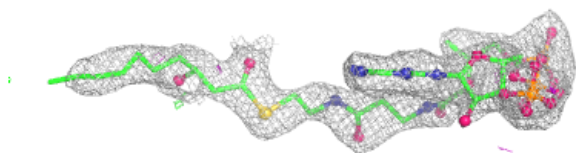
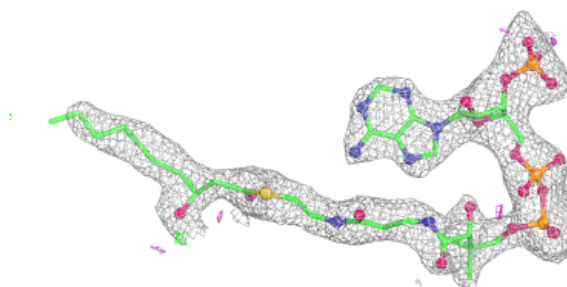
**Electron density around NAD A 801:**

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

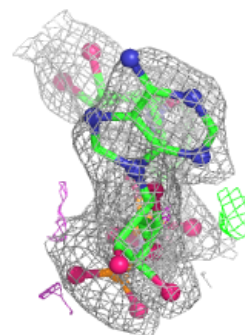
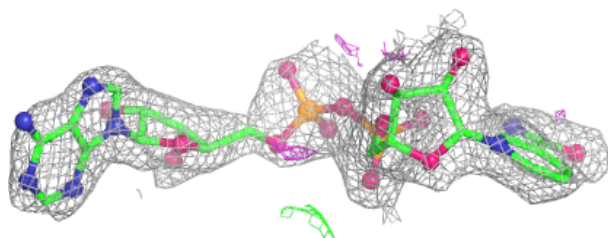
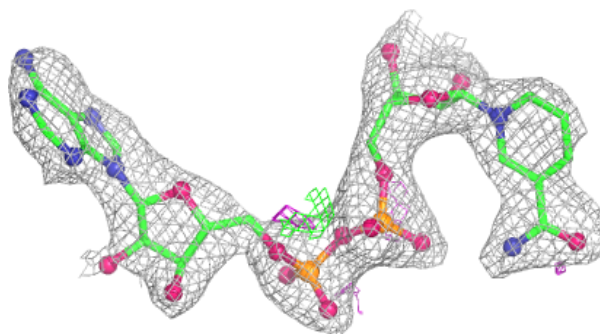


Electron density around A1JZ1 B 803:

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

**Electron density around NAD B 801:**

$2mF_o-DF_c$ (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.