



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 04:47 PM UTC

PDB ID : 4H03 / pdb_00004h03
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

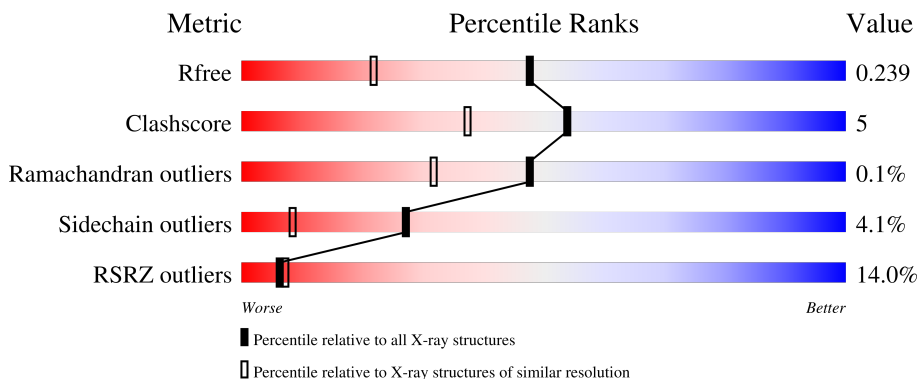
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 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	418	16% 90% 7% ..
2	B	375	11% 81% 13% • 5%

2 Entry composition

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	C	N	O	S	0	0	0
			3371	2151	554	662	4			

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.

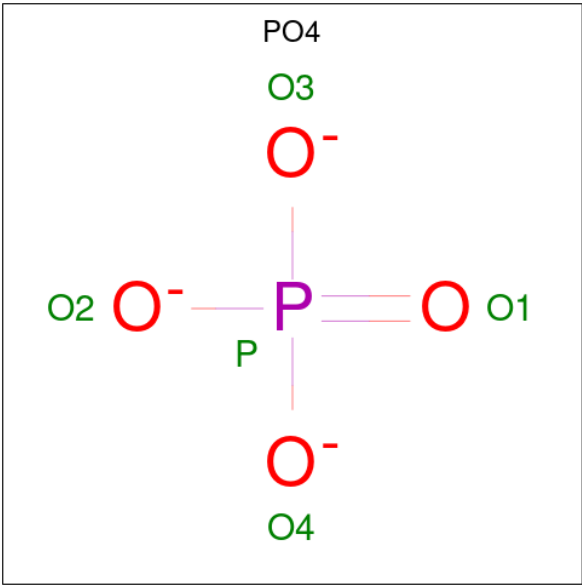
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	358	Total	C	N	O	S	0	0	0
			2800	1775	469	537	19			

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



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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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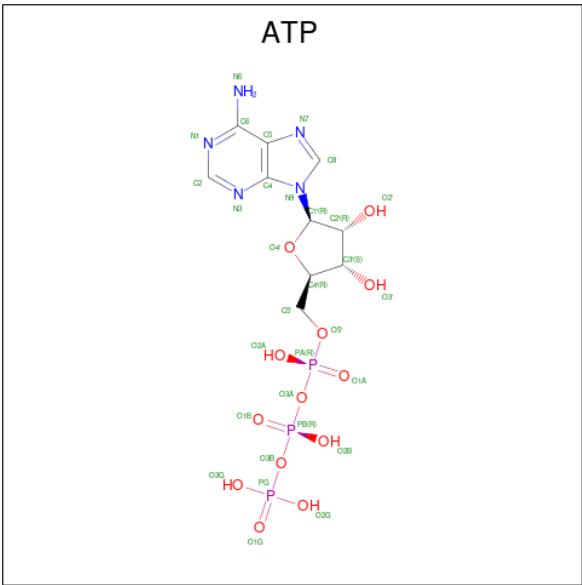
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

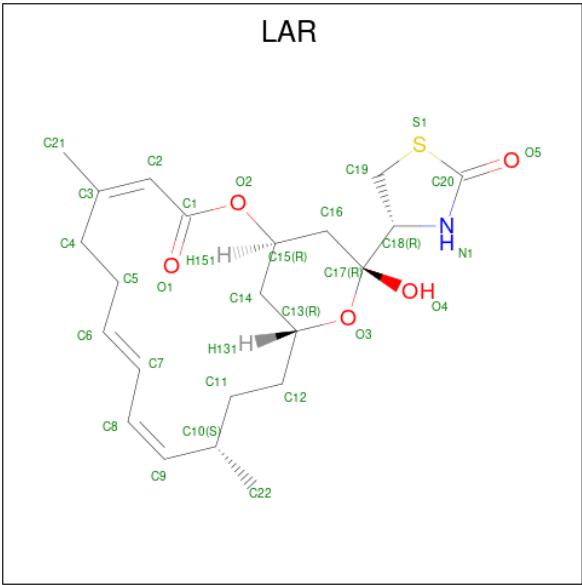
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Ca 1 1	0	0

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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 (CCD ID: LAR) (formula: C₂₂H₃₁NO₅S).



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

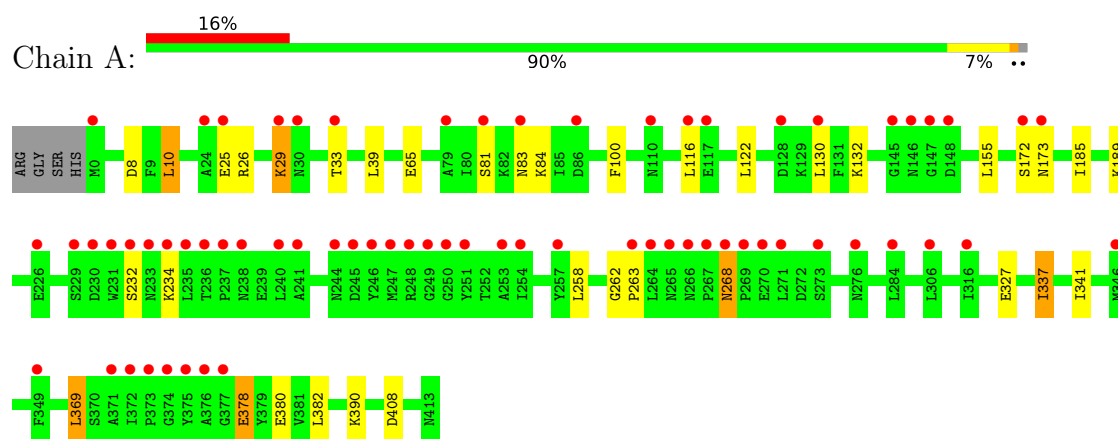
- Molecule 9 is water.

