



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:32 PM UTC

PDB ID : 4H0X / pdb_00004h0x
Title : Crystal structure of NAD⁺-Ia(E380A)-actin complex
Authors : Tsurumura, T.; Oda, M.; Nagahama, M.; Tsuge, H.
Deposited on : 2012-09-10
Resolution : 2.33 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

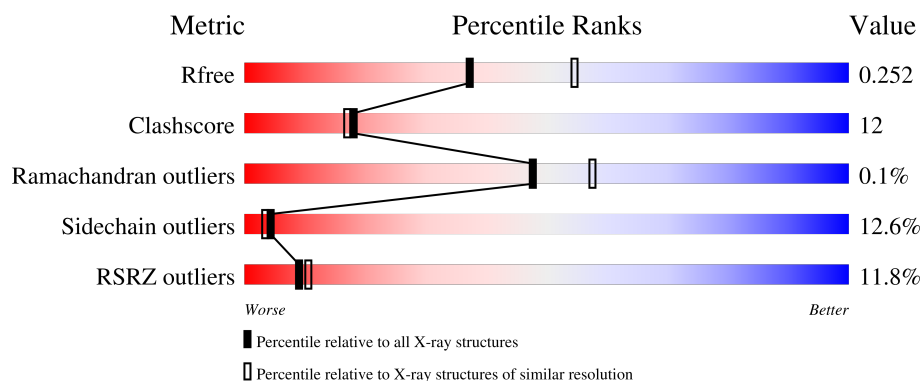
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	
2	B	375	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	511	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6567 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
			3360	2144	553	660	3			

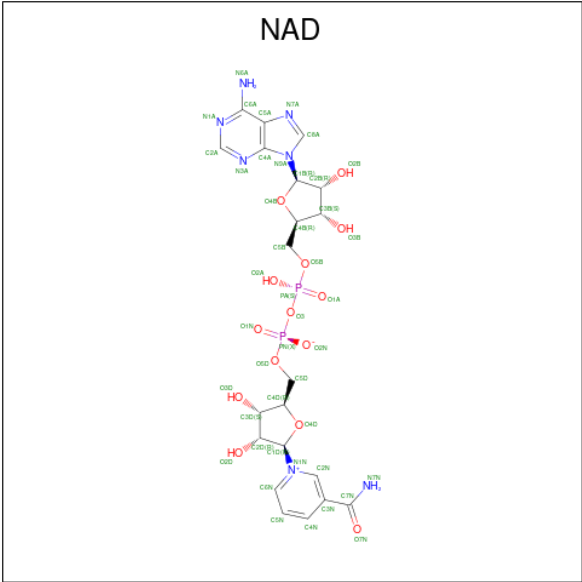
There are 6 discrepancies between the modelled and reference sequences:

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	380	ALA	GLU	engineered mutation	UNP Q46220

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

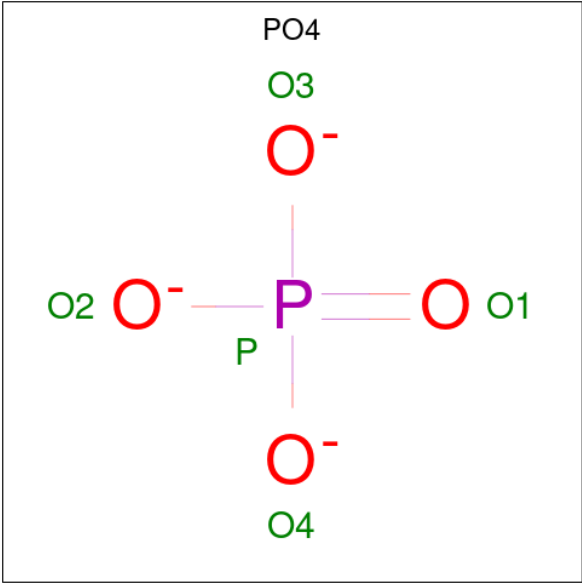
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	358	Total	C	N	O	S	0	0	0
			2799	1774	469	537	19			

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



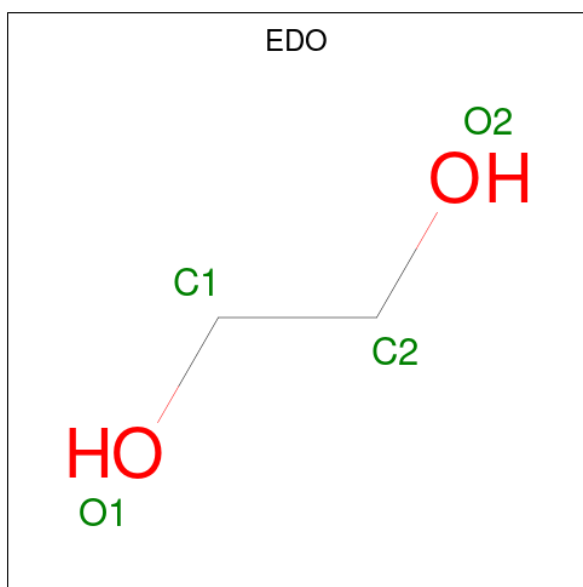
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- 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	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		

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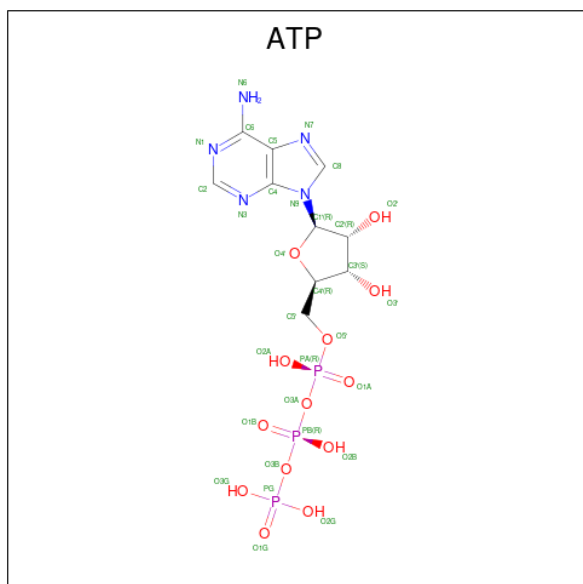
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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

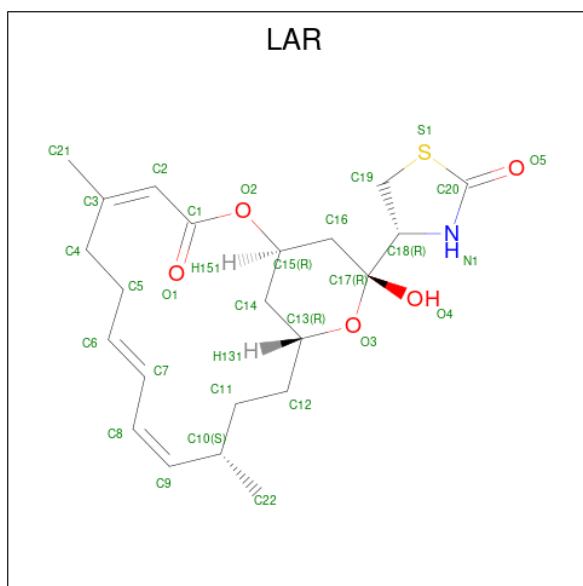
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		

- 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: $C_{22}H_{31}NO_5S$).

