



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 06:13 AM UTC

PDB ID : 4H0V / pdb_00004h0v
Title : Crystal structure of NAD⁺-Ia(E378S)-actin complex
Authors : Tsurumura, T.; Oda, M.; Nagahama, M.; Tsuge, H.
Deposited on : 2012-09-10
Resolution : 2.03 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

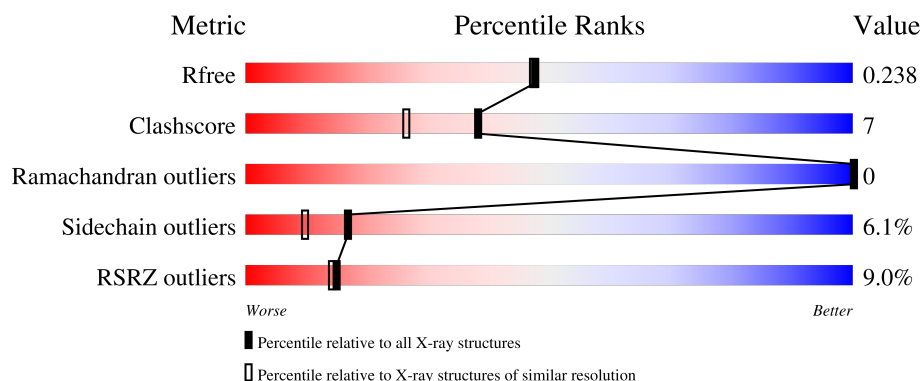
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	8% 87% 11% ..
2	B	375	9% 76% 16% .. 5%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6621 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	413	Total	C	N	O	S	0	0	0
			3361	2144	553	661	3			

There are 6 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
A	378	SER	GLU	engineered mutation	UNP Q46220

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

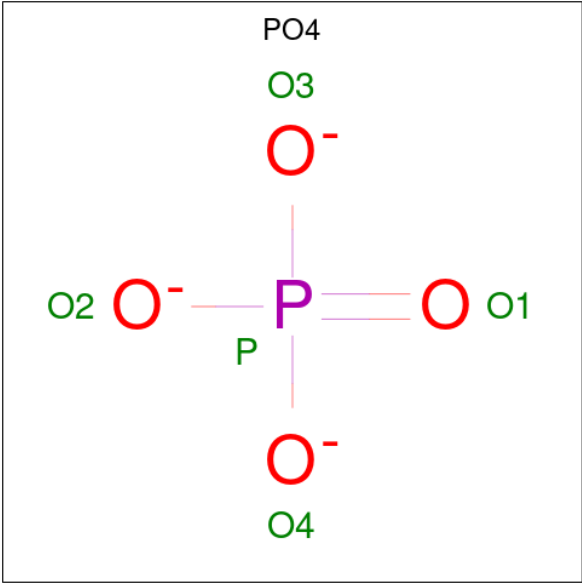
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	355	Total	C	N	O	S	0	0	0
			2776	1761	465	531	19			

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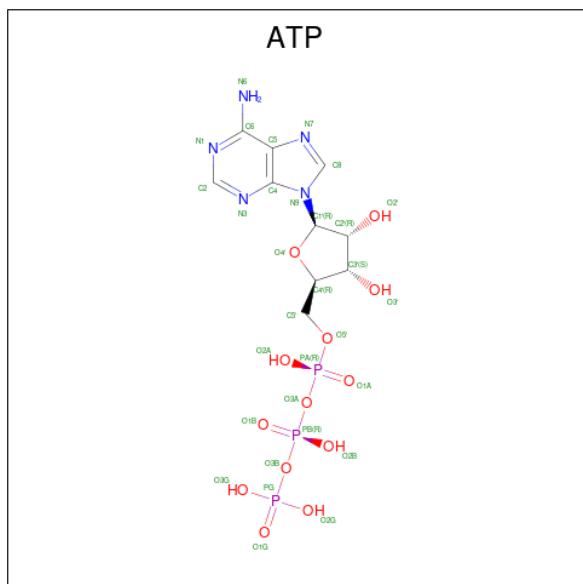
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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

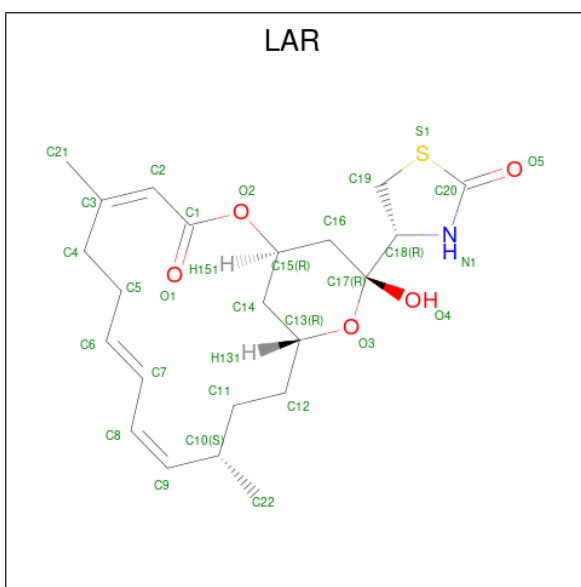
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		

- 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		

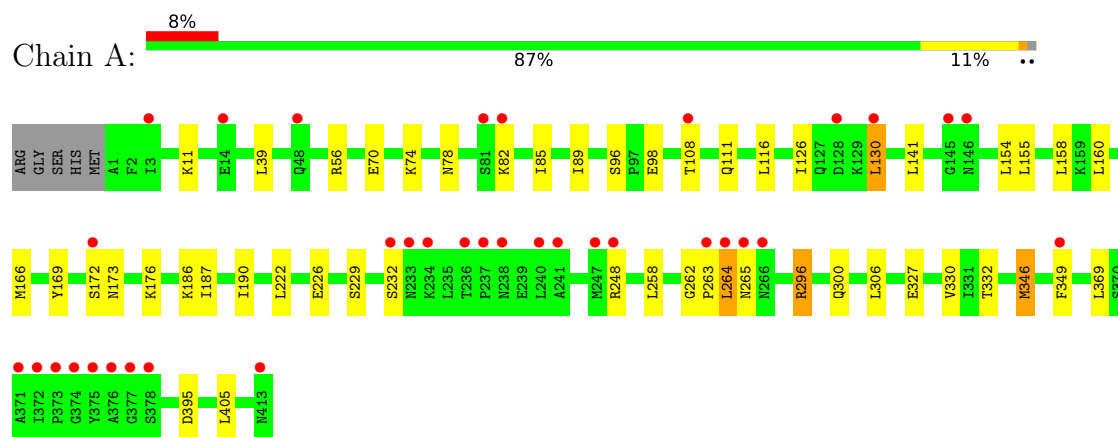
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	124	Total	O	0	0
			124	124		
9	B	94	Total	O	0	0
			94	94		

