



Full wwPDB X-ray Structure Validation Report

Jul 11, 2014 – 07:06 PM EDT

PDB ID : 4C4O
Title : Structure of carbonyl reductase CPCR2 from *Candida parapsilosis* in complex with NADH
Authors : Man, H.; Loderer, C.; Ansorge-Schumacher, M.; Grogan, G.
Deposited on : 2013-09-06
Resolution : 2.05 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>

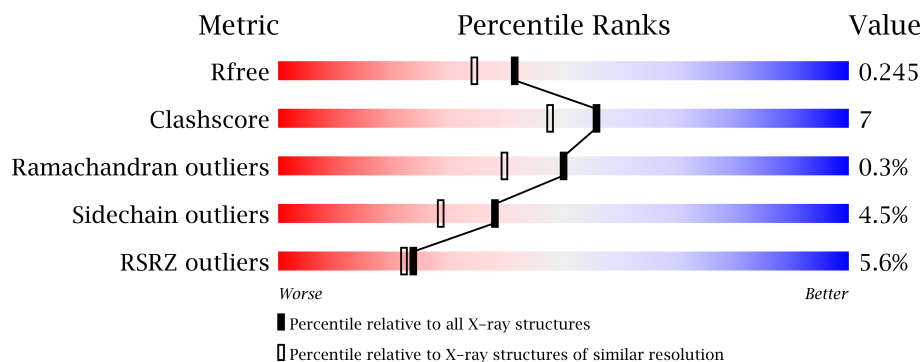
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
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) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 2.05 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	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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	336	
1	B	336	
1	C	336	
1	D	336	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	ZN	B	500	-	X
4	EDO	A	1337	-	X
4	EDO	B	1337	-	X
4	EDO	B	1338	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	EDO	B	1339	-	X
4	EDO	C	1337	-	X
4	EDO	C	1338	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9234 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.

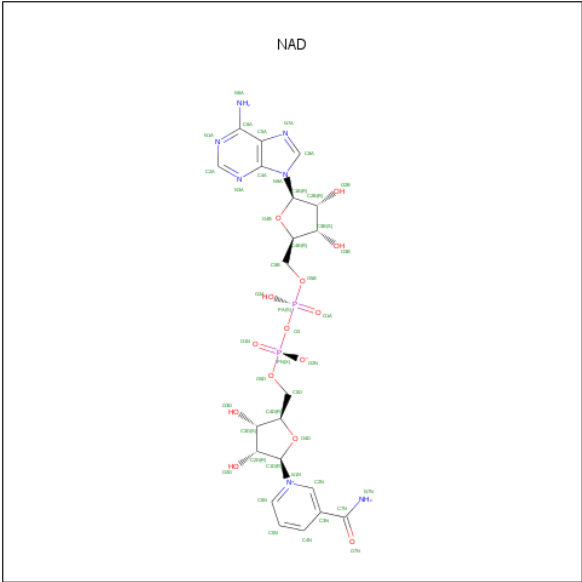
- Molecule 1 is a protein called CARBONYL REDUCTASE CPR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2318	1468	397	443	10			
1	B	335	Total	C	N	O	S	0	1	0
			2502	1590	424	476	12			
1	C	302	Total	C	N	O	S	0	0	0
			2111	1329	365	407	10			
1	D	270	Total	C	N	O	S	0	0	0
			1855	1165	320	361	9			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

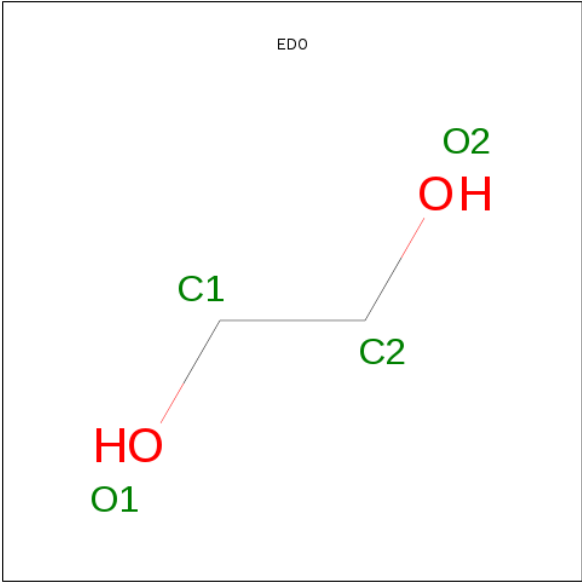
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Zn	0	0
			3	3		
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- 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
			36	15	6	13	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is water.