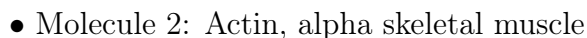


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	S	0	0
			29	22	1	5	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	110	Total	O	0	0
			110	110		
9	B	100	Total	O	0	0
			100	100		

- Molecule 1: Iota toxin component Ia



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.08Å 134.65Å 152.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.58 – 2.33 28.58 – 2.33	Depositor EDS
% Data completeness (in resolution range)	97.3 (28.58-2.33) 97.4 (28.58-2.33)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.77 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.224 , 0.251 (Not available) , 0.252	Depositor DCC
R_{free} test set	2394 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6567	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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, EDO, LAR, PO4, CA, ATP

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	0.50	0/3429	0.85	5/4632 (0.1%)
2	B	0.64	1/2857 (0.0%)	0.87	5/3870 (0.1%)
All	All	0.57	1/6286 (0.0%)	0.86	10/8502 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	71	ILE	C-O	-6.10	1.17	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	MET	N-CA-C	8.05	119.75	110.97
1	A	2	PHE	N-CA-C	6.32	118.88	110.53
2	B	365	ALA	N-CA-C	-6.09	101.19	110.14
2	B	62	ARG	N-CA-C	-5.46	105.93	112.59
1	A	247	MET	CB-CA-C	-5.42	102.61	110.96
1	A	249	GLY	N-CA-C	-5.35	104.85	112.55
2	B	370	VAL	CB-CA-C	-5.13	105.22	112.14
1	A	371	ALA	N-CA-C	-5.12	106.88	113.23
2	B	51	ASP	N-CA-C	5.07	118.89	111.34
2	B	148	THR	N-CA-C	-5.00	107.04	114.64

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	3360	0	3345	79	0
2	B	2799	0	2772	78	1
3	A	44	0	26	2	0
4	A	5	0	0	0	0
5	A	36	0	54	4	0
5	B	52	0	78	11	0
6	B	1	0	0	0	0
7	B	31	0	12	1	0
8	B	29	0	31	0	0
9	A	110	0	0	2	0
9	B	100	0	0	3	1
All	All	6567	0	6318	155	1

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 12.