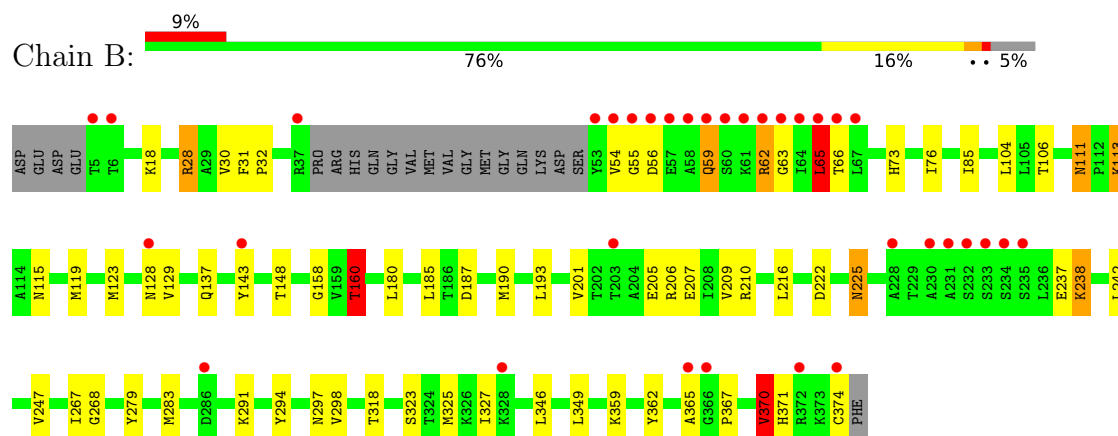
3 Residue-property plots [i](#)

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: 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	53.88Å 134.94Å 153.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.02 – 2.03 30.02 – 2.03	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.02-2.03) 97.4 (30.02-2.03)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.09 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.216 , 0.234 0.224 , 0.238	Depositor DCC
R_{free} test set	3623 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.9	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	0.93	EDS
Total number of atoms	6621	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.43	0/3430	0.83	6/4633 (0.1%)
2	B	0.55	1/2835 (0.0%)	0.84	5/3843 (0.1%)
All	All	0.49	1/6265 (0.0%)	0.83	11/8476 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	160	THR	CB-OG1	13.12	1.64	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ARG	CG-CD-NE	-7.90	94.62	112.00
2	B	370	VAL	CB-CA-C	-7.85	101.55	112.14
1	A	296	ARG	NE-CZ-NH2	-7.20	112.72	119.20
2	B	65	LEU	N-CA-C	6.98	120.02	109.41
1	A	296	ARG	CD-NE-CZ	6.95	134.12	124.40
1	A	296	ARG	NE-CZ-NH1	6.14	127.64	121.50
2	B	370	VAL	N-CA-CB	5.94	118.61	110.54
1	A	296	ARG	CB-CG-CD	5.53	124.03	111.30
1	A	82	LYS	CB-CA-C	-5.27	102.05	110.79
2	B	111	ASN	CA-C-N	-5.10	114.52	119.78
2	B	111	ASN	C-N-CA	-5.10	114.52	119.78

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3361	0	3345	31	0
2	B	2776	0	2751	55	0
3	A	44	0	26	0	0
4	A	5	0	0	0	0
5	A	76	0	114	4	0
5	B	80	0	120	13	0
6	B	1	0	0	0	0
7	B	31	0	12	0	0
8	B	29	0	31	2	0
9	A	124	0	0	1	0
9	B	94	0	0	0	0
All	All	6621	0	6399	88	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (88) 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:160:THR:CB	2:B:160:THR:OG1	1.64	1.44
2:B:283:MET:HE1	5:B:408:EDO:O2	1.61	1.00
1:A:56:ARG:NH1	1:A:70:GLU:OE1	2.05	0.89
1:A:56:ARG:HH12	1:A:70:GLU:CD	1.79	0.89
2:B:160:THR:HG23	2:B:180:LEU:O	1.76	0.84
1:A:85:ILE:HD13	1:A:166:MET:HE3	1.61	0.82
2:B:190:MET:CG	2:B:209:VAL:HG11	2.12	0.80
2:B:111:ASN:HD21	2:B:119:MET:HE1	1.47	0.79
1:A:56:ARG:NH1	1:A:70:GLU:CD	2.42	0.78
2:B:207:GLU:OE1	2:B:210:ARG:NH1	2.19	0.75
1:A:346:MET:HG3	1:A:349:PHE:CZ	2.22	0.75
8:B:403:LAR:H91	8:B:403:LAR:H131	1.73	0.71
2:B:190:MET:HG2	2:B:209:VAL:HG11	1.73	0.70
2:B:111:ASN:HD21	2:B:119:MET:CE	2.06	0.69
1:A:264:LEU:HD12	1:A:264:LEU:C	2.19	0.68
2:B:298:VAL:CG1	5:B:407:EDO:H21	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:MET:CE	5:B:408:EDO:O2	2.41	0.66
2:B:59:GLN:HA	2:B:62:ARG:HB3	1.78	0.66
2:B:362:TYR:O	2:B:365:ALA:O	2.14	0.66
2:B:123:MET:HE3	2:B:129:VAL:HG11	1.79	0.64
2:B:111:ASN:ND2	2:B:119:MET:HE1	2.12	0.63
2:B:160:THR:CG2	2:B:180:LEU:O	2.46	0.63
2:B:216:LEU:HD22	2:B:238:LYS:HG2	1.82	0.62
2:B:318:THR:HG23	5:B:409:EDO:H21	1.81	0.61
2:B:160:THR:CB	2:B:160:THR:HG1	2.08	0.61
2:B:207:GLU:CD	2:B:210:ARG:HH12	2.09	0.61
2:B:76:ILE:HD12	2:B:119:MET:HE2	1.82	0.60
2:B:148:THR:H	5:B:411:EDO:H12	1.66	0.60
2:B:32:PRO:HG2	2:B:55:GLY:HA2	1.84	0.59
2:B:323:SER:HA	5:B:409:EDO:H22	1.87	0.57
2:B:28:ARG:HH11	2:B:28:ARG:CB	2.19	0.56
2:B:28:ARG:HH11	2:B:28:ARG:HB2	1.69	0.56
2:B:207:GLU:CD	2:B:210:ARG:NH1	2.64	0.56
1:A:56:ARG:NH1	1:A:70:GLU:OE2	2.25	0.55
1:A:85:ILE:HD13	1:A:166:MET:CE	2.35	0.55
2:B:205:GLU:O	2:B:209:VAL:HG12	2.07	0.55
1:A:89:ILE:CG2	1:A:166:MET:HE1	2.37	0.53
2:B:190:MET:HG3	2:B:209:VAL:HG11	1.87	0.53
2:B:104:LEU:C	2:B:104:LEU:HD23	2.34	0.53
2:B:143:TYR:OH	2:B:349:LEU:HD11	2.09	0.53
2:B:115:ASN:HB3	2:B:119:MET:HE3	1.93	0.50
1:A:346:MET:HG3	1:A:349:PHE:CE1	2.46	0.50
2:B:54:VAL:HG13	2:B:85:ILE:HD13	1.94	0.50
1:A:89:ILE:HG22	1:A:166:MET:HE1	1.95	0.49
2:B:298:VAL:HG13	5:B:407:EDO:H21	1.93	0.49
2:B:180:LEU:HD13	2:B:267:ILE:HD11	1.95	0.49
2:B:28:ARG:HH11	2:B:28:ARG:CG	2.25	0.49
2:B:279:TYR:CE1	2:B:283:MET:HE3	2.48	0.48
2:B:187:ASP:OD1	2:B:206:ARG:HD2	2.13	0.48
2:B:113:LYS:HE2	2:B:371:HIS:CD2	2.48	0.48
2:B:106:THR:HB	2:B:137:GLN:HG3	1.96	0.48
2:B:367:PRO:O	2:B:370:VAL:HG22	2.14	0.47
2:B:222:ASP:CG	2:B:225:ASN:HB2	2.40	0.47
5:B:420:EDO:H22	5:B:421:EDO:O1	2.15	0.47
2:B:294:TYR:CD1	2:B:327:ILE:HD12	2.49	0.47
1:A:172:SER:OG	1:A:173:ASN:N	2.49	0.46
1:A:264:LEU:C	1:A:264:LEU:CD1	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:THR:HG23	1:A:111:GLN:H	1.81	0.46
2:B:237:GLU:HG2	5:B:418:EDO:H12	1.98	0.46
1:A:306:LEU:HD22	2:B:268:GLY:HA2	1.98	0.45
1:A:108:THR:HG22	1:A:111:GLN:CD	2.41	0.45
1:A:229:SER:O	1:A:232:SER:HB2	2.15	0.45
1:A:296:ARG:HD3	1:A:349:PHE:CE1	2.52	0.45
1:A:126:ILE:HD12	1:A:187:ILE:HD13	1.97	0.45
2:B:207:GLU:HA	2:B:210:ARG:NH1	2.33	0.44
2:B:148:THR:N	5:B:411:EDO:H12	2.32	0.44
1:A:169:TYR:CE2	1:A:176:LYS:HB2	2.52	0.44
1:A:327:GLU:OE1	5:A:507:EDO:H21	2.17	0.44
1:A:300:GLN:NE2	9:A:681:HOH:O	2.42	0.44
2:B:148:THR:H	5:B:411:EDO:C1	2.29	0.43
1:A:296:ARG:HD3	5:A:503:EDO:O2	2.18	0.43
2:B:31:PHE:HB2	2:B:32:PRO:HD2	2.01	0.43
1:A:264:LEU:HG	1:A:265:ASN:N	2.33	0.43
2:B:158:GLY:HA2	5:B:404:EDO:H11	2.01	0.43
1:A:262:GLY:N	1:A:263:PRO:CD	2.82	0.42
2:B:370:VAL:O	2:B:374:CYS:N	2.49	0.42
1:A:296:ARG:CD	5:A:503:EDO:O2	2.67	0.42
8:B:403:LAR:H81	8:B:403:LAR:H223	1.57	0.42
2:B:128:ASN:ND2	2:B:359:LYS:HE3	2.34	0.42
1:A:130:LEU:HD12	1:A:130:LEU:HA	1.95	0.42
1:A:126:ILE:HD11	1:A:190:ILE:HG21	2.01	0.42
1:A:160:LEU:HD13	1:A:166:MET:HE2	2.01	0.42
2:B:325:MET:HG3	2:B:327:ILE:HD13	2.01	0.42
2:B:63:GLY:C	2:B:65:LEU:N	2.77	0.41
1:A:96:SER:HB3	1:A:98:GLU:OE2	2.20	0.41
2:B:18:LYS:N	2:B:18:LYS:HD3	2.36	0.41
1:A:395:ASP:OD1	5:A:506:EDO:O1	2.35	0.40
2:B:73:HIS:CE1	5:B:404:EDO:H21	2.57	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	411/418 (98%)	399 (97%)	12 (3%)	0	100	100
2	B	351/375 (94%)	343 (98%)	8 (2%)	0	100	100
All	All	762/793 (96%)	742 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	376/380 (99%)	355 (94%)	21 (6%)	19	12
2	B	301/318 (95%)	281 (93%)	20 (7%)	15	8
All	All	677/698 (97%)	636 (94%)	41 (6%)	17	10

