



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:18 am GMT

PDB ID : 4H0V
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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

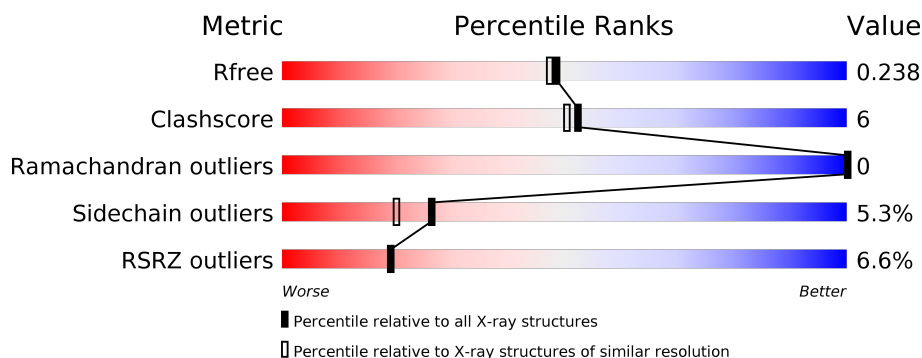
1 Overall quality at a glance

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}	100719	8396 (2.04-2.00)
Clashscore	112137	9678 (2.04-2.00)
Ramachandran outliers	110173	9566 (2.04-2.00)
Sidechain outliers	110143	9565 (2.04-2.00)
RSRZ outliers	101464	8490 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>7%</div> <div>88%</div> <div>10% ..</div> </div>
2	B	375	<div> <div>6%</div> <div>77%</div> <div>16% .. 5%</div> </div>

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	507	-	-	-	X
5	EDO	A	511	-	-	-	X
5	EDO	A	513	-	-	-	X
5	EDO	A	515	-	-	-	X
5	EDO	A	516	-	-	-	X
5	EDO	A	517	-	-	-	X
5	EDO	A	519	-	-	-	X
5	EDO	B	404	-	-	-	X
5	EDO	B	405	-	-	-	X
5	EDO	B	408	-	-	-	X
5	EDO	B	409	-	-	-	X
5	EDO	B	410	-	-	-	X
5	EDO	B	414	-	-	-	X
5	EDO	B	416	-	-	-	X
5	EDO	B	419	-	-	-	X
5	EDO	B	420	-	-	-	X
5	EDO	B	421	-	-	-	X
5	EDO	B	422	-	-	-	X

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			

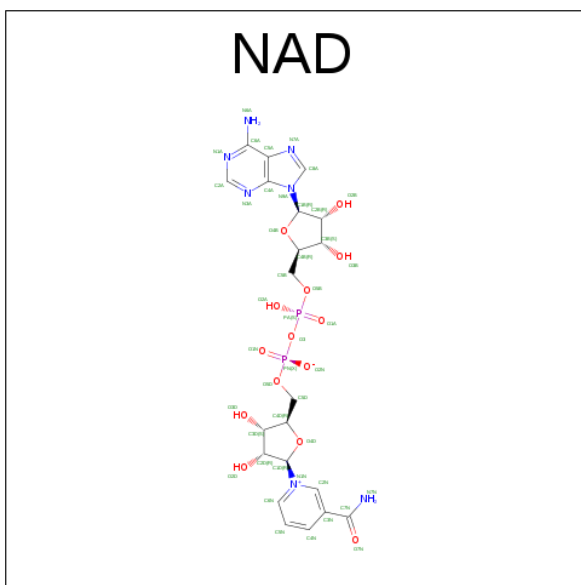
There are 6 discrepancies between the modelled and reference sequences:

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 (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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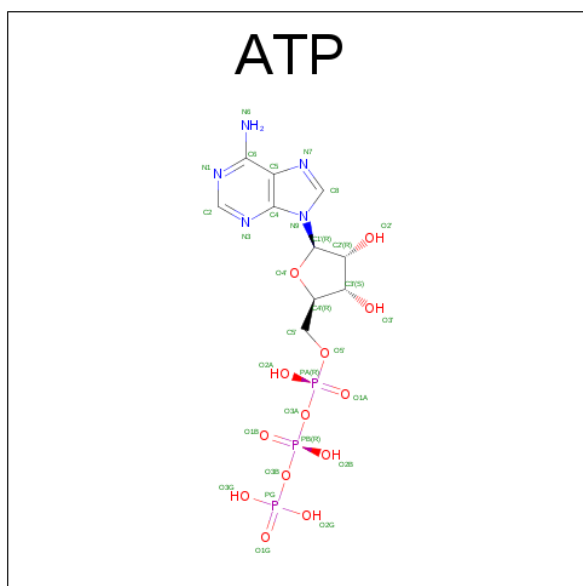
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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

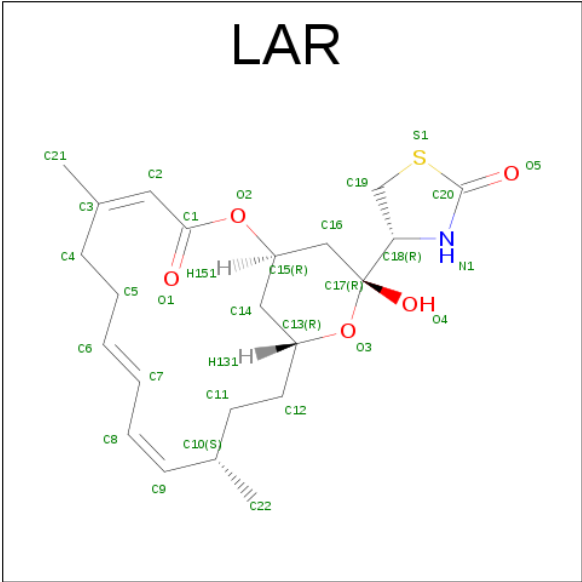
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: 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 (three-letter code: LAR) (formula: C₂₂H₃₁NO₅S).



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

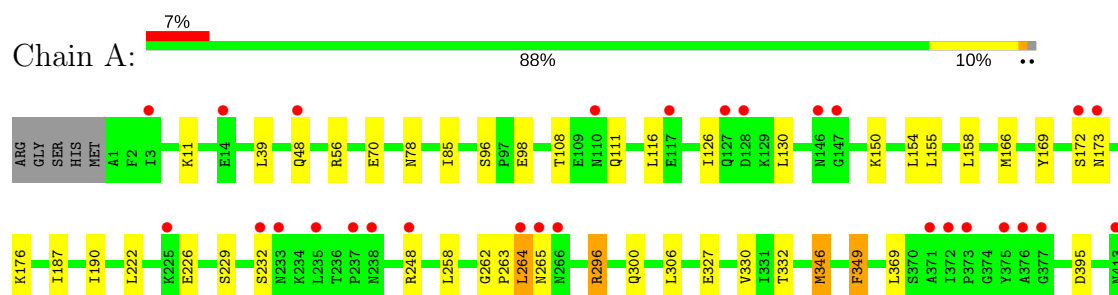
- Molecule 9 is water.

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

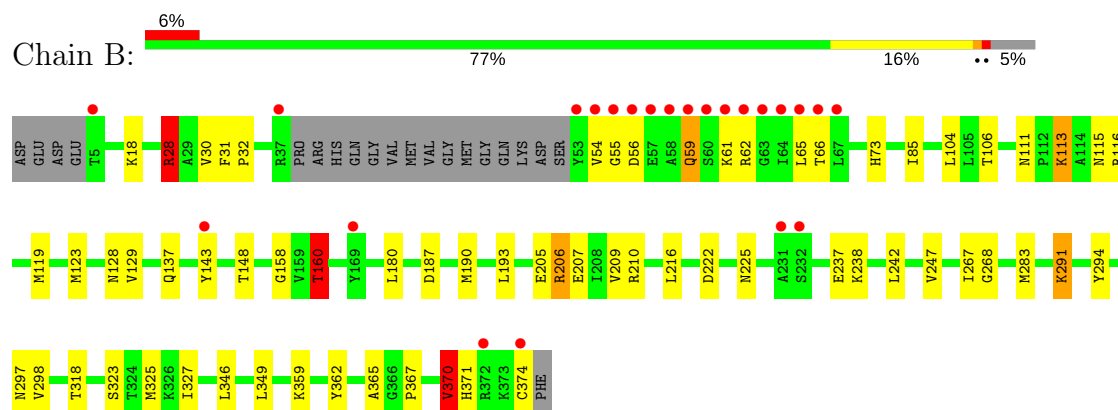
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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