All (155) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:MET:HE1	1:A:372:ILE:HG21	1.22	1.13
1:A:245:ASP:O	1:A:249:GLY:HA3	1.51	1.11
1:A:236:THR:OG1	1:A:239:GLU:HG3	1.57	1.02
2:B:274:ILE:HG23	2:B:313:MET:HE1	1.42	0.99
1:A:292:ILE:CD1	1:A:359:ASN:ND2	2.35	0.89
1:A:245:ASP:O	1:A:249:GLY:CA	2.21	0.88
1:A:236:THR:HB	1:A:237:PRO:HD2	1.56	0.85
2:B:283:MET:HE1	5:B:407:EDO:O2	1.80	0.82
1:A:370:SER:HA	1:A:376:ALA:HA	1.61	0.80
2:B:160:THR:HG23	2:B:180:LEU:O	1.82	0.80
2:B:105:LEU:HD21	2:B:123:MET:HE2	1.63	0.79
1:A:347:SER:OG	2:B:176:MET:HE2	1.83	0.78
2:B:310:ALA:HB1	2:B:329:ILE:HD13	1.65	0.78
2:B:216:LEU:O	2:B:254:ARG:HD2	1.83	0.78
1:A:347:SER:HB2	2:B:176:MET:CE	2.16	0.76
2:B:291:LYS:HG3	2:B:325:MET:HE1	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:ARG:HD3	2:B:214:GLU:OE1	1.88	0.72
2:B:190:MET:HG2	2:B:209:VAL:HG11	1.72	0.72
2:B:279:TYR:CE1	2:B:283:MET:HE3	2.25	0.72
1:A:57:GLN:HG2	1:A:214:LYS:HD3	1.70	0.72
2:B:148:THR:HG23	2:B:167:GLU:HA	1.72	0.72
2:B:244:ASP:OD2	2:B:246:GLN:NE2	2.15	0.71
2:B:332:PRO:HG2	5:B:406:EDO:H12	1.72	0.71
1:A:370:SER:CA	1:A:376:ALA:HA	2.22	0.69
1:A:52:TYR:CZ	1:A:56:ARG:HG3	2.29	0.68
1:A:129:LYS:NZ	9:A:670:HOH:O	2.25	0.68
1:A:292:ILE:CD1	1:A:359:ASN:HD22	2.06	0.68
1:A:292:ILE:HD12	1:A:359:ASN:ND2	2.07	0.67
2:B:354:GLN:HA	2:B:354:GLN:OE1	1.95	0.67
2:B:61:LYS:HD3	2:B:64:ILE:HG22	1.77	0.67
1:A:238:ASN:HB3	1:A:277:ASN:ND2	2.10	0.66
1:A:247:MET:HE1	1:A:372:ILE:CG2	2.13	0.65
2:B:362:TYR:O	2:B:365:ALA:O	2.15	0.65
1:A:337:ILE:HG23	1:A:383:LEU:HB2	1.79	0.64
2:B:160:THR:CG2	2:B:180:LEU:O	2.44	0.64
1:A:372:ILE:HG22	1:A:372:ILE:O	1.97	0.64
1:A:370:SER:O	1:A:376:ALA:HB1	1.98	0.64
1:A:370:SER:CB	1:A:376:ALA:HA	2.27	0.64
2:B:329:ILE:O	2:B:329:ILE:HD12	1.98	0.63
1:A:236:THR:HB	1:A:237:PRO:CD	2.28	0.62
2:B:111:ASN:HD21	2:B:119:MET:CE	2.13	0.61
1:A:347:SER:CB	2:B:176:MET:HE2	2.31	0.61
1:A:132:LYS:HE3	1:A:359:ASN:ND2	2.15	0.61
1:A:292:ILE:HD12	1:A:359:ASN:HD22	1.66	0.60
2:B:210:ARG:HG3	2:B:210:ARG:HH11	1.66	0.60
1:A:96:SER:HB3	1:A:98:GLU:OE2	2.00	0.60
2:B:188:TYR:CD1	2:B:267:ILE:HD11	2.37	0.60
2:B:274:ILE:CG2	2:B:313:MET:HE1	2.27	0.59
1:A:296:ARG:H	3:A:501:NAD:H72N	1.49	0.59
2:B:323:SER:HA	5:B:408:EDO:H22	1.84	0.59
1:A:244:ASN:HA	1:A:247:MET:HB2	1.83	0.59
2:B:196:ARG:HH21	2:B:249:THR:HG22	1.67	0.59
2:B:300:SER:HA	2:B:335:ARG:HG2	1.82	0.59
1:A:292:ILE:CD1	1:A:359:ASN:HD21	2.12	0.59
2:B:232:SER:OG	2:B:233:SER:N	2.35	0.58
1:A:302:PHE:HZ	1:A:356:LEU:HD11	1.67	0.58
2:B:367:PRO:O	2:B:370:VAL:HG22	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:SER:CB	2:B:176:MET:CE	2.80	0.58
1:A:5:ARG:NH2	1:A:88:PRO:O	2.35	0.57
1:A:236:THR:OG1	1:A:239:GLU:CG	2.43	0.57
1:A:183:TYR:HA	5:A:511:EDO:H12	1.87	0.57
2:B:90:PHE:HZ	2:B:123:MET:HE3	1.68	0.57
2:B:34:ILE:HD12	2:B:67:LEU:HD22	1.88	0.55
2:B:244:ASP:CG	2:B:246:GLN:HE22	2.12	0.55
2:B:54:VAL:HG13	2:B:85:ILE:HD13	1.88	0.55
1:A:302:PHE:CZ	1:A:356:LEU:HD11	2.43	0.54
2:B:210:ARG:CD	2:B:214:GLU:OE1	2.54	0.54
1:A:172:SER:OG	1:A:173:ASN:N	2.37	0.54
2:B:298:VAL:CG1	5:B:406:EDO:H21	2.37	0.54
2:B:237:GLU:HG2	2:B:249:THR:HG23	1.89	0.53
1:A:183:TYR:CA	5:A:511:EDO:H12	2.39	0.53
1:A:300:GLN:NE2	3:A:501:NAD:O3B	2.42	0.53
2:B:90:PHE:CZ	2:B:123:MET:HE3	2.43	0.53
1:A:220:GLY:HA3	1:A:341:ILE:HD13	1.91	0.53
1:A:292:ILE:HD11	1:A:359:ASN:HD21	1.72	0.53
1:A:306:LEU:HD21	2:B:265:SER:HB2	1.91	0.52
2:B:188:TYR:HB2	2:B:267:ILE:HD11	1.91	0.52
2:B:6:THR:O	2:B:101:HIS:HD2	1.92	0.52
1:A:255:ASN:O	1:A:259:ILE:HG12	2.09	0.52
2:B:369:ILE:HD12	2:B:372:ARG:HD3	1.92	0.52
1:A:85:ILE:HD12	1:A:87:LYS:O	2.10	0.51
2:B:291:LYS:CG	2:B:325:MET:HE1	2.38	0.50
1:A:370:SER:O	1:A:376:ALA:CB	2.59	0.50
1:A:192:ARG:HD2	1:A:199:GLN:CD	2.37	0.49
5:A:511:EDO:H21	9:A:673:HOH:O	2.11	0.49
1:A:192:ARG:HD2	1:A:199:GLN:OE1	2.12	0.49
1:A:297:SER:HB2	1:A:301:GLU:CD	2.38	0.49
2:B:111:ASN:ND2	2:B:119:MET:CE	2.76	0.49
2:B:190:MET:HG2	2:B:209:VAL:CG1	2.42	0.49
2:B:318:THR:HG23	5:B:408:EDO:H21	1.95	0.49
1:A:133:GLN:HG3	1:A:185:ILE:HG12	1.94	0.48
1:A:295:ARG:HB2	1:A:339:THR:HG22	1.95	0.48
2:B:148:THR:H	5:B:409:EDO:H12	1.78	0.48
2:B:143:TYR:OH	2:B:349:LEU:HD11	2.14	0.48
2:B:252:ASN:HD22	2:B:253:GLU:N	2.12	0.47
1:A:52:TYR:CE2	1:A:56:ARG:HG3	2.49	0.47
2:B:210:ARG:HD2	2:B:214:GLU:CD	2.39	0.47
2:B:317:ILE:HG22	2:B:327:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:ASN:ND2	2:B:256:ARG:HH21	2.12	0.47
1:A:250:GLY:O	1:A:254:ILE:HD12	2.14	0.46
1:A:346:MET:HG3	1:A:349:PHE:CE1	2.51	0.46
1:A:126:ILE:HD11	1:A:190:ILE:HG21	1.97	0.46
2:B:61:LYS:HD3	2:B:64:ILE:CG2	2.46	0.46
1:A:222:LEU:O	1:A:226:GLU:HB2	2.16	0.46
2:B:274:ILE:HG23	2:B:313:MET:CE	2.28	0.46
1:A:378:GLU:HB2	1:A:380:ALA:HB2	1.97	0.46
1:A:346:MET:HG3	1:A:349:PHE:CZ	2.50	0.45
2:B:111:ASN:ND2	2:B:119:MET:HE1	2.31	0.45
5:B:404:EDO:H11	9:B:581:HOH:O	2.16	0.45
2:B:194:THR:HA	2:B:198:TYR:O	2.16	0.45
2:B:332:PRO:O	2:B:335:ARG:HB2	2.16	0.45
2:B:54:VAL:O	2:B:57:GLU:HB2	2.17	0.45
2:B:283:MET:CE	5:B:407:EDO:O2	2.58	0.45
1:A:292:ILE:HD11	5:A:511:EDO:H22	1.99	0.45
2:B:267:ILE:HD13	2:B:267:ILE:HA	1.68	0.45
2:B:30:VAL:HG21	9:B:557:HOH:O	2.16	0.45
1:A:370:SER:HA	1:A:376:ALA:CA	2.39	0.44
2:B:354:GLN:HB2	2:B:355:MET:HE2	1.99	0.43
1:A:160:LEU:HD23	1:A:207:ILE:HD12	1.99	0.43
1:A:292:ILE:HD11	1:A:359:ASN:ND2	2.25	0.43
1:A:94:PHE:CG	1:A:151:PRO:HD2	2.54	0.43
2:B:188:TYR:CD1	2:B:267:ILE:CD1	3.01	0.43
2:B:205:GLU:O	2:B:209:VAL:HG12	2.18	0.43
2:B:313:MET:HG3	2:B:317:ILE:HD12	1.99	0.43
1:A:5:ARG:HH21	1:A:7:GLU:HA	1.84	0.43
1:A:162:LYS:O	1:A:163:ASN:HB2	2.19	0.43
2:B:31:PHE:CE2	2:B:93:GLU:HG3	2.55	0.42
2:B:252:ASN:HD22	2:B:252:ASN:C	2.26	0.42
1:A:98:GLU:H	1:A:98:GLU:CD	2.27	0.42
1:A:377:GLY:C	1:A:379:TYR:H	2.27	0.42
2:B:210:ARG:HH11	2:B:210:ARG:CG	2.30	0.42
5:B:415:EDO:H22	5:B:416:EDO:H12	2.02	0.42
2:B:91:TYR:HA	9:B:548:HOH:O	2.19	0.41
2:B:291:LYS:HA	2:B:325:MET:HE1	2.02	0.41
1:A:23:GLU:OE2	1:A:23:GLU:HA	2.21	0.41
1:A:182:ASP:O	1:A:182:ASP:CG	2.63	0.41
1:A:337:ILE:CG2	1:A:383:LEU:HB2	2.47	0.41
1:A:21:LYS:HG3	1:A:175:VAL:HG21	2.01	0.41
1:A:57:GLN:HG2	1:A:214:LYS:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LYS:HB2	1:A:190:ILE:HD11	2.02	0.41
1:A:249:GLY:HA3	1:A:250:GLY:HA3	1.61	0.41
2:B:214:GLU:HG2	7:B:402:ATP:C5	2.56	0.41
1:A:129:LYS:HG2	1:A:392:ASN:HD22	1.84	0.41
1:A:372:ILE:CG2	1:A:372:ILE:O	2.66	0.41
1:A:238:ASN:HB3	1:A:277:ASN:HD22	1.80	0.41
1:A:368:TYR:CZ	1:A:370:SER:HB2	2.56	0.41
2:B:111:ASN:HD21	2:B:119:MET:HE3	1.84	0.41
2:B:161:HIS:CD2	2:B:177:ARG:HB2	2.56	0.41
2:B:189:LEU:O	2:B:193:LEU:HB2	2.21	0.41
2:B:322:PRO:HG2	5:B:407:EDO:H21	2.03	0.40
1:A:126:ILE:HD12	1:A:187:ILE:HD13	2.03	0.40
1:A:221:ASP:HB2	1:A:379:TYR:CE1	2.56	0.40
2:B:17:VAL:O	2:B:30:VAL:HA	2.21	0.40
1:A:240:LEU:HD22	1:A:240:LEU:HA	1.91	0.40
2:B:298:VAL:HG12	5:B:406:EDO:H21	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:GLN:NE2	9:B:548:HOH:O[4_445]	1.94	0.26