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

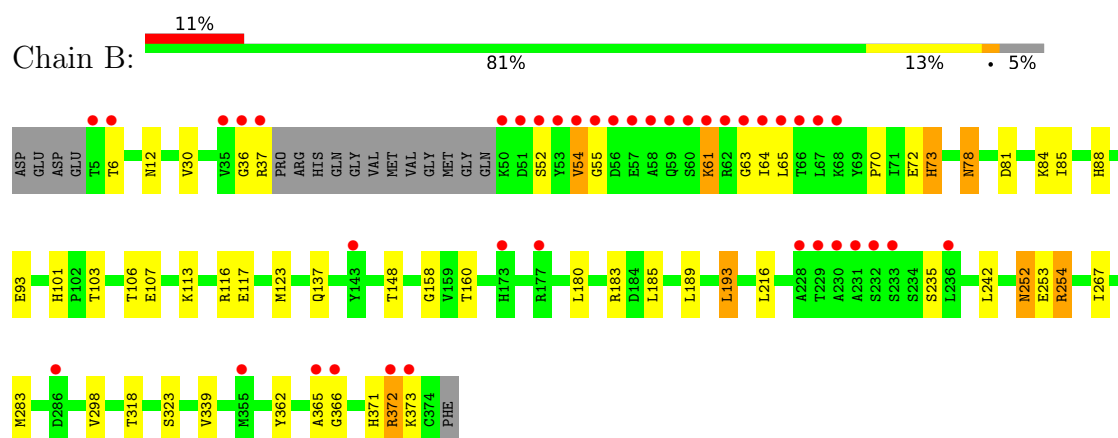
3 Residue-property plots

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: Iota toxin component Ia



- Molecule 2: Actin, alpha skeletal muscle



4 Data and refinement statistics

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) 96.4 (26.29-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.83%)	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 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/3440	0.75	0/4647
2	B	0.47	0/2846	0.80	3/3855 (0.1%)
All	All	0.45	0/6286	0.77	3/8502 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	254	ARG	NE-CZ-NH2	5.71	124.34	119.20
2	B	160	THR	OG1-CB-CG2	5.59	120.48	109.30
2	B	254	ARG	NE-CZ-NH1	-5.40	116.10	121.50

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	15	0
2	B	2800	0	2774	45	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	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
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	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 5.

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)
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
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
2:B:103:THR:HG21	2:B:123:MET:HE1	1.87	0.56
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
1:A:172:SER:OG	1:A:173:ASN:N	2.32	0.54
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
2:B:283:MET:HE2	5:B:426:EDO:H22	1.94	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:8:ASP:CG	1:A:10:LEU:HD13	2.40	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
2:B:103:THR:CG2	2:B:123:MET:HE1	2.46	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:CZ	2:B:372:ARG:HB2	2.48	0.43
1:A:268:ASN:C	1:A:268:ASN:HD22	2.27	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
2:B:63:GLY:C	2:B:65:LEU:H	2.28	0.42
2:B:84:LYS:HA	2:B:84:LYS:HD3	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:88:HIS:HE1	2:B:93:GLU:OE2	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: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

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	412/418 (99%)	402 (98%)	10 (2%)	0	100	100
2	B	353/375 (94%)	343 (97%)	9 (2%)	1 (0%)	36	21
All	All	765/793 (96%)	745 (97%)	19 (2%)	1 (0%)	48	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	54	VAL

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	377/380 (99%)	359 (95%)	18 (5%)	23	6
2	B	303/317 (96%)	293 (97%)	10 (3%)	33	13
All	All	680/697 (98%)	652 (96%)	28 (4%)	27	8

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	29	LYS
1	A	33	THR
1	A	39	LEU
1	A	116	LEU

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Mol	Chain	Res	Type
1	A	122	LEU
1	A	130	LEU
1	A	155	LEU
1	A	189	LYS
1	A	232	SER
1	A	234	LYS
1	A	258	LEU
1	A	268	ASN
1	A	337	ILE
1	A	341	ILE
1	A	369	LEU
1	A	378	GLU
1	A	390	LYS
2	B	12	ASN
2	B	37	ARG
2	B	61	LYS
2	B	78	ASN
2	B	185	LEU
2	B	193	LEU
2	B	235	SER
2	B	242	LEU
2	B	252	ASN
2	B	372	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	83	ASN
1	A	110	ASN
1	A	127	GLN
1	A	157	HIS
1	A	163	ASN
1	A	181	GLN
1	A	255	ASN
1	A	265	ASN
1	A	268	ASN
1	A	277	ASN
1	A	359	ASN
2	B	78	ASN
2	B	88	HIS
2	B	101	HIS

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Mol	Chain	Res	Type
2	B	121	GLN
2	B	128	ASN
2	B	137	GLN
2	B	173	HIS
2	B	252	ASN
2	B	371	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	10,11,12	1.69	2 (20%)	9,14,16	6.27	2 (22%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	73	HIC	CD2-NE2	-4.06	1.31	1.37
2	B	73	HIC	CG-ND1	-2.19	1.32	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	73	HIC	NE2-CE1-ND1	-14.12	107.25	112.66
2	B	73	HIC	CD2-NE2-CE1	11.92	111.42	106.71