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 (5.33%)	DCC
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 , 49.1	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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/3430	0.73	4/4633 (0.1%)
2	B	0.41	1/2835 (0.0%)	0.66	5/3843 (0.1%)
All	All	0.37	1/6265 (0.0%)	0.70	9/8476 (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	10.75	1.64	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ARG	NE-CZ-NH2	-15.16	112.72	120.30
1	A	296	ARG	NE-CZ-NH1	14.69	127.64	120.30
1	A	296	ARG	CG-CD-NE	-8.18	94.62	111.80
1	A	296	ARG	CD-NE-CZ	7.52	134.12	123.60
2	B	291	LYS	CD-CE-NZ	5.94	125.35	111.70
2	B	28	ARG	NE-CZ-NH1	5.66	123.13	120.30
2	B	206	ARG	NE-CZ-NH1	5.58	123.09	120.30
2	B	370	VAL	CB-CA-C	-5.19	101.55	111.40
2	B	206	ARG	NE-CZ-NH2	-5.17	117.72	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3361	0	3345	26	0
2	B	2776	0	2751	52	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	14	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	80	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 6.

All (80) 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
1:A:85:ILE:HD13	1:A:166:MET:HE3	1.41	1.03
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	0.84
2:B:160:THR:HG23	2:B:180:LEU:O	1.76	0.84
2:B:190:MET:CG	2:B:209:VAL:HG11	2.12	0.80
2:B:111:ASN:HD21	2:B:119:MET:HE3	1.45	0.79
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
1:A:56:ARG:NH1	1:A:70:GLU:CD	2.42	0.73
8:B:403:LAR:H131	8:B:403:LAR:H91	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
2:B:283:MET:CE	5:B:408:EDO:O2	2.41	0.68
2:B:298:VAL:CG1	5:B:407:EDO:H21	2.25	0.67
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
1:A:264:LEU:HD12	1:A:264:LEU:C	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:THR:HG23	5:B:409:EDO:H21	1.81	0.61
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:283:MET:HE1	5:B:408:EDO:O2	2.03	0.59
2:B:283:MET:HE3	5:B:408:EDO:O2	2.01	0.59
2:B:160:THR:CB	2:B:160:THR:HG1	2.08	0.58
2:B:323:SER:HA	5:B:409:EDO:H22	1.87	0.57
2:B:207:GLU:CD	2:B:210:ARG:HH12	2.09	0.56
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
1:A:56:ARG:NH1	1:A:70:GLU:OE2	2.25	0.55
2:B:205:GLU:O	2:B:209:VAL:HG12	2.07	0.55
2:B:190:MET:HG3	2:B:209:VAL:HG11	1.87	0.53
2:B:143:TYR:OH	2:B:349:LEU:HD11	2.09	0.53
2:B:207:GLU:CD	2:B:210:ARG:NH1	2.64	0.51
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
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:CG	2:B:28:ARG:HH11	2.25	0.49
2:B:115:ASN:HB3	2:B:119:MET:HE3	1.96	0.48
2:B:104:LEU:HD23	2:B:104:LEU:C	2.34	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
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: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: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
2:B:123:MET:HE3	2:B:129:VAL:HG11	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:222:ASP:CG	2:B:225:ASN:HB2	2.40	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:H223	8:B:403:LAR:H81	1.57	0.42
2:B:128:ASN:ND2	2:B:359:LYS:HE3	2.34	0.42
1:A:130:LEU:HA	1:A:130:LEU:HD12	1.95	0.42
1:A:126:ILE:HD11	1:A:190:ILE:HG21	2.01	0.42
2:B:325:MET:HG3	2:B:327:ILE:HD13	2.01	0.42
1:A:96:SER:HB3	1:A:98:GLU:OE2	2.20	0.41
2:B:18:LYS:HD3	2:B:18:LYS:N	2.36	0.41
1:A:108:THR:HG22	1:A:111:GLN:CD	2.41	0.40
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%)	357 (95%)	19 (5%)	28	21
2	B	301/318 (95%)	284 (94%)	17 (6%)	25	18
All	All	677/698 (97%)	641 (95%)	36 (5%)	26	20

