Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:49 PM GMT

PDB ID	:	4PZ2
Title	:	Structure of Zm ALDH2-6 (RF2F) in complex with NAD
Authors	:	Morera, S.; Vigouroux, A.; Kopecny, D.
Deposited on	:	2014-03-28
Resolution	:	2.40 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

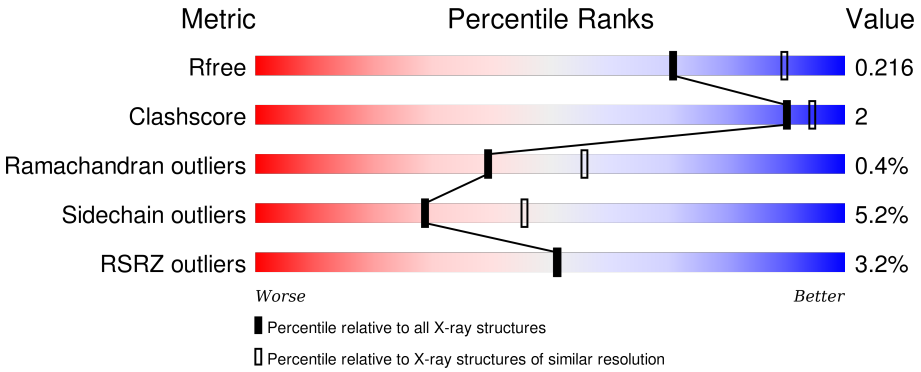
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 <=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	534	82% 9% • 8%
1	B	534	3% 84% 7% • 7%
1	C	534	84% 7% 8%
1	D	534	7% 83% 8% 8%