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 oligosaccharides 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	A	507	-	3,3,3	0.44	0	2,2,2	0.22	0
5	EDO	A	503	-	3,3,3	0.43	0	2,2,2	0.44	0
5	EDO	B	419	-	3,3,3	0.44	0	2,2,2	0.28	0
5	EDO	B	421	-	3,3,3	0.45	0	2,2,2	0.25	0
5	EDO	B	415	-	3,3,3	0.44	0	2,2,2	0.28	0
5	EDO	B	416	-	3,3,3	0.48	0	2,2,2	0.25	0
5	EDO	B	426	-	3,3,3	0.54	0	2,2,2	0.39	0
5	EDO	B	412	-	3,3,3	0.40	0	2,2,2	0.47	0
5	EDO	B	414	-	3,3,3	0.43	0	2,2,2	0.25	0
5	EDO	A	511	-	3,3,3	0.46	0	2,2,2	0.41	0
5	EDO	A	517	-	3,3,3	0.46	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	A	502	-	4,4,4	0.94	0	6,6,6	0.51	0
5	EDO	A	516	-	3,3,3	0.44	0	2,2,2	0.43	0
5	EDO	B	405	-	3,3,3	0.47	0	2,2,2	0.39	0
5	EDO	A	513	-	3,3,3	0.43	0	2,2,2	0.42	0
5	EDO	B	409	-	3,3,3	0.44	0	2,2,2	0.25	0
5	EDO	A	524	-	3,3,3	0.42	0	2,2,2	0.35	0
5	EDO	B	423	-	3,3,3	0.44	0	2,2,2	0.32	0
5	EDO	B	411	-	3,3,3	0.45	0	2,2,2	0.18	0
5	EDO	A	505	-	3,3,3	0.45	0	2,2,2	0.24	0
3	NAD	A	501	-	46,48,48	1.19	5 (10%)	64,73,73	1.72	13 (20%)
5	EDO	A	504	-	3,3,3	0.43	0	2,2,2	0.35	0
5	EDO	A	508	-	3,3,3	0.58	0	2,2,2	0.10	0
5	EDO	A	518	-	3,3,3	0.43	0	2,2,2	0.36	0
5	EDO	A	515	-	3,3,3	0.41	0	2,2,2	0.28	0
5	EDO	A	519	-	3,3,3	0.47	0	2,2,2	0.16	0
5	EDO	A	521	-	3,3,3	0.51	0	2,2,2	0.20	0
5	EDO	A	523	-	3,3,3	0.50	0	2,2,2	0.29	0
5	EDO	A	514	-	3,3,3	0.47	0	2,2,2	0.27	0
5	EDO	B	407	-	3,3,3	0.41	0	2,2,2	0.43	0
7	ATP	B	402	-	32,33,33	1.54	8 (25%)	48,52,52	1.68	10 (20%)
5	EDO	A	510	-	3,3,3	0.43	0	2,2,2	0.40	0
5	EDO	B	422	-	3,3,3	0.45	0	2,2,2	0.29	0
5	EDO	B	427	-	3,3,3	0.46	0	2,2,2	0.32	0
5	EDO	B	413	-	3,3,3	0.47	0	2,2,2	0.36	0
5	EDO	B	428	-	3,3,3	0.48	0	2,2,2	0.34	0
5	EDO	A	509	-	3,3,3	0.48	0	2,2,2	0.21	0
5	EDO	B	424	-	3,3,3	0.43	0	2,2,2	0.26	0
8	LAR	B	403	-	30,31,31	1.57	2 (6%)	32,43,43	2.62	13 (40%)
5	EDO	B	420	-	3,3,3	0.46	0	2,2,2	0.22	0
5	EDO	A	522	-	3,3,3	0.50	0	2,2,2	0.39	0
5	EDO	B	418	-	3,3,3	0.46	0	2,2,2	0.29	0
5	EDO	B	404	-	3,3,3	0.60	0	2,2,2	0.18	0
5	EDO	B	408	-	3,3,3	0.46	0	2,2,2	0.41	0
5	EDO	B	425	-	3,3,3	0.61	0	2,2,2	0.52	0
5	EDO	A	512	-	3,3,3	0.41	0	2,2,2	0.28	0
5	EDO	B	417	-	3,3,3	0.43	0	2,2,2	0.37	0
5	EDO	A	506	-	3,3,3	0.42	0	2,2,2	0.53	0
5	EDO	B	406	-	3,3,3	0.46	0	2,2,2	0.16	0
5	EDO	A	520	-	3,3,3	0.43	0	2,2,2	0.26	0
5	EDO	B	410	-	3,3,3	0.36	0	2,2,2	0.47	0
5	EDO	A	525	-	3,3,3	0.43	0	2,2,2	0.27	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	A	507	-	-	0/1/1/1	-
5	EDO	A	503	-	-	0/1/1/1	-
5	EDO	B	419	-	-	0/1/1/1	-
5	EDO	B	421	-	-	1/1/1/1	-
5	EDO	B	415	-	-	0/1/1/1	-
5	EDO	B	416	-	-	1/1/1/1	-
5	EDO	B	426	-	-	1/1/1/1	-
5	EDO	B	412	-	-	0/1/1/1	-
5	EDO	B	414	-	-	0/1/1/1	-
5	EDO	A	511	-	-	1/1/1/1	-
5	EDO	A	517	-	-	1/1/1/1	-
5	EDO	A	516	-	-	0/1/1/1	-
5	EDO	B	405	-	-	1/1/1/1	-
5	EDO	A	513	-	-	0/1/1/1	-
5	EDO	B	409	-	-	0/1/1/1	-
5	EDO	A	524	-	-	0/1/1/1	-
5	EDO	B	423	-	-	1/1/1/1	-
5	EDO	B	411	-	-	1/1/1/1	-
5	EDO	A	505	-	-	0/1/1/1	-
3	NAD	A	501	-	-	2/30/62/62	0/5/5/5
5	EDO	A	504	-	-	1/1/1/1	-
5	EDO	A	508	-	-	1/1/1/1	-
5	EDO	A	518	-	-	0/1/1/1	-
5	EDO	A	515	-	-	0/1/1/1	-
5	EDO	A	519	-	-	1/1/1/1	-
5	EDO	A	521	-	-	0/1/1/1	-
5	EDO	A	523	-	-	1/1/1/1	-
5	EDO	A	514	-	-	1/1/1/1	-
5	EDO	B	407	-	-	0/1/1/1	-
7	ATP	B	402	-	-	3/22/38/38	0/3/3/3
5	EDO	A	510	-	-	0/1/1/1	-
5	EDO	B	422	-	-	0/1/1/1	-
5	EDO	B	427	-	-	1/1/1/1	-
5	EDO	B	413	-	-	1/1/1/1	-
5	EDO	B	428	-	-	1/1/1/1	-
5	EDO	A	509	-	-	0/1/1/1	-
5	EDO	B	424	-	-	0/1/1/1	-
8	LAR	B	403	-	-	5/23/51/51	0/2/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	420	-	-	1/1/1/1	-
5	EDO	A	522	-	-	0/1/1/1	-
5	EDO	B	418	-	-	1/1/1/1	-
5	EDO	B	404	-	-	1/1/1/1	-
5	EDO	B	408	-	-	0/1/1/1	-
5	EDO	B	425	-	-	1/1/1/1	-
5	EDO	A	512	-	-	0/1/1/1	-
5	EDO	B	417	-	-	0/1/1/1	-
5	EDO	A	506	-	-	0/1/1/1	-
5	EDO	B	406	-	-	1/1/1/1	-
5	EDO	A	520	-	-	1/1/1/1	-
5	EDO	B	410	-	-	1/1/1/1	-
5	EDO	A	525	-	-	0/1/1/1	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	403	LAR	O2-C1	5.40	1.45	1.34
8	B	403	LAR	C20-S1	-5.26	1.66	1.77
7	B	402	ATP	C5-C4	4.53	1.47	1.39
3	A	501	NAD	C5A-C4A	4.51	1.47	1.39
7	B	402	ATP	PB-O3B	3.39	1.63	1.59
7	B	402	ATP	C5-C6	2.54	1.48	1.41
3	A	501	NAD	C5A-C6A	2.51	1.48	1.41
7	B	402	ATP	C5-N7	-2.44	1.34	1.39
7	B	402	ATP	C4-N9	-2.44	1.32	1.37
3	A	501	NAD	C5A-N7A	-2.34	1.34	1.39
7	B	402	ATP	C8-N7	2.30	1.36	1.31
3	A	501	NAD	O4D-C1D	2.29	1.43	1.40
7	B	402	ATP	PB-O3A	2.28	1.62	1.59
3	A	501	NAD	C8A-N7A	2.28	1.36	1.31
7	B	402	ATP	PA-O3A	2.20	1.61	1.59