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	39	LEU
1	A	48	GLN
1	A	78	ASN
1	A	116	LEU
1	A	150	LYS
1	A	154	LEU
1	A	155	LEU
1	A	158	LEU
1	A	222	LEU
1	A	226	GLU
1	A	248	ARG
1	A	258	LEU
1	A	264	LEU
1	A	330	VAL
1	A	332	THR
1	A	346	MET
1	A	349	PHE
1	A	369	LEU
2	B	28	ARG
2	B	30	VAL
2	B	56	ASP
2	B	59	GLN
2	B	61	LYS
2	B	65	LEU
2	B	66	THR
2	B	113	LYS

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Mol	Chain	Res	Type
2	B	116	ARG
2	B	160	THR
2	B	193	LEU
2	B	242	LEU
2	B	247	VAL
2	B	291	LYS
2	B	297	ASN
2	B	346	LEU
2	B	370	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	110	ASN
1	A	111	GLN
1	A	127	GLN
2	B	87	HIS
2	B	111	ASN
2	B	128	ASN
2	B	263	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	NAD	A	501	-	41,48,48	0.90	2 (4%)	43,73,73	1.66	7 (16%)
4	PO4	A	502	-	4,4,4	0.81	0	6,6,6	0.37	0
5	EDO	A	503	-	3,3,3	0.57	0	2,2,2	0.50	0
5	EDO	A	504	-	3,3,3	0.43	0	2,2,2	0.39	0
5	EDO	A	505	-	3,3,3	0.48	0	2,2,2	0.15	0
5	EDO	A	506	-	3,3,3	0.45	0	2,2,2	0.38	0
5	EDO	A	507	-	3,3,3	0.47	0	2,2,2	0.21	0
5	EDO	A	508	-	3,3,3	0.49	0	2,2,2	0.14	0
5	EDO	A	509	-	3,3,3	0.49	0	2,2,2	0.21	0
5	EDO	A	510	-	3,3,3	0.45	0	2,2,2	0.28	0
5	EDO	A	511	-	3,3,3	0.48	0	2,2,2	0.50	0
5	EDO	A	512	-	3,3,3	0.49	0	2,2,2	0.55	0
5	EDO	A	513	-	3,3,3	0.48	0	2,2,2	0.40	0
5	EDO	A	514	-	3,3,3	0.51	0	2,2,2	0.09	0
5	EDO	A	515	-	3,3,3	0.47	0	2,2,2	0.30	0
5	EDO	A	516	-	3,3,3	0.53	0	2,2,2	0.39	0
5	EDO	A	517	-	3,3,3	0.43	0	2,2,2	0.21	0
5	EDO	A	518	-	3,3,3	0.44	0	2,2,2	0.29	0
5	EDO	A	519	-	3,3,3	0.48	0	2,2,2	0.29	0
5	EDO	A	520	-	3,3,3	0.57	0	2,2,2	0.32	0
5	EDO	A	521	-	3,3,3	0.50	0	2,2,2	0.28	0
7	ATP	B	402	-	27,33,33	0.95	1 (3%)	25,52,52	1.67	2 (8%)
8	LAR	B	403	-	30,31,31	1.67	3 (10%)	36,43,43	1.70	8 (22%)
5	EDO	B	404	-	3,3,3	0.62	0	2,2,2	0.14	0
5	EDO	B	405	-	3,3,3	0.49	0	2,2,2	0.18	0
