



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:32 PM GMT

PDB ID : 4H0X
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 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/ValidationPDFNotes.html>

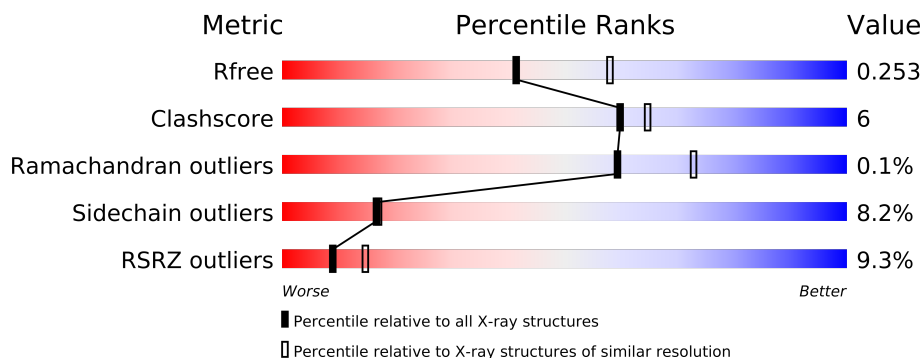
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	4049 (2.38-2.30)
Clashscore	79885	1094 (2.36-2.32)
Ramachandran outliers	78287	1080 (2.36-2.32)
Sidechain outliers	78261	1081 (2.36-2.32)
RSRZ outliers	66119	4050 (2.38-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	418	
2	B	375	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	EDO	A	504	-	X
5	EDO	A	508	-	X
5	EDO	A	509	-	X
5	EDO	A	510	-	X
5	EDO	A	511	-	X
5	EDO	B	404	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	EDO	B	405	-	X
5	EDO	B	407	-	X
5	EDO	B	408	-	X
5	EDO	B	409	-	X
5	EDO	B	411	-	X
5	EDO	B	414	-	X
5	EDO	B	415	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6567 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

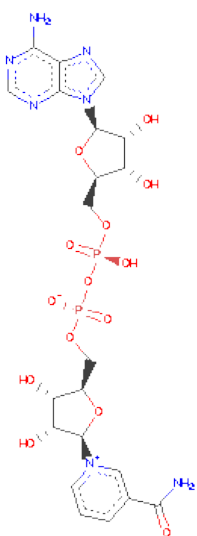
There are 6 discrepancies between the modelled and reference sequences:

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.

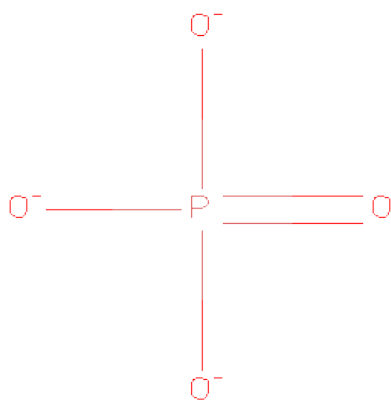
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	358	Total	C	N	O	S	0	0	0
			2799	1774	469	537	19			

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



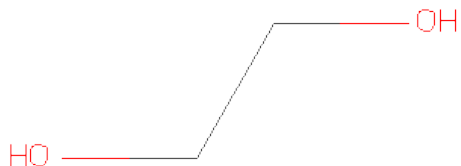
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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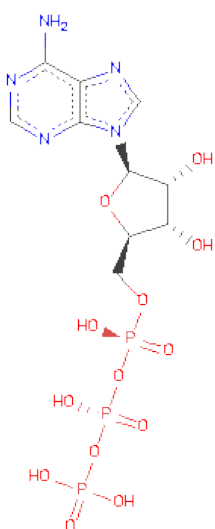
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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