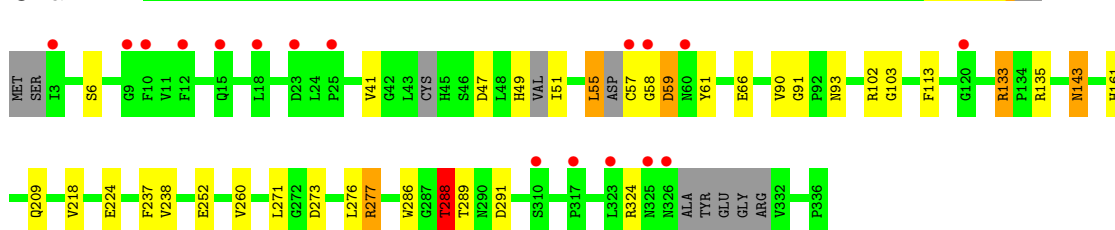
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	67	Total O 67 67	0	0
5	B	102	Total O 102 102	0	0
5	C	44	Total O 44 44	0	0
5	D	34	Total O 34 34	0	0

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.

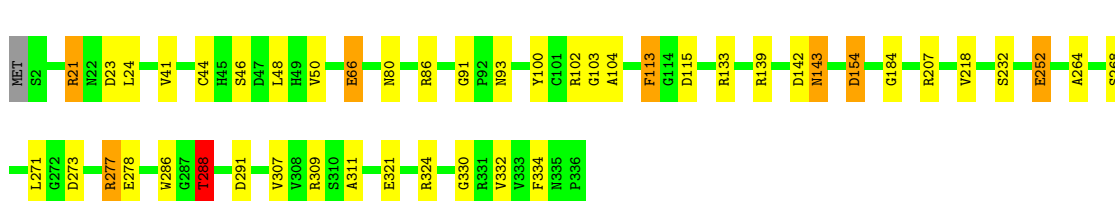
• Molecule 1: CARBONYL REDUCTASE CPR2

Chain A:



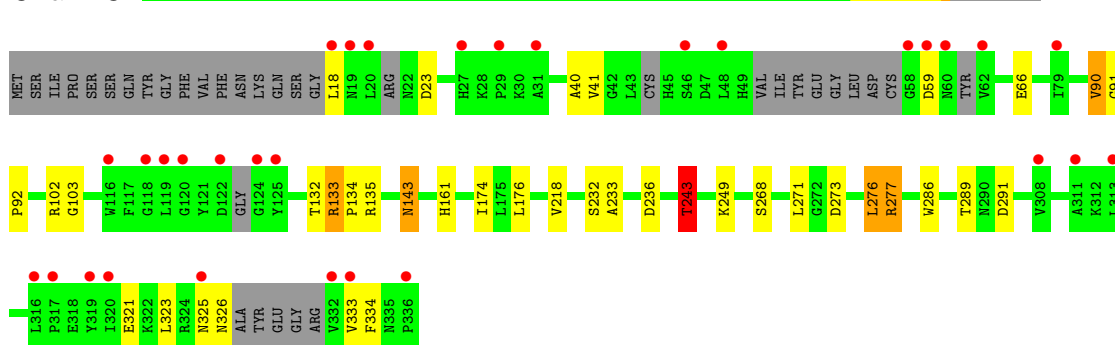
• Molecule 1: CARBONYL REDUCTASE CPR2

Chain B:



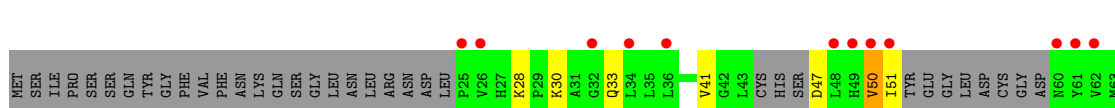
• Molecule 1: CARBONYL REDUCTASE CPR2

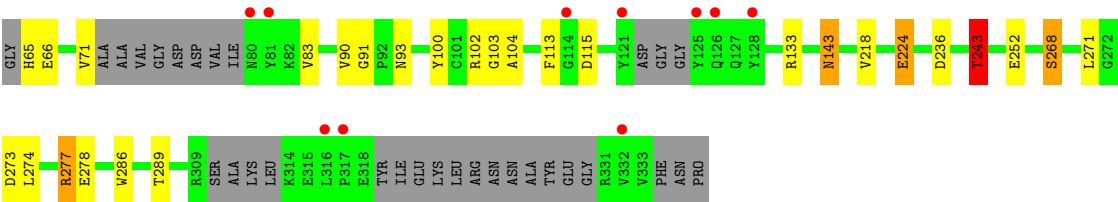
Chain C:



• Molecule 1: CARBONYL REDUCTASE CPR2

Chain D:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.72Å 88.84Å 118.20Å 90.00° 100.40° 90.00°	Depositor
Resolution (Å)	58.13 – 2.05 58.13 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.13-2.05) 99.8 (58.13-2.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0033	Depositor
R, R_{free}	0.205 , 0.241 0.215 , 0.245	Depositor DCC
R_{free} test set	4253 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.8	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	1 of 85078 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9234	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EDO, NAD

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	0.79	0/2359	0.96	8/3211 (0.2%)
1	B	0.94	3/2553 (0.1%)	1.02	15/3467 (0.4%)
1	C	0.78	0/2145	0.95	9/2922 (0.3%)
1	D	1.01	2/1880 (0.1%)	0.97	7/2559 (0.3%)
All	All	0.88	5/8937 (0.1%)	0.98	39/12159 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	50	VAL	C-N	-26.47	0.73	1.34
1	B	277	ARG	CD-NE	-6.70	1.35	1.46
1	B	66[A]	GLU	CG-CD	6.39	1.61	1.51
1	B	66[B]	GLU	CG-CD	6.39	1.61	1.51
1	D	268	SER	CB-OG	-5.04	1.35	1.42

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	ARG	NE-CZ-NH2	-17.62	111.49	120.30
1	A	277	ARG	NE-CZ-NH1	16.65	128.63	120.30
1	C	277	ARG	NE-CZ-NH1	16.33	128.47	120.30
1	A	277	ARG	NE-CZ-NH2	-15.99	112.31	120.30
1	C	277	ARG	NE-CZ-NH2	-15.60	112.50	120.30
1	B	277	ARG	NE-CZ-NH1	15.53	128.06	120.30
1	D	277	ARG	NE-CZ-NH2	-15.23	112.68	120.30
1	D	277	ARG	NE-CZ-NH1	15.11	127.86	120.30
1	A	133	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	B	154	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	D	50	VAL	O-C-N	7.16	134.15	122.70
1	B	66[A]	GLU	OE1-CD-OE2	-6.88	115.04	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66[B]	GLU	OE1-CD-OE2	-6.88	115.04	123.30
1	C	176	LEU	CB-CG-CD2	6.84	122.62	111.00
1	D	243	THR	N-CA-CB	-6.82	97.34	110.30
1	D	252	GLU	CB-CA-C	-6.76	96.88	110.40
1	A	252	GLU	CB-CA-C	-6.74	96.92	110.40
1	C	132	THR	N-CA-C	-6.48	93.52	111.00
1	C	243	THR	N-CA-CB	-6.47	98.00	110.30
1	A	288	THR	N-CA-CB	-6.46	98.03	110.30
1	B	44	CYS	CB-CA-C	-6.45	97.51	110.40
1	B	277	ARG	CD-NE-CZ	6.35	132.50	123.60
1	C	176	LEU	CA-CB-CG	6.25	129.69	115.30
1	B	288	THR	N-CA-CB	-6.23	98.47	110.30
1	D	277	ARG	CD-NE-CZ	6.04	132.05	123.60
1	B	86	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	135	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	C	276	LEU	CA-CB-CG	5.75	128.53	115.30
1	B	86	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	252	GLU	CB-CA-C	-5.72	98.96	110.40
1	A	135	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	D	50	VAL	CA-C-N	-5.60	104.88	117.20
1	B	102	ARG	N-CA-C	5.40	125.58	111.00
1	C	135	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	207	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	277	ARG	CD-NE-CZ	5.11	130.75	123.60
1	A	277	ARG	CD-NE-CZ	5.09	130.72	123.60
1	B	66[A]	GLU	CG-CD-OE2	5.00	128.31	118.30
1	B	66[B]	GLU	CG-CD-OE2	5.00	128.31	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	2318	0	2156	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2502	0	2459	33	1
1	C	2111	0	1944	34	1
1	D	1855	0	1664	30	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	36	0	20	0	0
3	B	44	0	26	0	0
3	C	44	0	26	0	0
3	D	44	0	26	0	0
4	A	4	0	6	0	0
4	B	12	0	18	9	0
4	C	8	0	12	8	0
5	A	67	0	0	1	0
5	B	102	0	0	2	0
5	C	44	0	0	0	0
5	D	34	0	0	1	0
All	All	9234	0	8357	115	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 7.

