Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 08:04 pm BST

PDB ID	:	4H03
Title	:	Crystal structure of NAD+-Ia-actin complex
Authors	:	Tsurumura, T.; Oda, M.; Nagahama, M.; Tsuge, H.
Deposited on	:	2012-09-07
Resolution	:	1.75 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

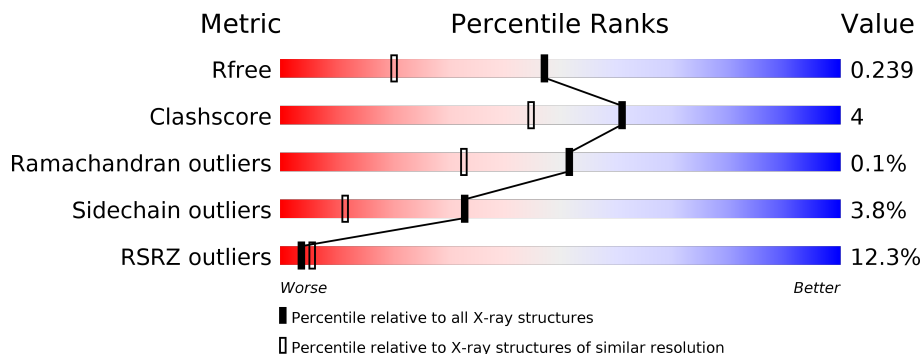|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1　Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	Percentile Ranks	Value
Rfree		0.239
Clashscore		4
Ramachandran outliers		0.1%
Sidechain outliers		3.8%
RSRZ outliers		12.3%

■ Percentile relative to all X-ray structures
⧠ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	418	13%　／　90%　　　8%　••
2	B	375	11%　／　82%　　　12%　•　5%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6745 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 Iota toxin component Ia.

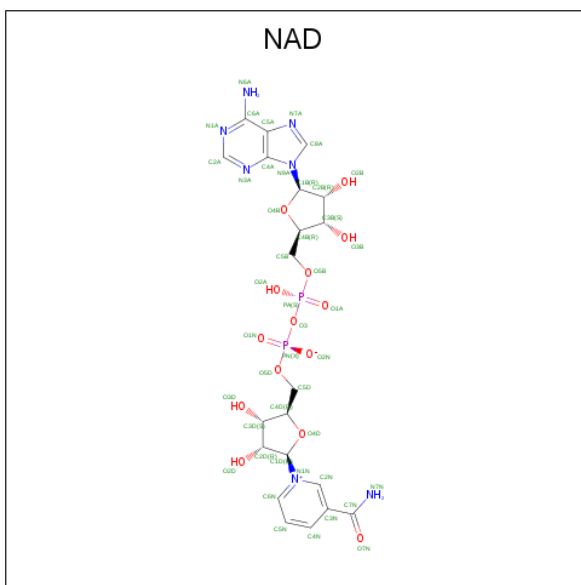| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total 3371	C 2151	N 554	O 662	S 4	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ARG	-	EXPRESSION TAG	UNP Q46220
A	-3	GLY	-	EXPRESSION TAG	UNP Q46220
A	-2	SER	-	EXPRESSION TAG	UNP Q46220
A	-1	HIS	-	EXPRESSION TAG	UNP Q46220
A	0	MET	-	EXPRESSION TAG	UNP Q46220

- Molecule 2 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	358	Total 2800	C 1775	N 469	O 537	S 19	0	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: 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		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
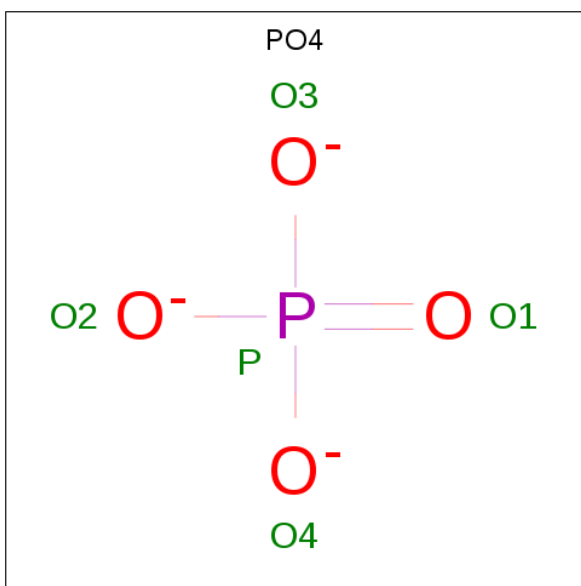
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

O2

OH

C1

C2

HO

O1

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0

W O R L D W I D E
PDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Ca 1	0	0

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

ATP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

• Molecule 8 is LATRUNCULIN A (three-letter code: LAR) (formula: $C_{22}H_{31}NO_5S$).

LAR

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	S	0	0
			29	22	1	5	1		

• Molecule 9 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	157	Total 157	O 157	0	0
9	B	115	Total 115	O 115	0	0

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: Iota toxin component Ia
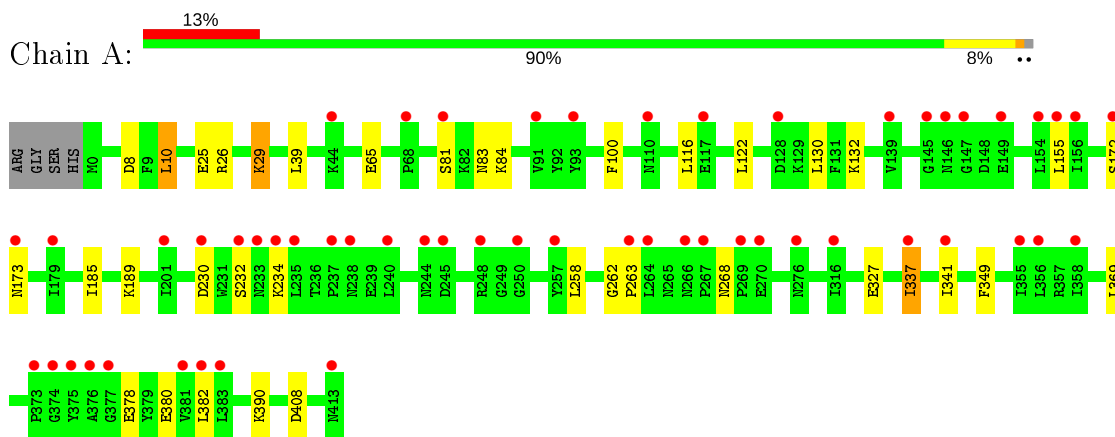
• Molecule 2: Actin, alpha skeletal muscle
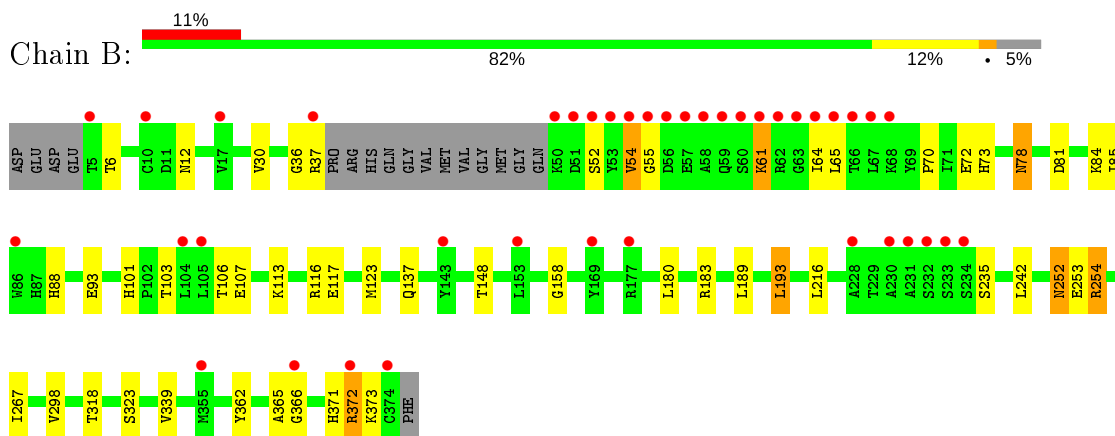
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	53.86Å 135.04Å 154.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.29 – 1.75 26.29 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.3 (26.29-1.75) 96.3 (26.29-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.32 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.216 , 0.233 0.224 , 0.239	Depositor DCC
R_{free} test set	5535 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	22.5	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 47.7	EDS
L-test for twinning[2]	$< |L| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6745	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, PO4, EDO, HIC, ATP, CA, LAR