5	EDO	B	406	-	3,3,3	0.43	0	2,2,2	0.40	0
5	EDO	B	407	-	3,3,3	0.50	0	2,2,2	0.47	0
5	EDO	B	408	-	3,3,3	0.50	0	2,2,2	0.18	0
5	EDO	B	409	-	3,3,3	0.42	0	2,2,2	0.37	0
5	EDO	B	410	-	3,3,3	0.53	0	2,2,2	0.22	0
5	EDO	B	411	-	3,3,3	0.42	0	2,2,2	0.37	0
5	EDO	B	412	-	3,3,3	0.45	0	2,2,2	0.32	0
5	EDO	B	413	-	3,3,3	0.48	0	2,2,2	0.28	0
5	EDO	B	414	-	3,3,3	0.53	0	2,2,2	0.37	0
5	EDO	B	415	-	3,3,3	0.45	0	2,2,2	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	416	-	3,3,3	0.46	0	2,2,2	0.25	0
5	EDO	B	417	-	3,3,3	0.48	0	2,2,2	0.27	0
5	EDO	B	418	-	3,3,3	0.48	0	2,2,2	0.17	0
5	EDO	B	419	-	3,3,3	0.48	0	2,2,2	0.22	0
5	EDO	B	420	-	3,3,3	0.44	0	2,2,2	0.25	0
5	EDO	B	421	-	3,3,3	0.42	0	2,2,2	0.70	0
5	EDO	B	422	-	3,3,3	0.44	0	2,2,2	0.26	0
5	EDO	B	423	-	3,3,3	0.48	0	2,2,2	0.23	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
3	NAD	A	501	-	-	0/22/62/62	0/5/5/5
4	PO4	A	502	-	-	0/0/0/0	0/0/0/0
5	EDO	A	503	-	-	0/1/1/1	0/0/0/0
5	EDO	A	504	-	-	0/1/1/1	0/0/0/0
5	EDO	A	505	-	-	0/1/1/1	0/0/0/0
5	EDO	A	506	-	-	0/1/1/1	0/0/0/0
5	EDO	A	507	-	-	0/1/1/1	0/0/0/0
5	EDO	A	508	-	-	0/1/1/1	0/0/0/0
5	EDO	A	509	-	-	0/1/1/1	0/0/0/0
5	EDO	A	510	-	-	0/1/1/1	0/0/0/0
5	EDO	A	511	-	-	0/1/1/1	0/0/0/0
5	EDO	A	512	-	-	0/1/1/1	0/0/0/0
5	EDO	A	513	-	-	0/1/1/1	0/0/0/0
5	EDO	A	514	-	-	0/1/1/1	0/0/0/0
5	EDO	A	515	-	-	0/1/1/1	0/0/0/0
5	EDO	A	516	-	-	0/1/1/1	0/0/0/0
5	EDO	A	517	-	-	0/1/1/1	0/0/0/0
5	EDO	A	518	-	-	0/1/1/1	0/0/0/0
5	EDO	A	519	-	-	0/1/1/1	0/0/0/0
5	EDO	A	520	-	-	0/1/1/1	0/0/0/0
5	EDO	A	521	-	-	0/1/1/1	0/0/0/0
7	ATP	B	402	-	-	0/18/38/38	0/3/3/3
8	LAR	B	403	-	-	0/23/51/51	0/1/3/3
5	EDO	B	404	-	-	0/1/1/1	0/0/0/0
5	EDO	B	405	-	-	0/1/1/1	0/0/0/0
5	EDO	B	406	-	-	0/1/1/1	0/0/0/0
5	EDO	B	407	-	-	0/1/1/1	0/0/0/0
5	EDO	B	408	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	409	-	-	0/1/1/1	0/0/0/0