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	39	LEU
1	A	74	LYS
1	A	78	ASN
1	A	116	LEU
1	A	130	LEU
1	A	141	LEU
1	A	154	LEU
1	A	155	LEU
1	A	158	LEU
1	A	186	LYS
1	A	222	LEU
1	A	226	GLU
1	A	248	ARG
1	A	258	LEU

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Mol	Chain	Res	Type
1	A	264	LEU
1	A	330	VAL
1	A	332	THR
1	A	346	MET
1	A	369	LEU
1	A	405	LEU
2	B	28	ARG
2	B	30	VAL
2	B	56	ASP
2	B	59	GLN
2	B	62	ARG
2	B	65	LEU
2	B	66	THR
2	B	113	LYS
2	B	160	THR
2	B	185	LEU
2	B	193	LEU
2	B	201	VAL
2	B	225	ASN
2	B	238	LYS
2	B	242	LEU
2	B	247	VAL
2	B	291	LYS
2	B	297	ASN
2	B	346	LEU
2	B	370	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	127	GLN
1	A	209	ASN
1	A	265	ASN
1	A	359	ASN
2	B	87	HIS
2	B	111	ASN
2	B	128	ASN
2	B	162	ASN
2	B	263	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 44 ligands modelled in this entry, 1 is monoatomic - leaving 43 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	415	-	3,3,3	0.42	0	2,2,2	0.50	0
5	EDO	A	512	-	3,3,3	0.48	0	2,2,2	0.56	0
5	EDO	B	407	-	3,3,3	0.48	0	2,2,2	0.46	0
5	EDO	A	503	-	3,3,3	0.56	0	2,2,2	0.50	0
5	EDO	A	510	-	3,3,3	0.43	0	2,2,2	0.30	0
5	EDO	A	516	-	3,3,3	0.51	0	2,2,2	0.41	0
5	EDO	B	417	-	3,3,3	0.45	0	2,2,2	0.29	0
5	EDO	B	406	-	3,3,3	0.40	0	2,2,2	0.42	0
5	EDO	A	519	-	3,3,3	0.46	0	2,2,2	0.31	0
5	EDO	A	520	-	3,3,3	0.56	0	2,2,2	0.33	0
5	EDO	B	412	-	3,3,3	0.42	0	2,2,2	0.34	0
5	EDO	B	419	-	3,3,3	0.46	0	2,2,2	0.25	0
7	ATP	B	402	-	32,33,33	1.51	8 (25%)	48,52,52	1.74	9 (18%)
5	EDO	B	404	-	3,3,3	0.60	0	2,2,2	0.16	0
5	EDO	B	409	-	3,3,3	0.40	0	2,2,2	0.39	0
5	EDO	A	521	-	3,3,3	0.48	0	2,2,2	0.30	0
5	EDO	B	414	-	3,3,3	0.50	0	2,2,2	0.35	0