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%)	390 (95%)	20 (5%)	1 (0%)	43	50
2	B	353/375 (94%)	343 (97%)	10 (3%)	0	100	100
All	All	764/793 (96%)	733 (96%)	30 (4%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	ARG

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
2	B	127/318 (40%)	111 (87%)	16 (13%)	4 3

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	232	SER
2	B	233	SER
2	B	235	SER
2	B	241	GLU
2	B	242	LEU
2	B	244	ASP
2	B	247	VAL
2	B	252	ASN
2	B	267	ILE
2	B	274	ILE
2	B	291	LYS
2	B	329	ILE
2	B	346	LEU
2	B	348	SER
2	B	354	GLN
2	B	370	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	252	ASN
2	B	360	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 27 ligands modelled in this entry, 1 is monoatomic - leaving 26 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	509	-	3,3,3	0.46	0	2,2,2	0.43	0
5	EDO	B	416	-	3,3,3	0.45	0	2,2,2	0.44	0
5	EDO	A	511	-	3,3,3	0.58	0	2,2,2	0.45	0
8	LAR	B	403	-	30,31,31	1.66	3 (10%)	32,43,43	2.60	7 (21%)
7	ATP	B	402	-	32,33,33	1.49	8 (25%)	48,52,52	1.71	9 (18%)
5	EDO	B	411	-	3,3,3	0.44	0	2,2,2	0.37	0
3	NAD	A	501	-	46,48,48	1.22	6 (13%)	64,73,73	1.60	12 (18%)
5	EDO	A	507	-	3,3,3	0.44	0	2,2,2	0.40	0
5	EDO	A	503	-	3,3,3	0.63	0	2,2,2	0.42	0
5	EDO	A	510	-	3,3,3	0.42	0	2,2,2	0.40	0
5	EDO	A	508	-	3,3,3	0.48	0	2,2,2	0.45	0
5	EDO	B	410	-	3,3,3	0.45	0	2,2,2	0.41	0
5	EDO	B	412	-	3,3,3	0.51	0	2,2,2	0.42	0
5	EDO	B	405	-	3,3,3	0.55	0	2,2,2	0.28	0
5	EDO	B	409	-	3,3,3	0.48	0	2,2,2	0.40	0
5	EDO	B	414	-	3,3,3	0.44	0	2,2,2	0.29	0
5	EDO	B	407	-	3,3,3	0.63	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	B	406	-	3,3,3	0.47	0	2,2,2	0.42	0
5	EDO	B	404	-	3,3,3	0.49	0	2,2,2	0.35	0
5	EDO	B	408	-	3,3,3	0.40	0	2,2,2	0.43	0
4	PO4	A	502	-	4,4,4	0.85	0	6,6,6	0.57	0
5	EDO	A	505	-	3,3,3	0.45	0	2,2,2	0.31	0
5	EDO	A	506	-	3,3,3	0.48	0	2,2,2	0.37	0
5	EDO	A	504	-	3,3,3	0.48	0	2,2,2	0.40	0
5	EDO	B	413	-	3,3,3	0.44	0	2,2,2	0.37	0
5	EDO	B	415	-	3,3,3	0.47	0	2,2,2	0.21	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	509	-	-	0/1/1/1	-
5	EDO	B	416	-	-	1/1/1/1	-
5	EDO	A	511	-	-	1/1/1/1	-
8	LAR	B	403	-	-	5/23/51/51	0/2/3/3
7	ATP	B	402	-	-	4/22/38/38	0/3/3/3
5	EDO	B	411	-	-	1/1/1/1	-
3	NAD	A	501	-	-	12/30/62/62	0/5/5/5
5	EDO	A	507	-	-	0/1/1/1	-
5	EDO	A	503	-	-	0/1/1/1	-
5	EDO	A	510	-	-	1/1/1/1	-
5	EDO	A	508	-	-	1/1/1/1	-
5	EDO	B	410	-	-	0/1/1/1	-
5	EDO	B	412	-	-	0/1/1/1	-
5	EDO	B	405	-	-	1/1/1/1	-
5	EDO	B	409	-	-	1/1/1/1	-
5	EDO	B	414	-	-	1/1/1/1	-
5	EDO	B	407	-	-	1/1/1/1	-
5	EDO	B	406	-	-	1/1/1/1	-
5	EDO	B	404	-	-	1/1/1/1	-
5	EDO	B	408	-	-	1/1/1/1	-
5	EDO	A	505	-	-	0/1/1/1	-
5	EDO	A	506	-	-	0/1/1/1	-
5	EDO	A	504	-	-	0/1/1/1	-
5	EDO	B	413	-	-	0/1/1/1	-
5	EDO	B	415	-	-	1/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	403	LAR	O2-C1	6.19	1.47	1.34
8	B	403	LAR	C20-S1	-5.23	1.66	1.77
3	A	501	NAD	C5A-C4A	4.67	1.47	1.39
7	B	402	ATP	C5-C4	4.65	1.47	1.39
7	B	402	ATP	PB-O3B	2.98	1.62	1.59
3	A	501	NAD	C5A-C6A	2.94	1.49	1.41
7	B	402	ATP	C5-C6	2.60	1.48	1.41
3	A	501	NAD	C8A-N7A	2.55	1.36	1.31
3	A	501	NAD	O4D-C1D	2.34	1.44	1.40
7	B	402	ATP	C5-N7	-2.25	1.35	1.39
7	B	402	ATP	C8-N7	2.23	1.36	1.31
7	B	402	ATP	PA-O3A	2.22	1.61	1.59
7	B	402	ATP	C4-N9	-2.20	1.33	1.37
3	A	501	NAD	C4A-N9A	-2.10	1.33	1.37
3	A	501	NAD	C5A-N7A	-2.07	1.35	1.39
7	B	402	ATP	PB-O3A	2.05	1.61	1.59
8	B	403	LAR	O4-C17	2.05	1.44	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	403	LAR	C4-C5-C6	-7.30	96.71	112.57
8	B	403	LAR	C10-C9-C8	-6.99	105.43	126.42
8	B	403	LAR	O2-C1-C2	5.38	123.68	111.20
3	A	501	NAD	C5A-C4A-N3A	-5.21	119.55	126.72
7	B	402	ATP	C5-C4-N3	-5.17	119.60	126.72
8	B	403	LAR	C8-C7-C6	-4.66	99.76	125.30
7	B	402	ATP	N3-C4-N9	4.50	134.83	127.17
3	A	501	NAD	N3A-C4A-N9A	4.06	134.08	127.17
3	A	501	NAD	N3A-C2A-N1A	-3.87	122.73	128.58
3	A	501	NAD	C2A-N3A-C4A	3.85	121.24	111.83
7	B	402	ATP	N3-C2-N1	-3.59	123.15	128.58
7	B	402	ATP	C2-N3-C4	3.50	120.37	111.83
3	A	501	NAD	C4A-C5A-N7A	-3.49	106.59	110.58
7	B	402	ATP	C4-N9-C8	3.47	109.38	105.74
8	B	403	LAR	O1-C1-C2	-3.27	118.09	126.23
8	B	403	LAR	O2-C1-O1	-3.19	118.23	123.34
3	A	501	NAD	C4A-N9A-C8A	3.02	108.91	105.74
7	B	402	ATP	C4-C5-N7	-2.98	107.17	110.58
3	A	501	NAD	C6A-C5A-N7A	2.73	137.35	132.09
8	B	403	LAR	C19-S1-C20	2.69	93.60	92.04
3	A	501	NAD	C6N-N1N-C2N	-2.59	119.67	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NAD	C5A-N7A-C8A	2.52	107.41	103.45
7	B	402	ATP	C5-N7-C8	2.33	107.12	103.45
7	B	402	ATP	C2-N1-C6	2.27	122.46	118.73
3	A	501	NAD	N9A-C8A-N7A	-2.27	110.72	113.94
7	B	402	ATP	N9-C8-N7	-2.24	110.75	113.94
3	A	501	NAD	C2A-N1A-C6A	2.06	122.12	118.73
3	A	501	NAD	C5N-C4N-C3N	-2.00	118.39	120.36

