Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:46 pm BST

PDB ID	:	4H0Y
Title	:	Crystal structure of NAD+-Ia(E380S)-actin complex
Authors	:	Tsurumura, T.; Oda, M.; Nagahama, M.; Tsuge, H.
Deposited on	:	2012-09-10
Resolution	:	1.94 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 following versions of software and data (see references ⓘ) were used in the production of this report:

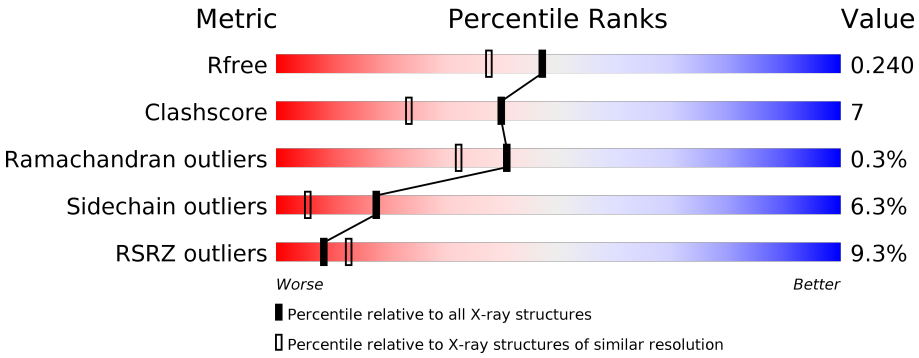
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.94 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}	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	418	9% 83% 13%
2	B	375	9% 79% 14% 5%

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	521	-	-	-	X
5	EDO	B	426	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6739 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
			Total	C	N	O	S			
1	A	413	3361	2144	553	661	3	0	0	0

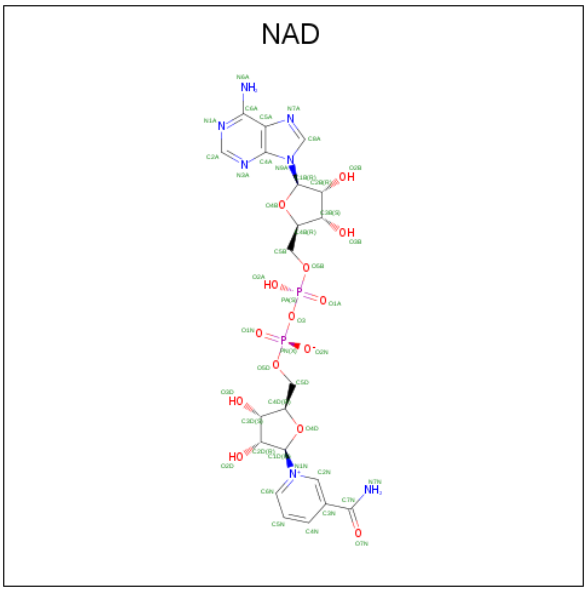
There are 6 discrepancies between the modelled and reference sequences:

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	SER	GLU	ENGINEERED MUTATION	UNP Q46220

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

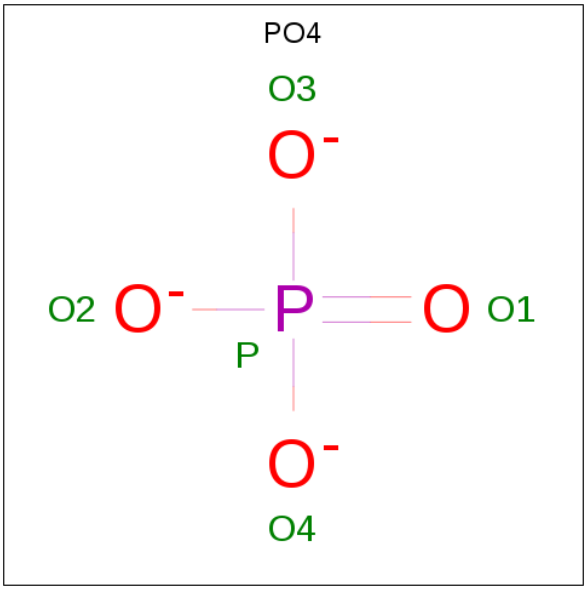
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	358	2799	1774	469	537	19	0	0	0

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



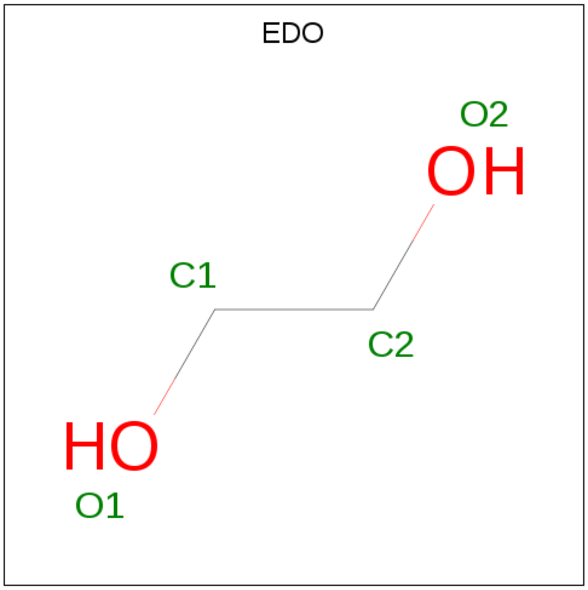
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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



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

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

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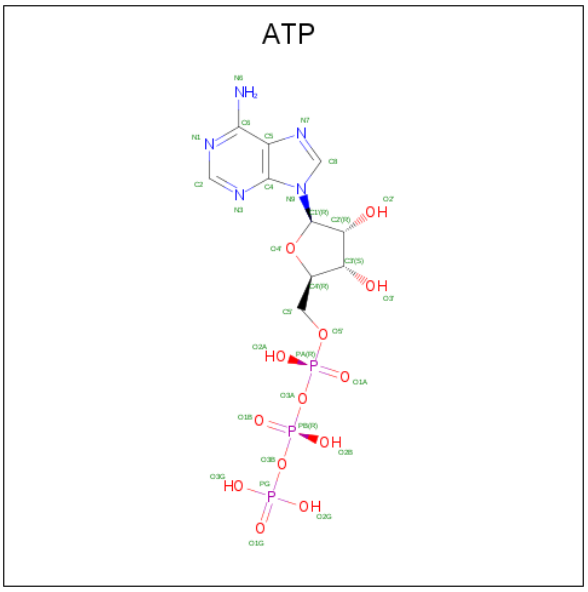
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
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
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 (three-letter code: CA) (formula: Ca).