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	0.24	0
3	NAD	A	501	-	46,48,48	1.19	6 (13%)	64,73,73	1.74	13 (20%)
5	EDO	A	518	-	3,3,3	0.42	0	2,2,2	0.31	0
5	EDO	B	420	-	3,3,3	0.41	0	2,2,2	0.26	0
5	EDO	B	422	-	3,3,3	0.41	0	2,2,2	0.28	0
8	LAR	B	403	-	30,31,31	1.66	2 (6%)	32,43,43	1.77	6 (18%)
5	EDO	A	505	-	3,3,3	0.46	0	2,2,2	0.17	0
5	EDO	A	509	-	3,3,3	0.47	0	2,2,2	0.23	0
4	PO4	A	502	-	4,4,4	1.00	0	6,6,6	0.44	0
5	EDO	B	408	-	3,3,3	0.48	0	2,2,2	0.21	0
5	EDO	A	517	-	3,3,3	0.41	0	2,2,2	0.23	0
5	EDO	B	413	-	3,3,3	0.46	0	2,2,2	0.29	0
5	EDO	A	508	-	3,3,3	0.46	0	2,2,2	0.17	0
5	EDO	B	410	-	3,3,3	0.50	0	2,2,2	0.25	0
5	EDO	B	411	-	3,3,3	0.41	0	2,2,2	0.38	0
5	EDO	B	418	-	3,3,3	0.46	0	2,2,2	0.19	0
5	EDO	A	506	-	3,3,3	0.43	0	2,2,2	0.40	0
5	EDO	A	513	-	3,3,3	0.46	0	2,2,2	0.42	0
5	EDO	A	511	-	3,3,3	0.46	0	2,2,2	0.51	0
5	EDO	A	515	-	3,3,3	0.45	0	2,2,2	0.32	0
5	EDO	A	504	-	3,3,3	0.40	0	2,2,2	0.41	0
5	EDO	B	416	-	3,3,3	0.43	0	2,2,2	0.27	0
5	EDO	B	423	-	3,3,3	0.46	0	2,2,2	0.25	0
5	EDO	B	405	-	3,3,3	0.46	0	2,2,2	0.21	0
5	EDO	B	421	-	3,3,3	0.40	0	2,2,2	0.70	0
5	EDO	A	514	-	3,3,3	0.48	0	2,2,2	0.07	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	415	-	-	0/1/1/1	-
5	EDO	A	512	-	-	0/1/1/1	-
5	EDO	B	407	-	-	0/1/1/1	-
5	EDO	A	503	-	-	0/1/1/1	-
5	EDO	A	510	-	-	0/1/1/1	-
5	EDO	A	516	-	-	1/1/1/1	-
5	EDO	B	417	-	-	0/1/1/1	-
5	EDO	B	406	-	-	0/1/1/1	-
5	EDO	A	519	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	520	-	-	1/1/1/1	-
5	EDO	B	412	-	-	0/1/1/1	-
5	EDO	B	419	-	-	0/1/1/1	-
7	ATP	B	402	-	-	2/22/38/38	0/3/3/3
5	EDO	B	404	-	-	1/1/1/1	-
5	EDO	B	409	-	-	1/1/1/1	-
5	EDO	A	521	-	-	1/1/1/1	-
5	EDO	B	414	-	-	1/1/1/1	-
5	EDO	A	507	-	-	1/1/1/1	-
3	NAD	A	501	-	-	2/30/62/62	0/5/5/5
5	EDO	A	518	-	-	0/1/1/1	-
5	EDO	B	420	-	-	0/1/1/1	-
5	EDO	B	422	-	-	1/1/1/1	-
8	LAR	B	403	-	-	11/23/51/51	0/2/3/3
5	EDO	A	505	-	-	1/1/1/1	-
5	EDO	A	509	-	-	0/1/1/1	-
5	EDO	B	408	-	-	0/1/1/1	-
5	EDO	A	517	-	-	1/1/1/1	-
5	EDO	B	413	-	-	1/1/1/1	-
5	EDO	A	508	-	-	1/1/1/1	-
5	EDO	B	410	-	-	1/1/1/1	-
5	EDO	B	411	-	-	1/1/1/1	-
5	EDO	B	418	-	-	1/1/1/1	-
5	EDO	A	506	-	-	1/1/1/1	-
5	EDO	A	513	-	-	1/1/1/1	-
5	EDO	A	511	-	-	0/1/1/1	-
5	EDO	A	515	-	-	0/1/1/1	-
5	EDO	A	504	-	-	1/1/1/1	-
5	EDO	B	416	-	-	1/1/1/1	-
5	EDO	B	423	-	-	1/1/1/1	-
5	EDO	B	405	-	-	1/1/1/1	-
5	EDO	B	421	-	-	1/1/1/1	-
5	EDO	A	514	-	-	1/1/1/1	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	403	LAR	O2-C1	6.04	1.47	1.34
8	B	403	LAR	C20-S1	-5.37	1.66	1.77
3	A	501	NAD	C5A-C4A	4.46	1.47	1.39
7	B	402	ATP	C5-C4	4.39	1.46	1.39
7	B	402	ATP	PB-O3B	3.47	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	NAD	C5A-C6A	2.56	1.48	1.41
7	B	402	ATP	C4-N9	-2.47	1.32	1.37
7	B	402	ATP	C5-N7	-2.42	1.34	1.39
7	B	402	ATP	C5-C6	2.41	1.47	1.41
3	A	501	NAD	C8A-N7A	2.37	1.36	1.31
7	B	402	ATP	PB-O3A	2.29	1.62	1.59
3	A	501	NAD	C5A-N7A	-2.26	1.35	1.39
3	A	501	NAD	O4D-C1D	2.25	1.43	1.40
3	A	501	NAD	C4A-N9A	-2.16	1.33	1.37
7	B	402	ATP	C8-N7	2.15	1.35	1.31
7	B	402	ATP	PA-O3A	2.09	1.61	1.59

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NAD	C5A-C4A-N3A	-5.12	119.66	126.72
7	B	402	ATP	C5-C4-N3	-5.01	119.82	126.72
8	B	403	LAR	O2-C1-C2	4.89	122.55	111.20
7	B	402	ATP	N3-C4-N9	4.65	135.07	127.17
3	A	501	NAD	N3A-C4A-N9A	4.50	134.81	127.17
7	B	402	ATP	C4-N9-C8	4.06	110.01	105.74
3	A	501	NAD	N3A-C2A-N1A	-4.03	122.48	128.58
3	A	501	NAD	C3N-C7N-N7N	3.83	122.45	117.74
3	A	501	NAD	C4A-N9A-C8A	3.78	109.71	105.74
3	A	501	NAD	C2A-N3A-C4A	3.73	120.94	111.83
8	B	403	LAR	C22-C10-C9	-3.62	103.27	110.82
7	B	402	ATP	N3-C2-N1	-3.60	123.13	128.58
7	B	402	ATP	C2-N3-C4	3.52	120.43	111.83
8	B	403	LAR	O1-C1-C2	-3.13	118.43	126.23
3	A	501	NAD	C4A-C5A-N7A	-2.99	107.16	110.58
8	B	403	LAR	C19-S1-C20	2.84	93.68	92.04
8	B	403	LAR	C10-C9-C8	-2.74	118.18	126.42
8	B	403	LAR	O2-C1-O1	-2.70	119.02	123.34
3	A	501	NAD	N9A-C8A-N7A	-2.68	110.14	113.94
7	B	402	ATP	C4-C5-N7	-2.64	107.56	110.58
3	A	501	NAD	C5D-C4D-C3D	-2.61	105.80	115.21
7	B	402	ATP	N9-C8-N7	-2.59	110.27	113.94
3	A	501	NAD	C5A-N7A-C8A	2.55	107.46	103.45
7	B	402	ATP	C5-N7-C8	2.30	107.06	103.45
3	A	501	NAD	O7N-C7N-N7N	-2.28	119.32	122.62
3	A	501	NAD	C2A-N1A-C6A	2.25	122.43	118.73
3	A	501	NAD	C6A-C5A-N7A	2.19	136.31	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	402	ATP	C6-C5-N7	2.05	136.05	132.09