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	403	LAR	C4-C5-C6	-7.40	96.50	112.57
8	B	403	LAR	C10-C9-C8	-6.49	106.91	126.42
3	A	501	NAD	C5A-C4A-N3A	-5.53	119.11	126.72
3	A	501	NAD	N3A-C4A-N9A	5.01	135.69	127.17
8	B	403	LAR	O2-C1-C2	4.94	122.65	111.20
7	B	402	ATP	C5-C4-N3	-4.88	120.00	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	403	LAR	C8-C7-C6	-4.46	100.89	125.30
7	B	402	ATP	N3-C4-N9	4.22	134.35	127.17
3	A	501	NAD	N3A-C2A-N1A	-3.93	122.64	128.58
3	A	501	NAD	C2A-N3A-C4A	3.78	121.07	111.83
3	A	501	NAD	C4A-N9A-C8A	3.76	109.69	105.74
7	B	402	ATP	C4-N9-C8	3.65	109.57	105.74
8	B	403	LAR	C19-S1-C20	3.41	94.02	92.04
7	B	402	ATP	N3-C2-N1	-3.28	123.61	128.58
7	B	402	ATP	C2-N3-C4	3.27	119.81	111.83
8	B	403	LAR	O1-C1-C2	-3.15	118.37	126.23
7	B	402	ATP	C4-C5-N7	-3.07	107.07	110.58
8	B	403	LAR	O3-C17-C18	2.89	107.95	104.25
3	A	501	NAD	C4A-C5A-N7A	-2.78	107.41	110.58
8	B	403	LAR	O2-C1-O1	-2.73	118.97	123.34
3	A	501	NAD	N9A-C8A-N7A	-2.61	110.24	113.94
3	A	501	NAD	C5A-N7A-C8A	2.55	107.45	103.45
7	B	402	ATP	N9-C8-N7	-2.46	110.45	113.94
3	A	501	NAD	C3N-C7N-N7N	2.45	120.75	117.74
8	B	403	LAR	C7-C8-C9	2.45	140.57	124.25
7	B	402	ATP	C5-N7-C8	2.42	107.25	103.45
8	B	403	LAR	C5-C6-C7	2.42	137.53	125.66
8	B	403	LAR	C22-C10-C9	2.32	115.66	110.82
3	A	501	NAD	O5D-C5D-C4D	-2.28	101.22	108.99
3	A	501	NAD	C5D-C4D-C3D	-2.27	107.04	115.21
7	B	402	ATP	C2-N1-C6	2.19	122.32	118.73
3	A	501	NAD	N6A-C6A-N1A	2.15	123.17	118.38
8	B	403	LAR	C21-C3-C2	-2.12	116.65	122.90
3	A	501	NAD	C2A-N1A-C6A	2.10	122.17	118.73
8	B	403	LAR	C4-C3-C2	2.06	127.85	121.90
7	B	402	ATP	C6-C5-N7	2.05	136.04	132.09

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	523	EDO	O1-C1-C2-O2
5	B	404	EDO	O1-C1-C2-O2
5	B	411	EDO	O1-C1-C2-O2
5	B	416	EDO	O1-C1-C2-O2
5	B	420	EDO	O1-C1-C2-O2
5	A	504	EDO	O1-C1-C2-O2
5	B	418	EDO	O1-C1-C2-O2

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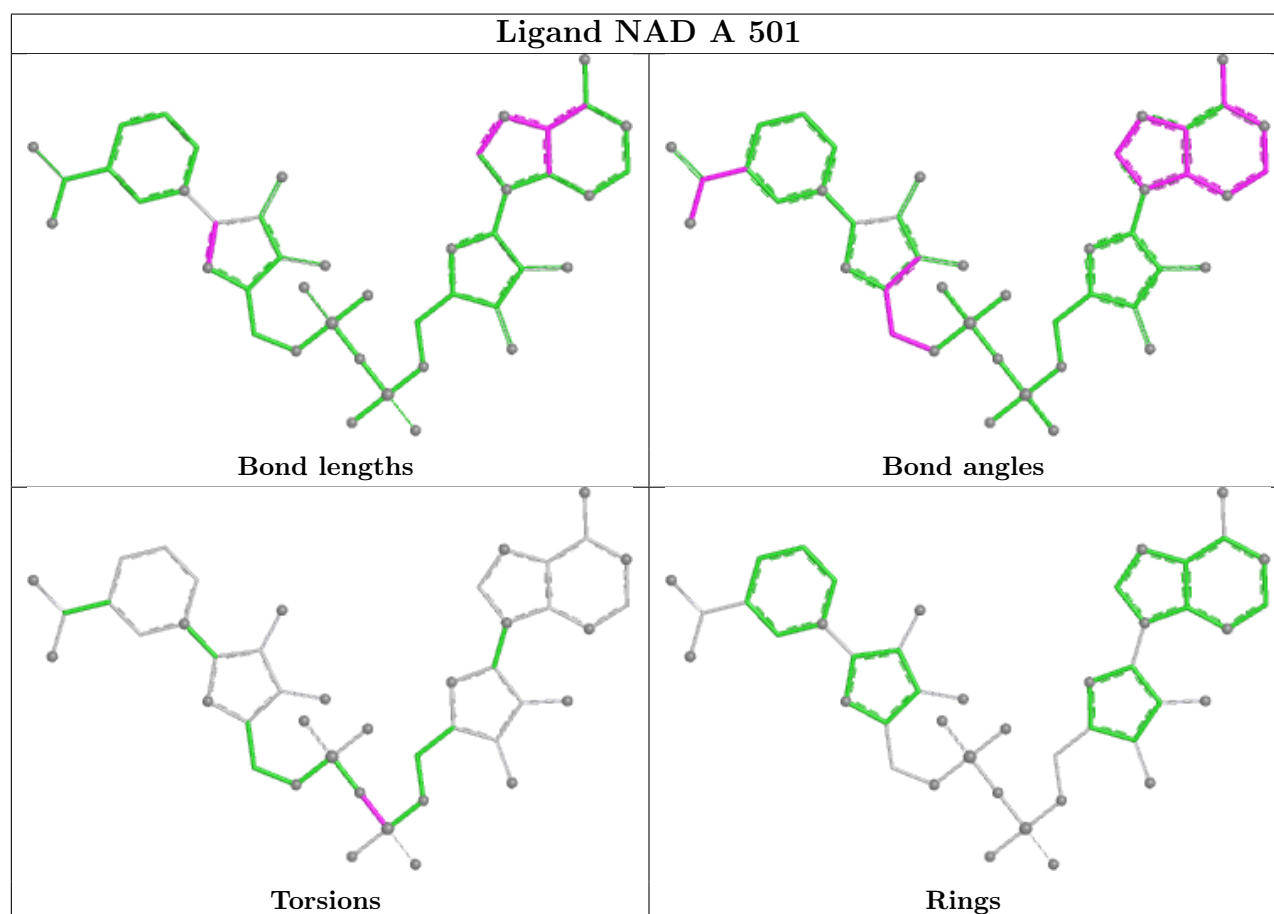
Mol	Chain	Res	Type	Atoms
5	B	421	EDO	O1-C1-C2-O2
5	B	423	EDO	O1-C1-C2-O2
5	B	425	EDO	O1-C1-C2-O2
5	B	427	EDO	O1-C1-C2-O2
3	A	501	NAD	PN-O3-PA-O2A
8	B	403	LAR	O2-C1-C2-C3
5	A	514	EDO	O1-C1-C2-O2
5	A	520	EDO	O1-C1-C2-O2
5	B	406	EDO	O1-C1-C2-O2
5	B	410	EDO	O1-C1-C2-O2
8	B	403	LAR	C10-C11-C12-C13
7	B	402	ATP	PB-O3B-PG-O2G
8	B	403	LAR	C4-C5-C6-C7
5	A	511	EDO	O1-C1-C2-O2
5	A	519	EDO	O1-C1-C2-O2
5	B	413	EDO	O1-C1-C2-O2
5	B	428	EDO	O1-C1-C2-O2
7	B	402	ATP	PG-O3B-PB-O1B
7	B	402	ATP	PG-O3B-PB-O2B
8	B	403	LAR	O1-C1-C2-C3
5	A	508	EDO	O1-C1-C2-O2
5	A	517	EDO	O1-C1-C2-O2
5	B	426	EDO	O1-C1-C2-O2
8	B	403	LAR	C3-C4-C5-C6
5	B	405	EDO	O1-C1-C2-O2
3	A	501	NAD	PN-O3-PA-O1A