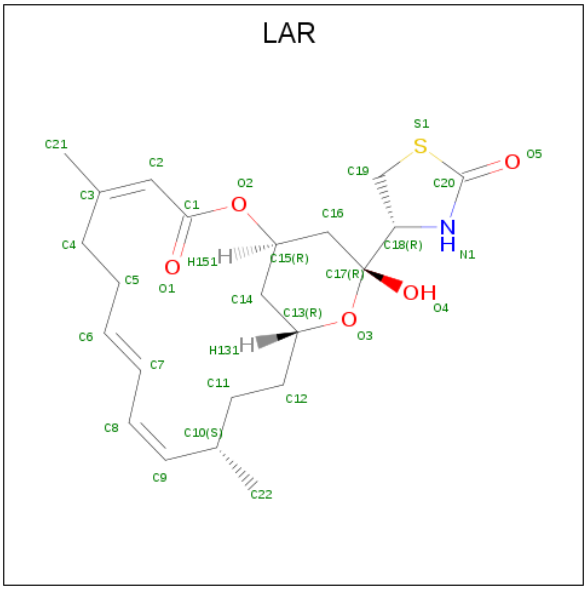
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Ca 1 1	0	0

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



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

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



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

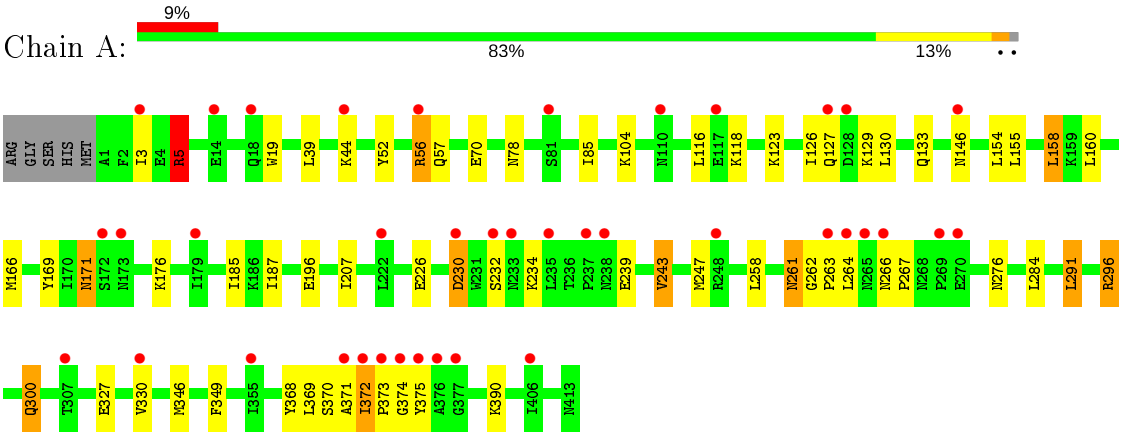
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	149	Total O 149 149	0	0
9	B	112	Total O 112 112	0	0

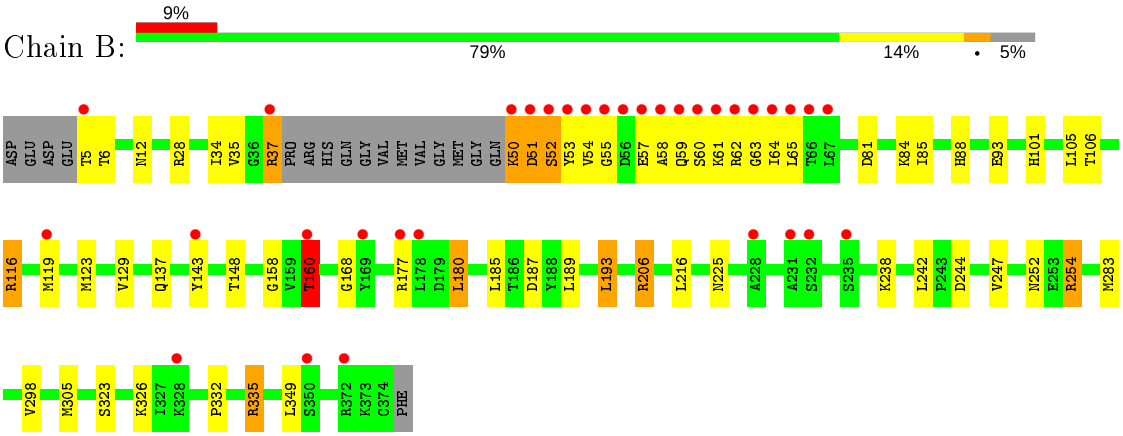
3 Residue-property plots (i)

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

- Molecule 1: Iota toxin component Ia



- Molecule 2: Actin, alpha skeletal muscle



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	53.87Å 134.94Å 154.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.91 – 1.94 30.91 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.91-1.94) 99.6 (30.91-1.94)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.220 , 0.233 0.228 , 0.240	Depositor DCC
R_{free} test set	4182 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6739	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.35	0/3430	0.81	8/4633 (0.2%)
2	B	0.42	1/2858 (0.0%)	0.65	3/3873 (0.1%)
All	All	0.38	1/6288 (0.0%)	0.74	11/8506 (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	12.83	1.69	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	5	ARG	NE-CZ-NH2	-16.57	112.01	120.30
1	A	296	ARG	NE-CZ-NH2	-15.27	112.67	120.30
1	A	296	ARG	NE-CZ-NH1	14.11	127.36	120.30
1	A	5	ARG	NE-CZ-NH1	13.01	126.80	120.30
2	B	254	ARG	NE-CZ-NH1	-8.66	115.97	120.30
1	A	296	ARG	CG-CD-NE	-7.82	95.38	111.80
2	B	254	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	A	296	ARG	CD-NE-CZ	7.06	133.49	123.60
1	A	291	LEU	CA-CB-CG	5.73	128.49	115.30
2	B	206	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	5	ARG	CD-NE-CZ	5.38	131.13	123.60

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	3361	0	3343	40	0
2	B	2799	0	2773	54	1
3	A	44	0	26	0	0
4	A	5	0	0	1	0
5	A	104	0	155	4	0
5	B	104	0	156	10	0
6	B	1	0	0	0	0
7	B	31	0	12	0	0
8	B	29	0	31	1	0
9	A	149	0	0	1	0
9	B	112	0	0	1	0
All	All	6739	0	6496	95	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 7.