All (115) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:50:VAL:CA	1:D:51:ILE:N	1.84	1.39
1:D:50:VAL:C	1:D:51:ILE:CA	1.92	1.36
1:D:47:ASP:O	1:D:51:ILE:HG12	1.34	1.22
1:C:323:LEU:O	1:C:326:ASN:HB2	1.39	1.20
1:D:50:VAL:O	1:D:51:ILE:N	1.81	1.11
1:A:55:LEU:C	1:A:57:CYS:N	2.14	0.99
1:A:58:GLY:HA3	1:A:61:TYR:HE2	1.28	0.97
1:A:58:GLY:HA3	1:A:61:TYR:CE2	1.99	0.96
1:C:323:LEU:O	1:C:326:ASN:CB	2.24	0.85
1:B:113:PHE:CE1	1:B:113:PHE:CE2	2.60	0.83
1:A:288:THR:HG21	5:A:2019:HOH:O	1.81	0.81
1:A:276:LEU:HD21	1:B:113:PHE:CE1	2.16	0.79
1:D:115:ASP:OD2	1:D:133:ARG:NH2	2.16	0.78
1:B:115:ASP:OD2	1:B:133:ARG:NH2	2.17	0.78
1:C:321:GLU:O	1:C:325:ASN:ND2	2.16	0.78
1:D:50:VAL:C	1:D:51:ILE:N	0.73	0.78
1:B:288:THR:HG22	1:B:291:ASP:H	1.51	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:104:ALA:HA	1:C:102:ARG:O	1.87	0.75
1:D:93:ASN:O	1:D:133:ARG:NH1	2.19	0.74
1:B:184:GLY:HA3	4:B:1337:EDO:H21	1.67	0.73
1:D:224:GLU:CD	1:D:224:GLU:H	1.91	0.73
1:B:93:ASN:O	1:B:133:ARG:NH1	2.21	0.73
1:A:55:LEU:O	1:A:57:CYS:N	2.23	0.72
1:B:288:THR:HG21	5:B:2034:HOH:O	1.89	0.72
1:C:249:LYS:HB2	4:C:1337:EDO:H11	1.72	0.71
1:D:50:VAL:O	1:D:51:ILE:CA	2.32	0.70
1:A:288:THR:HG22	1:A:291:ASP:H	1.56	0.70
1:D:71:VAL:HG12	1:D:83:VAL:HA	1.74	0.69
1:A:58:GLY:O	1:A:59:ASP:HB2	1.92	0.69
1:C:233:ALA:HB2	4:C:1338:EDO:H21	1.75	0.69
1:B:80:ASN:O	1:B:139:ARG:NH2	2.26	0.68
1:B:307:VAL:HG22	1:B:330:GLY:HA3	1.75	0.68
1:C:236:ASP:OD2	1:C:243:THR:HG23	1.95	0.67
1:C:90:VAL:HG11	1:C:289:THR:HA	1.77	0.66
1:D:50:VAL:N	1:D:51:ILE:N	2.44	0.66
1:C:161:HIS:HE1	1:D:278:GLU:OE2	1.78	0.65
1:D:236:ASP:OD2	1:D:243:THR:HG23	1.97	0.65
1:C:233:ALA:HB2	4:C:1338:EDO:C2	2.26	0.65
1:D:90:VAL:HG21	1:D:289:THR:HG22	1.79	0.64
1:C:90:VAL:HG23	1:C:92:PRO:HD2	1.79	0.64
1:A:58:GLY:CA	1:A:61:TYR:HE2	2.08	0.64
1:A:161:HIS:HE1	1:B:278:GLU:OE2	1.81	0.63
1:A:161:HIS:HD2	1:A:291:ASP:OD2	1.81	0.63
1:A:90:VAL:HG21	1:A:289:THR:HG22	1.81	0.62
1:D:50:VAL:CB	1:D:51:ILE:N	2.62	0.62
1:A:237:PHE:CE1	1:A:260:VAL:HG21	2.36	0.61
1:C:90:VAL:HG11	1:C:289:THR:HG22	1.83	0.60
1:C:236:ASP:OD2	1:C:243:THR:CG2	2.50	0.59
1:D:50:VAL:O	1:D:51:ILE:HA	2.02	0.58
1:D:236:ASP:OD2	1:D:243:THR:CG2	2.51	0.58
1:A:47:ASP:O	1:A:51:ILE:CB	2.52	0.58
1:A:161:HIS:CD2	1:A:291:ASP:OD2	2.58	0.57
1:A:102:ARG:O	1:D:104:ALA:HA	2.04	0.57
1:B:113:PHE:CE1	4:B:1339:EDO:H11	2.40	0.56
1:C:161:HIS:CD2	1:C:291:ASP:OD2	2.59	0.56
1:C:249:LYS:HB2	4:C:1337:EDO:C1	2.35	0.56
1:B:113:PHE:CD1	4:B:1339:EDO:H11	2.41	0.56
1:C:161:HIS:HD2	1:C:291:ASP:OD2	1.90	0.55