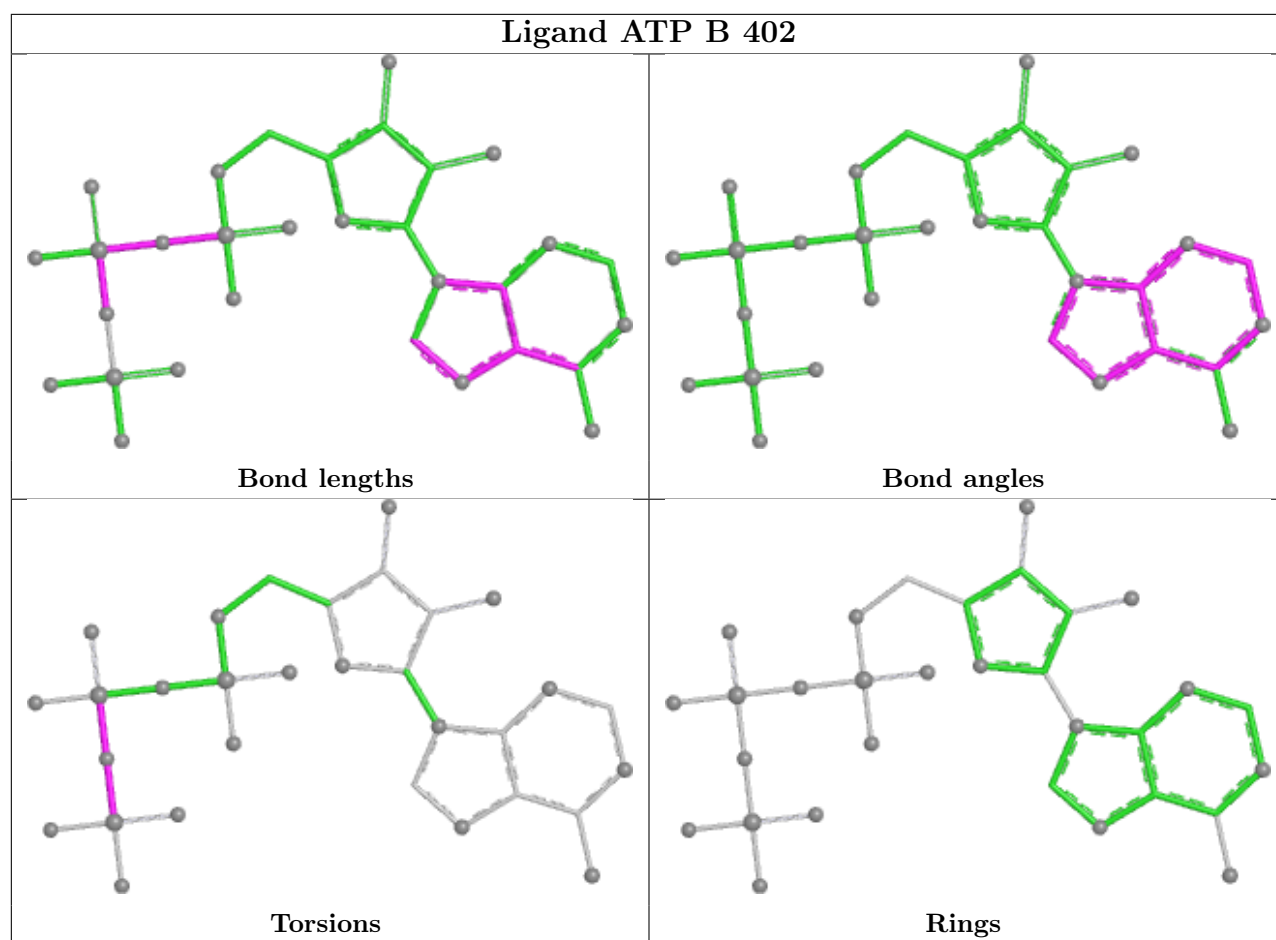
There are no ring outliers.