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	604	-	-	-	X
5	EDO	A	606	-	-	-	X
5	EDO	C	602	-	-	-	X
5	EDO	C	603	-	-	-	X
5	EDO	D	602	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15179 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 ZmALDH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3713	2350	650	692	21			
1	B	494	Total	C	N	O	S	0	0	0
			3734	2363	653	697	21			
1	C	491	Total	C	N	O	S	0	0	0
			3713	2350	650	692	21			
1	D	491	Total	C	N	O	S	0	0	0
			3712	2350	649	692	21			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	GLY	-	EXPRESSION TAG	UNP K7VEU7
A	-13	SER	-	EXPRESSION TAG	UNP K7VEU7
A	-12	SER	-	EXPRESSION TAG	UNP K7VEU7
A	-11	HIS	-	EXPRESSION TAG	UNP K7VEU7
A	-10	HIS	-	EXPRESSION TAG	UNP K7VEU7
A	-9	HIS	-	EXPRESSION TAG	UNP K7VEU7
A	-8	HIS	-	EXPRESSION TAG	UNP K7VEU7
A	-7	HIS	-	EXPRESSION TAG	UNP K7VEU7
A	-6	HIS	-	EXPRESSION TAG	UNP K7VEU7
A	-5	SER	-	EXPRESSION TAG	UNP K7VEU7
A	-4	GLN	-	EXPRESSION TAG	UNP K7VEU7
A	-3	ASP	-	EXPRESSION TAG	UNP K7VEU7
A	-2	PRO	-	EXPRESSION TAG	UNP K7VEU7
A	-1	ASN	-	EXPRESSION TAG	UNP K7VEU7
A	0	SER	-	EXPRESSION TAG	UNP K7VEU7
A	18	GLU	-	EXPRESSION TAG	UNP K7VEU7
A	19	GLU	-	EXPRESSION TAG	UNP K7VEU7
A	20	LYS	-	EXPRESSION TAG	UNP K7VEU7
A	54	ASP	GLU	SEE REMARK 999	UNP K7VEU7
A	113	HIS	ARG	SEE REMARK 999	UNP K7VEU7
A	115	GLY	ASP	SEE REMARK 999	UNP K7VEU7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ARG	SER	SEE REMARK 999	UNP K7VEU7
A	391	ALA	GLY	SEE REMARK 999	UNP K7VEU7
B	-14	GLY	-	EXPRESSION TAG	UNP K7VEU7
B	-13	SER	-	EXPRESSION TAG	UNP K7VEU7
B	-12	SER	-	EXPRESSION TAG	UNP K7VEU7
B	-11	HIS	-	EXPRESSION TAG	UNP K7VEU7
B	-10	HIS	-	EXPRESSION TAG	UNP K7VEU7
B	-9	HIS	-	EXPRESSION TAG	UNP K7VEU7
B	-8	HIS	-	EXPRESSION TAG	UNP K7VEU7
B	-7	HIS	-	EXPRESSION TAG	UNP K7VEU7
B	-6	HIS	-	EXPRESSION TAG	UNP K7VEU7
B	-5	SER	-	EXPRESSION TAG	UNP K7VEU7
B	-4	GLN	-	EXPRESSION TAG	UNP K7VEU7
B	-3	ASP	-	EXPRESSION TAG	UNP K7VEU7
B	-2	PRO	-	EXPRESSION TAG	UNP K7VEU7
B	-1	ASN	-	EXPRESSION TAG	UNP K7VEU7
B	0	SER	-	EXPRESSION TAG	UNP K7VEU7
B	18	GLU	-	EXPRESSION TAG	UNP K7VEU7
B	19	GLU	-	EXPRESSION TAG	UNP K7VEU7
B	20	LYS	-	EXPRESSION TAG	UNP K7VEU7
B	54	ASP	GLU	SEE REMARK 999	UNP K7VEU7
B	113	HIS	ARG	SEE REMARK 999	UNP K7VEU7
B	115	GLY	ASP	SEE REMARK 999	UNP K7VEU7
B	354	ARG	SER	SEE REMARK 999	UNP K7VEU7
B	391	ALA	GLY	SEE REMARK 999	UNP K7VEU7
C	-14	GLY	-	EXPRESSION TAG	UNP K7VEU7
C	-13	SER	-	EXPRESSION TAG	UNP K7VEU7
C	-12	SER	-	EXPRESSION TAG	UNP K7VEU7
C	-11	HIS	-	EXPRESSION TAG	UNP K7VEU7
C	-10	HIS	-	EXPRESSION TAG	UNP K7VEU7
C	-9	HIS	-	EXPRESSION TAG	UNP K7VEU7
C	-8	HIS	-	EXPRESSION TAG	UNP K7VEU7
C	-7	HIS	-	EXPRESSION TAG	UNP K7VEU7
C	-6	HIS	-	EXPRESSION TAG	UNP K7VEU7
C	-5	SER	-	EXPRESSION TAG	UNP K7VEU7
C	-4	GLN	-	EXPRESSION TAG	UNP K7VEU7
C	-3	ASP	-	EXPRESSION TAG	UNP K7VEU7
C	-2	PRO	-	EXPRESSION TAG	UNP K7VEU7
C	-1	ASN	-	EXPRESSION TAG	UNP K7VEU7
C	0	SER	-	EXPRESSION TAG	UNP K7VEU7
C	18	GLU	-	EXPRESSION TAG	UNP K7VEU7
C	19	GLU	-	EXPRESSION TAG	UNP K7VEU7