1:C:40:ALA:HB1	1:C:333:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:21:ARG:NH1	1:B:23:ASP:OD1	2.40	0.54
1:D:50:VAL:C	1:D:51:ILE:HA	2.13	0.53
1:B:309:ARG:CG	1:B:332:VAL:HG22	2.40	0.52
1:C:236:ASP:CG	1:C:243:THR:HG23	2.30	0.51
1:B:143:ASN:H	1:B:143:ASN:HD22	1.58	0.51
1:A:93:ASN:O	1:A:133:ARG:NH1	2.45	0.50
1:B:330:GLY:HA2	4:B:1337:EDO:C1	2.41	0.50
1:D:47:ASP:O	1:D:51:ILE:CG1	2.30	0.49
1:D:236:ASP:CG	1:D:243:THR:HG23	2.33	0.48
1:D:65:HIS:CE1	5:D:2003:HOH:O	2.66	0.48
1:C:249:LYS:CB	4:C:1337:EDO:H11	2.42	0.48
1:B:309:ARG:HG3	1:B:332:VAL:HG22	1.96	0.48
1:C:40:ALA:HB1	1:C:333:VAL:CG2	2.43	0.48
1:C:91:GLY:HA3	1:C:286:TRP:CZ2	2.49	0.47
1:D:91:GLY:HA3	1:D:286:TRP:CZ2	2.49	0.47
1:A:161:HIS:CE1	1:B:278:GLU:OE2	2.65	0.47
1:C:232:SER:OG	4:C:1338:EDO:H11	2.15	0.47
1:C:90:VAL:CG1	1:C:289:THR:HG22	2.45	0.46
1:B:91:GLY:HA3	1:B:286:TRP:CZ2	2.50	0.46
1:C:102:ARG:N	1:C:103:GLY:HA3	2.31	0.46
1:B:46:SER:O	1:B:50:VAL:HG23	2.15	0.46
1:A:143:ASN:H	1:A:143:ASN:HD22	1.63	0.45
1:A:91:GLY:HA3	1:A:286:TRP:CZ2	2.52	0.45
1:D:30:LYS:HA	1:D:33:GLN:HB2	1.98	0.45
1:B:330:GLY:HA2	4:B:1337:EDO:H11	1.97	0.45
1:C:161:HIS:CE1	1:D:278:GLU:OE2	2.65	0.45
1:A:49:HIS:HB3	1:A:55:LEU:HD23	1.99	0.44
1:C:41:VAL:C	1:C:333:VAL:HG23	2.38	0.44
1:D:41:VAL:HA	1:D:66:GLU:O	2.19	0.43
1:B:273:ASP:OD1	1:B:277:ARG:HD3	2.19	0.43
1:C:41:VAL:HA	1:C:66:GLU:O	2.19	0.43
1:D:143:ASN:H	1:D:143:ASN:HD22	1.64	0.43
1:C:273:ASP:OD1	1:C:277:ARG:HD3	2.19	0.43
1:D:273:ASP:OD1	1:D:277:ARG:HD3	2.18	0.42
1:B:100:TYR:O	1:B:103:GLY:HA3	2.19	0.42
1:B:288:THR:CG2	1:B:291:ASP:H	2.28	0.42
1:B:252:GLU:OE2	4:B:1338:EDO:C2	2.67	0.42
1:C:143:ASN:H	1:C:143:ASN:HD22	1.67	0.42
1:A:90:VAL:HG21	1:A:289:THR:HA	2.02	0.42
1:C:249:LYS:N	4:C:1337:EDO:H11	2.35	0.42
1:B:232:SER:HB3	4:B:1338:EDO:C2	2.49	0.41
1:D:100:TYR:O	1:D:103:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:252:GLU:OE2	4:B:1338:EDO:H22	2.20	0.41
1:B:264:ALA:HB2	5:B:2087:HOH:O	2.19	0.41
1:A:41:VAL:HA	1:A:66:GLU:O	2.20	0.41
1:B:66[A]:GLU:HG2	1:B:154:ASP:CB	2.51	0.41
1:A:273:ASP:OD1	1:A:277:ARG:HD3	2.21	0.41
1:C:249:LYS:CA	4:C:1337:EDO:H11	2.51	0.41
1:A:102:ARG:N	1:A:103:GLY:HA3	2.35	0.41
1:D:102:ARG:N	1:D:103:GLY:HA3	2.36	0.41
1:C:133:ARG:N	1:C:134:PRO:HD3	2.36	0.41
1:B:311:ALA:O	1:B:334:PHE:HA	2.21	0.41
1:B:307:VAL:HG13	4:B:1337:EDO:H22	2.02	0.40
1:C:174:ILE:HG21	1:C:174:ILE:HD13	1.81	0.40
1:C:40:ALA:HA	1:C:334:PHE:O	2.22	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	Distance(Å)	Clash(Å)
1:B:142:ASP:OD2	1:C:23:ASP:O[2_545]	2.15	0.05