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	NAD	C5D-O5D-PN-O1N
3	A	501	NAD	O4D-C4D-C5D-O5D
3	A	501	NAD	C3D-C4D-C5D-O5D
8	B	403	LAR	O3-C17-C18-C19
5	A	510	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
7	B	402	ATP	PB-O3B-PG-O3G
3	A	501	NAD	C2N-C3N-C7N-N7N
3	A	501	NAD	C4D-C5D-O5D-PN
3	A	501	NAD	C5D-O5D-PN-O3
3	A	501	NAD	C5D-O5D-PN-O2N
3	A	501	NAD	C2N-C3N-C7N-O7N
8	B	403	LAR	O2-C1-C2-C3
5	B	408	EDO	O1-C1-C2-O2
3	A	501	NAD	C4N-C3N-C7N-N7N
8	B	403	LAR	C3-C4-C5-C6
3	A	501	NAD	PA-O3-PN-O1N
7	B	402	ATP	PG-O3B-PB-O1B
5	A	508	EDO	O1-C1-C2-O2
5	B	405	EDO	O1-C1-C2-O2
5	B	406	EDO	O1-C1-C2-O2
5	B	409	EDO	O1-C1-C2-O2
3	A	501	NAD	C4N-C3N-C7N-O7N
7	B	402	ATP	PB-O3B-PG-O2G
8	B	403	LAR	O1-C1-C2-C3
5	B	415	EDO	O1-C1-C2-O2
8	B	403	LAR	C4-C5-C6-C7
3	A	501	NAD	PA-O3-PN-O2N

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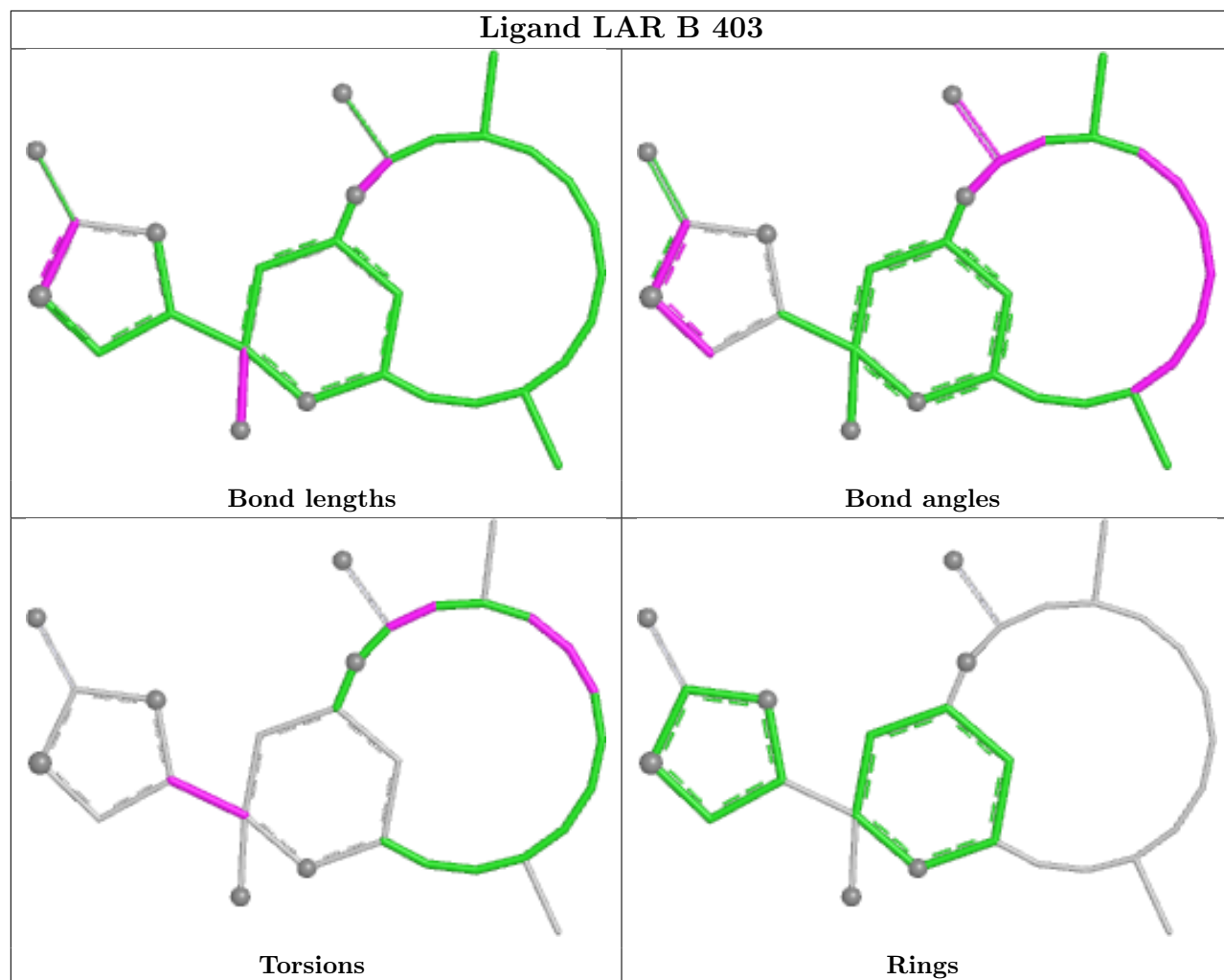
Mol	Chain	Res	Type	Atoms
7	B	402	ATP	PG-O3B-PB-O2B
5	B	407	EDO	O1-C1-C2-O2
5	B	414	EDO	O1-C1-C2-O2
5	A	511	EDO	O1-C1-C2-O2