All (95) 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	1.68	1.41
1:A:104:LYS:NZ	5:A:519:EDO:O1	1.67	1.24
2:B:51:ASP:O	2:B:52:SER:HB3	1.51	1.08
2:B:116:ARG:NH1	9:B:586:HOH:O	1.98	0.96
2:B:216:LEU:O	2:B:254:ARG:HD2	1.69	0.92
2:B:160:THR:HG23	2:B:180:LEU:O	1.72	0.89
2:B:332:PRO:O	2:B:335:ARG:HG2	1.74	0.88
2:B:51:ASP:O	2:B:52:SER:CB	2.29	0.81
2:B:283:MET:CE	5:B:409:EDO:O2	2.30	0.80
1:A:146:ASN:HA	1:A:196:GLU:HG3	1.65	0.78
2:B:61:LYS:HD3	2:B:64:ILE:HG22	1.67	0.77
2:B:283:MET:HE1	5:B:409:EDO:O2	1.85	0.76
2:B:298:VAL:CG1	5:B:408:EDO:H21	2.17	0.75
1:A:56:ARG:NH2	1:A:57:GLN:HB3	2.10	0.67
1:A:372:ILE:HG22	1:A:372:ILE:O	1.95	0.67
1:A:129:LYS:HE2	1:A:390:LYS:HE2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ILE:HD13	1:A:166:MET:HE3	1.79	0.64
1:A:261:ASN:HD21	1:A:264:LEU:HD12	1.64	0.62
2:B:216:LEU:HD22	2:B:238:LYS:HG2	1.80	0.62
1:A:5:ARG:HD3	4:A:502:PO4:O3	1.99	0.62
2:B:216:LEU:O	2:B:254:ARG:CD	2.46	0.62
1:A:230:ASP:N	1:A:230:ASP:OD2	2.19	0.61
1:A:247:MET:HE1	1:A:372:ILE:HG21	1.82	0.61
1:A:56:ARG:HH21	1:A:57:GLN:HB3	1.63	0.61
1:A:5:ARG:HD2	1:A:19:TRP:CZ2	2.37	0.60
2:B:54:VAL:HG13	2:B:85:ILE:HD13	1.83	0.60
1:A:158:LEU:HD21	1:A:185:ILE:HD12	1.84	0.59
2:B:283:MET:HE3	5:B:409:EDO:O2	2.03	0.59
1:A:239:GLU:O	1:A:243:VAL:HG13	2.02	0.58
1:A:371:ALA:O	1:A:373:PRO:HD3	2.02	0.58
2:B:52:SER:HB2	2:B:84:LYS:HG3	1.85	0.57
2:B:143:TYR:OH	2:B:349:LEU:HD11	2.04	0.57
2:B:53:TYR:CE2	2:B:60:SER:CB	2.88	0.57
2:B:298:VAL:HG12	5:B:408:EDO:H21	1.87	0.56
2:B:6:THR:O	2:B:101:HIS:HD2	1.88	0.56
2:B:148:THR:H	5:B:413:EDO:H12	1.71	0.56
1:A:78:ASN:ND2	9:A:609:HOH:O	2.38	0.56
1:A:146:ASN:HA	1:A:196:GLU:CG	2.37	0.55
2:B:323:SER:HA	5:B:410:EDO:H22	1.89	0.55
2:B:160:THR:CG2	2:B:180:LEU:O	2.52	0.54
2:B:50:LYS:O	2:B:51:ASP:C	2.45	0.54
1:A:346:MET:HG3	1:A:349:PHE:CE1	2.44	0.53
2:B:148:THR:OG1	2:B:168:GLY:N	2.41	0.53
2:B:51:ASP:O	2:B:84:LYS:HE3	2.10	0.52
2:B:37:ARG:NH1	2:B:81:ASP:OD1	2.43	0.51
1:A:123:LYS:O	1:A:127:GLN:HB2	2.10	0.51
2:B:158:GLY:HA2	5:B:404:EDO:H11	1.92	0.51
2:B:53:TYR:CD2	2:B:60:SER:HB2	2.45	0.51
2:B:53:TYR:HB3	2:B:58:ALA:HA	1.92	0.51
1:A:126:ILE:HD12	1:A:187:ILE:HD13	1.93	0.51
1:A:263:PRO:O	1:A:267:PRO:HG3	2.12	0.50
1:A:296:ARG:HD3	1:A:349:PHE:CE1	2.46	0.50
2:B:50:LYS:O	2:B:51:ASP:O	2.29	0.49
2:B:35:VAL:HA	2:B:53:TYR:O	2.12	0.49
2:B:106:THR:HB	2:B:137:GLN:HG3	1.95	0.49
1:A:133:GLN:HG3	1:A:185:ILE:HG12	1.95	0.48
2:B:53:TYR:CE2	2:B:60:SER:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:MET:HG3	1:A:349:PHE:CZ	2.49	0.48
2:B:53:TYR:CD2	2:B:60:SER:CB	2.96	0.48
2:B:52:SER:O	2:B:53:TYR:CD1	2.67	0.48
1:A:171:ASN:HD22	1:A:171:ASN:C	2.17	0.47
1:A:160:LEU:HD13	1:A:166:MET:HE2	1.97	0.47
1:A:327:GLU:OE1	5:A:507:EDO:H21	2.15	0.47
1:A:52:TYR:CZ	1:A:56:ARG:HB3	2.49	0.47
2:B:187:ASP:OD1	2:B:206:ARG:HD2	2.15	0.46
1:A:5:ARG:HD2	1:A:19:TRP:CH2	2.50	0.46
1:A:3:ILE:O	1:A:3:ILE:HG22	2.14	0.46
1:A:374:GLY:O	1:A:375:TYR:CD1	2.69	0.46
2:B:50:LYS:C	2:B:51:ASP:O	2.53	0.46
2:B:63:GLY:N	2:B:65:LEU:O	2.50	0.45
1:A:185:ILE:CD1	1:A:207:ILE:HG22	2.47	0.45
2:B:61:LYS:HD3	2:B:64:ILE:CG2	2.43	0.44
1:A:368:TYR:CZ	1:A:370:SER:HB2	2.53	0.44
2:B:298:VAL:HG11	5:B:408:EDO:H21	1.98	0.44
1:A:300:GLN:NE2	1:A:300:GLN:H	2.16	0.43
1:A:5:ARG:CD	1:A:19:TRP:CZ2	3.00	0.43
2:B:53:TYR:HD2	2:B:57:GLU:O	2.00	0.43
1:A:104:LYS:NZ	5:A:519:EDO:C1	2.75	0.43
2:B:305:MET:SD	2:B:335:ARG:HG3	2.58	0.43
2:B:105:LEU:CD1	2:B:119:MET:HG2	2.48	0.42
2:B:34:ILE:HD11	2:B:55:GLY:O	2.19	0.42
2:B:206:ARG:HG2	8:B:403:LAR:S1	2.59	0.42
2:B:54:VAL:HG13	2:B:85:ILE:CD1	2.46	0.42
1:A:169:TYR:CE2	1:A:176:LYS:HB2	2.55	0.42
1:A:262:GLY:N	1:A:263:PRO:CD	2.82	0.42
5:B:411:EDO:H21	5:B:412:EDO:O2	2.19	0.42
1:A:70:GLU:OE2	5:A:525:EDO:O1	2.37	0.41
2:B:160:THR:CB	2:B:160:THR:HG1	2.12	0.41
2:B:88:HIS:HE1	2:B:93:GLU:OE2	2.03	0.41
2:B:119:MET:HB2	2:B:119:MET:HE2	1.93	0.41
2:B:189:LEU:HG	2:B:193:LEU:HD22	2.03	0.41
1:A:146:ASN:HD22	1:A:196:GLU:HG3	1.84	0.41
2:B:54:VAL:HA	2:B:58:ALA:HB2	2.03	0.41
2:B:123:MET:CE	2:B:129:VAL:HG11	2.51	0.40
2:B:62:ARG:C	2:B:65:LEU:O	2.60	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:244:ASP:OD1	2:B:326:LYS:NZ[1_655]	2.10	0.10

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	411/418 (98%)	396 (96%)	15 (4%)	0	100 100
2	B	354/375 (94%)	347 (98%)	5 (1%)	2 (1%)	25 13
All	All	765/793 (96%)	743 (97%)	20 (3%)	2 (0%)	41 32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	ASP
2	B	52	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	376/380 (99%)	350 (93%)	26 (7%)	15 4
2	B	304/318 (96%)	287 (94%)	17 (6%)	21 8
All	All	680/698 (97%)	637 (94%)	43 (6%)	18 5