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	316/336 (94%)	301 (95%)	14 (4%)	1 (0%)	50	39
1	B	334/336 (99%)	320 (96%)	14 (4%)	0	100	100
1	C	288/336 (86%)	274 (95%)	12 (4%)	2 (1%)	30	16
1	D	254/336 (76%)	239 (94%)	14 (6%)	1 (0%)	43	32
All	All	1192/1344 (89%)	1134 (95%)	54 (4%)	4 (0%)	50	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ASP

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Mol	Chain	Res	Type
1	C	59	ASP
1	D	28	LYS
1	C	133	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	223/270 (83%)	212 (95%)	11 (5%)	35	25
1	B	261/270 (97%)	250 (96%)	11 (4%)	40	32
1	C	201/270 (74%)	193 (96%)	8 (4%)	42	33
1	D	168/270 (62%)	160 (95%)	8 (5%)	35	25
All	All	853/1080 (79%)	815 (96%)	38 (4%)	38	28

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	55	LEU
1	A	113	PHE
1	A	143	ASN
1	A	209	GLN
1	A	218	VAL
1	A	224	GLU
1	A	238	VAL
1	A	271	LEU
1	A	288	THR
1	A	324	ARG
1	B	21	ARG
1	B	24	LEU
1	B	48	LEU
1	B	113	PHE
1	B	143	ASN
1	B	218	VAL
1	B	268	SER
1	B	271	LEU

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Mol	Chain	Res	Type
1	B	288	THR
1	B	321	GLU
1	B	324	ARG
1	C	18	LEU
1	C	90	VAL
1	C	143	ASN
1	C	218	VAL
1	C	243	THR
1	C	268	SER
1	C	271	LEU
1	C	276	LEU
1	D	113	PHE
1	D	143	ASN
1	D	218	VAL
1	D	224	GLU
1	D	243	THR
1	D	268	SER
1	D	271	LEU
1	D	274	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	143	ASN
1	A	161	HIS
1	B	93	ASN
1	B	143	ASN
1	C	143	ASN
1	C	161	HIS
1	C	266	ASN
1	D	143	ASN

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 19 ligands modelled in this entry, 9 are monoatomic - leaving 10 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	1000	-	38,39,48	1.23	5 (13%)	58,60,73	2.24	10 (17%)
4	EDO	A	1337	-	3,3,3	0.48	0	2,2,2	0.47	0
3	NAD	B	1000	-	48,48,48	1.06	3 (6%)	73,73,73	2.09	9 (12%)
4	EDO	B	1337	-	3,3,3	0.64	0	2,2,2	0.41	0
4	EDO	B	1338	-	3,3,3	0.66	0	2,2,2	0.33	0
4	EDO	B	1339	-	3,3,3	1.49	0	2,2,2	1.01	0
3	NAD	C	1000	-	48,48,48	1.11	4 (8%)	73,73,73	1.96	12 (16%)
4	EDO	C	1337	-	3,3,3	0.38	0	2,2,2	0.79	0
4	EDO	C	1338	-	3,3,3	0.57	0	2,2,2	0.41	0
3	NAD	D	1000	-	48,48,48	1.34	9 (18%)	73,73,73	2.13	15 (20%)

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	1000	-	-	0/22/54/62	0/4/4/5
4	EDO	A	1337	-	-	0/1/1/1	0/0/0/0
3	NAD	B	1000	-	-	0/30/62/62	0/5/5/5
4	EDO	B	1337	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1338	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1339	-	-	0/1/1/1	0/0/0/0
3	NAD	C	1000	-	-	0/30/62/62	0/5/5/5
4	EDO	C	1337	-	-	0/1/1/1	0/0/0/0
4	EDO	C	1338	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	D	1000	-	-	0/30/62/62	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	NAD	O4B-C1B	3.54	1.45	1.41
3	C	1000	NAD	O4D-C1D	3.43	1.45	1.41
3	A	1000	NAD	C5A-C4A	3.43	1.48	1.40
3	D	1000	NAD	C5A-C4A	3.40	1.48	1.40
3	B	1000	NAD	PA-O3	3.12	1.65	1.59
3	D	1000	NAD	PA-O3	2.89	1.65	1.59
3	A	1000	NAD	C2A-N3A	2.84	1.37	1.32
3	C	1000	NAD	C5A-C4A	2.51	1.46	1.40
3	B	1000	NAD	C2A-N3A	2.48	1.36	1.32
3	D	1000	NAD	C2A-N1A	2.46	1.38	1.33
3	D	1000	NAD	C3N-C7N	2.43	1.54	1.50
3	D	1000	NAD	C4A-N9A	-2.39	1.34	1.37
3	D	1000	NAD	PN-O1N	2.33	1.54	1.48
3	D	1000	NAD	C2A-N3A	2.23	1.36	1.32
3	C	1000	NAD	PA-O3	2.22	1.63	1.59
3	B	1000	NAD	PN-O2N	2.21	1.53	1.48
3	A	1000	NAD	C4A-N9A	-2.16	1.34	1.37
3	D	1000	NAD	PN-O2N	2.12	1.53	1.48
3	C	1000	NAD	PN-O3	2.04	1.64	1.60
3	D	1000	NAD	C2N-C3N	2.02	1.42	1.39
3	A	1000	NAD	PN-O3	2.01	1.64	1.60