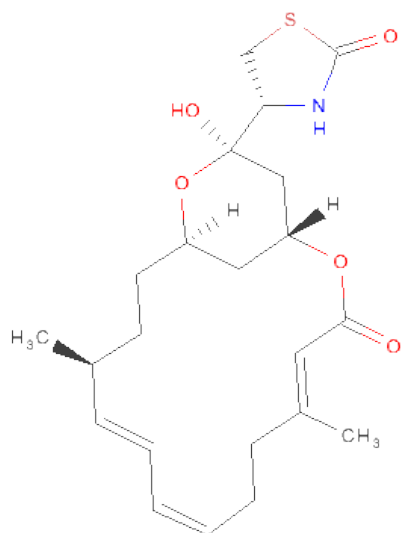
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		

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



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

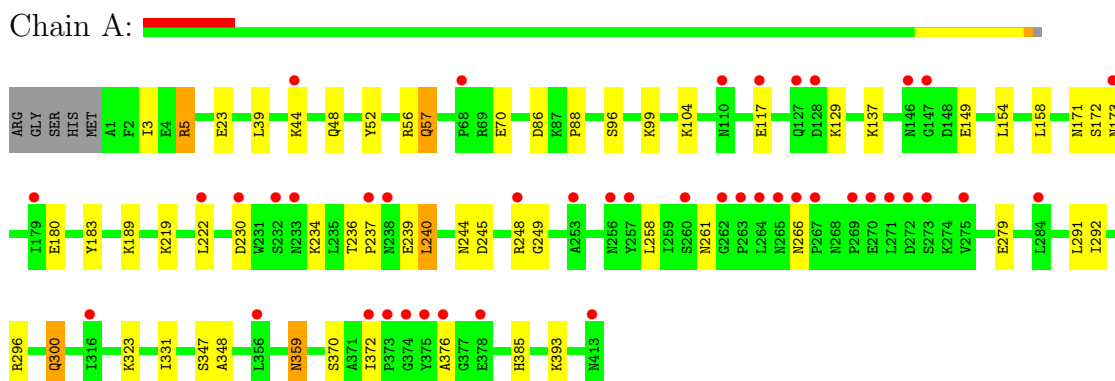
- Molecule 9 is water.

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

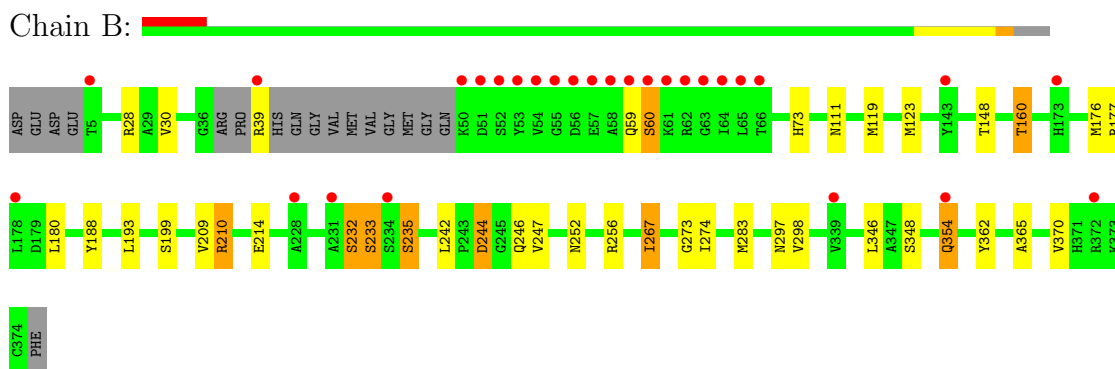
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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	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) 97.3 (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 0.229 , 0.253	Depositor DCC
R_{free} test set	2394 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 47441 reflections	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.