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	39	LEU
1	A	44	LYS
1	A	56	ARG
1	A	116	LEU
1	A	118	LYS
1	A	130	LEU
1	A	154	LEU
1	A	155	LEU
1	A	158	LEU
1	A	171	ASN
1	A	226	GLU
1	A	230	ASP
1	A	232	SER
1	A	234	LYS
1	A	243	VAL
1	A	258	LEU
1	A	261	ASN
1	A	266	ASN
1	A	276	ASN
1	A	284	LEU
1	A	291	LEU
1	A	300	GLN
1	A	330	VAL
1	A	369	LEU
1	A	372	ILE
2	B	5	THR
2	B	12	ASN
2	B	28	ARG
2	B	37	ARG
2	B	50	LYS
2	B	59	GLN
2	B	116	ARG
2	B	160	THR
2	B	177	ARG
2	B	180	LEU
2	B	185	LEU
2	B	193	LEU
2	B	225	ASN
2	B	242	LEU
2	B	247	VAL
2	B	252	ASN
2	B	335	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	51	ASN
1	A	54	GLN
1	A	78	ASN
1	A	90	ASN
1	A	146	ASN
1	A	157	HIS
1	A	171	ASN
1	A	181	GLN
1	A	209	ASN
1	A	244	ASN
1	A	256	ASN
1	A	261	ASN
1	A	266	ASN
1	A	300	GLN
1	A	392	ASN
2	B	73	HIS
2	B	88	HIS
2	B	101	HIS
2	B	128	ASN
2	B	162	ASN
2	B	252	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 57 ligands modelled in this entry, 1 is monoatomic - leaving 56 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	$\#\|Z\| > 2$
4	PO4	A	502	-	4,4,4	0.91	0	6,6,6	0.30	0
5	EDO	A	520	-	3,3,3	0.44	0	2,2,2	0.22	0
5	EDO	B	407	-	3,3,3	0.44	0	2,2,2	0.31	0
5	EDO	B	424	-	3,3,3	0.44	0	2,2,2	0.22	0
5	EDO	A	506	-	3,3,3	0.44	0	2,2,2	0.35	0
5	EDO	B	425	-	3,3,3	0.43	0	2,2,2	0.36	0
5	EDO	A	518	-	3,3,3	0.47	0	2,2,2	0.23	0
5	EDO	A	515	-	3,3,3	0.49	0	2,2,2	0.15	0
7	ATP	B	402	-	26,33,33	0.91	1 (3%)	31,52,52	1.26	3 (9%)
5	EDO	A	521	-	3,3,3	0.48	0	2,2,2	0.16	0
5	EDO	A	507	-	3,3,3	0.46	0	2,2,2	0.25	0
5	EDO	B	404	-	3,3,3	0.51	0	2,2,2	0.03	0
5	EDO	A	504	-	3,3,3	0.47	0	2,2,2	0.28	0
5	EDO	B	423	-	3,3,3	0.48	0	2,2,2	0.22	0
5	EDO	A	512	-	3,3,3	0.46	0	2,2,2	0.15	0
5	EDO	A	517	-	3,3,3	0.47	0	2,2,2	0.26	0
5	EDO	B	409	-	3,3,3	0.42	0	2,2,2	0.46	0
5	EDO	A	519	-	3,3,3	0.39	0	2,2,2	0.61	0
5	EDO	B	416	-	3,3,3	0.52	0	2,2,2	0.32	0
5	EDO	B	421	-	3,3,3	0.49	0	2,2,2	0.28	0
5	EDO	B	406	-	3,3,3	0.49	0	2,2,2	0.14	0
5	EDO	B	429	-	3,3,3	0.50	0	2,2,2	0.21	0
5	EDO	B	422	-	3,3,3	0.47	0	2,2,2	0.24	0
5	EDO	B	427	-	3,3,3	0.51	0	2,2,2	0.26	0
5	EDO	A	503	-	3,3,3	0.50	0	2,2,2	0.31	0
5	EDO	A	509	-	3,3,3	0.50	0	2,2,2	0.20	0
5	EDO	A	522	-	3,3,3	0.48	0	2,2,2	0.25	0
5	EDO	B	420	-	3,3,3	0.50	0	2,2,2	0.17	0
5	EDO	B	419	-	3,3,3	0.48	0	2,2,2	0.21	0
5	EDO	B	412	-	3,3,3	0.43	0	2,2,2	0.39	0
5	EDO	A	511	-	3,3,3	0.46	0	2,2,2	0.26	0
5	EDO	B	418	-	3,3,3	0.46	0	2,2,2	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	A	525	-	3,3,3	0.70	0	2,2,2	0.30	0
5	EDO	A	528	-	3,3,3	0.48	0	2,2,2	0.25	0
5	EDO	A	523	-	3,3,3	0.47	0	2,2,2	0.24	0
3	NAD	A	501	-	42,48,48	0.89	3 (7%)	50,73,73	1.30	6 (12%)
5	EDO	A	510	-	3,3,3	0.45	0	2,2,2	0.25	0
5	EDO	B	408	-	3,3,3	0.46	0	2,2,2	0.30	0
5	EDO	A	527	-	3,3,3	0.49	0	2,2,2	0.14	0
5	EDO	B	417	-	3,3,3	0.45	0	2,2,2	0.33	0
5	EDO	A	513	-	3,3,3	0.45	0	2,2,2	0.29	0
5	EDO	B	413	-	3,3,3	0.42	0	2,2,2	0.21	0
5	EDO	A	505	-	3,3,3	0.48	0	2,2,2	0.21	0
5	EDO	A	524	-	3,3,3	0.44	0	2,2,2	0.30	0
5	EDO	A	516	-	3,3,3	0.46	0	2,2,2	0.13	0
5	EDO	B	405	-	3,3,3	0.47	0	2,2,2	0.28	0
5	EDO	B	415	-	3,3,3	0.46	0	2,2,2	0.24	0
5	EDO	B	414	-	3,3,3	0.46	0	2,2,2	0.23	0
5	EDO	B	411	-	3,3,3	0.48	0	2,2,2	0.12	0
5	EDO	B	426	-	3,3,3	0.48	0	2,2,2	0.20	0
5	EDO	B	410	-	3,3,3	0.38	0	2,2,2	0.32	0
5	EDO	A	526	-	3,3,3	0.45	0	2,2,2	0.25	0
5	EDO	B	428	-	3,3,3	0.45	0	2,2,2	0.24	0
5	EDO	A	508	-	3,3,3	0.48	0	2,2,2	0.19	0
5	EDO	A	514	-	3,3,3	0.48	0	2,2,2	0.24	0
8	LAR	B	403	-	30,31,31	1.63	3 (10%)	32,43,43	2.41	10 (31%)

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	420	-	-	1/1/1/1	-
5	EDO	A	520	-	-	0/1/1/1	-
5	EDO	B	407	-	-	0/1/1/1	-
5	EDO	B	424	-	-	0/1/1/1	-
5	EDO	A	506	-	-	0/1/1/1	-
5	EDO	B	425	-	-	1/1/1/1	-
5	EDO	A	518	-	-	0/1/1/1	-
5	EDO	A	515	-	-	1/1/1/1	-
7	ATP	B	402	-	-	2/18/38/38	0/3/3/3
5	EDO	A	521	-	-	1/1/1/1	-
5	EDO	A	507	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	404	-	-	1/1/1/1	-
5	EDO	A	504	-	-	1/1/1/1	-
5	EDO	B	423	-	-	1/1/1/1	-
5	EDO	A	512	-	-	0/1/1/1	-
5	EDO	A	517	-	-	0/1/1/1	-
5	EDO	B	409	-	-	0/1/1/1	-
5	EDO	A	519	-	-	0/1/1/1	-
5	EDO	B	416	-	-	1/1/1/1	-
5	EDO	B	421	-	-	1/1/1/1	-
5	EDO	B	406	-	-	1/1/1/1	-
5	EDO	B	429	-	-	1/1/1/1	-
5	EDO	B	422	-	-	0/1/1/1	-
5	EDO	B	427	-	-	0/1/1/1	-
5	EDO	A	503	-	-	0/1/1/1	-
5	EDO	A	509	-	-	0/1/1/1	-
5	EDO	A	522	-	-	1/1/1/1	-
3	NAD	A	501	-	-	2/26/62/62	0/5/5/5
5	EDO	B	419	-	-	0/1/1/1	-
5	EDO	B	412	-	-	0/1/1/1	-
5	EDO	A	511	-	-	1/1/1/1	-
5	EDO	B	418	-	-	1/1/1/1	-
5	EDO	A	525	-	-	0/1/1/1	-
5	EDO	A	528	-	-	1/1/1/1	-
5	EDO	A	523	-	-	0/1/1/1	-
5	EDO	A	510	-	-	0/1/1/1	-
5	EDO	B	408	-	-	0/1/1/1	-
5	EDO	A	527	-	-	0/1/1/1	-
5	EDO	B	417	-	-	0/1/1/1	-
5	EDO	A	513	-	-	0/1/1/1	-
5	EDO	B	413	-	-	0/1/1/1	-
5	EDO	A	505	-	-	0/1/1/1	-
5	EDO	A	524	-	-	0/1/1/1	-
5	EDO	A	516	-	-	1/1/1/1	-
5	EDO	B	405	-	-	0/1/1/1	-
5	EDO	B	415	-	-	0/1/1/1	-
5	EDO	B	414	-	-	0/1/1/1	-
5	EDO	B	411	-	-	1/1/1/1	-
5	EDO	B	426	-	-	1/1/1/1	-
5	EDO	B	410	-	-	1/1/1/1	-
5	EDO	A	526	-	-	1/1/1/1	-
5	EDO	B	428	-	-	1/1/1/1	-
5	EDO	A	508	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	514	-	-	1/1/1/1	-
8	LAR	B	403	-	-	3/23/51/51	0/2/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	403	LAR	O2-C1	5.73	1.46	1.34
8	B	403	LAR	C20-S1	-5.06	1.66	1.77
7	B	402	ATP	C5-C4	2.38	1.47	1.40
3	A	501	NAD	C5A-C4A	2.30	1.47	1.40
3	A	501	NAD	O4D-C1D	2.14	1.44	1.41
3	A	501	NAD	O4B-C1B	2.13	1.44	1.41
8	B	403	LAR	O4-C17	2.01	1.44	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	403	LAR	C4-C5-C6	-8.33	94.60	112.59
8	B	403	LAR	O2-C1-C2	4.70	122.30	111.27
8	B	403	LAR	C8-C7-C6	-4.39	100.25	125.51
8	B	403	LAR	C19-S1-C20	4.01	94.15	92.00
3	A	501	NAD	N3A-C2A-N1A	-3.90	122.58	128.68
7	B	402	ATP	N3-C2-N1	-3.43	123.32	128.68
3	A	501	NAD	C3N-C7N-N7N	3.16	121.55	117.75
8	B	403	LAR	O1-C1-C2	-3.02	118.63	126.23
3	A	501	NAD	C5D-C4D-C3D	-2.78	104.76	115.18
8	B	403	LAR	O2-C1-O1	-2.63	119.07	123.35
8	B	403	LAR	C5-C6-C7	2.55	138.34	125.90
8	B	403	LAR	O3-C17-C18	2.36	107.28	104.25
7	B	402	ATP	C2-N1-C6	2.32	122.73	118.75
8	B	403	LAR	O5-C20-N1	-2.26	124.34	126.81
7	B	402	ATP	PA-O3A-PB	-2.21	125.23	132.83
3	A	501	NAD	C4A-C5A-N7A	-2.20	107.10	109.40
3	A	501	NAD	C2A-N1A-C6A	2.12	122.37	118.75
3	A	501	NAD	C1B-N9A-C4A	-2.11	122.94	126.64
8	B	403	LAR	O2-C15-C16	2.05	112.71	107.59