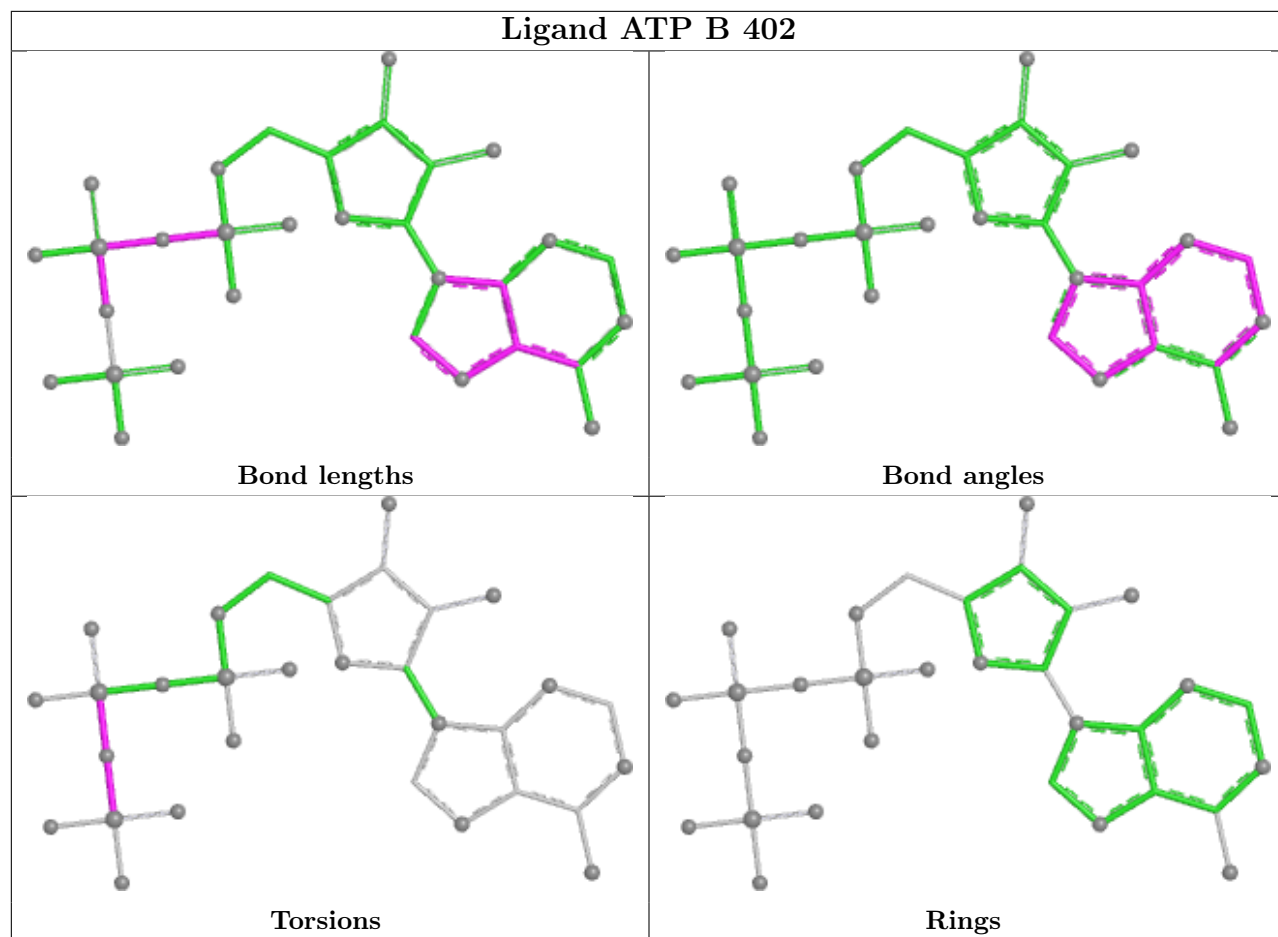
There are no ring outliers.