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	0.46	1/3429 (0.0%)	0.61	0/4632
2	B	0.52	2/2857 (0.1%)	0.61	0/3870
All	All	0.49	3/6286 (0.0%)	0.61	0/8502

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	60	SER	CB-OG	7.29	1.51	1.42
1	A	96	SER	CB-OG	5.61	1.49	1.42
2	B	235	SER	CB-OG	5.30	1.49	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3360	0	0	21	0
2	B	2799	0	0	17	1
3	A	44	0	0	1	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	36	0	54	5	0
5	B	52	0	78	6	0
6	B	1	0	0	0	0
7	B	31	0	0	0	0
8	B	29	0	0	0	0
9	A	110	0	0	5	0
9	B	100	0	0	3	1
All	All	6567	0	132	39	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (39) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	0.89
2:B:244:ASP:OD2	2:B:246:GLN:NE2	2.15	0.79
1:A:129:LYS:NZ	9:A:670:HOH:O	2.25	0.68
2:B:273:GLY:N	5:B:416:EDO:HO2	1.94	0.66
1:A:236:THR:OG1	1:A:239:GLU:CG	2.43	0.66
2:B:362:TYR:O	2:B:365:ALA:O	2.15	0.65
2:B:160:THR:CG2	2:B:180:LEU:O	2.44	0.64
1:A:348:ALA:N	5:A:504:EDO:HO2	1.98	0.61
1:A:5:ARG:NH2	1:A:88:PRO:O	2.35	0.59
1:A:347:SER:CB	2:B:176:MET:CE	2.80	0.59
2:B:232:SER:OG	2:B:233:SER:N	2.35	0.58
1:A:172:SER:OG	1:A:173:ASN:N	2.37	0.56
2:B:210:ARG:CD	2:B:214:GLU:OE1	2.54	0.56
1:A:180:GLU:N	5:A:506:EDO:HO2	2.03	0.55
2:B:298:VAL:CG1	5:B:406:EDO:H21	2.37	0.54
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:199:SER:N	5:B:413:EDO:HO1	2.06	0.53
2:B:283:MET:CE	5:B:407:EDO:O2	2.58	0.51
1:A:370:SER:O	1:A:376:ALA:CB	2.59	0.50
5:A:511:EDO:H21	9:A:673:HOH:O	2.11	0.49
2:B:111:ASN:ND2	2:B:119:MET:CE	2.76	0.49
5:A:504:EDO:HO1	2:B:177:ARG:N	2.13	0.47
5:B:404:EDO:H11	9:B:581:HOH:O	2.16	0.45
1:A:236:THR:CB	1:A:237:PRO:CD	2.94	0.45
2:B:256:ARG:NH1	9:B:535:HOH:O	2.49	0.45
1:A:57:GLN:NE2	9:A:647:HOH:O	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:354:GLN:OE1	2:B:354:GLN:CA	2.62	0.45
1:A:240:LEU:O	1:A:244:ASN:ND2	2.50	0.45
1:A:52:TYR:OH	1:A:70:GLU:OE1	2.36	0.43
2:B:188:TYR:CD1	2:B:267:ILE:CD1	3.01	0.43
1:A:372:ILE:CG2	1:A:372:ILE:O	2.66	0.42
2:B:73:HIS:N	9:B:532:HOH:O	2.53	0.42
5:B:415:EDO:H22	5:B:416:EDO:H12	2.02	0.42
1:A:99:LYS:NZ	9:A:613:HOH:O	2.52	0.42
1:A:279:GLU:OE2	1:A:385:HIS:NE2	2.53	0.41
1:A:347:SER:OG	2:B:176:MET:CE	2.69	0.41
1:A:323:LYS:NZ	9:A:685:HOH:O	2.53	0.41

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	Distance(Å)	Clash(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%)	56	67
2	B	353/375 (94%)	343 (97%)	10 (3%)	0	100	100
All	All	764/793 (96%)	733 (96%)	30 (4%)	1 (0%)	59	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	ARG

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	375/379 (99%)	344 (92%)	31 (8%)	16	16
2	B	304/318 (96%)	279 (92%)	25 (8%)	17	17
All	All	679/697 (97%)	623 (92%)	56 (8%)	17	17