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	420	EDO	O1-C1-C2-O2
5	B	429	EDO	O1-C1-C2-O2
5	B	425	EDO	O1-C1-C2-O2
5	B	404	EDO	O1-C1-C2-O2
5	A	504	EDO	O1-C1-C2-O2
5	B	421	EDO	O1-C1-C2-O2
5	B	411	EDO	O1-C1-C2-O2
5	B	426	EDO	O1-C1-C2-O2
5	B	423	EDO	O1-C1-C2-O2
5	B	416	EDO	O1-C1-C2-O2
5	A	528	EDO	O1-C1-C2-O2
5	A	514	EDO	O1-C1-C2-O2
5	A	515	EDO	O1-C1-C2-O2
5	A	522	EDO	O1-C1-C2-O2
5	B	418	EDO	O1-C1-C2-O2
5	A	526	EDO	O1-C1-C2-O2
5	B	428	EDO	O1-C1-C2-O2
3	A	501	NAD	PN-O3-PA-O2A
5	B	406	EDO	O1-C1-C2-O2
8	B	403	LAR	O2-C1-C2-C3
7	B	402	ATP	PG-O3B-PB-O1B
7	B	402	ATP	PG-O3B-PB-O2B
5	A	521	EDO	O1-C1-C2-O2
5	A	516	EDO	O1-C1-C2-O2
5	B	410	EDO	O1-C1-C2-O2
3	A	501	NAD	PN-O3-PA-O1A
8	B	403	LAR	C9-C10-C11-C12
5	A	511	EDO	O1-C1-C2-O2
8	B	403	LAR	O1-C1-C2-C3

There are no ring outliers.

12 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	PO4	1	0
5	A	507	EDO	1	0
5	B	404	EDO	1	0
5	B	409	EDO	3	0
5	A	519	EDO	2	0
5	B	412	EDO	1	0
5	A	525	EDO	1	0
5	B	408	EDO	3	0
5	B	413	EDO	1	0

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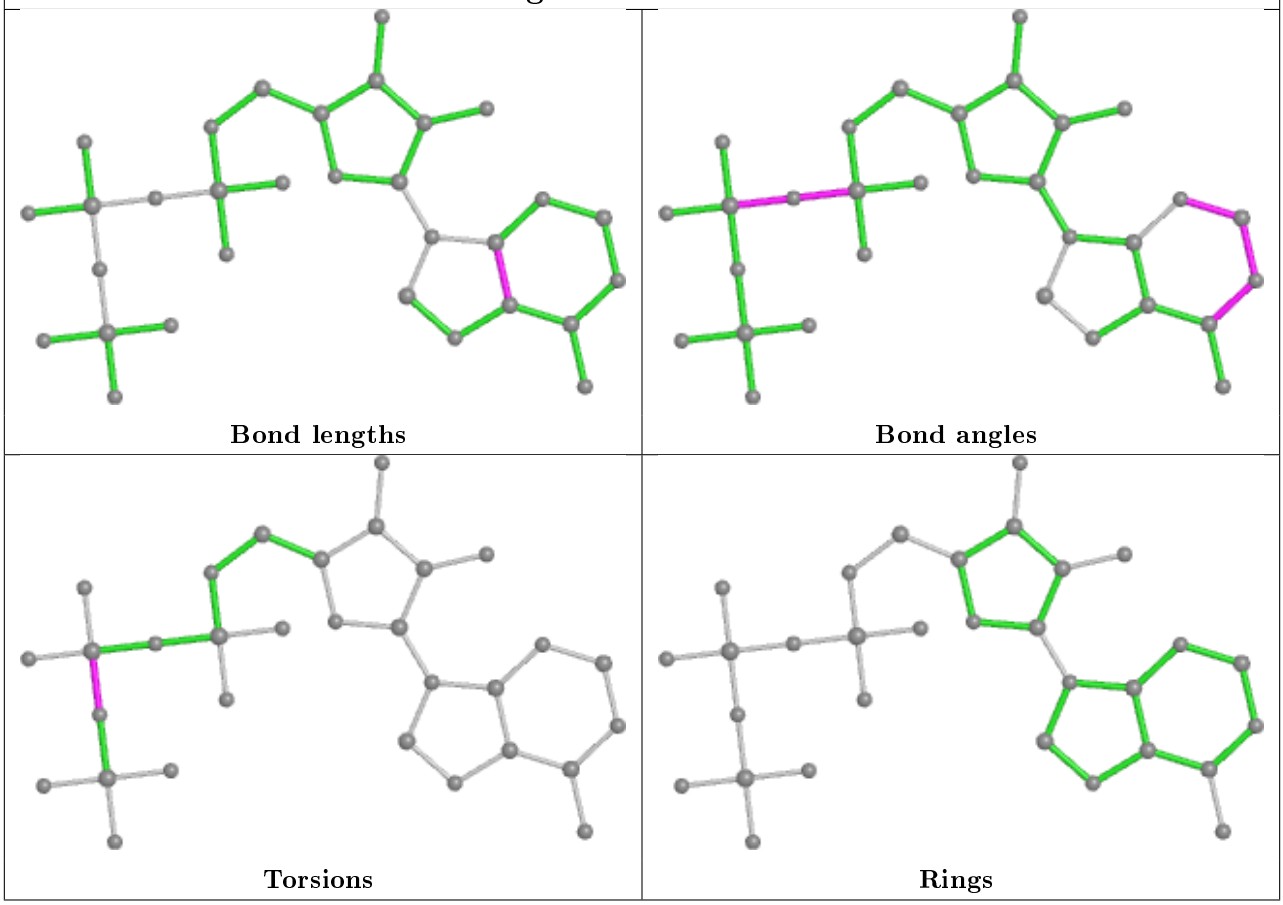
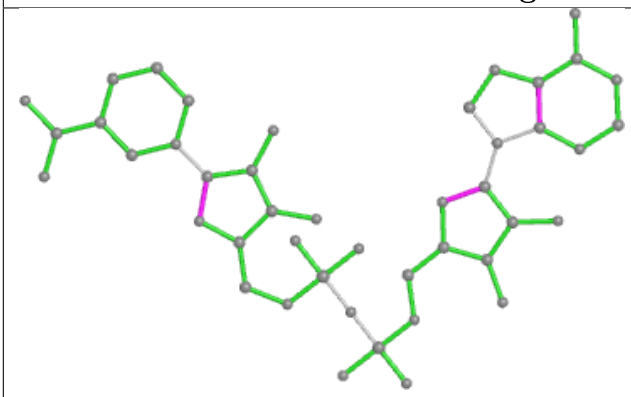
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	411	EDO	1	0
5	B	410	EDO	1	0
8	B	403	LAR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