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	0.34	0/3440	0.61	0/4647
2	B	0.36	0/2846	0.64	2/3855 (0.1%)
All	All	0.35	0/6286	0.62	2/8502 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	254	ARG	NE-CZ-NH1	-8.40	116.10	120.30
2	B	254	ARG	NE-CZ-NH2	8.08	124.34	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3371	0	3355	14	0
2	B	2800	0	2774	41	0
3	A	44	0	26	0	0
4	A	5	0	0	0	0
5	A	92	0	138	3	0
5	B	100	0	150	11	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	31	0	12	0	0
8	B	29	0	31	0	0
9	A	157	0	0	2	0
9	B	115	0	0	5	0
All	All	6745	0	6486	58	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 4.

All (58) 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)
2:B:216:LEU:O	2:B:254:ARG:HD2	1.63	0.96
1:A:337:ILE:HD11	9:A:641:HOH:O	1.70	0.91
2:B:298:VAL:CG1	5:B:408:EDO:H21	2.17	0.74
2:B:113:LYS:HG3	2:B:371:HIS:NE2	2.04	0.72
2:B:362:TYR:O	2:B:365:ALA:O	2.11	0.68
2:B:366:GLY:HA3	9:B:501:HOH:O	1.98	0.64
1:A:100:PHE:CE2	1:A:185:ILE:HD11	2.34	0.62
1:A:172:SER:OG	1:A:173:ASN:N	2.32	0.61
2:B:64:ILE:HG23	2:B:65:LEU:HD13	1.86	0.58
2:B:148:THR:H	5:B:413:EDO:H12	1.70	0.57
5:B:411:EDO:H21	5:B:412:EDO:O2	2.05	0.55
2:B:54:VAL:HG12	2:B:55:GLY:N	2.22	0.55
2:B:216:LEU:O	2:B:254:ARG:CD	2.47	0.54
2:B:298:VAL:HG12	5:B:408:EDO:H21	1.89	0.54
2:B:323:SER:HA	5:B:410:EDO:H22	1.90	0.54
2:B:36:GLY:O	2:B:52:SER:HB3	2.08	0.53
2:B:116:ARG:NE	9:B:586:HOH:O	2.42	0.53
2:B:70:PRO:HG2	2:B:85:ILE:CD1	2.40	0.52
1:A:81:SER:O	1:A:84:LYS:NZ	2.43	0.51
2:B:70:PRO:HG2	2:B:85:ILE:HD12	1.93	0.51
1:A:25:GLU:O	1:A:29:LYS:HD3	2.12	0.50
1:A:327:GLU:OE1	5:A:507:EDO:H21	2.12	0.49
2:B:6:THR:O	2:B:101:HIS:HD2	1.94	0.49
2:B:113:LYS:CG	2:B:371:HIS:CE1	2.95	0.49
2:B:113:LYS:CG	2:B:371:HIS:NE2	2.75	0.49
2:B:158:GLY:HA2	5:B:404:EDO:H11	1.95	0.48
1:A:26:ARG:HH22	1:A:83:ASN:HD21	1.61	0.48
2:B:30:VAL:HG11	9:B:561:HOH:O	2.13	0.48
2:B:372:ARG:HB3	2:B:373:LYS:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:ASN:HD22	2:B:81:ASP:H	1.62	0.47
2:B:61:LYS:HB3	2:B:65:LEU:HD22	1.97	0.47
2:B:107:GLU:OE1	2:B:116:ARG:CZ	2.63	0.46
2:B:180:LEU:HD13	2:B:267:ILE:HD11	1.98	0.46
1:A:378:GLU:HB2	1:A:380:GLU:HB2	1.97	0.45
2:B:252:ASN:HD22	2:B:253:GLU:N	2.15	0.45
1:A:337:ILE:HD12	1:A:337:ILE:N	2.32	0.45
1:A:262:GLY:N	1:A:263:PRO:CD	2.80	0.44
2:B:189:LEU:HG	2:B:193:LEU:HD22	1.99	0.44
2:B:183:ARG:N	9:B:585:HOH:O	2.51	0.44
2:B:78:ASN:ND2	2:B:81:ASP:H	2.15	0.44
1:A:369:LEU:HD22	1:A:382:LEU:HB2	2.00	0.43
2:B:372:ARG:HB2	2:B:372:ARG:CZ	2.48	0.43
2:B:106:THR:HB	2:B:137:GLN:HG3	2.01	0.43
2:B:318:THR:HG23	5:B:410:EDO:H21	2.01	0.42
1:A:8:ASP:CG	1:A:10:LEU:HD13	2.40	0.42
2:B:84:LYS:HD3	2:B:84:LYS:HA	1.83	0.41
2:B:298:VAL:HG11	5:B:408:EDO:H21	2.02	0.41
1:A:65:GLU:HG3	5:A:524:EDO:C2	2.50	0.41
1:A:132:LYS:NZ	1:A:408:ASP:OD2	2.48	0.41
2:B:117:GLU:OE2	2:B:371:HIS:HE1	2.04	0.40
2:B:103:THR:HB	2:B:123:MET:CE	2.51	0.40
5:B:411:EDO:C2	5:B:412:EDO:O2	2.67	0.40
2:B:88:HIS:HE1	2:B:93:GLU:OE2	2.04	0.40
2:B:72:GLU:O	2:B:73:HIC:C	2.70	0.40
2:B:148:THR:N	5:B:413:EDO:H12	2.34	0.40
5:A:521:EDO:C2	9:A:622:HOH:O	2.70	0.40
2:B:148:THR:H	5:B:413:EDO:C1	2.32	0.40
2:B:339:VAL:HG23	9:B:524:HOH:O	2.22	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	412/418 (99%)	402 (98%)	10 (2%)	0	100	100
2	B	353/375 (94%)	343 (97%)	9 (2%)	1 (0%)	41	22
All	All	765/793 (96%)	745 (97%)	19 (2%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	54	VAL