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	403	LAR	C22-C10-C11-C12
8	B	403	LAR	O3-C17-C18-C19
8	B	403	LAR	C3-C4-C5-C6
8	B	403	LAR	C6-C7-C8-C9
5	B	404	EDO	O1-C1-C2-O2
5	A	504	EDO	O1-C1-C2-O2
5	A	513	EDO	O1-C1-C2-O2
5	A	514	EDO	O1-C1-C2-O2
5	A	516	EDO	O1-C1-C2-O2
5	B	409	EDO	O1-C1-C2-O2
5	B	410	EDO	O1-C1-C2-O2
5	B	423	EDO	O1-C1-C2-O2
5	B	414	EDO	O1-C1-C2-O2
5	B	416	EDO	O1-C1-C2-O2
5	B	418	EDO	O1-C1-C2-O2
5	A	521	EDO	O1-C1-C2-O2
5	A	506	EDO	O1-C1-C2-O2
5	B	421	EDO	O1-C1-C2-O2
3	A	501	NAD	PN-O3-PA-O2A
7	B	402	ATP	PG-O3B-PB-O1B
8	B	403	LAR	C9-C10-C11-C12
8	B	403	LAR	C22-C10-C9-C8
8	B	403	LAR	O2-C1-C2-C3
7	B	402	ATP	PG-O3B-PB-O2B
5	A	507	EDO	O1-C1-C2-O2
5	B	422	EDO	O1-C1-C2-O2
8	B	403	LAR	C10-C11-C12-C13
5	A	520	EDO	O1-C1-C2-O2
5	B	413	EDO	O1-C1-C2-O2
3	A	501	NAD	PN-O3-PA-O1A
8	B	403	LAR	C21-C3-C4-C5
5	A	505	EDO	O1-C1-C2-O2
5	A	508	EDO	O1-C1-C2-O2
5	A	517	EDO	O1-C1-C2-O2
8	B	403	LAR	O1-C1-C2-C3
5	B	405	EDO	O1-C1-C2-O2

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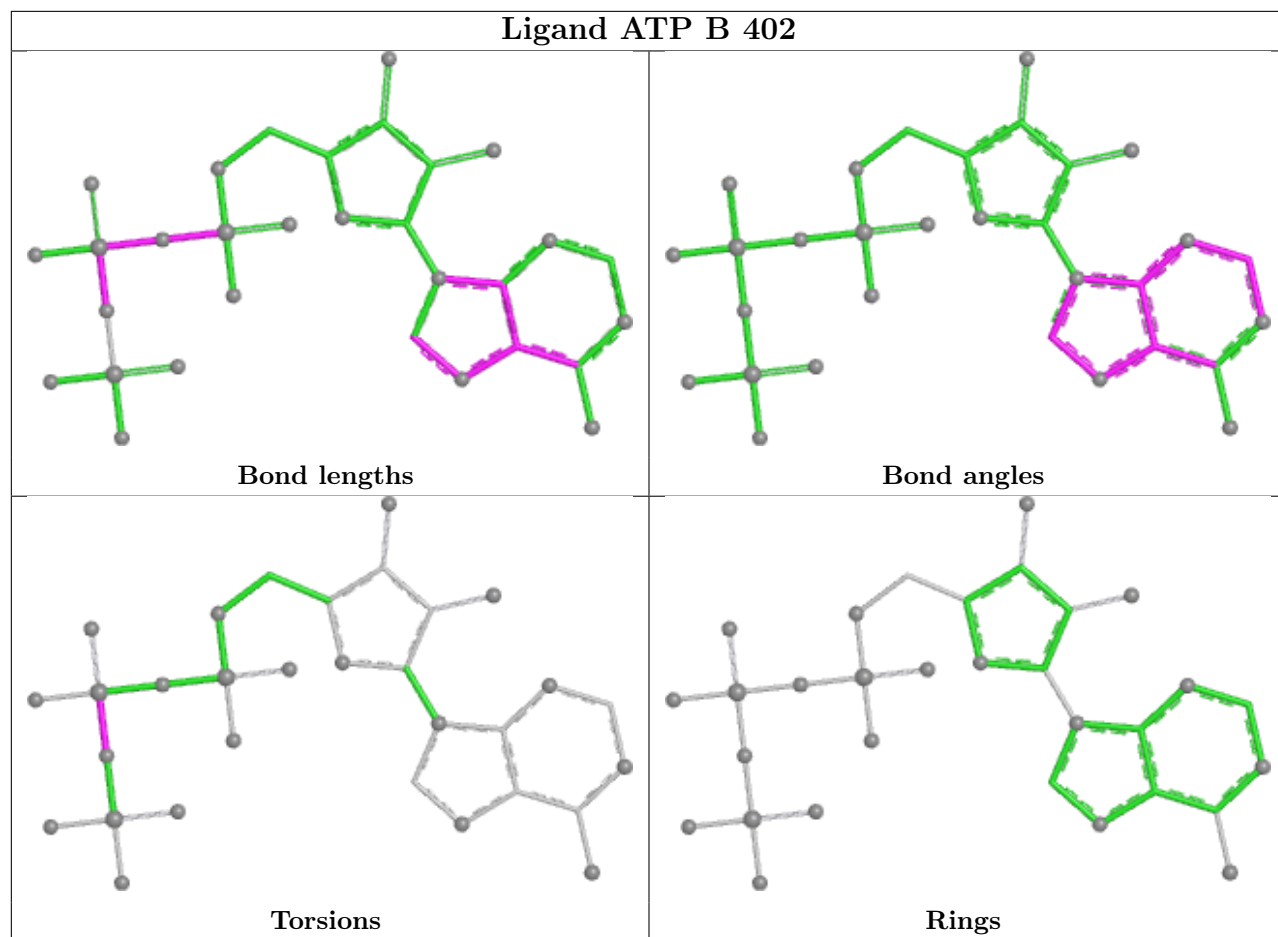
Mol	Chain	Res	Type	Atoms
5	A	519	EDO	O1-C1-C2-O2
8	B	403	LAR	C4-C5-C6-C7
5	B	411	EDO	O1-C1-C2-O2