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1000	NAD	C5A-C4A-N3A	-9.85	116.37	125.98
3	A	1000	NAD	C5A-C4A-N3A	-8.57	117.62	125.98
3	C	1000	NAD	C5A-C4A-N3A	-7.68	118.49	125.98
3	C	1000	NAD	N3A-C2A-N1A	-7.60	122.20	128.89
3	A	1000	NAD	N3A-C2A-N1A	-7.57	122.23	128.89
3	D	1000	NAD	N3A-C2A-N1A	-7.53	122.26	128.89
3	D	1000	NAD	N3A-C4A-N9A	7.31	137.94	125.39
3	A	1000	NAD	N3A-C4A-N9A	7.31	137.93	125.39
3	B	1000	NAD	N3A-C4A-N9A	7.22	137.77	125.39
3	D	1000	NAD	C5A-C4A-N3A	-6.80	119.35	125.98
3	B	1000	NAD	N3A-C2A-N1A	-6.56	123.12	128.89
3	C	1000	NAD	N3A-C4A-N9A	5.65	135.09	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1000	NAD	O3-PN-O1N	4.86	120.52	108.77
3	D	1000	NAD	C8A-N9A-C4A	4.66	110.75	106.96
3	A	1000	NAD	C8A-N9A-C4A	4.48	110.60	106.96
3	D	1000	NAD	C2D-C1D-N1N	4.46	122.40	113.48
3	C	1000	NAD	O4D-C1D-N1N	4.33	112.89	108.13
3	B	1000	NAD	C4D-O4D-C1D	-3.50	105.88	109.72
3	B	1000	NAD	O4D-C1D-N1N	-3.48	104.31	108.13
3	D	1000	NAD	N6A-C6A-N1A	3.38	126.28	119.11
3	C	1000	NAD	C4A-C5A-N7A	-3.36	106.16	109.41
3	B	1000	NAD	C2A-N3A-C4A	3.35	122.92	113.27
3	A	1000	NAD	C2A-N3A-C4A	3.27	122.70	113.27
3	D	1000	NAD	C5A-C4A-N9A	-3.19	102.67	107.09
3	B	1000	NAD	C4B-O4B-C1B	-3.10	106.31	109.72
3	C	1000	NAD	O7N-C7N-C3N	3.08	123.03	119.59
3	D	1000	NAD	C5A-C6A-N6A	-2.99	113.95	120.72
3	C	1000	NAD	O3-PN-O1N	2.99	116.01	108.77
3	C	1000	NAD	C8A-N9A-C4A	2.98	109.38	106.96
3	B	1000	NAD	C8A-N9A-C4A	2.97	109.37	106.96
3	C	1000	NAD	C2A-N3A-C4A	2.91	121.66	113.27
3	A	1000	NAD	C8A-N9A-C1B	-2.82	120.85	126.15
3	A	1000	NAD	C4A-C5A-N7A	-2.72	106.78	109.41
3	D	1000	NAD	C2A-N3A-C4A	2.50	120.48	113.27
3	A	1000	NAD	C3D-C2D-C1D	2.47	106.29	101.38
3	C	1000	NAD	C4D-O4D-C1D	-2.38	107.11	109.72
3	D	1000	NAD	O4B-C1B-C2B	-2.31	103.32	106.69
3	C	1000	NAD	O4B-C1B-C2B	-2.29	103.36	106.69
3	D	1000	NAD	C3N-C7N-N7N	2.27	120.31	117.78
3	D	1000	NAD	O4D-C1D-C2D	-2.23	103.44	106.69
3	B	1000	NAD	O2A-PA-O1A	2.22	124.45	112.14
3	D	1000	NAD	C8A-N9A-C1B	-2.17	122.06	126.15
3	A	1000	NAD	PN-O3-PA	-2.15	124.53	133.17
3	A	1000	NAD	O2A-PA-O1A	2.14	123.99	112.14
3	C	1000	NAD	O7N-C7N-N7N	-2.02	119.70	122.59
3	D	1000	NAD	O3D-C3D-C4D	-2.01	105.15	111.07

There are no chirality outliers.