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	377/380 (99%)	360 (96%)	17 (4%)	27	8
2	B	303/317 (96%)	294 (97%)	9 (3%)	41	18
All	All	680/697 (98%)	654 (96%)	26 (4%)	33	11

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	29	LYS
1	A	39	LEU
1	A	116	LEU
1	A	122	LEU
1	A	130	LEU
1	A	155	LEU
1	A	189	LYS
1	A	230	ASP
1	A	232	SER
1	A	234	LYS
1	A	258	LEU
1	A	268	ASN
1	A	337	ILE
1	A	341	ILE

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Mol	Chain	Res	Type
1	A	349	PHE
1	A	390	LYS
2	B	12	ASN
2	B	37	ARG
2	B	61	LYS
2	B	78	ASN
2	B	193	LEU
2	B	235	SER
2	B	242	LEU
2	B	252	ASN
2	B	372	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	83	ASN
1	A	90	ASN
1	A	110	ASN
1	A	157	HIS
1	A	163	ASN
1	A	181	GLN
1	A	209	ASN
1	A	268	ASN
1	A	277	ASN
1	A	392	ASN
2	B	78	ASN
2	B	88	HIS
2	B	101	HIS
2	B	121	GLN
2	B	252	ASN
2	B	263	GLN
2	B	371	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	HIC	B	73	2	8,11,12	1.89	1 (12%)	6,14,16	1.30	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HIC	B	73	2	-	0/5/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	73	HIC	CD2-NE2	-4.75	1.31	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	73	HIC	CD2-NE2-CE1	2.15	111.42	107.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	73	HIC	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 53 ligands modelled in this entry, 1 is monoatomic - leaving 52 for Mogul analysis.