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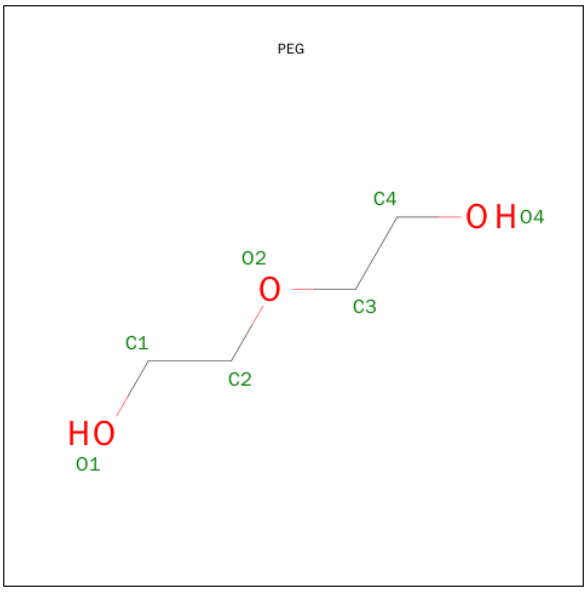
Chain	Residue	Modelled	Actual	Comment	Reference
C	20	LYS	-	EXPRESSION TAG	UNP K7VEU7
C	54	ASP	GLU	SEE REMARK 999	UNP K7VEU7
C	113	HIS	ARG	SEE REMARK 999	UNP K7VEU7
C	115	GLY	ASP	SEE REMARK 999	UNP K7VEU7
C	354	ARG	SER	SEE REMARK 999	UNP K7VEU7
C	391	ALA	GLY	SEE REMARK 999	UNP K7VEU7
D	-14	GLY	-	EXPRESSION TAG	UNP K7VEU7
D	-13	SER	-	EXPRESSION TAG	UNP K7VEU7
D	-12	SER	-	EXPRESSION TAG	UNP K7VEU7
D	-11	HIS	-	EXPRESSION TAG	UNP K7VEU7
D	-10	HIS	-	EXPRESSION TAG	UNP K7VEU7
D	-9	HIS	-	EXPRESSION TAG	UNP K7VEU7
D	-8	HIS	-	EXPRESSION TAG	UNP K7VEU7
D	-7	HIS	-	EXPRESSION TAG	UNP K7VEU7
D	-6	HIS	-	EXPRESSION TAG	UNP K7VEU7
D	-5	SER	-	EXPRESSION TAG	UNP K7VEU7
D	-4	GLN	-	EXPRESSION TAG	UNP K7VEU7
D	-3	ASP	-	EXPRESSION TAG	UNP K7VEU7
D	-2	PRO	-	EXPRESSION TAG	UNP K7VEU7
D	-1	ASN	-	EXPRESSION TAG	UNP K7VEU7
D	0	SER	-	EXPRESSION TAG	UNP K7VEU7
D	18	GLU	-	EXPRESSION TAG	UNP K7VEU7
D	19	GLU	-	EXPRESSION TAG	UNP K7VEU7
D	20	LYS	-	EXPRESSION TAG	UNP K7VEU7
D	54	ASP	GLU	SEE REMARK 999	UNP K7VEU7
D	113	HIS	ARG	SEE REMARK 999	UNP K7VEU7
D	115	GLY	ASP	SEE REMARK 999	UNP K7VEU7
D	354	ARG	SER	SEE REMARK 999	UNP K7VEU7
D	391	ALA	GLY	SEE REMARK 999	UNP K7VEU7

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

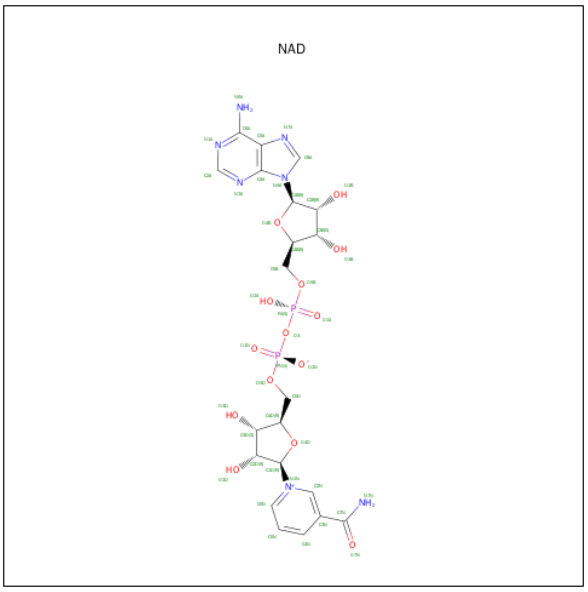
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