5	EDO	B	410	-	-	0/1/1/1	0/0/0/0
5	EDO	B	411	-	-	0/1/1/1	0/0/0/0
5	EDO	B	412	-	-	0/1/1/1	0/0/0/0
5	EDO	B	413	-	-	0/1/1/1	0/0/0/0
5	EDO	B	414	-	-	0/1/1/1	0/0/0/0
5	EDO	B	415	-	-	0/1/1/1	0/0/0/0
5	EDO	B	416	-	-	0/1/1/1	0/0/0/0
5	EDO	B	417	-	-	0/1/1/1	0/0/0/0
5	EDO	B	418	-	-	0/1/1/1	0/0/0/0
5	EDO	B	419	-	-	0/1/1/1	0/0/0/0
5	EDO	B	420	-	-	0/1/1/1	0/0/0/0
5	EDO	B	421	-	-	0/1/1/1	0/0/0/0
5	EDO	B	422	-	-	0/1/1/1	0/0/0/0
5	EDO	B	423	-	-	0/1/1/1	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	403	LAR	C20-S1	-4.99	1.66	1.78
8	B	403	LAR	C20-N1	-2.71	1.32	1.36
3	A	501	NAD	O4B-C1B	2.03	1.44	1.41
7	B	402	ATP	C5-C4	2.84	1.46	1.40
3	A	501	NAD	C5A-C4A	2.90	1.47	1.40
8	B	403	LAR	O2-C1	5.94	1.47	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NAD	N3A-C2A-N1A	-7.33	122.48	128.86
7	B	402	ATP	N3-C2-N1	-6.57	123.13	128.86
8	B	403	LAR	C22-C10-C9	-3.33	103.27	110.83
8	B	403	LAR	O1-C1-C2	-2.99	118.43	126.20
3	A	501	NAD	C1B-N9A-C4A	-2.51	122.29	126.64
3	A	501	NAD	C5D-C4D-C3D	-2.49	105.80	115.29
8	B	403	LAR	O2-C1-O1	-2.45	119.02	123.32
3	A	501	NAD	C4A-C5A-N7A	-2.33	107.16	109.41
3	A	501	NAD	O7N-C7N-N7N	-2.29	119.32	122.58
7	B	402	ATP	C1'-N9-C4	-2.11	123.00	126.64
8	B	403	LAR	C18-N1-C20	2.04	116.29	113.28
3	A	501	NAD	C2A-N1A-C6A	2.09	122.43	118.77
8	B	403	LAR	S1-C20-N1	2.26	113.14	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	403	LAR	C8-C7-C6	2.61	135.95	124.62
8	B	403	LAR	C19-S1-C20	3.15	93.68	92.00
3	A	501	NAD	C3N-C7N-N7N	4.10	122.45	117.77
8	B	403	LAR	O2-C1-C2	4.61	122.55	111.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	EDO	2	0
5	A	506	EDO	1	0
5	A	507	EDO	1	0
8	B	403	LAR	2	0
5	B	404	EDO	2	0
5	B	407	EDO	2	0
5	B	408	EDO	3	0
5	B	409	EDO	2	0
5	B	411	EDO	3	0
5	B	418	EDO	1	0
5	B	420	EDO	1	0
5	B	421	EDO	1	0