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	$\#|Z| > 2$
5	EDO	B	414	-	3,3,3	0.47	0	2,2,2	0.20	0
5	EDO	A	508	-	3,3,3	0.61	0	2,2,2	0.17	0
5	EDO	B	423	-	3,3,3	0.47	0	2,2,2	0.28	0
5	EDO	A	504	-	3,3,3	0.47	0	2,2,2	0.30	0
5	EDO	B	404	-	3,3,3	0.62	0	2,2,2	0.16	0
5	EDO	A	517	-	3,3,3	0.50	0	2,2,2	0.10	0
5	EDO	B	405	-	3,3,3	0.49	0	2,2,2	0.35	0
5	EDO	A	522	-	3,3,3	0.53	0	2,2,2	0.35	0
5	EDO	B	420	-	3,3,3	0.49	0	2,2,2	0.19	0
5	EDO	A	505	-	3,3,3	0.48	0	2,2,2	0.21	0
5	EDO	A	518	-	3,3,3	0.47	0	2,2,2	0.31	0
5	EDO	A	506	-	3,3,3	0.45	0	2,2,2	0.50	0
5	EDO	A	523	-	3,3,3	0.53	0	2,2,2	0.25	0
5	EDO	A	510	-	3,3,3	0.46	0	2,2,2	0.36	0
5	EDO	A	515	-	3,3,3	0.43	0	2,2,2	0.23	0
7	ATP	B	402	-	26,33,33	0.90	<mark>1 (3%)</mark>	31,52,52	1.25	<mark>4 (12%)</mark>
5	EDO	A	503	-	3,3,3	0.46	0	2,2,2	0.40	0
5	EDO	B	422	-	3,3,3	0.49	0	2,2,2	0.24	0
5	EDO	B	410	-	3,3,3	0.39	0	2,2,2	0.43	0
4	PO4	A	502	-	4,4,4	0.90	0	6,6,6	0.48	0
5	EDO	A	519	-	3,3,3	0.50	0	2,2,2	0.11	0
5	EDO	B	424	-	3,3,3	0.45	0	2,2,2	0.22	0
5	EDO	B	415	-	3,3,3	0.47	0	2,2,2	0.24	0
5	EDO	A	521	-	3,3,3	0.54	0	2,2,2	0.22	0
5	EDO	B	411	-	3,3,3	0.49	0	2,2,2	0.14	0
5	EDO	B	418	-	3,3,3	0.49	0	2,2,2	0.26	0
5	EDO	B	407	-	3,3,3	0.44	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	B	428	-	3,3,3	0.51	0	2,2,2	0.29	0
5	EDO	A	513	-	3,3,3	0.46	0	2,2,2	0.38	0
5	EDO	B	417	-	3,3,3	0.46	0	2,2,2	0.32	0
5	EDO	B	416	-	3,3,3	0.51	0	2,2,2	0.22	0
5	EDO	B	413	-	3,3,3	0.48	0	2,2,2	0.31	0
5	EDO	B	412	-	3,3,3	0.42	0	2,2,2	0.43	0
5	EDO	A	512	-	3,3,3	0.44	0	2,2,2	0.23	0
3	NAD	A	501	-	42,48,48	0.90	4 (9%)	50,73,73	1.26	5 (10%)
5	EDO	A	525	-	3,3,3	0.46	0	2,2,2	0.22	0
5	EDO	A	511	-	3,3,3	0.49	0	2,2,2	0.37	0
5	EDO	B	426	-	3,3,3	0.56	0	2,2,2	0.36	0
5	EDO	A	507	-	3,3,3	0.47	0	2,2,2	0.18	0
5	EDO	A	514	-	3,3,3	0.51	0	2,2,2	0.22	0
5	EDO	B	408	-	3,3,3	0.49	0	2,2,2	0.41	0
5	EDO	B	409	-	3,3,3	0.46	0	2,2,2	0.21	0
5	EDO	A	509	-	3,3,3	0.51	0	2,2,2	0.17	0
5	EDO	B	427	-	3,3,3	0.49	0	2,2,2	0.27	0
5	EDO	A	524	-	3,3,3	0.45	0	2,2,2	0.35	0
5	EDO	B	419	-	3,3,3	0.47	0	2,2,2	0.24	0
5	EDO	A	520	-	3,3,3	0.46	0	2,2,2	0.22	0
5	EDO	A	516	-	3,3,3	0.47	0	2,2,2	0.39	0
5	EDO	B	406	-	3,3,3	0.50	0	2,2,2	0.12	0
5	EDO	B	421	-	3,3,3	0.48	0	2,2,2	0.23	0
8	LAR	B	403	-	30,31,31	1.56	2 (6%)	32,43,43	2.37	14 (43%)
5	EDO	B	425	-	3,3,3	0.62	0	2,2,2	0.49	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
5	EDO	B	414	-	-	0/1/1/1	-
5	EDO	A	508	-	-	1/1/1/1	-
5	EDO	B	423	-	-	1/1/1/1	-
5	EDO	A	504	-	-	1/1/1/1	-
5	EDO	B	404	-	-	1/1/1/1	-
5	EDO	A	517	-	-	1/1/1/1	-
5	EDO	B	405	-	-	0/1/1/1	-
5	EDO	A	522	-	-	0/1/1/1	-
5	EDO	B	420	-	-	1/1/1/1	-
5	EDO	A	505	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	518	-	-	0/1/1/1	-
5	EDO	A	506	-	-	0/1/1/1	-
5	EDO	A	523	-	-	1/1/1/1	-
5	EDO	A	510	-	-	0/1/1/1	-
5	EDO	A	515	-	-	0/1/1/1	-
7	ATP	B	402	-	-	3/18/38/38	0/3/3/3
5	EDO	A	503	-	-	0/1/1/1	-
5	EDO	B	422	-	-	0/1/1/1	-
5	EDO	B	410	-	-	1/1/1/1	-
5	EDO	A	519	-	-	1/1/1/1	-
5	EDO	B	424	-	-	0/1/1/1	-
5	EDO	B	415	-	-	0/1/1/1	-
5	EDO	A	521	-	-	0/1/1/1	-
5	EDO	B	411	-	-	1/1/1/1	-
5	EDO	B	418	-	-	1/1/1/1	-
5	EDO	B	407	-	-	0/1/1/1	-
5	EDO	B	428	-	-	1/1/1/1	-
5	EDO	A	513	-	-	0/1/1/1	-
5	EDO	B	417	-	-	0/1/1/1	-
5	EDO	B	416	-	-	1/1/1/1	-
5	EDO	B	413	-	-	1/1/1/1	-
5	EDO	B	412	-	-	0/1/1/1	-
5	EDO	A	512	-	-	0/1/1/1	-
3	NAD	A	501	-	-	1/26/62/62	0/5/5/5
5	EDO	A	525	-	-	0/1/1/1	-
5	EDO	A	511	-	-	1/1/1/1	-
5	EDO	B	426	-	-	1/1/1/1	-
5	EDO	A	507	-	-	0/1/1/1	-
5	EDO	A	514	-	-	1/1/1/1	-
5	EDO	B	408	-	-	0/1/1/1	-
5	EDO	B	409	-	-	0/1/1/1	-
5	EDO	A	509	-	-	0/1/1/1	-
5	EDO	B	427	-	-	1/1/1/1	-
5	EDO	A	524	-	-	0/1/1/1	-
5	EDO	B	419	-	-	0/1/1/1	-
5	EDO	A	520	-	-	1/1/1/1	-
5	EDO	A	516	-	-	0/1/1/1	-
5	EDO	B	406	-	-	1/1/1/1	-
5	EDO	B	421	-	-	1/1/1/1	-
8	LAR	B	403	-	-	6/23/51/51	0/2/3/3
5	EDO	B	425	-	-	1/1/1/1	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	403	LAR	O2-C1	5.41	1.45	1.34
8	B	403	LAR	C20-S1	-4.95	1.66	1.77
7	B	402	ATP	C5-C4	2.36	1.47	1.40
3	A	501	NAD	C5A-C4A	2.34	1.47	1.40
3	A	501	NAD	O4B-C1B	2.17	1.44	1.41
3	A	501	NAD	C2A-N3A	2.07	1.35	1.32
3	A	501	NAD	O4D-C1D	2.02	1.43	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	403	LAR	C4-C5-C6	-7.45	96.50	112.59
8	B	403	LAR	O2-C1-C2	4.85	122.65	111.27
8	B	403	LAR	C8-C7-C6	-4.28	100.89	125.51
3	A	501	NAD	N3A-C2A-N1A	-3.87	122.64	128.68
8	B	403	LAR	C19-S1-C20	3.76	94.02	92.00
7	B	402	ATP	N3-C2-N1	-3.24	123.61	128.68
8	B	403	LAR	O1-C1-C2	-3.12	118.37	126.23
8	B	403	LAR	O3-C17-C18	2.89	107.95	104.25
8	B	403	LAR	O2-C1-O1	-2.69	118.97	123.35
3	A	501	NAD	C3N-C7N-N7N	2.50	120.75	117.75
8	B	403	LAR	C5-C6-C7	2.38	137.53	125.90
8	B	403	LAR	C7-C8-C9	2.26	140.57	124.42
3	A	501	NAD	O5D-C5D-C4D	-2.26	101.22	108.99
7	B	402	ATP	C4-C5-N7	-2.24	107.07	109.40
3	A	501	NAD	N6A-C6A-N1A	2.21	123.17	118.57
8	B	403	LAR	C22-C10-C9	2.17	115.66	110.86
3	A	501	NAD	C5D-C4D-C3D	-2.17	107.04	115.18
7	B	402	ATP	PA-O3A-PB	-2.17	125.38	132.83
7	B	402	ATP	C2-N1-C6	2.09	122.32	118.75
8	B	403	LAR	O5-C20-N1	-2.08	124.54	126.81
8	B	403	LAR	C21-C3-C2	-2.04	116.65	122.77
8	B	403	LAR	O2-C15-C16	2.02	112.63	107.59
8	B	403	LAR	C4-C3-C2	2.00	127.85	121.87

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	411	EDO	O1-C1-C2-O2
5	A	504	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	B	404	EDO	O1-C1-C2-O2
5	B	420	EDO	O1-C1-C2-O2
5	A	523	EDO	O1-C1-C2-O2
5	B	418	EDO	O1-C1-C2-O2
5	B	416	EDO	O1-C1-C2-O2
5	B	427	EDO	O1-C1-C2-O2
5	B	421	EDO	O1-C1-C2-O2
5	B	425	EDO	O1-C1-C2-O2
5	B	423	EDO	O1-C1-C2-O2
3	A	501	NAD	PN-O3-PA-O2A
5	A	514	EDO	O1-C1-C2-O2
5	A	520	EDO	O1-C1-C2-O2
8	B	403	LAR	O2-C1-C2-C3
5	B	406	EDO	O1-C1-C2-O2
8	B	403	LAR	C4-C5-C6-C7
5	B	410	EDO	O1-C1-C2-O2
5	B	426	EDO	O1-C1-C2-O2
7	B	402	ATP	PB-O3B-PG-O2G
7	B	402	ATP	PG-O3B-PB-O1B
7	B	402	ATP	PG-O3B-PB-O2B
8	B	403	LAR	O1-C1-C2-C3
8	B	403	LAR	C9-C10-C11-C12
8	B	403	LAR	C3-C4-C5-C6
5	A	508	EDO	O1-C1-C2-O2
5	A	517	EDO	O1-C1-C2-O2
5	A	519	EDO	O1-C1-C2-O2
5	B	428	EDO	O1-C1-C2-O2
5	B	413	EDO	O1-C1-C2-O2
5	A	511	EDO	O1-C1-C2-O2
8	B	403	LAR	C10-C11-C12-C13