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	5	ARG
1	A	23	GLU
1	A	39	LEU
1	A	44	LYS
1	A	48	GLN
1	A	57	GLN
1	A	86	ASP
1	A	104	LYS
1	A	117	GLU
1	A	137	LYS
1	A	149	GLU
1	A	154	LEU
1	A	158	LEU
1	A	171	ASN
1	A	189	LYS
1	A	219	LYS
1	A	222	LEU
1	A	230	ASP
1	A	234	LYS
1	A	240	LEU
1	A	248	ARG
1	A	258	LEU
1	A	261	ASN
1	A	266	ASN
1	A	291	LEU
1	A	296	ARG
1	A	300	GLN
1	A	331	ILE

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Mol	Chain	Res	Type
1	A	359	ASN
1	A	393	LYS
2	B	28	ARG
2	B	30	VAL
2	B	39	ARG
2	B	59	GLN
2	B	60	SER
2	B	123	MET
2	B	148	THR
2	B	160	THR
2	B	193	LEU
2	B	209	VAL
2	B	210	ARG
2	B	232	SER
2	B	233	SER
2	B	235	SER
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	297	ASN
2	B	346	LEU
2	B	348	SER
2	B	354	GLN
2	B	370	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	$\# Z > 2$
3	NAD	A	501	-	48,48,48	0.92	2 (4%)	73,73,73	1.75	11 (15%)
4	PO4	A	502	-	4,4,4	0.23	0	6,6,6	0.32	0
5	EDO	A	503	-	3,3,3	0.70	0	2,2,2	0.42	0
5	EDO	A	504	-	3,3,3	0.58	0	2,2,2	0.40	0
5	EDO	A	505	-	3,3,3	0.56	0	2,2,2	0.30	0
5	EDO	A	506	-	3,3,3	0.59	0	2,2,2	0.36	0
5	EDO	A	507	-	3,3,3	0.55	0	2,2,2	0.40	0
5	EDO	A	508	-	3,3,3	0.57	0	2,2,2	0.45	0
5	EDO	A	509	-	3,3,3	0.57	0	2,2,2	0.43	0
5	EDO	A	510	-	3,3,3	0.54	0	2,2,2	0.40	0
5	EDO	A	511	-	3,3,3	0.65	0	2,2,2	0.45	0
7	ATP	B	402	-	33,33,33	1.10	2 (6%)	52,52,52	1.67	7 (13%)
8	LAR	B	403	-	31,31,31	1.53	2 (6%)	43,43,43	2.17	9 (20%)
5	EDO	B	404	-	3,3,3	0.58	0	2,2,2	0.34	0
5	EDO	B	405	-	3,3,3	0.64	0	2,2,2	0.27	0
5	EDO	B	406	-	3,3,3	0.58	0	2,2,2	0.42	0
5	EDO	B	407	-	3,3,3	0.71	0	2,2,2	0.35	0
5	EDO	B	408	-	3,3,3	0.51	0	2,2,2	0.44	0
5	EDO	B	409	-	3,3,3	0.57	0	2,2,2	0.40	0
5	EDO	B	410	-	3,3,3	0.56	0	2,2,2	0.40	0
5	EDO	B	411	-	3,3,3	0.55	0	2,2,2	0.37	0
5	EDO	B	412	-	3,3,3	0.61	0	2,2,2	0.42	0
5	EDO	B	413	-	3,3,3	0.56	0	2,2,2	0.37	0
5	EDO	B	414	-	3,3,3	0.55	0	2,2,2	0.28	0