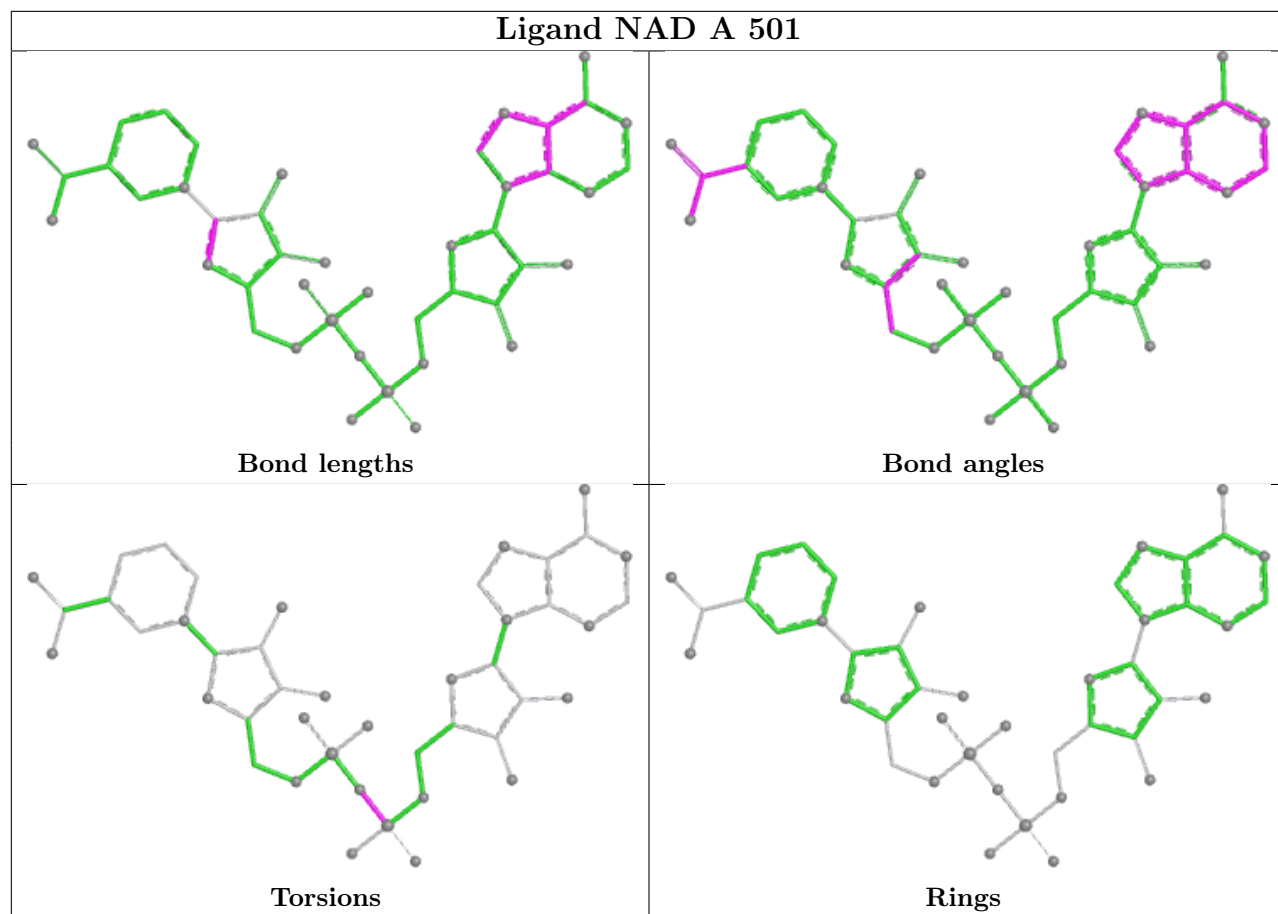
There are no ring outliers.