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	404	EDO	1	0
5	B	410	EDO	2	0
5	A	521	EDO	1	0
5	B	411	EDO	2	0
5	B	413	EDO	3	0
5	B	412	EDO	2	0
5	A	507	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	408	EDO	3	0
5	A	524	EDO	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 then 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 ATP B 402

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand LAR B 403

Bond lengths

Bond angles

Torsions

Rings
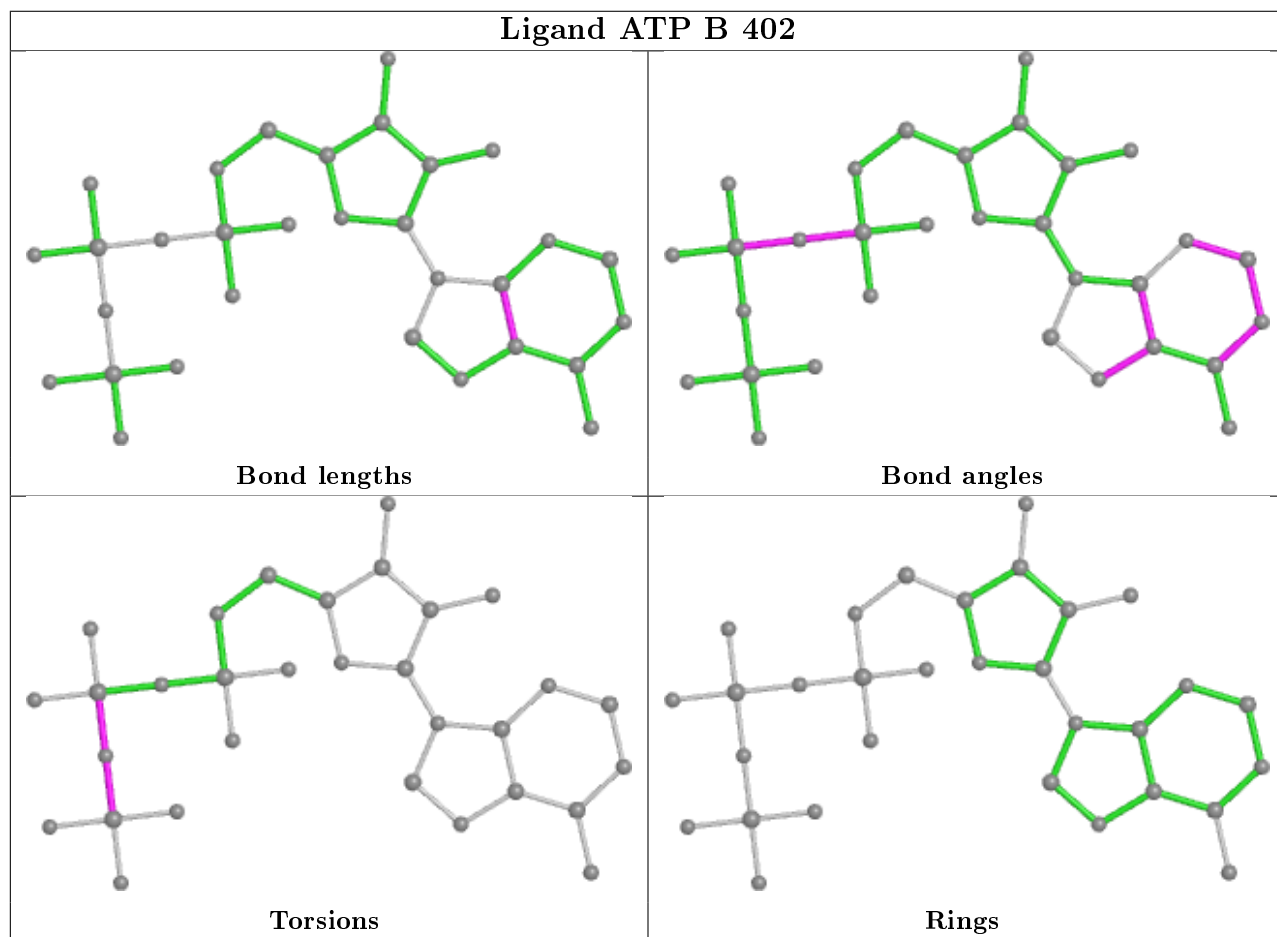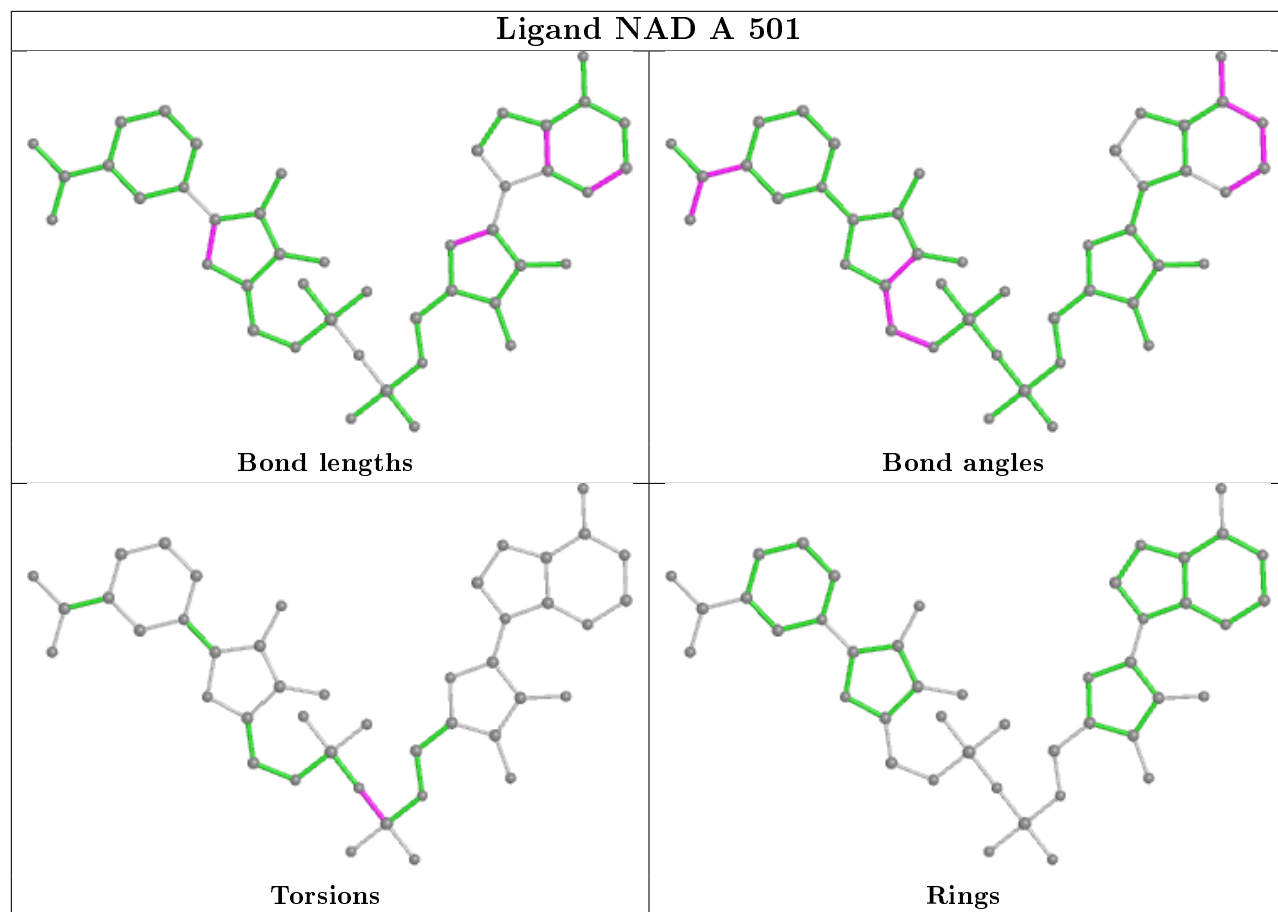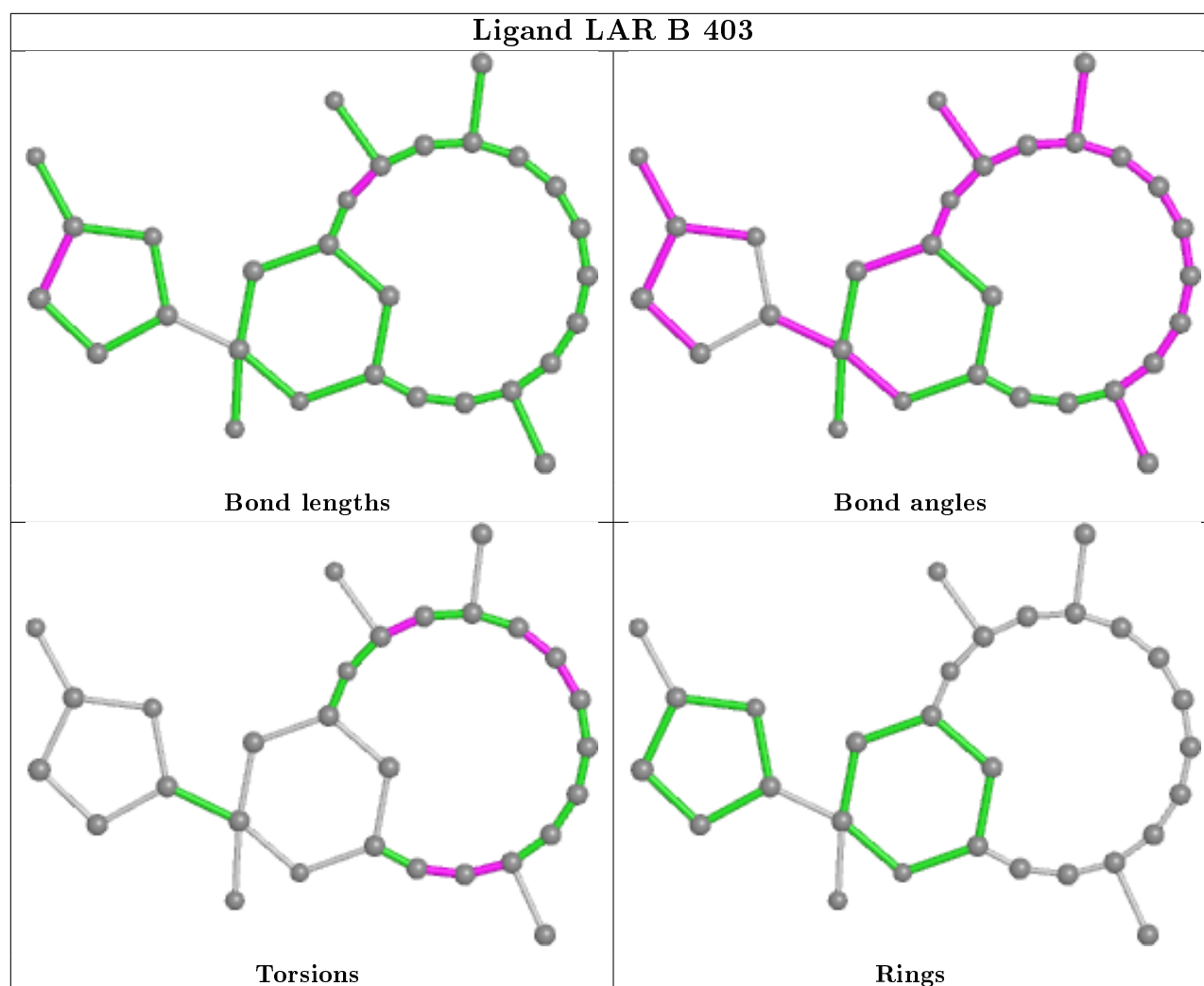
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	414/418 (99%)	0.79	55 (13%)	3	4	19, 30, 54, 86	0
2	B	357/375 (95%)	0.76	40 (11%)	5	7	13, 20, 57, 114	0
All	All	771/793 (97%)	0.77	95 (12%)	4	6	13, 25, 56, 114	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	376	ALA	10.4
2	B	60	SER	10.0
2	B	52	SER	9.7
2	B	53	TYR	9.0
2	B	59	GLN	9.0
2	B	50	LYS	8.2
1	A	375	TYR	8.1
2	B	63	GLY	7.7
2	B	58	ALA	7.6
2	B	57	GLU	6.8
2	B	61	LYS	6.8
2	B	51	ASP	6.8
2	B	54	VAL	6.6
2	B	37	ARG	6.5
2	B	64	ILE	6.0
2	B	55	GLY	5.6
1	A	264	LEU	5.6
2	B	56	ASP	5.1
2	B	372	ARG	4.9
1	A	110	ASN	4.6
2	B	62	ARG	4.5
2	B	66	THR	4.5
2	B	232	SER	4.5
1	A	173	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	237	PRO	4.4