5	EDO	B	415	-	3,3,3	0.58	0	2,2,2	0.20	0
5	EDO	B	416	-	3,3,3	0.55	0	2,2,2	0.44	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	-	-	0/30/62/62	0/3/5/5
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
7	ATP	B	402	-	-	0/22/38/38	0/1/3/3
8	LAR	B	403	-	-	1/28/51/51	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
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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	403	LAR	O2-C1	5.84	1.47	1.34
8	B	403	LAR	C20-S1	-4.51	1.66	1.78
7	B	402	ATP	C4-N9	-3.18	1.33	1.37
3	A	501	NAD	C5A-C4A	3.06	1.47	1.40
7	B	402	ATP	C5-C4	3.05	1.47	1.40
3	A	501	NAD	C4A-N9A	-3.03	1.33	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NAD	N3A-C2A-N1A	-7.15	122.73	128.71
3	A	501	NAD	O4D-C1D-N1N	6.97	115.08	107.95
7	B	402	ATP	N3-C2-N1	-6.65	123.15	128.71
8	B	403	LAR	C4-C5-C6	-6.18	96.71	112.74
8	B	403	LAR	C10-C9-C8	-6.17	105.43	126.70
8	B	403	LAR	C8-C7-C6	-5.30	99.76	124.23
7	B	402	ATP	N3-C4-N9	5.20	134.83	125.43
3	A	501	NAD	N3A-C4A-N9A	4.79	134.08	125.43
8	B	403	LAR	O2-C1-C2	4.78	123.68	111.66
3	A	501	NAD	C4A-C5A-N7A	-3.42	106.59	109.52
8	B	403	LAR	O5-C20-N1	-3.41	124.01	126.57
7	B	402	ATP	C8-N9-C4	3.25	109.38	106.90
8	B	403	LAR	O1-C1-C2	-3.12	118.09	126.28
3	A	501	NAD	PN-O3-PA	-2.93	120.38	132.95
8	B	403	LAR	C19-S1-C20	2.92	93.60	91.97
3	A	501	NAD	C5A-C4A-N3A	-2.83	119.55	125.70
7	B	402	ATP	C5-C4-N3	-2.80	119.60	125.70
8	B	403	LAR	S1-C20-N1	2.80	114.01	111.26
3	A	501	NAD	O4B-C1B-N9A	2.75	111.00	108.44
8	B	403	LAR	O2-C1-O1	-2.74	118.23	123.24
7	B	402	ATP	C4-C5-N7	-2.74	107.17	109.52
3	A	501	NAD	C8A-N9A-C4A	2.63	108.91	106.90
3	A	501	NAD	C1B-N9A-C4A	-2.59	122.17	126.64
3	A	501	NAD	C2A-N3A-C4A	2.54	121.24	114.01
7	B	402	ATP	C2-N3-C4	2.23	120.37	114.01
3	A	501	NAD	C6N-N1N-C2N	-2.09	119.67	122.04
7	B	402	ATP	C2-N1-C6	2.04	122.46	118.77