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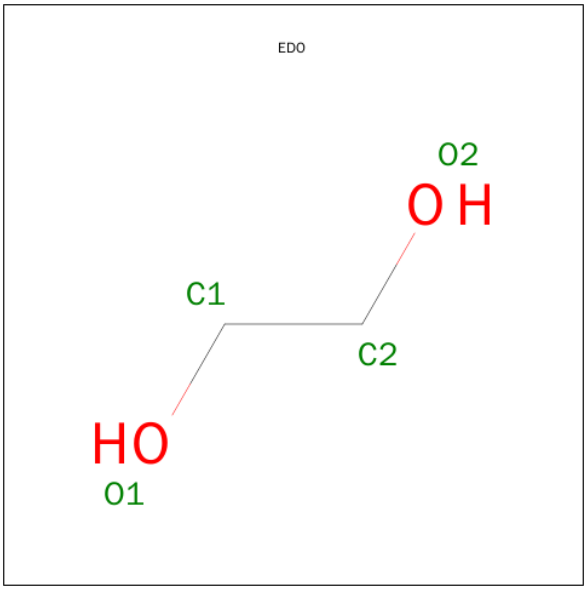
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- 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	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

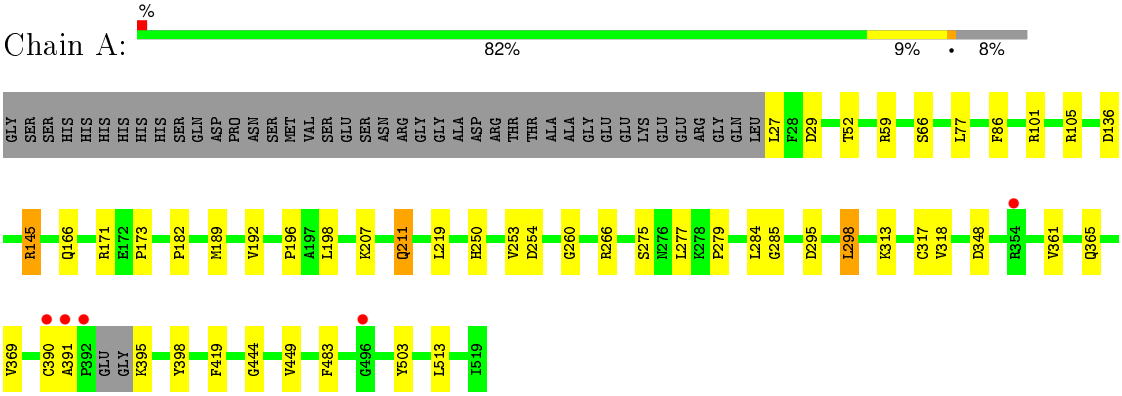
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	25	Total O 25 25	0	0
6	B	22	Total O 22 22	0	0
6	C	23	Total O 23 23	0	0
6	D	18	Total O 18 18	0	0

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 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.

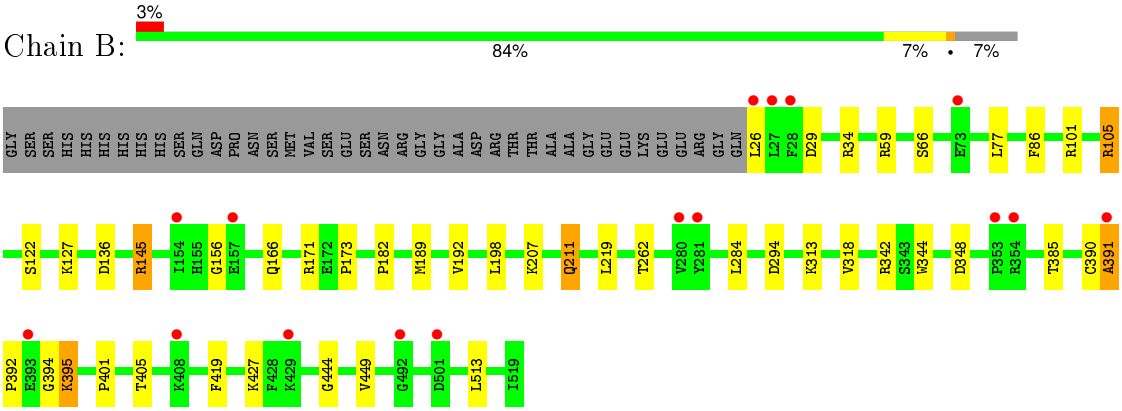
- Molecule 1: ZmALDH

Chain A:



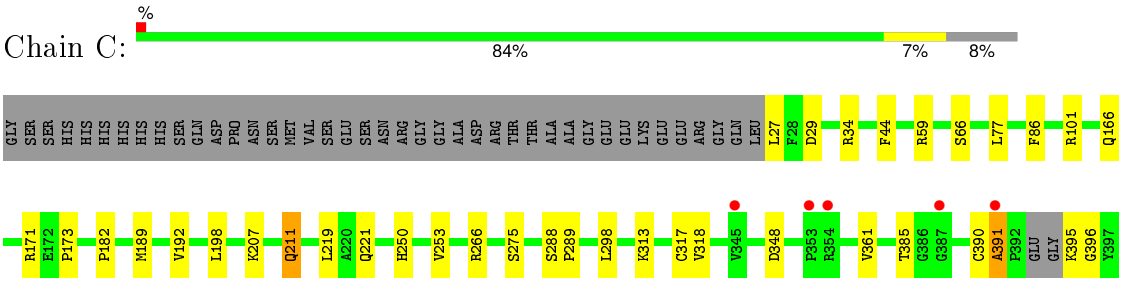
- Molecule 1: ZmALDH

Chain B:



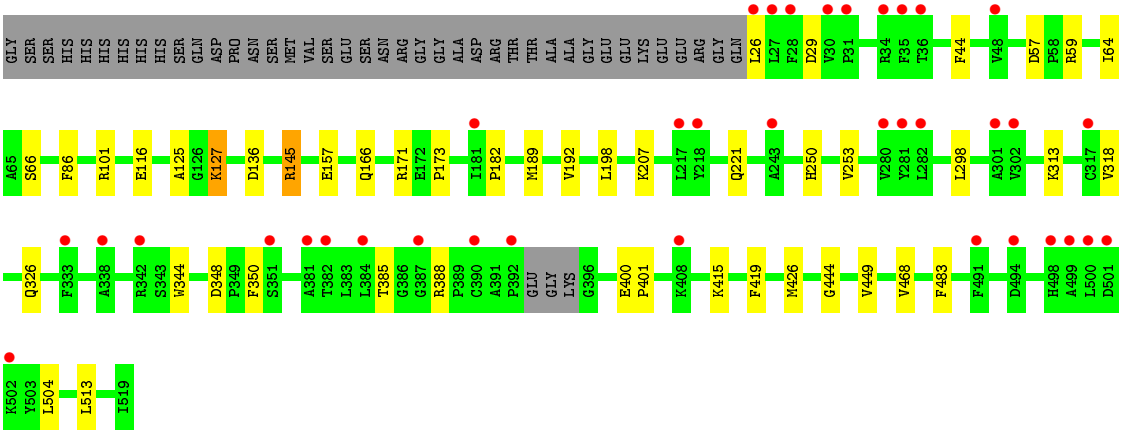
- Molecule 1: ZmALDH

Chain C:



• Molecule 1: ZmALDH

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	233.88Å 233.88Å 82.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.81 – 2.40 46.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.81-2.40) 99.7 (46.81-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.190 , 0.213 0.191 , 0.216	Depositor DCC
R_{free} test set	4380 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	67.5	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 49.9	EDS
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 87610 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15179	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, PEG, 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	0.47	0/3790	0.71	0/5133
1	B	0.46	0/3812	0.72	0/5164
1	C	0.45	0/3790	0.70	0/5133
1	D	0.46	0/3789	0.71	0/5133
All	All	0.46	0/15181	0.71	0/20563

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3713	0	3693	23	0
1	B	3734	0	3714	20	0
1	C	3713	0	3693	15	0
1	D	3712	0	3691	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	7	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	44	0	26	5	0
4	B	44	0	26	1	0
4	C	44	0	26	1	0
4	D	44	0	26	2	0
5	A	12	0	18	0	0
5	C	16	0	24	0	0
5	D	4	0	6	0	0
6	A	25	0	0	0	0
6	B	22	0	0	0	0
6	C	23	0	0	0	0
6	D	18	0	0	1	0
All	All	15179	0	14953	68	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 2.