1	A	269	PRO	4.4
1	A	374	GLY	4.2
2	B	231	ALA	4.2
1	A	238	ASN	4.1
1	A	128	ASP	4.1
1	A	233	ASN	4.0
1	A	377	GLY	3.7
2	B	65	LEU	3.7
1	A	146	ASN	3.7
1	A	81	SER	3.4
1	A	248	ARG	3.3
2	B	5	THR	3.3
1	A	337	ILE	3.2
1	A	373	PRO	3.2
1	A	230	ASP	3.2
2	B	143	TYR	3.2
2	B	105	LEU	3.1
1	A	117	GLU	3.1
1	A	201	ILE	3.1
1	A	270	GLU	3.0
1	A	266	ASN	3.0
1	A	179	ILE	3.0
2	B	86	TRP	3.0
1	A	91	VAL	3.0
1	A	235	LEU	2.9
1	A	172	SER	2.9
1	A	145	GLY	2.8
1	A	244	ASN	2.8
1	A	156	ILE	2.8
1	A	382	LEU	2.8
1	A	155	LEU	2.8
1	A	68	PRO	2.7
2	B	374	CYS	2.7
1	A	139	VAL	2.6
2	B	169	TYR	2.6
1	A	316	ILE	2.6
1	A	257	TYR	2.6
2	B	230	ALA	2.6
1	A	44	LYS	2.6
1	A	267	PRO	2.6
1	A	240	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	104	LEU	2.5
1	A	234	LYS	2.5
2	B	228	ALA	2.4
1	A	147	GLY	2.4
1	A	381	VAL	2.4
1	A	250	GLY	2.4
2	B	233	SER	2.4
2	B	10	CYS	2.4
1	A	263	PRO	2.3
1	A	413	ASN	2.3
1	A	93	TYR	2.3
1	A	232	SER	2.3
1	A	356	LEU	2.3
2	B	67	LEU	2.3
1	A	355	ILE	2.3
1	A	383	LEU	2.2
2	B	355	MET	2.2
2	B	234	SER	2.2
1	A	154	LEU	2.2
1	A	245	ASP	2.2
1	A	149	GLU	2.2
1	A	358	ILE	2.1
1	A	276	ASN	2.1
1	A	341	ILE	2.1
2	B	153	LEU	2.0
2	B	366	GLY	2.0
2	B	68	LYS	2.0
2	B	177	ARG	2.0
2	B	17	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HIC	B	73	11/12	0.93	0.11	20,23,28,28	0