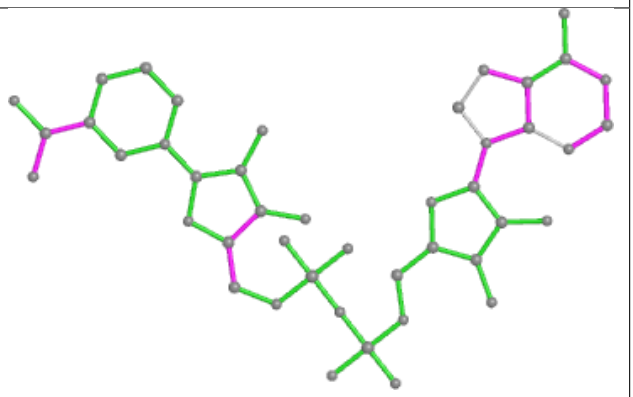
Ligand ATP B 402



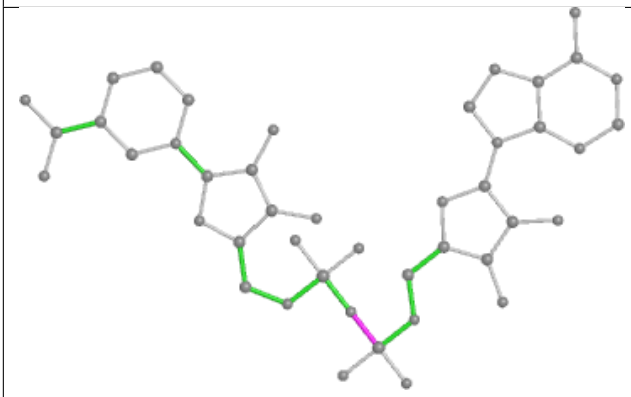
Ligand NAD A 501



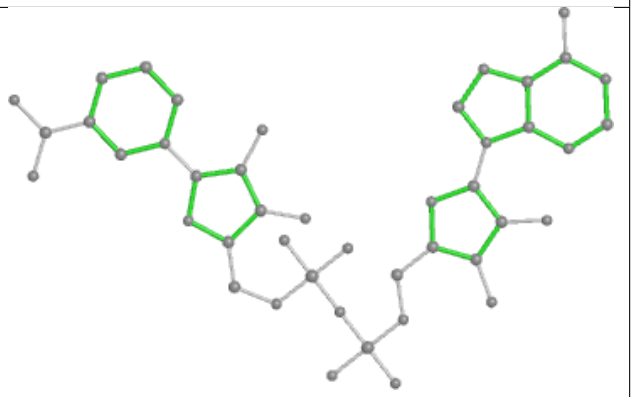
Bond lengths



Bond angles

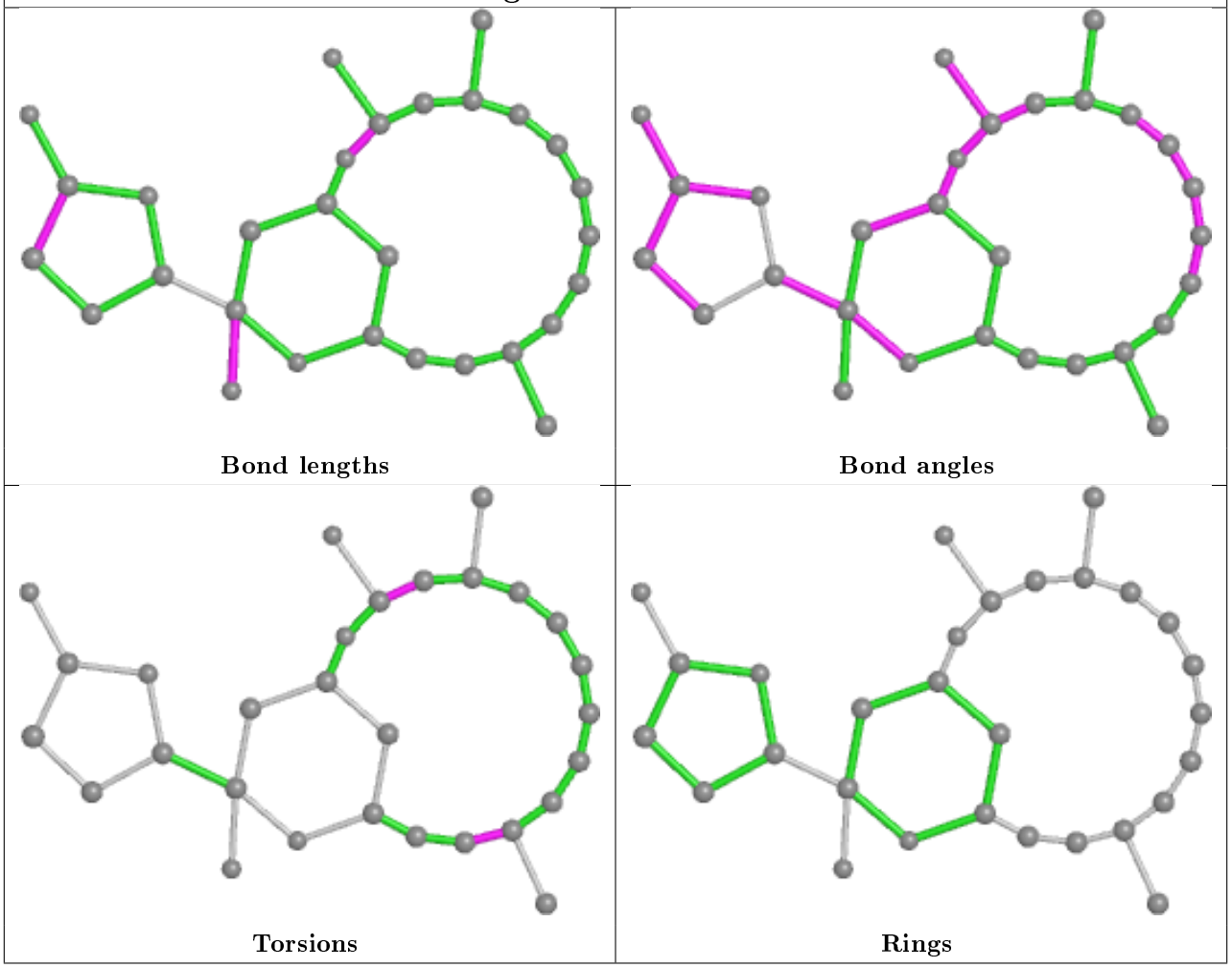


Torsions



Rings

Ligand LAR B 403



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, 95^{th} 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%)	0.74	39 (9%)	8	12	23, 33, 63, 98	0
2	B	358/375 (95%)	0.73	33 (9%)	9	13	15, 23, 59, 119	0
All	All	771/793 (97%)	0.73	72 (9%)	8	13	15, 29, 61, 119	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	63	GLY	12.9
2	B	60	SER	12.8
1	A	376	ALA	9.5
2	B	57	GLU	9.4
2	B	52	SER	9.4
2	B	51	ASP	9.1
2	B	56	ASP	8.2
2	B	62	ARG	8.0
2	B	53	TYR	8.0
2	B	59	GLN	7.1
2	B	64	ILE	7.0
1	A	375	TYR	6.5
1	A	372	ILE	6.2
2	B	54	VAL	5.8
2	B	61	LYS	5.7
2	B	50	LYS	5.0
2	B	58	ALA	4.8
1	A	373	PRO	4.7
2	B	66	THR	4.6
1	A	237	PRO	4.5
2	B	65	LEU	4.5
2	B	37	ARG	4.5
1	A	238	ASN	4.3
1	A	264	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	232	SER	4.0
1	A	44	LYS	3.8
2	B	55	GLY	3.7
1	A	371	ALA	3.6
1	A	173	ASN	3.6
1	A	117	GLU	3.5
2	B	231	ALA	3.5
1	A	377	GLY	3.4
1	A	222	LEU	3.2
1	A	110	ASN	3.2
1	A	128	ASP	3.1
1	A	270	GLU	3.1
1	A	233	ASN	3.1
1	A	266	ASN	3.0
1	A	330	VAL	2.9
1	A	374	GLY	2.9
1	A	179	ILE	2.9
1	A	307	THR	2.8
2	B	143	TYR	2.7
2	B	119	MET	2.6
2	B	67	LEU	2.6
1	A	230	ASP	2.5
1	A	56	ARG	2.5
2	B	169	TYR	2.5
1	A	265	ASN	2.5
1	A	235	LEU	2.5
1	A	3	ILE	2.5
1	A	127	GLN	2.4
2	B	372	ARG	2.4
2	B	160	THR	2.4
2	B	350	SER	2.4
1	A	146	ASN	2.3
2	B	328	LYS	2.3
1	A	355	ILE	2.3
2	B	228	ALA	2.3
1	A	269	PRO	2.3
2	B	235	SER	2.2
1	A	263	PRO	2.1
1	A	406	ILE	2.1
1	A	81	SER	2.1
1	A	248	ARG	2.1
1	A	14	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	232	SER	2.1
1	A	172	SER	2.0
2	B	177	ARG	2.0
2	B	178	LEU	2.0
1	A	18	GLN	2.0
2	B	5	THR	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	406	4/4	0.62	0.37	45,45,45,45	0
5	EDO	B	424	4/4	0.65	0.32	37,37,37,37	0
5	EDO	A	519	4/4	0.67	0.24	46,46,47,47	0
5	EDO	A	507	4/4	0.67	0.28	38,38,38,38	0
5	EDO	A	525	4/4	0.70	0.31	40,41,41,41	0
5	EDO	A	528	4/4	0.70	0.28	35,35,35,36	0
5	EDO	A	518	4/4	0.72	0.28	37,38,38,38	0