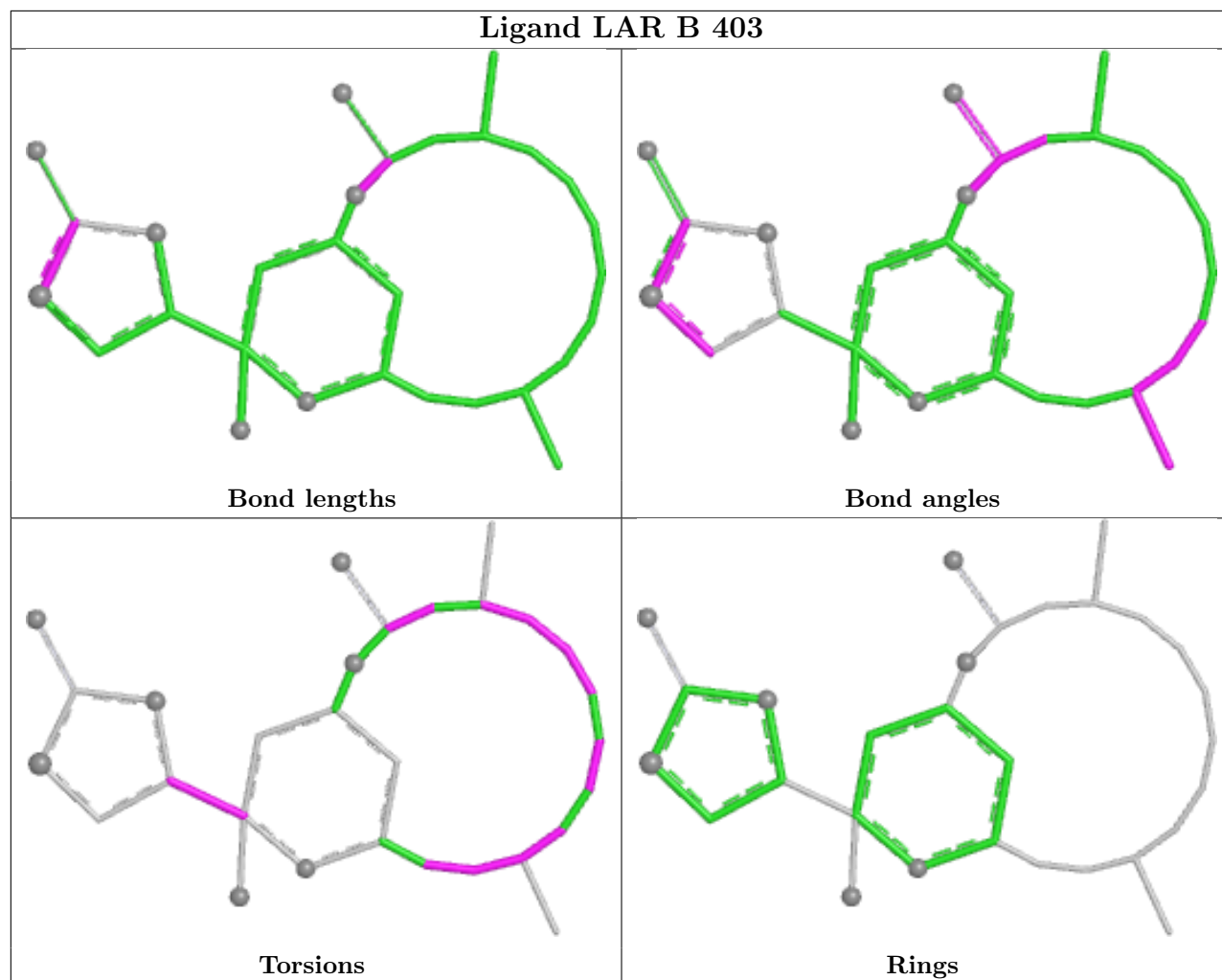
12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	407	EDO	2	0
5	A	503	EDO	2	0
5	B	404	EDO	2	0
5	B	409	EDO	2	0
5	A	507	EDO	1	0
5	B	420	EDO	1	0
8	B	403	LAR	2	0
5	B	408	EDO	2	0
5	B	411	EDO	3	0
5	B	418	EDO	1	0
5	A	506	EDO	1	0
5	B	421	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 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	413/418 (98%)	0.66	35 (8%) 16 16	22, 34, 59, 95	0
2	B	355/375 (94%)	0.39	34 (9%) 13 12	17, 25, 57, 121	0
All	All	768/793 (96%)	0.53	69 (8%) 15 14	17, 29, 59, 121	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	61	LYS	7.6
1	A	376	ALA	7.0
2	B	55	GLY	6.5
2	B	54	VAL	6.4
1	A	375	TYR	6.0
2	B	64	ILE	5.5
2	B	53	TYR	5.5
2	B	58	ALA	5.0
1	A	264	LEU	4.7
2	B	62	ARG	4.7
1	A	377	GLY	4.6
2	B	63	GLY	4.6
2	B	60	SER	4.4
2	B	66	THR	4.4
2	B	56	ASP	4.3
1	A	374	GLY	4.2
2	B	57	GLU	4.1
1	A	3	ILE	4.1
1	A	373	PRO	3.9
2	B	59	GLN	3.9
2	B	233	SER	3.8
2	B	37	ARG	3.7
1	A	372	ILE	3.7
1	A	378	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	248	ARG	3.5
1	A	266	ASN	3.4
1	A	172	SER	3.2
2	B	67	LEU	3.2
2	B	231	ALA	3.1
2	B	374	CYS	3.1
1	A	14	GLU	3.1
1	A	48	GLN	3.1
1	A	81	SER	3.0
2	B	5	THR	3.0
2	B	366	GLY	3.0
1	A	232	SER	2.9
2	B	232	SER	2.9
2	B	65	LEU	2.8
1	A	237	PRO	2.8
2	B	143	TYR	2.8
1	A	238	ASN	2.7
1	A	265	ASN	2.7
2	B	235	SER	2.7
1	A	240	LEU	2.7
2	B	228	ALA	2.7
1	A	82	LYS	2.7
2	B	286	ASP	2.6
1	A	371	ALA	2.6
1	A	241	ALA	2.5
1	A	234	LYS	2.5
1	A	108	THR	2.4
1	A	233	ASN	2.4
1	A	263	PRO	2.4
1	A	413	ASN	2.3
2	B	128	ASN	2.3
1	A	145	GLY	2.3
2	B	203	THR	2.3
2	B	234	SER	2.2
1	A	236	THR	2.2
2	B	6	THR	2.2
2	B	365	ALA	2.2
1	A	130	LEU	2.2
2	B	372	ARG	2.2
1	A	128	ASP	2.2
1	A	247	MET	2.1
1	A	146	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	349	PHE	2.0
2	B	230	ALA	2.0
2	B	328	LYS	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(Å ²)	Q<0.9
5	EDO	B	418	4/4	0.61	0.26	41,42,43,43	0
5	EDO	A	516	4/4	0.68	0.24	43,44,45,45	0
5	EDO	A	520	4/4	0.70	0.24	48,48,48,49	0
5	EDO	A	513	4/4	0.72	0.23	44,44,45,45	0
5	EDO	B	411	4/4	0.74	0.20	40,41,41,42	0
5	EDO	A	506	4/4	0.75	0.20	48,49,49,49	0
5	EDO	B	416	4/4	0.76	0.22	47,47,47,47	0
5	EDO	B	410	4/4	0.76	0.22	47,47,47,48	0
5	EDO	B	422	4/4	0.77	0.21	46,46,46,47	0
5	EDO	A	511	4/4	0.78	0.22	43,44,44,44	0
5	EDO	B	405	4/4	0.81	0.20	48,49,49,49	0
5	EDO	A	517	4/4	0.81	0.18	44,44,44,44	0
5	EDO	B	404	4/4	0.81	0.20	35,36,36,37	0
5	EDO	B	414	4/4	0.82	0.19	42,42,43,43	0
5	EDO	B	421	4/4	0.83	0.17	38,38,38,39	0
5	EDO	B	423	4/4	0.83	0.16	39,40,41,41	0
5	EDO	A	503	4/4	0.84	0.14	26,26,26,26	0
5	EDO	A	521	4/4	0.84	0.17	43,43,43,43	0
5	EDO	A	510	4/4	0.84	0.16	43,43,43,43	0
5	EDO	B	409	4/4	0.85	0.23	38,39,39,39	0

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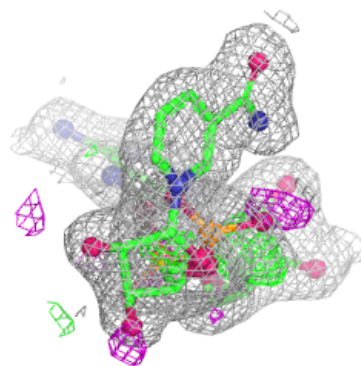
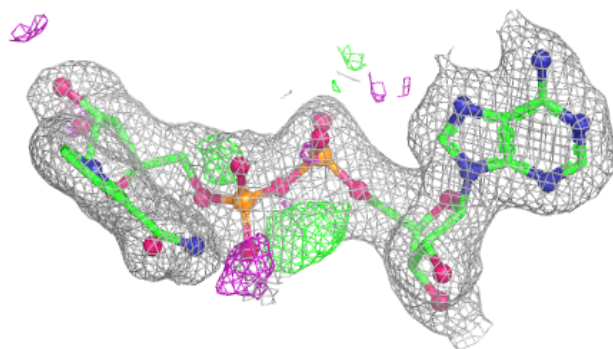
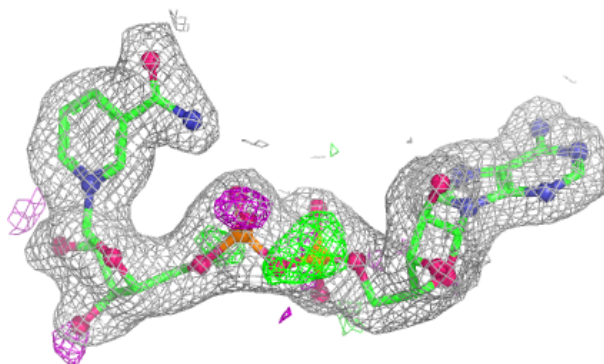
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	B	420	4/4	0.86	0.16	40,41,42,42	0
5	EDO	A	519	4/4	0.87	0.15	43,44,44,44	0
5	EDO	A	514	4/4	0.88	0.15	44,44,44,44	0
5	EDO	B	412	4/4	0.88	0.12	33,34,34,34	0
5	EDO	A	509	4/4	0.88	0.11	29,29,29,29	0
5	EDO	B	408	4/4	0.88	0.15	38,38,39,39	0
5	EDO	A	515	4/4	0.89	0.13	36,36,36,37	0
5	EDO	A	508	4/4	0.89	0.12	33,33,33,33	0
5	EDO	A	504	4/4	0.89	0.11	32,32,32,33	0
5	EDO	A	507	4/4	0.89	0.13	43,43,43,43	0
5	EDO	B	407	4/4	0.90	0.12	25,25,25,25	0
5	EDO	B	413	4/4	0.90	0.12	42,43,43,44	0
3	NAD	A	501	44/44	0.91	0.09	30,32,36,36	0
8	LAR	B	403	29/29	0.91	0.12	24,28,35,35	0
5	EDO	B	417	4/4	0.92	0.11	40,40,40,40	0
4	PO4	A	502	5/5	0.92	0.13	44,45,45,45	0
5	EDO	A	505	4/4	0.93	0.11	32,32,32,32	0
5	EDO	A	512	4/4	0.93	0.12	40,41,41,41	0
5	EDO	B	415	4/4	0.94	0.11	29,29,29,29	0
5	EDO	B	406	4/4	0.94	0.09	26,26,26,27	0
5	EDO	A	518	4/4	0.95	0.08	32,32,33,33	0
5	EDO	B	419	4/4	0.96	0.11	30,30,30,30	0
7	ATP	B	402	31/31	0.99	0.04	17,18,18,18	0
6	CA	B	401	1/1	0.99	0.03	17,17,17,17	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.