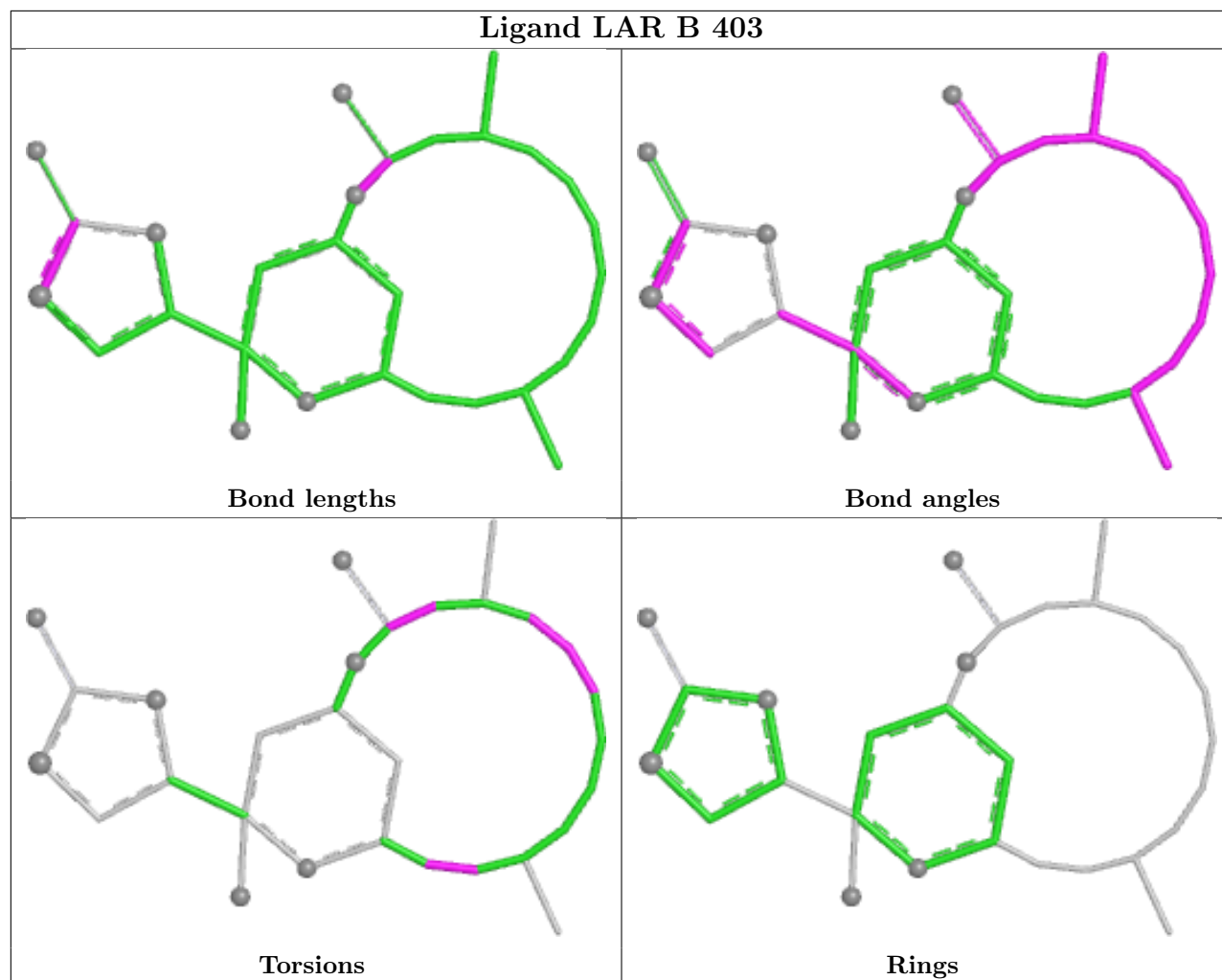
10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	507	EDO	1	0
5	B	426	EDO	1	0
5	B	412	EDO	2	0
5	A	524	EDO	1	0
5	B	411	EDO	2	0
5	A	521	EDO	1	0
5	B	413	EDO	3	0
5	B	404	EDO	1	0
5	B	408	EDO	3	0
5	B	410	EDO	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	414/418 (99%)	1.00	68 (16%) 4 4	19, 30, 54, 86	0
2	B	357/375 (95%)	0.62	40 (11%) 10 11	13, 20, 57, 114	0
All	All	771/793 (97%)	0.82	108 (14%) 6 7	13, 25, 56, 114	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	58	ALA	7.7
1	A	376	ALA	7.6
1	A	375	TYR	7.1
2	B	63	GLY	7.0
2	B	55	GLY	6.8
2	B	60	SER	6.7
2	B	54	VAL	6.4
2	B	64	ILE	6.3
2	B	52	SER	6.1
2	B	56	ASP	5.9
1	A	377	GLY	5.9
2	B	59	GLN	5.7
2	B	66	THR	5.0
2	B	53	TYR	5.0
1	A	264	LEU	4.9
2	B	62	ARG	4.7
2	B	61	LYS	4.7
1	A	237	PRO	4.6
1	A	374	GLY	4.5
2	B	65	LEU	4.5
2	B	51	ASP	4.3
1	A	250	GLY	4.2
1	A	240	LEU	4.2
2	B	233	SER	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	5	THR	4.1
1	A	145	GLY	4.0
2	B	67	LEU	4.0
2	B	143	TYR	4.0
2	B	366	GLY	4.0
1	A	265	ASN	4.0
2	B	231	ALA	3.8
1	A	372	ILE	3.7
1	A	236	THR	3.7
2	B	37	ARG	3.6
1	A	241	ALA	3.6
1	A	238	ASN	3.5
1	A	284	LEU	3.5
1	A	83	ASN	3.4
2	B	57	GLU	3.4
1	A	244	ASN	3.4
1	A	232	SER	3.3
1	A	266	ASN	3.3
1	A	234	LYS	3.3
1	A	271	LEU	3.1
1	A	349	PHE	3.1
1	A	248	ARG	3.1
1	A	81	SER	3.1
2	B	372	ARG	3.1
2	B	230	ALA	3.0
1	A	147	GLY	3.0
1	A	269	PRO	3.0
1	A	110	ASN	3.0
1	A	270	GLU	3.0
1	A	245	ASP	2.9
1	A	257	TYR	2.9
1	A	371	ALA	2.9
1	A	146	ASN	2.9
2	B	50	LYS	2.8
2	B	355	MET	2.8
1	A	373	PRO	2.8
2	B	232	SER	2.8
1	A	230	ASP	2.8
2	B	373	LYS	2.8
1	A	273	SER	2.8
1	A	276	ASN	2.8
1	A	263	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	35	VAL	2.8
1	A	86	ASP	2.8
2	B	286	ASP	2.8
1	A	268	ASN	2.7
1	A	267	PRO	2.6
2	B	36	GLY	2.6
1	A	116	LEU	2.6
1	A	128	ASP	2.6
1	A	235	LEU	2.6
1	A	249	GLY	2.6
1	A	254	ILE	2.6
1	A	29	LYS	2.5
2	B	236	LEU	2.5
1	A	251	TYR	2.5
2	B	6	THR	2.5
1	A	130	LEU	2.5
2	B	228	ALA	2.5
1	A	172	SER	2.5
1	A	231	TRP	2.4
1	A	233	ASN	2.4
1	A	306	LEU	2.4
1	A	148	ASP	2.4
1	A	30	ASN	2.3
1	A	253	ALA	2.3
2	B	68	LYS	2.3
1	A	173	ASN	2.3
1	A	25	GLU	2.3
1	A	24	ALA	2.2
1	A	229	SER	2.2
1	A	0	MET	2.2
1	A	117	GLU	2.2
1	A	246	TYR	2.2
1	A	226	GLU	2.1
1	A	316	ILE	2.1
2	B	365	ALA	2.1
2	B	173	HIS	2.1
1	A	346	MET	2.1
2	B	177	ARG	2.1
1	A	33	THR	2.1
1	A	79	ALA	2.0
2	B	229	THR	2.0
1	A	247	MET	2.0