5	EDO	B	413	4/4	0.72	0.30	32,32,32,32	0
5	EDO	A	526	4/4	0.72	0.38	43,43,44,44	0
5	EDO	A	506	4/4	0.73	0.29	43,43,43,44	0
5	EDO	B	423	4/4	0.74	0.25	45,45,45,46	0
5	EDO	A	522	4/4	0.74	0.30	34,34,34,34	0
5	EDO	A	514	4/4	0.74	0.39	36,36,36,36	0
5	EDO	B	428	4/4	0.75	0.22	38,38,38,38	0
5	EDO	B	420	4/4	0.75	0.36	40,40,40,40	0
5	EDO	B	426	4/4	0.76	0.51	43,43,43,43	0
5	EDO	A	521	4/4	0.77	0.41	47,47,47,47	0

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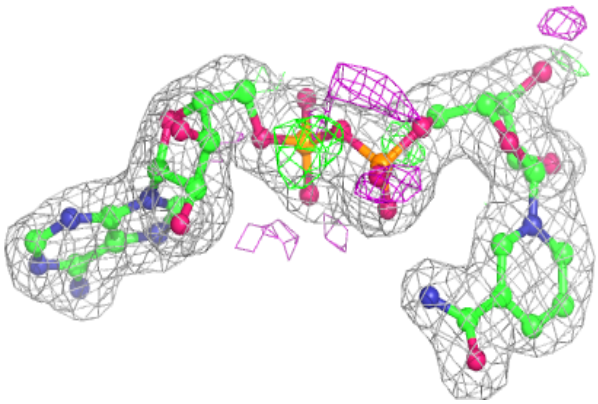
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	B	411	4/4	0.77	0.20	42,42,42,42	0
5	EDO	A	527	4/4	0.77	0.30	46,46,46,46	0
5	EDO	B	425	4/4	0.78	0.34	31,31,32,32	0
5	EDO	B	421	4/4	0.78	0.19	38,38,38,39	0
5	EDO	B	418	4/4	0.78	0.27	39,39,39,39	0
5	EDO	B	427	4/4	0.79	0.22	46,46,46,46	0
5	EDO	B	408	4/4	0.80	0.20	22,22,22,23	0
5	EDO	A	508	4/4	0.80	0.21	30,30,30,30	0
5	EDO	A	512	4/4	0.80	0.29	40,40,40,40	0
5	EDO	A	513	4/4	0.81	0.17	38,38,38,38	0
5	EDO	A	511	4/4	0.81	0.24	42,42,42,42	0
5	EDO	B	416	4/4	0.83	0.33	37,38,38,38	0
5	EDO	B	429	4/4	0.84	0.20	39,39,39,39	0
5	EDO	A	523	4/4	0.84	0.24	36,36,36,36	0
5	EDO	A	515	4/4	0.84	0.31	48,48,48,48	0
5	EDO	B	412	4/4	0.84	0.21	48,48,48,48	0
5	EDO	A	516	4/4	0.86	0.20	37,37,37,37	0
5	EDO	B	415	4/4	0.86	0.24	40,40,40,40	0
5	EDO	A	520	4/4	0.86	0.21	37,37,37,37	0
5	EDO	A	524	4/4	0.86	0.44	41,41,41,41	0
5	EDO	B	405	4/4	0.87	0.27	43,43,43,43	0
5	EDO	A	503	4/4	0.87	0.19	27,27,27,27	0
5	EDO	B	404	4/4	0.88	0.22	33,33,34,34	0
5	EDO	B	419	4/4	0.88	0.15	31,32,32,32	0
5	EDO	A	504	4/4	0.89	0.15	31,31,31,31	0
5	EDO	A	509	4/4	0.89	0.14	27,27,27,27	0
5	EDO	A	517	4/4	0.90	0.17	34,34,34,34	0
5	EDO	A	505	4/4	0.90	0.15	30,30,30,30	0
5	EDO	B	409	4/4	0.90	0.19	34,35,35,35	0
5	EDO	B	410	4/4	0.92	0.36	32,32,32,32	0
3	NAD	A	501	44/44	0.93	0.13	29,34,38,38	0
5	EDO	B	414	4/4	0.93	0.14	27,27,27,27	0
5	EDO	B	407	4/4	0.93	0.11	27,27,27,27	0
8	LAR	B	403	29/29	0.93	0.12	23,25,30,30	0
4	PO4	A	502	5/5	0.94	0.21	42,42,42,42	0
5	EDO	A	510	4/4	0.94	0.12	43,43,43,43	0
5	EDO	B	417	4/4	0.95	0.15	26,26,26,26	0
5	EDO	B	422	4/4	0.97	0.22	23,24,24,24	0
7	ATP	B	402	31/31	0.98	0.12	17,17,17,17	0
6	CA	B	401	1/1	1.00	0.09	17,17,17,17	0