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%)	0.39	28 (6%) 18 18	22, 34, 59, 95	0
2	B	355/375 (94%)	0.38	23 (6%) 20 20	17, 25, 57, 121	0
All	All	768/793 (96%)	0.39	51 (6%) 19 19	17, 29, 59, 121	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	60	SER	9.9
1	A	376	ALA	9.3
2	B	61	LYS	8.6
2	B	63	GLY	8.4
2	B	53	TYR	8.0
2	B	57	GLU	7.7
2	B	64	ILE	6.8
2	B	56	ASP	6.1
2	B	54	VAL	5.6
2	B	59	GLN	5.5
2	B	62	ARG	5.4
2	B	66	THR	5.1
2	B	65	LEU	4.7
1	A	375	TYR	4.6
2	B	58	ALA	4.3
1	A	264	LEU	4.2
1	A	377	GLY	3.9
2	B	55	GLY	3.7
2	B	37	ARG	3.7
1	A	233	ASN	3.6
1	A	128	ASP	3.5
1	A	173	ASN	3.3
1	A	248	ARG	3.1
2	B	5	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	237	PRO	3.0
1	A	373	PRO	3.0
2	B	372	ARG	2.9
2	B	374	CYS	2.9
1	A	266	ASN	2.9
2	B	67	LEU	2.9
2	B	231	ALA	2.7
1	A	238	ASN	2.6
1	A	110	ASN	2.5
1	A	3	ILE	2.5
1	A	146	ASN	2.5
1	A	127	GLN	2.4
1	A	172	SER	2.4
2	B	232	SER	2.4
1	A	371	ALA	2.4
1	A	48	GLN	2.3
2	B	169	TYR	2.3
1	A	14	GLU	2.3
1	A	232	SER	2.2
1	A	413	ASN	2.2
1	A	147	GLY	2.2
1	A	117	GLU	2.2
1	A	265	ASN	2.1
2	B	143	TYR	2.1
1	A	225	LYS	2.1
1	A	372	ILE	2.0
1	A	235	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(Å ²)	Q<0.9
5	EDO	B	421	4/4	0.86	0.23	11.36	38,38,38,39	0
5	EDO	B	409	4/4	0.89	0.43	11.33	38,39,39,39	0
5	EDO	A	516	4/4	0.70	0.30	9.88	43,44,45,45	0
5	EDO	A	513	4/4	0.73	0.27	9.47	44,44,45,45	0
5	EDO	B	419	4/4	0.95	0.22	8.49	30,30,30,30	0
5	EDO	B	405	4/4	0.62	0.30	5.61	48,49,49,49	0
5	EDO	B	420	4/4	0.87	0.17	5.32	40,41,42,42	0
5	EDO	A	515	4/4	0.88	0.21	5.22	36,36,36,37	0
5	EDO	B	408	4/4	0.87	0.19	5.18	38,38,39,39	0
5	EDO	B	416	4/4	0.79	0.22	5.11	47,47,47,47	0
5	EDO	A	517	4/4	0.86	0.23	4.90	44,44,44,44	0
5	EDO	B	404	4/4	0.83	0.23	4.84	35,36,36,37	0
5	EDO	B	410	4/4	0.81	0.17	3.87	47,47,47,48	0
5	EDO	A	511	4/4	0.80	0.26	3.64	43,44,44,44	0
5	EDO	B	414	4/4	0.81	0.30	3.24	42,42,43,43	0
5	EDO	B	422	4/4	0.82	0.20	3.20	46,46,46,47	0
5	EDO	A	507	4/4	0.77	0.23	3.03	43,43,43,43	0
5	EDO	A	519	4/4	0.89	0.18	2.13	43,44,44,44	0
5	EDO	B	423	4/4	0.87	0.19	1.74	39,40,41,41	0
5	EDO	A	503	4/4	0.88	0.19	1.43	26,26,26,26	0
5	EDO	A	514	4/4	0.84	0.21	1.41	44,44,44,44	0
5	EDO	B	418	4/4	0.71	0.24	1.41	41,42,43,43	0
5	EDO	A	512	4/4	0.96	0.14	1.19	40,41,41,41	0
5	EDO	A	509	4/4	0.89	0.17	1.02	29,29,29,29	0
5	EDO	B	415	4/4	0.97	0.15	0.92	29,29,29,29	0
5	EDO	B	417	4/4	0.90	0.15	0.73	40,40,40,40	0
5	EDO	A	505	4/4	0.95	0.15	0.73	32,32,32,32	0
4	PO4	A	502	5/5	0.96	0.17	0.37	44,45,45,45	0
5	EDO	B	413	4/4	0.94	0.16	0.21	42,43,43,44	0
5	EDO	B	407	4/4	0.90	0.16	0.10	25,25,25,25	0
5	EDO	A	504	4/4	0.94	0.15	0.01	32,32,32,33	0
5	EDO	A	510	4/4	0.91	0.15	-0.26	43,43,43,43	0
8	LAR	B	403	29/29	0.90	0.15	-0.31	24,28,35,35	0
5	EDO	B	412	4/4	0.94	0.12	-0.34	33,34,34,34	0
5	EDO	A	508	4/4	0.95	0.12	-0.38	33,33,33,33	0
5	EDO	A	518	4/4	0.95	0.12	-0.51	32,32,33,33	0
3	NAD	A	501	44/44	0.93	0.11	-0.81	30,32,36,36	0
7	ATP	B	402	31/31	0.98	0.11	-0.85	17,18,18,18	0
5	EDO	B	406	4/4	0.95	0.08	-1.81	26,26,26,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	EDO	A	520	4/4	0.81	0.29	-	48,48,48,49	0
6	CA	B	401	1/1	0.99	0.09	-	17,17,17,17	0
5	EDO	A	506	4/4	0.79	0.26	-	48,49,49,49	0
5	EDO	B	411	4/4	0.78	0.20	-	40,41,41,42	0
5	EDO	A	521	4/4	0.85	0.18	-	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.