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

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	0.92	0.09	20,23,28,28	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	0.58	0.28	42,44,44,44	0
5	EDO	B	421	4/4	0.71	0.21	38,38,39,39	0
5	EDO	A	519	4/4	0.72	0.23	47,48,48,48	0
5	EDO	B	406	4/4	0.73	0.27	45,45,45,45	0
5	EDO	A	521	4/4	0.73	0.25	46,46,46,46	0
5	EDO	B	413	4/4	0.74	0.18	30,33,33,33	0
5	EDO	B	411	4/4	0.75	0.20	40,41,41,41	0
5	EDO	B	426	4/4	0.76	0.18	45,45,45,45	0
5	EDO	A	524	4/4	0.77	0.25	40,41,41,41	0
5	EDO	B	425	4/4	0.78	0.19	31,32,33,33	0
5	EDO	B	427	4/4	0.78	0.21	45,45,46,46	0
5	EDO	A	511	4/4	0.79	0.17	41,41,42,42	0
5	EDO	B	404	4/4	0.79	0.19	34,34,34,35	0
5	EDO	A	516	4/4	0.79	0.18	45,46,46,46	0
5	EDO	B	423	4/4	0.80	0.16	46,46,46,47	0
5	EDO	B	420	4/4	0.81	0.18	39,41,42,42	0
5	EDO	B	416	4/4	0.81	0.17	37,37,38,38	0
5	EDO	A	510	4/4	0.82	0.17	43,43,43,44	0
5	EDO	B	418	4/4	0.83	0.16	39,39,39,39	0
5	EDO	B	428	4/4	0.83	0.17	47,47,47,47	0
5	EDO	B	412	4/4	0.85	0.15	47,48,48,48	0

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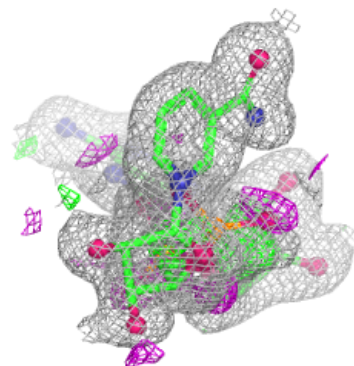
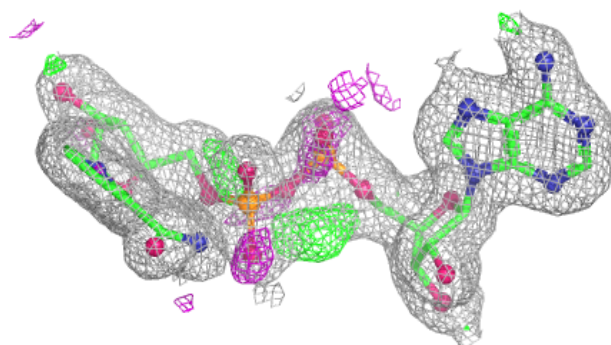
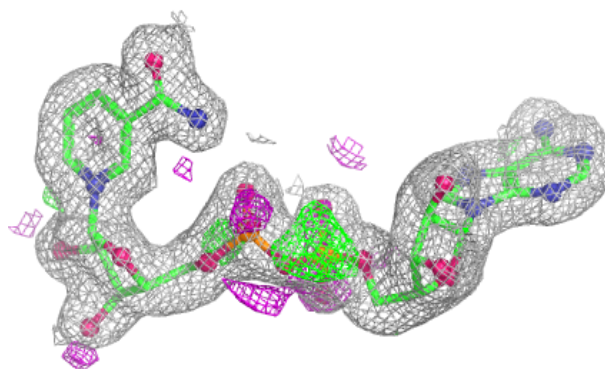
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	B	424	4/4	0.85	0.16	37,38,38,39	0
5	EDO	A	515	4/4	0.85	0.15	38,38,38,38	0
5	EDO	B	410	4/4	0.86	0.23	33,33,33,33	0
5	EDO	A	512	4/4	0.86	0.16	38,39,39,39	0
5	EDO	A	503	4/4	0.87	0.14	26,27,27,27	0
5	EDO	B	408	4/4	0.87	0.14	22,22,22,23	0
5	EDO	A	522	4/4	0.88	0.15	36,36,36,36	0
5	EDO	A	523	4/4	0.88	0.17	36,36,36,36	0
5	EDO	A	507	4/4	0.88	0.13	38,38,38,38	0
5	EDO	A	518	4/4	0.88	0.13	34,34,34,34	0
5	EDO	A	517	4/4	0.89	0.14	36,36,36,36	0
5	EDO	A	508	4/4	0.90	0.12	29,29,29,29	0
5	EDO	B	414	4/4	0.90	0.13	27,27,27,27	0
5	EDO	A	509	4/4	0.90	0.09	26,26,26,27	0
5	EDO	A	504	4/4	0.91	0.11	31,32,32,32	0
3	NAD	A	501	44/44	0.91	0.10	26,30,33,34	0
5	EDO	B	409	4/4	0.91	0.11	35,35,35,35	0
5	EDO	A	514	4/4	0.92	0.13	47,48,48,48	0
5	EDO	B	405	4/4	0.92	0.11	43,44,44,44	0
4	PO4	A	502	5/5	0.92	0.13	40,42,42,42	0
5	EDO	A	513	4/4	0.92	0.11	38,38,38,38	0
5	EDO	B	415	4/4	0.92	0.11	38,40,40,40	0
5	EDO	A	520	4/4	0.92	0.11	33,34,34,34	0
5	EDO	A	525	4/4	0.92	0.12	40,40,40,40	0
5	EDO	B	419	4/4	0.92	0.10	31,31,31,31	0
8	LAR	B	403	29/29	0.93	0.10	20,22,28,28	0
5	EDO	B	407	4/4	0.94	0.09	26,26,26,26	0
5	EDO	B	422	4/4	0.95	0.14	23,23,23,23	0
5	EDO	A	505	4/4	0.95	0.08	30,30,30,30	0
5	EDO	B	417	4/4	0.96	0.09	26,26,26,26	0
7	ATP	B	402	31/31	0.98	0.05	14,15,15,15	0
6	CA	B	401	1/1	0.99	0.04	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.