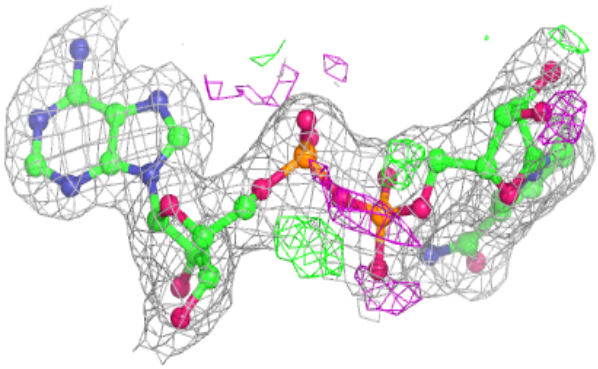
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

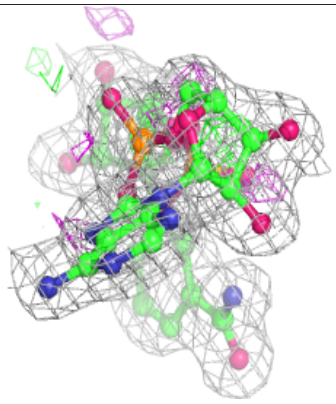
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

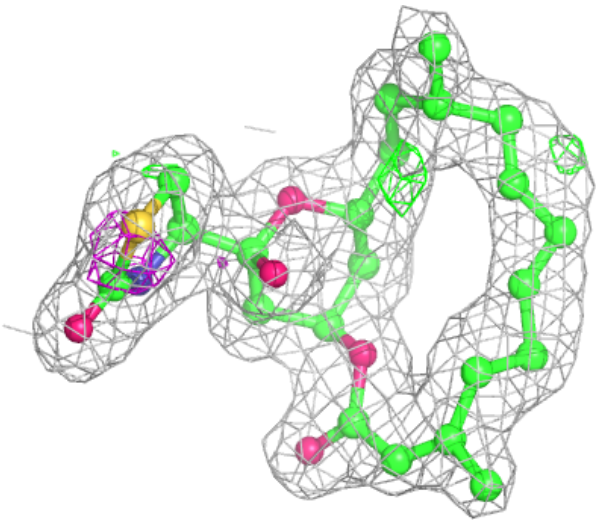


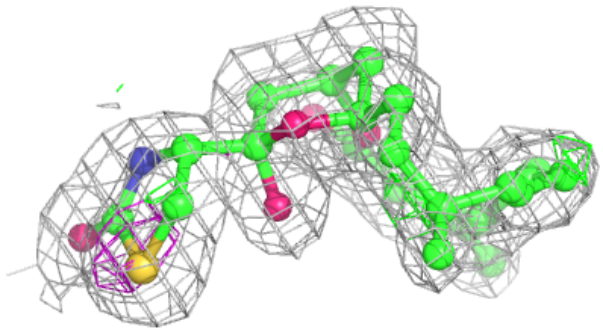


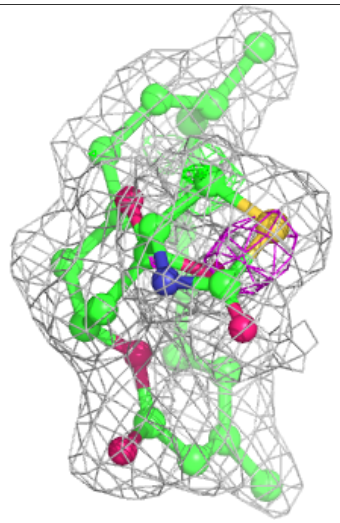


Electron density around LAR B 403:

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

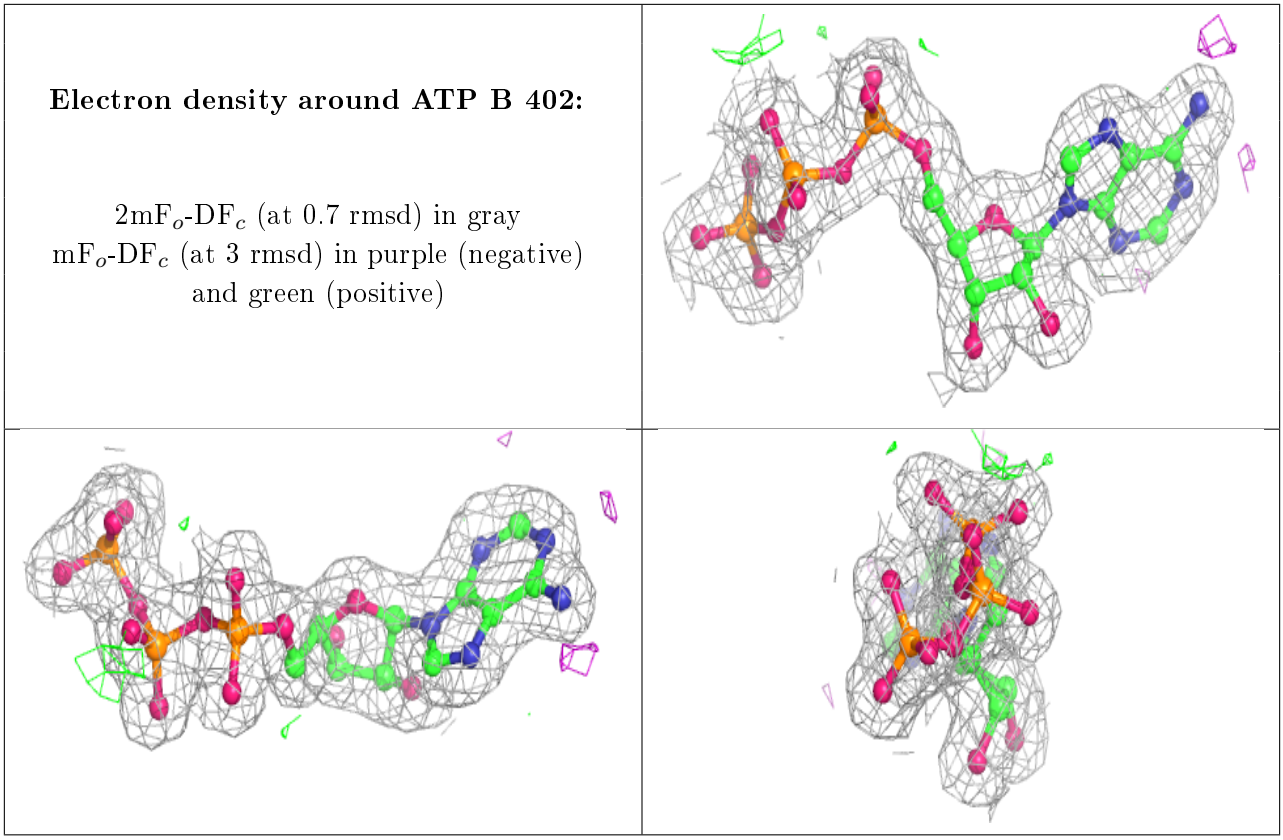






Electron density around ATP B 402:

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



6.5 Other polymers (i)

There are no such residues in this entry.