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(Å^2)	Q<0.9
5	EDO	A	506	4/4	0.62	0.27	42,44,44,44	0
5	EDO	B	406	4/4	0.66	0.29	45,45,45,45	0
5	EDO	A	507	4/4	0.69	0.19	38,38,38,38	0
5	EDO	B	423	4/4	0.70	0.19	46,46,46,47	0
5	EDO	A	511	4/4	0.73	0.17	41,41,42,42	0
5	EDO	B	421	4/4	0.73	0.22	38,38,39,39	0
5	EDO	A	519	4/4	0.74	0.21	47,48,48,48	0
5	EDO	B	420	4/4	0.74	0.33	39,41,42,42	0
5	EDO	B	426	4/4	0.75	0.26	45,45,45,45	0
5	EDO	A	521	4/4	0.76	0.22	46,46,46,46	0
5	EDO	B	411	4/4	0.76	0.22	40,41,41,41	0
5	EDO	B	416	4/4	0.77	0.21	37,37,38,38	0
5	EDO	B	413	4/4	0.77	0.24	30,33,33,33	0
5	EDO	B	424	4/4	0.77	0.20	37,38,38,39	0
5	EDO	B	428	4/4	0.78	0.19	47,47,47,47	0
5	EDO	B	404	4/4	0.79	0.22	34,34,34,35	0
5	EDO	B	425	4/4	0.79	0.19	31,32,33,33	0
5	EDO	A	510	4/4	0.80	0.14	43,43,43,44	0
5	EDO	A	516	4/4	0.82	0.20	45,46,46,46	0
5	EDO	A	524	4/4	0.82	0.31	40,41,41,41	0
5	EDO	B	418	4/4	0.83	0.17	39,39,39,39	0
5	EDO	B	427	4/4	0.85	0.32	45,45,46,46	0
5	EDO	A	512	4/4	0.85	0.23	38,39,39,39	0
5	EDO	A	522	4/4	0.86	0.19	36,36,36,36	0
5	EDO	B	412	4/4	0.86	0.17	47,48,48,48	0
5	EDO	A	514	4/4	0.86	0.19	47,48,48,48	0
5	EDO	B	408	4/4	0.87	0.17	22,22,22,23	0
5	EDO	A	518	4/4	0.87	0.16	34,34,34,34	0
5	EDO	A	515	4/4	0.87	0.14	38,38,38,38	0
5	EDO	A	517	4/4	0.87	0.11	36,36,36,36	0
5	EDO	A	523	4/4	0.88	0.26	36,36,36,36	0
5	EDO	A	508	4/4	0.88	0.14	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
5	EDO	A	503	4/4	0.89	0.14	26,27,27,27	0