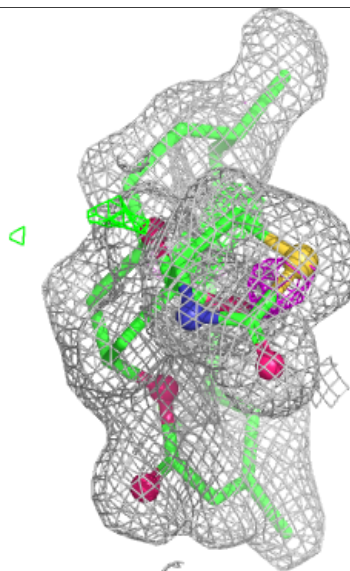
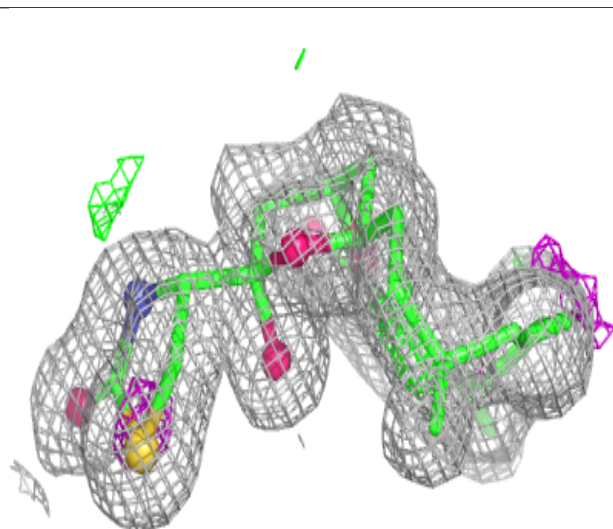
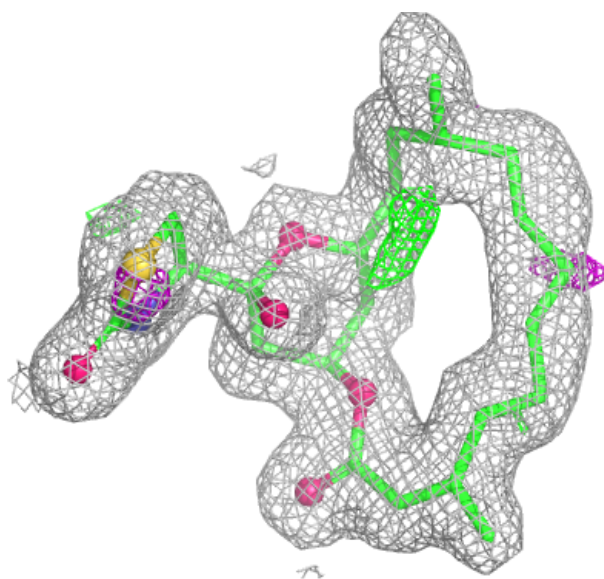
Electron density around NAD A 501:

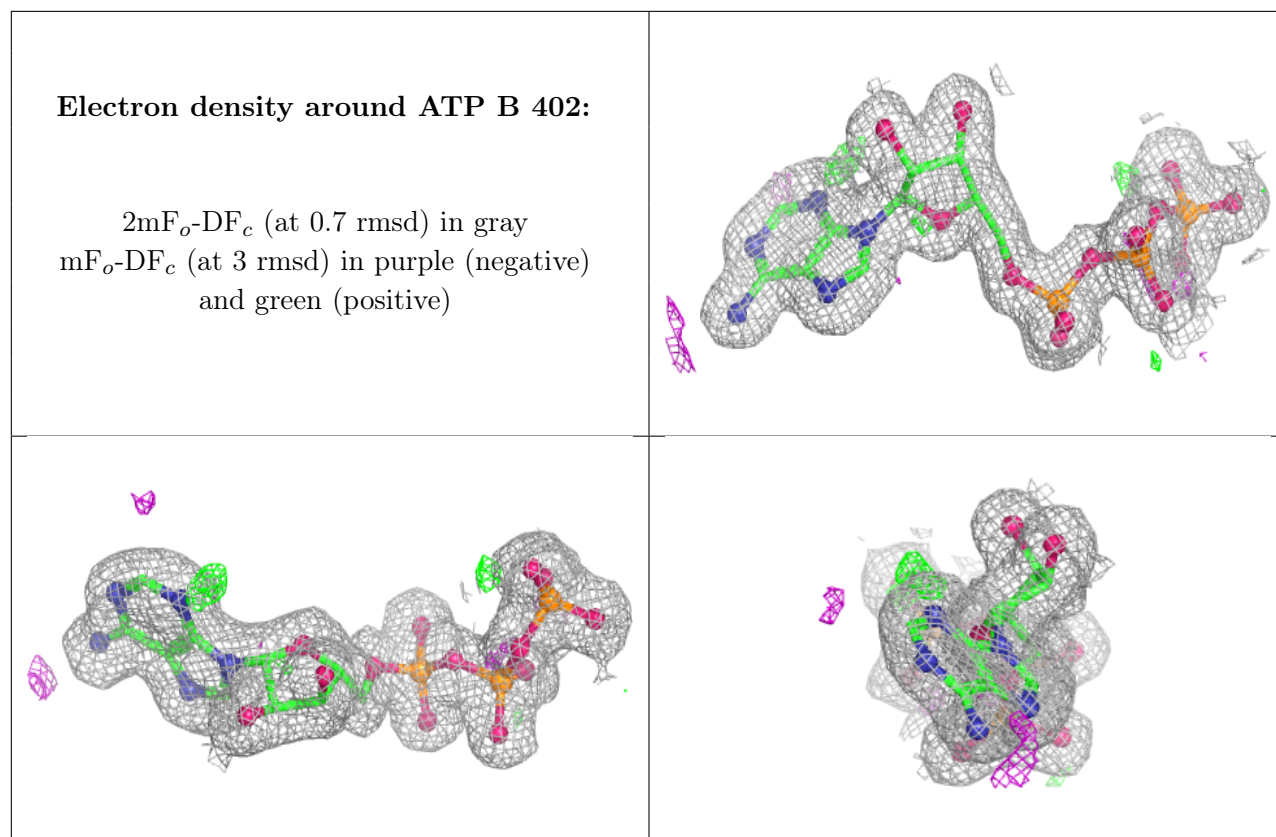
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.