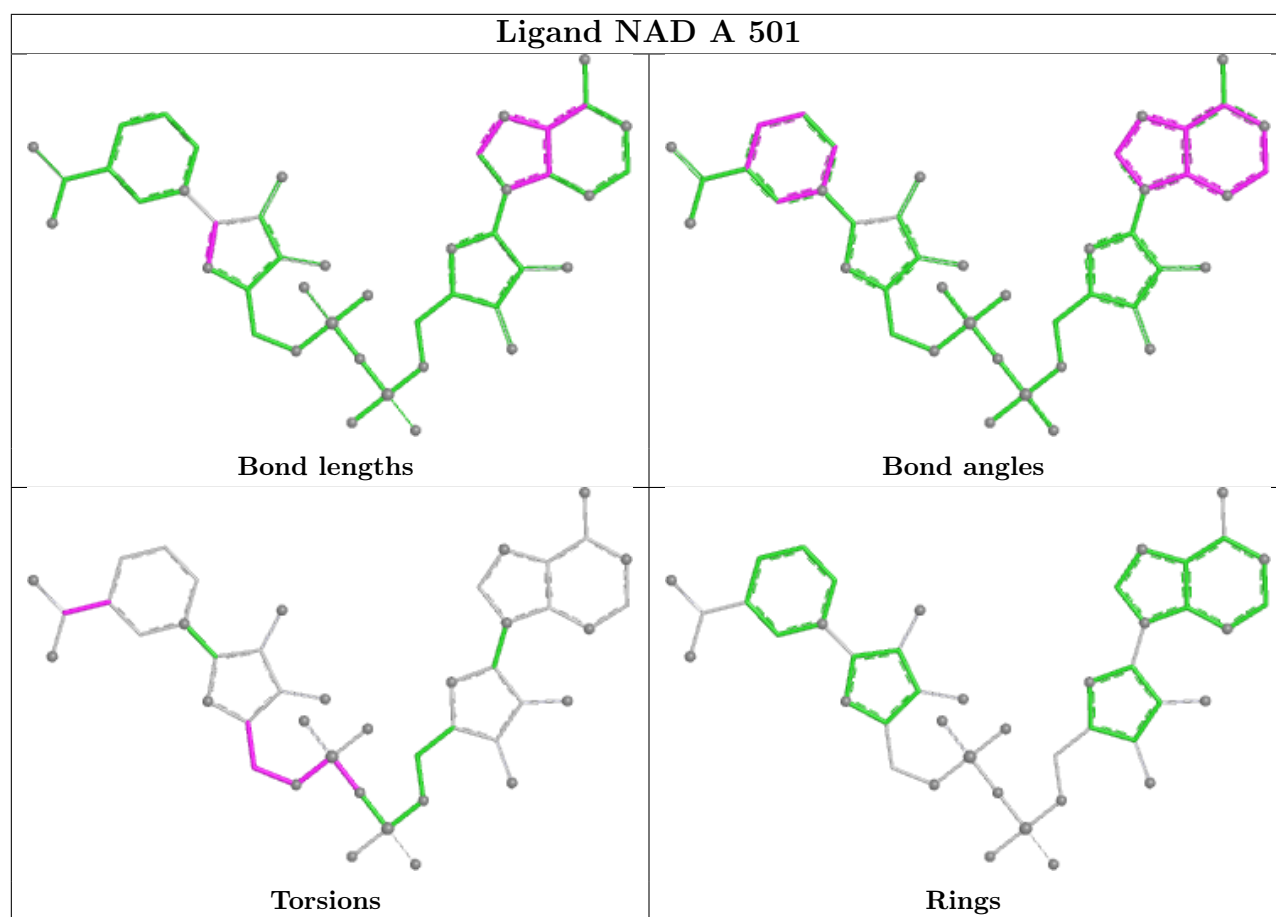
10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	416	EDO	1	0
5	A	511	EDO	4	0
7	B	402	ATP	1	0
3	A	501	NAD	2	0
5	B	409	EDO	1	0
5	B	407	EDO	3	0
5	B	406	EDO	3	0
5	B	404	EDO	1	0
5	B	408	EDO	2	0
5	B	415	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%)	0.92	53 (12%) 7 9	28, 46, 83, 101	0
2	B	358/375 (95%)	0.41	38 (10%) 11 13	19, 28, 73, 141	0
All	All	771/793 (97%)	0.68	91 (11%) 9 10	19, 37, 81, 141	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	376	ALA	6.4
2	B	52	SER	6.2
2	B	64	ILE	6.1
1	A	372	ILE	5.7
2	B	62	ARG	5.6
2	B	63	GLY	5.4
2	B	50	LYS	5.2
2	B	51	ASP	5.1
1	A	373	PRO	5.1
1	A	284	LEU	5.1
2	B	55	GLY	5.0
1	A	375	TYR	5.0
1	A	269	PRO	4.7
2	B	59	GLN	4.6
1	A	374	GLY	4.4
1	A	236	THR	4.3
2	B	233	SER	4.2
1	A	264	LEU	4.2
1	A	246	TYR	4.0
2	B	354	GLN	4.0
2	B	39	ARG	3.9
2	B	56	ASP	3.8
2	B	329	ILE	3.8
2	B	54	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	61	LYS	3.7
2	B	173	HIS	3.5
2	B	5	THR	3.5
1	A	377	GLY	3.5
2	B	66	THR	3.4
1	A	271	LEU	3.4
1	A	1	ALA	3.4
1	A	413	ASN	3.4
1	A	378	GLU	3.3
2	B	57	GLU	3.3
1	A	145	GLY	3.3
2	B	228	ALA	3.3
1	A	275	VAL	3.3
1	A	267	PRO	3.2
1	A	273	SER	3.1
2	B	60	SER	3.1
1	A	232	SER	3.0
1	A	241	ALA	3.0
1	A	265	ASN	3.0
1	A	237	PRO	3.0
1	A	3	ILE	2.9
2	B	53	TYR	2.8
1	A	234	LYS	2.8
1	A	257	TYR	2.8
1	A	83	ASN	2.7
1	A	268	ASN	2.7
2	B	232	SER	2.7
2	B	246	GLN	2.7
2	B	123	MET	2.7
1	A	249	GLY	2.6
1	A	276	ASN	2.6
1	A	251	TYR	2.6
2	B	234	SER	2.6
1	A	266	ASN	2.6
1	A	359	ASN	2.6
1	A	331	ILE	2.6
2	B	231	ALA	2.5
2	B	65	LEU	2.5
1	A	272	ASP	2.5
2	B	58	ALA	2.5
2	B	374	CYS	2.4
1	A	173	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	247	MET	2.4
2	B	143	TYR	2.4
2	B	128	ASN	2.4
1	A	330	VAL	2.4
1	A	369	LEU	2.4
2	B	365	ALA	2.3
1	A	238	ASN	2.3
1	A	371	ALA	2.3
2	B	241	GLU	2.3
1	A	285	THR	2.3
1	A	324	GLU	2.2
1	A	78	ASN	2.2
2	B	67	LEU	2.1
1	A	233	ASN	2.1
2	B	244	ASP	2.1
1	A	263	PRO	2.1
1	A	248	ARG	2.1
1	A	207	ILE	2.1
1	A	260	SER	2.1
1	A	98	GLU	2.0
1	A	235	LEU	2.0
2	B	178	LEU	2.0
1	A	337	ILE	2.0
2	B	225	ASN	2.0
1	A	278	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

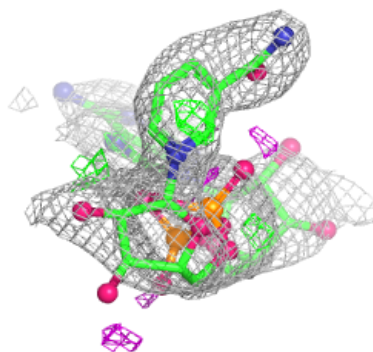
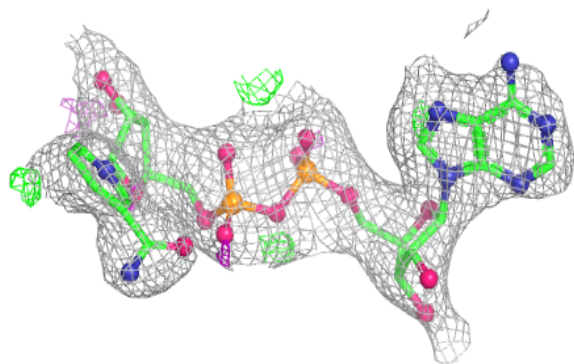
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	511	4/4	0.70	0.33	43,43,43,44	0
5	EDO	B	407	4/4	0.73	0.19	38,38,39,39	0
5	EDO	A	504	4/4	0.75	0.18	35,35,35,35	0
5	EDO	B	406	4/4	0.77	0.21	26,27,28,29	0
5	EDO	A	508	4/4	0.79	0.16	40,41,41,41	0
5	EDO	A	510	4/4	0.80	0.13	44,44,45,45	0
5	EDO	B	409	4/4	0.81	0.17	40,40,41,49	0
5	EDO	A	509	4/4	0.82	0.16	46,46,46,47	0
3	NAD	A	501	44/44	0.82	0.15	59,70,74,77	0
5	EDO	B	411	4/4	0.83	0.17	48,49,49,50	0
5	EDO	B	413	4/4	0.83	0.12	38,38,38,39	0
5	EDO	B	404	4/4	0.84	0.18	37,39,39,40	0
5	EDO	B	405	4/4	0.85	0.16	49,49,49,50	0
5	EDO	B	416	4/4	0.85	0.13	36,36,37,38	0
5	EDO	A	506	4/4	0.86	0.12	38,38,39,39	0
5	EDO	B	412	4/4	0.88	0.12	34,34,34,35	0
5	EDO	A	503	4/4	0.88	0.13	39,39,39,40	0
5	EDO	B	415	4/4	0.88	0.22	39,40,45,46	0
5	EDO	A	507	4/4	0.88	0.15	43,43,44,44	0
5	EDO	B	408	4/4	0.89	0.20	37,38,39,39	0
5	EDO	B	410	4/4	0.90	0.11	38,38,38,39	0
4	PO4	A	502	5/5	0.91	0.16	56,57,57,60	0
8	LAR	B	403	29/29	0.91	0.11	29,31,34,34	0
5	EDO	B	414	4/4	0.93	0.14	27,28,28,28	0
5	EDO	A	505	4/4	0.94	0.09	38,39,39,39	0
7	ATP	B	402	31/31	0.98	0.05	20,20,21,21	0
6	CA	B	401	1/1	0.99	0.04	21,21,21,21	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.