There are no torsion outliers.

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	326/336 (97%)	0.13	17 (5%) 26 25	23, 46, 77, 96	0
1	B	335/336 (99%)	-0.25	0 100 100	22, 33, 54, 73	0
1	C	302/336 (89%)	0.35	31 (10%) 7 6	27, 49, 84, 108	0
1	D	270/336 (80%)	0.26	22 (8%) 12 11	25, 47, 93, 110	0
All	All	1233/1344 (91%)	0.11	70 (5%) 24 21	22, 43, 83, 110	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	49	HIS	5.4
1	D	80	ASN	5.0
1	D	48	LEU	5.0
1	D	125	TYR	4.8
1	D	36	LEU	4.8
1	C	20	LEU	4.6
1	D	316	LEU	4.4
1	C	332	VAL	4.2
1	D	62	VAL	4.1
1	C	308	VAL	4.0
1	C	125	TYR	3.8
1	C	317	PRO	3.8
1	C	333	VAL	3.7
1	D	61	TYR	3.7
1	C	325	ASN	3.6
1	C	311	ALA	3.6
1	C	62	VAL	3.4
1	C	319	TYR	3.4
1	D	25	PRO	3.4
1	A	57	CYS	3.4
1	C	59	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	48	LEU	3.4
1	D	51	ILE	3.4
1	D	26	VAL	3.3
1	A	323	LEU	3.2
1	A	325	ASN	3.1
1	C	19	ASN	3.1
1	D	114	GLY	3.0
1	C	320	ILE	3.0
1	D	121	TYR	3.0
1	D	34	LEU	2.9
1	D	317	PRO	2.9
1	D	50	VAL	2.8
1	C	116	TRP	2.8
1	D	332	VAL	2.8
1	C	60	ASN	2.8
1	C	27	HIS	2.8
1	C	122	ASP	2.7
1	A	12	PHE	2.7
1	A	317	PRO	2.7
1	C	313	LEU	2.6
1	D	32	GLY	2.6
1	D	60	ASN	2.6
1	C	316	LEU	2.6
1	C	118	GLY	2.5
1	A	326	ASN	2.5
1	A	9	GLY	2.5
1	A	3	ILE	2.5
1	C	124	GLY	2.4
1	C	336	PRO	2.4
1	C	58	GLY	2.4
1	D	81	TYR	2.4
1	C	31	ALA	2.4
1	C	79	ILE	2.4
1	C	46	SER	2.3
1	A	15	GLN	2.3
1	D	126	GLN	2.3
1	A	18	LEU	2.3
1	A	25	PRO	2.3
1	A	310	SER	2.3
1	A	120	GLY	2.3
1	C	29	PRO	2.2
1	C	119	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	120	GLY	2.2
1	A	10	PHE	2.1
1	A	58	GLY	2.1
1	A	23	ASP	2.1
1	C	18	LEU	2.1
1	A	60	ASN	2.1
1	D	128	TYR	2.1

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
4	EDO	B	1337	4/4	0.33	13.38	38,40,42,47	0
4	EDO	C	1337	4/4	0.18	9.69	51,51,53,54	0
4	EDO	A	1337	4/4	0.25	5.14	46,53,59,62	0
4	EDO	C	1338	4/4	0.20	4.65	41,43,45,48	0
4	EDO	B	1338	4/4	0.20	4.38	40,41,43,46	0
2	ZN	B	500	1/1	0.15	3.78	28,28,28,28	1
4	EDO	B	1339	4/4	0.18	2.74	46,48,48,56	0
3	NAD	D	1000	44/44	0.13	1.11	43,51,58,67	0
2	ZN	B	499	1/1	0.11	0.44	37,37,37,37	1
3	NAD	A	1000	36/44	0.13	0.37	40,58,91,94	0
3	NAD	C	1000	44/44	0.11	-0.21	42,55,69,72	0
2	ZN	B	600	1/1	0.09	-0.51	36,36,36,36	0
3	NAD	B	1000	44/44	0.09	-0.93	23,27,31,32	0
2	ZN	A	600	1/1	0.04	-1.68	38,38,38,38	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	C	600	1/1	0.02	-2.39	49,49,49,49	0
2	ZN	D	500	1/1	0.07	-2.45	92,92,92,92	0
2	ZN	D	600	1/1	0.03	-3.70	50,50,50,50	0
2	ZN	C	500	1/1	0.03	-4.26	60,60,60,60	1
2	ZN	A	500	1/1	0.04	-8.29	45,45,45,45	1

6.5 Other polymers

There are no such residues in this entry.