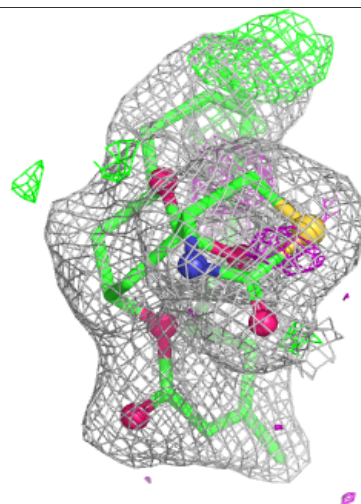
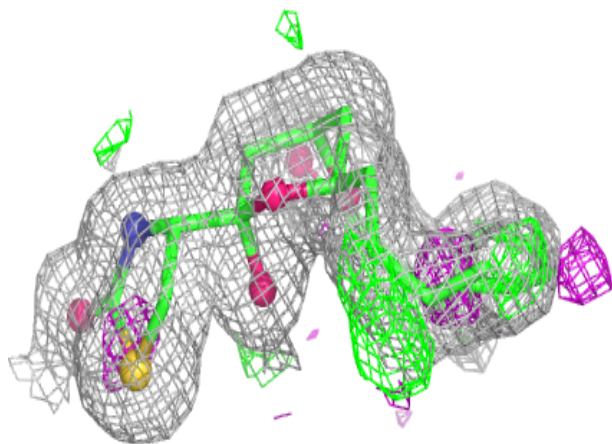
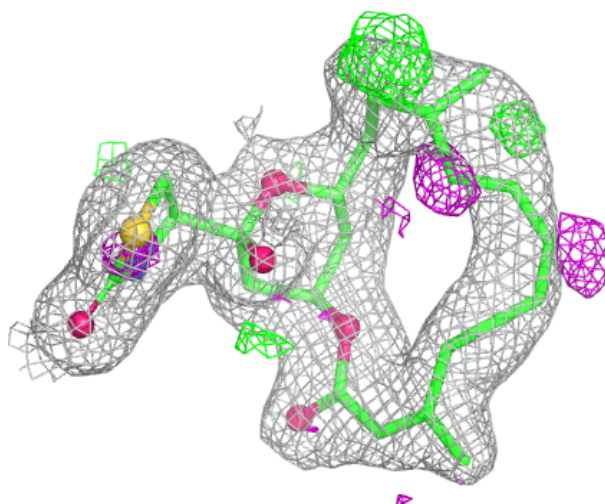
Electron density around NAD A 501:

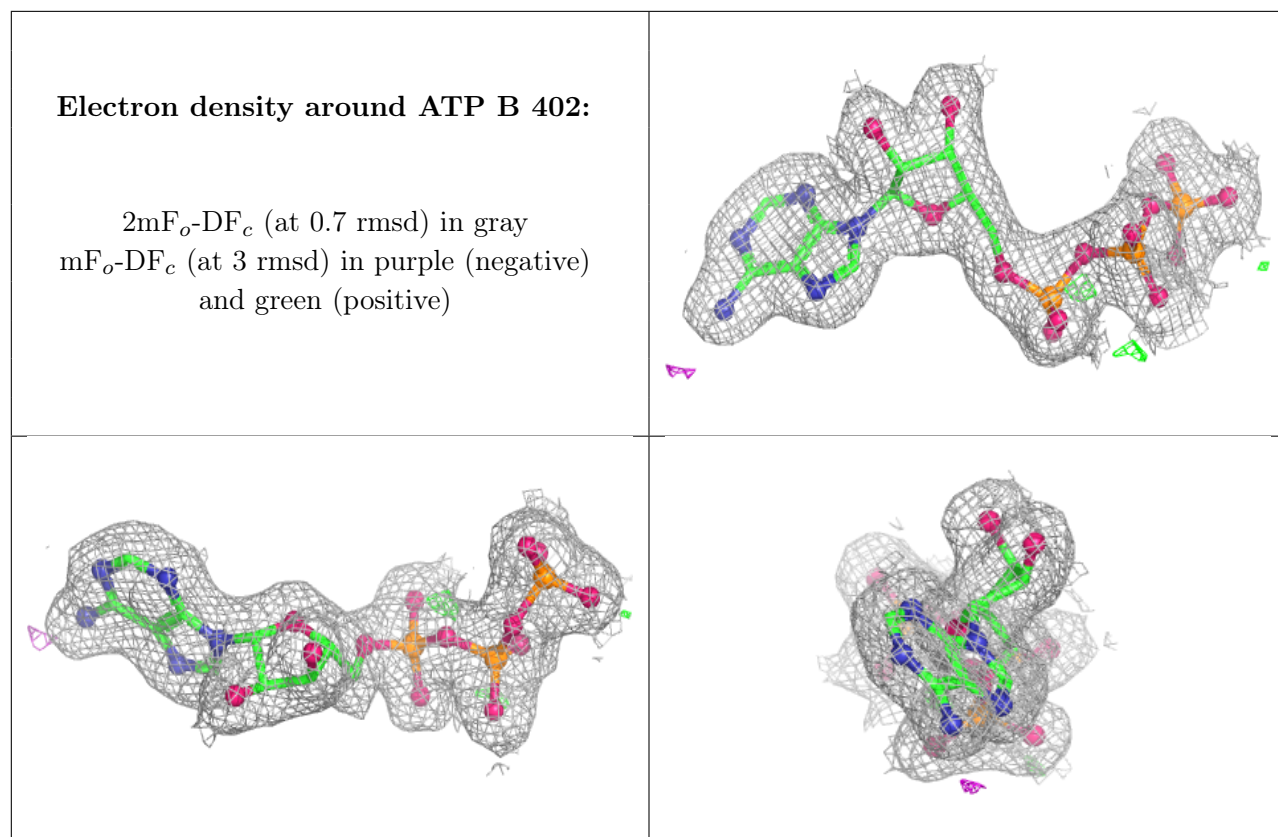
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.