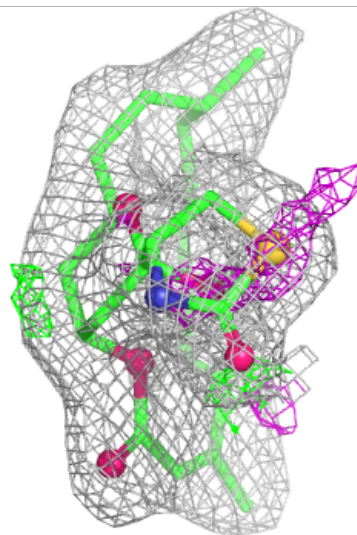
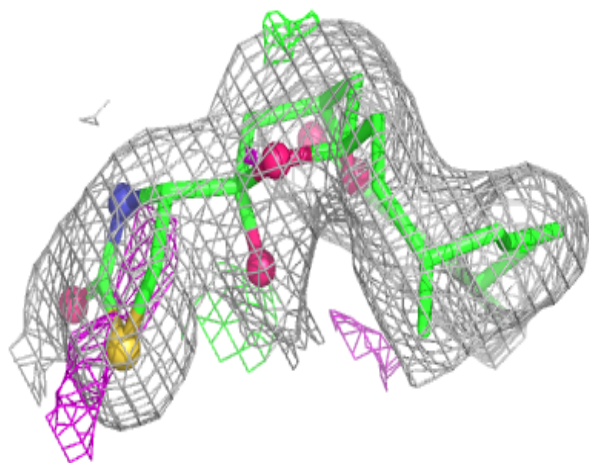
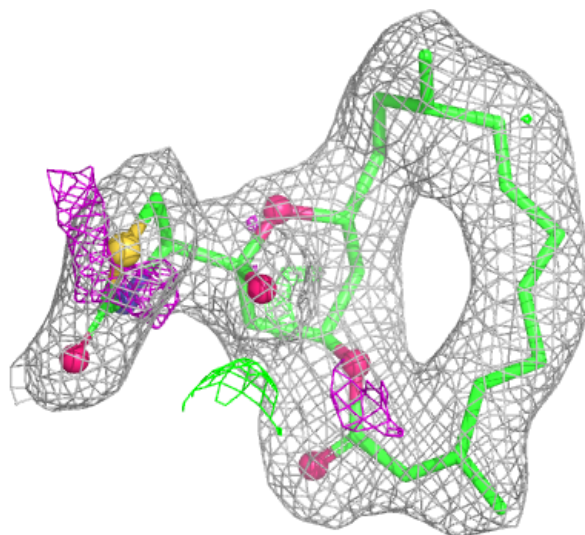
Electron density around NAD A 501:

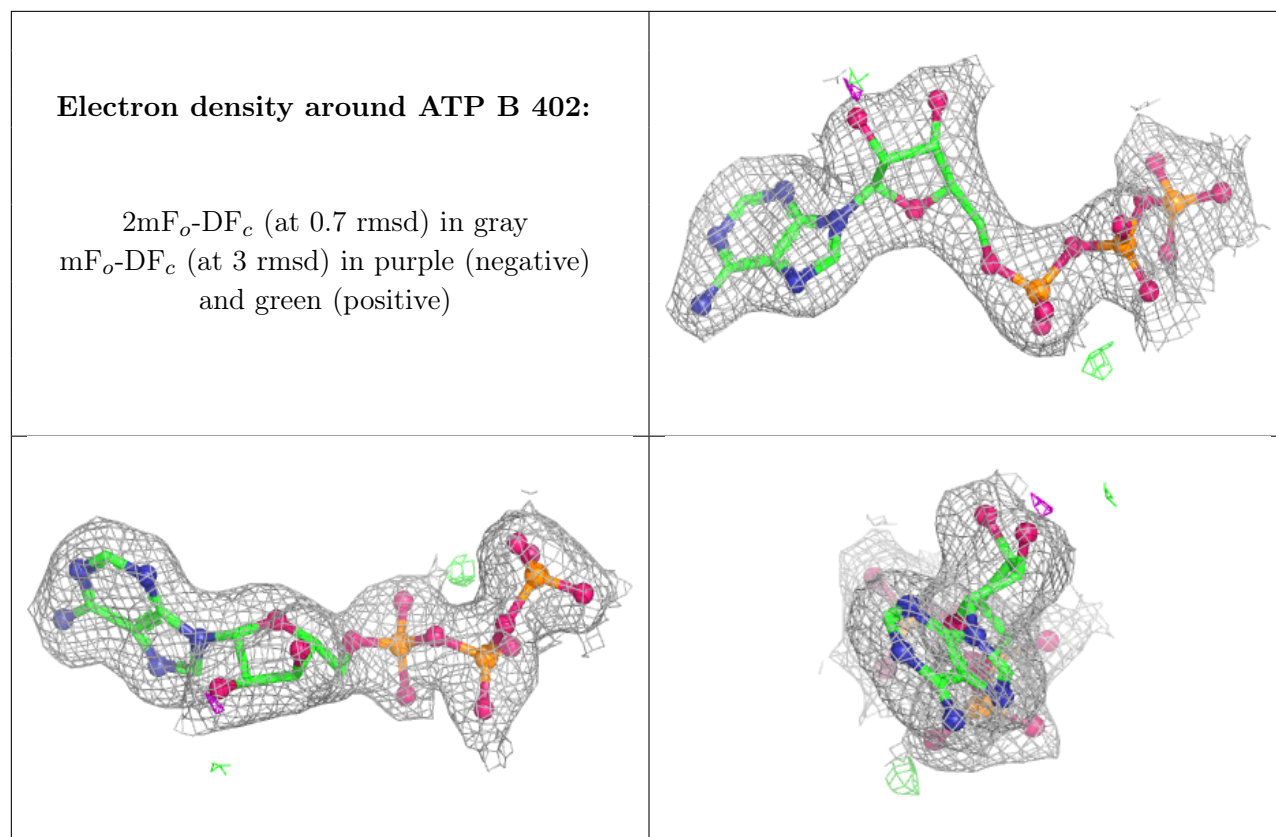
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.