3	NAD	A	501	44/44	0.90	0.11	26,30,33,34	0
5	EDO	A	520	4/4	0.91	0.13	33,34,34,34	0
5	EDO	B	410	4/4	0.91	0.32	33,33,33,33	0
5	EDO	B	415	4/4	0.91	0.14	38,40,40,40	0
5	EDO	A	513	4/4	0.92	0.14	38,38,38,38	0
5	EDO	B	409	4/4	0.92	0.14	35,35,35,35	0
8	LAR	B	403	29/29	0.93	0.11	20,22,28,28	0
5	EDO	A	525	4/4	0.93	0.22	40,40,40,40	0
5	EDO	B	405	4/4	0.94	0.21	43,44,44,44	0
5	EDO	B	414	4/4	0.94	0.11	27,27,27,27	0
4	PO4	A	502	5/5	0.95	0.13	40,42,42,42	0
5	EDO	A	509	4/4	0.95	0.09	26,26,26,27	0
5	EDO	B	422	4/4	0.95	0.15	23,23,23,23	0
5	EDO	B	419	4/4	0.95	0.09	31,31,31,31	0
5	EDO	B	407	4/4	0.95	0.07	26,26,26,26	0
5	EDO	A	504	4/4	0.96	0.09	31,32,32,32	0
5	EDO	A	505	4/4	0.96	0.11	30,30,30,30	0
5	EDO	B	417	4/4	0.97	0.09	26,26,26,26	0
7	ATP	B	402	31/31	0.98	0.10	14,15,15,15	0
6	CA	B	401	1/1	0.99	0.06	15,15,15,15	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.
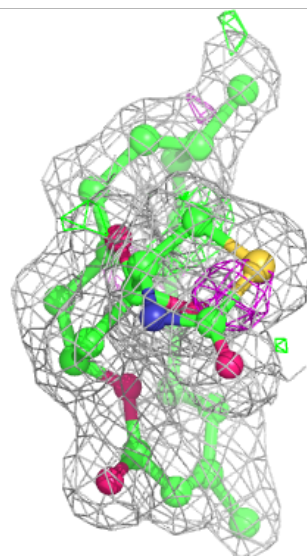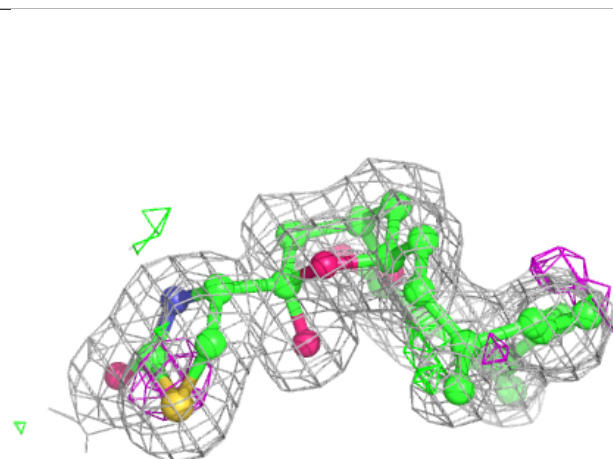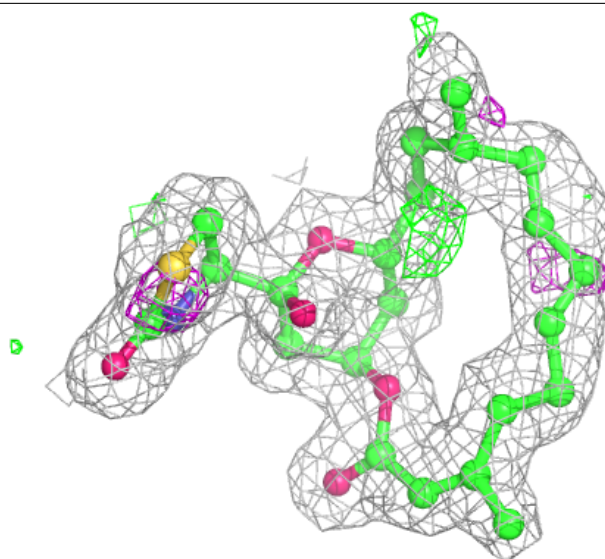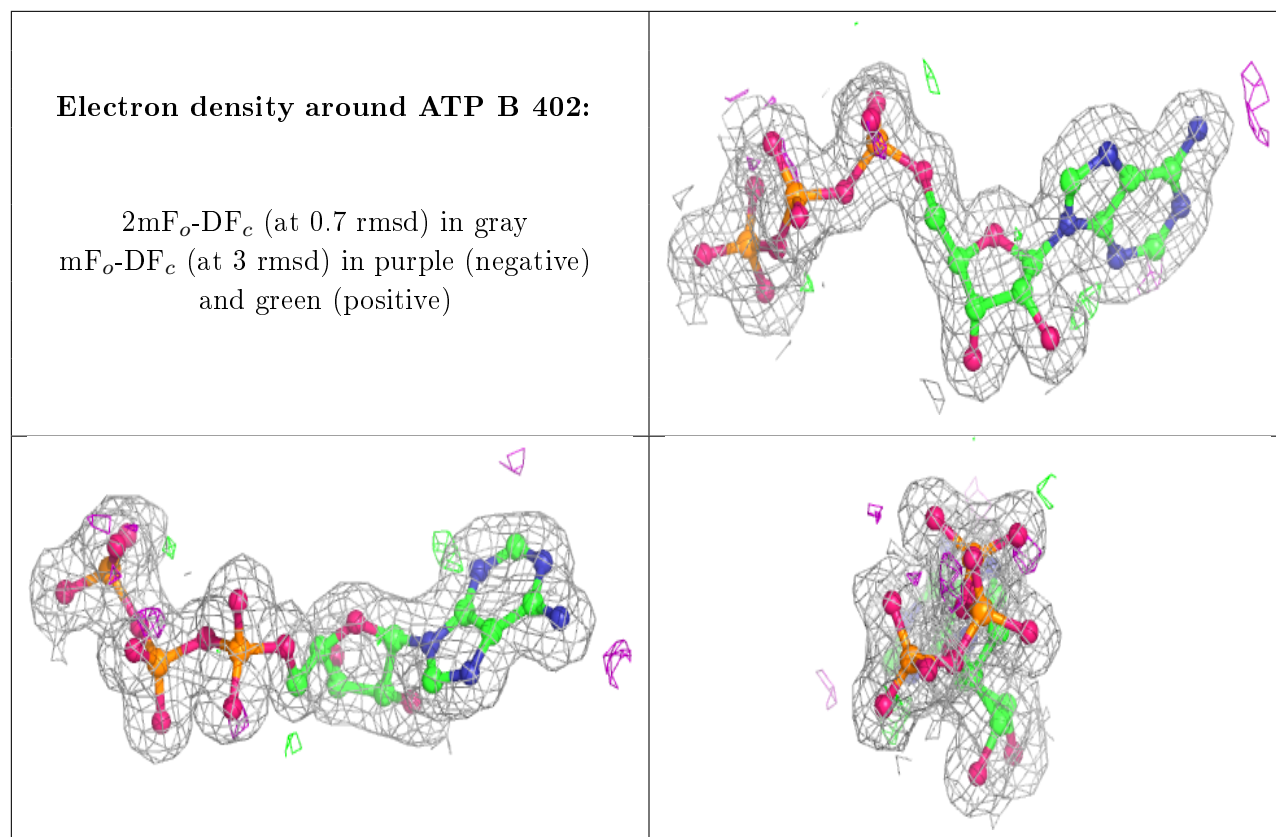
Electron density around NAD A 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
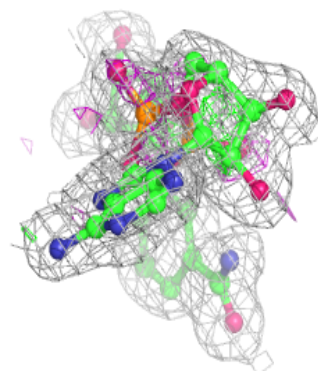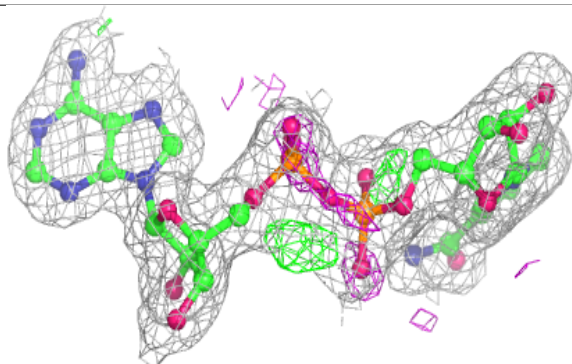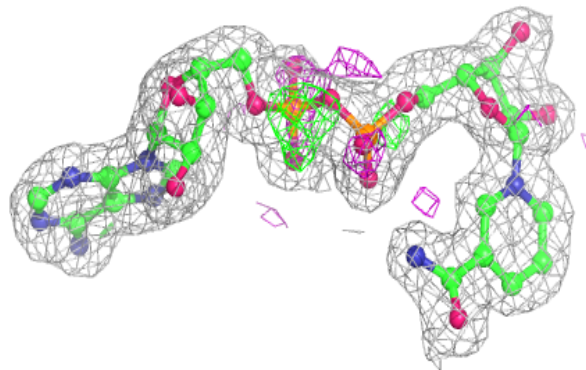
Electron density around LAR B 403:

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

Electron density around ATP B 402:

$2mF_o$-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 ⓘ

There are no such residues in this entry.