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	403	LAR	C19-C18-C17-C16

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.68	43 (10%) 7 11	28, 46, 83, 101	0
2	B	358/375 (95%)	0.55	28 (7%) 13 20	19, 28, 73, 141	0
All	All	771/793 (97%)	0.62	71 (9%) 9 15	19, 37, 81, 141	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	60	SER	15.9
2	B	50	LYS	12.5
2	B	39	ARG	12.3
1	A	376	ALA	10.6
2	B	51	ASP	10.4
2	B	52	SER	7.7
2	B	64	ILE	7.2
1	A	264	LEU	6.6
2	B	57	GLU	6.5
2	B	53	TYR	6.1
2	B	62	ARG	6.0
2	B	63	GLY	5.7
1	A	375	TYR	5.7
2	B	56	ASP	5.6
1	A	372	ILE	5.2
2	B	61	LYS	4.9
2	B	59	GLN	4.9
1	A	269	PRO	4.8
1	A	232	SER	4.4
1	A	284	LEU	4.4
1	A	233	ASN	4.3
1	A	173	ASN	3.9
1	A	260	SER	3.8
1	A	222	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	54	VAL	3.6
2	B	66	THR	3.6
1	A	267	PRO	3.5
1	A	128	ASP	3.3
1	A	271	LEU	3.3
1	A	263	PRO	3.2
1	A	117	GLU	3.2
1	A	272	ASP	3.1
2	B	234	SER	3.0
1	A	262	GLY	3.0
1	A	373	PRO	3.0
1	A	179	ILE	3.0
2	B	65	LEU	2.9
1	A	237	PRO	2.9
1	A	68	PRO	2.8
2	B	55	GLY	2.8
2	B	5	THR	2.8
1	A	266	ASN	2.8
1	A	257	TYR	2.8
1	A	238	ASN	2.6
1	A	316	ILE	2.6
1	A	265	ASN	2.6
1	A	256	ASN	2.6
2	B	228	ALA	2.5
1	A	253	ALA	2.5
2	B	58	ALA	2.5
1	A	147	GLY	2.5
1	A	374	GLY	2.4
2	B	354	GLN	2.4
2	B	339	VAL	2.4
1	A	378	GLU	2.4
1	A	110	ASN	2.4
2	B	372	ARG	2.4
1	A	230	ASP	2.3
2	B	143	TYR	2.3
1	A	413	ASN	2.3
2	B	173	HIS	2.3
1	A	270	GLU	2.3
1	A	248	ARG	2.3
2	B	178	LEU	2.3
1	A	127	GLN	2.2
1	A	356	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	231	ALA	2.2
1	A	273	SER	2.2
1	A	44	LYS	2.1
1	A	275	VAL	2.0
1	A	146	ASN	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 carbohydrates 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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	EDO	B	415	4/4	0.39	8.38	39,40,45,46	0
5	EDO	B	405	4/4	0.43	7.98	49,49,49,50	0
5	EDO	A	511	4/4	0.52	7.47	43,43,43,44	0
5	EDO	B	409	4/4	0.26	7.03	40,40,41,49	0
5	EDO	B	407	4/4	0.29	6.07	38,38,39,39	0
5	EDO	B	408	4/4	0.39	5.82	37,38,39,39	0
5	EDO	B	411	4/4	0.42	5.53	48,49,49,50	0
5	EDO	B	414	4/4	0.22	5.20	27,28,28,28	0
5	EDO	A	509	4/4	0.25	3.85	46,46,46,47	0
5	EDO	A	508	4/4	0.22	3.57	40,41,41,41	0
5	EDO	A	504	4/4	0.25	3.43	35,35,35,35	0
5	EDO	B	404	4/4	0.25	2.99	37,39,39,40	0
5	EDO	A	510	4/4	0.24	2.97	44,44,45,45	0
5	EDO	B	406	4/4	0.24	1.65	26,27,28,29	0
5	EDO	A	505	4/4	0.17	0.92	38,39,39,39	0
5	EDO	A	507	4/4	0.18	0.91	43,43,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	EDO	B	413	4/4	0.13	0.60	38,38,38,39	0
5	EDO	B	412	4/4	0.16	0.43	34,34,34,35	0
3	NAD	A	501	44/44	0.19	0.40	59,70,74,77	0
4	PO4	A	502	5/5	0.17	0.06	56,57,57,60	0
5	EDO	B	410	4/4	0.14	-0.20	38,38,38,39	0
5	EDO	A	506	4/4	0.15	-0.40	38,38,39,39	0
8	LAR	B	403	29/29	0.13	-0.59	29,31,34,34	0
7	ATP	B	402	31/31	0.13	-0.63	20,20,21,21	0
5	EDO	B	416	4/4	0.13	-0.79	36,36,37,38	0
5	EDO	A	503	4/4	0.14	-0.97	39,39,39,40	0
6	CA	B	401	1/1	0.12	-2.69	21,21,21,21	0

6.5 Other polymers ⓘ

There are no such residues in this entry.