All (68) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:ASP:HB2	1:D:64:ILE:HD11	1.53	0.88
1:A:211:GLN:HE21	1:A:211:GLN:H	1.28	0.79
1:B:211:GLN:H	1:B:211:GLN:HE21	1.30	0.78
1:C:211:GLN:HE21	1:C:211:GLN:H	1.31	0.77
1:B:391:ALA:HB3	1:B:392:PRO:HD3	1.71	0.72
1:D:326:GLN:HG2	6:D:711:HOH:O	1.97	0.64
1:A:101:ARG:HD3	1:B:145:ARG:HD3	1.83	0.59
1:B:394:GLY:CA	1:B:395:LYS:HB3	2.32	0.59
1:C:391:ALA:HB1	1:C:395:LYS:HA	1.88	0.56
1:A:145:ARG:HD3	1:B:101:ARG:HD3	1.88	0.55
1:B:390:CYS:HB2	1:B:391:ALA:HA	1.88	0.55
1:B:390:CYS:HB2	1:B:391:ALA:CA	2.39	0.53
1:D:171:ARG:HG3	1:D:504:LEU:HD13	1.90	0.52
1:D:26:LEU:HD13	1:D:350:PHE:HB3	1.92	0.52
1:C:101:ARG:HD3	1:D:145:ARG:HD3	1.92	0.51
1:A:52:THR:H	3:A:602:PEG:H12	1.74	0.51
1:B:394:GLY:HA3	1:B:395:LYS:HB3	1.94	0.49
1:A:391:ALA:H	1:A:398:TYR:HB2	1.78	0.48
1:D:182:PRO:HD2	1:D:189:MET:HG3	1.95	0.48
1:A:182:PRO:HD2	1:A:189:MET:HG3	1.96	0.48
1:C:182:PRO:HD2	1:C:189:MET:HG3	1.96	0.47
1:B:156:GLY:HA2	1:B:171:ARG:HH11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ARG:HD2	1:A:348:ASP:OD1	2.15	0.47
1:C:391:ALA:H	1:C:398:TYR:HB2	1.80	0.47
1:B:166:GLN:HB2	1:B:513:LEU:HD21	1.97	0.47
1:A:483:PHE:HE2	4:A:603:NAD:H72N	1.63	0.46
1:A:317:CYS:SG	4:A:603:NAD:C4N	3.03	0.46
1:D:125:ALA:HB3	1:D:127:LYS:HD3	1.96	0.46
1:B:390:CYS:HB2	1:B:391:ALA:HB2	1.96	0.46
1:B:59:ARG:HD2	1:B:348:ASP:OD1	2.15	0.46
1:D:388:ARG:O	1:D:400:GLU:HG2	2.16	0.45
1:D:44:PHE:HE2	1:D:221:GLN:HE21	1.63	0.45
1:C:166:GLN:HB2	1:C:513:LEU:HD21	1.99	0.45
1:D:59:ARG:HD2	1:D:348:ASP:OD1	2.17	0.45
1:C:44:PHE:HE2	1:C:221:GLN:HE21	1.64	0.44
1:A:285:GLY:HA2	4:A:603:NAD:O2D	2.17	0.44
1:A:196:PRO:HG2	1:A:503:TYR:HE2	1.82	0.44
1:C:86:PHE:HE1	1:C:173:PRO:HB2	1.83	0.44
1:D:166:GLN:HB2	1:D:513:LEU:HD21	2.00	0.44
1:A:419:PHE:CE1	4:A:603:NAD:H2D	2.53	0.44
1:A:166:GLN:HB2	1:A:513:LEU:HD21	2.00	0.44
1:B:182:PRO:HD2	1:B:189:MET:HG3	1.99	0.44
1:A:86:PHE:HE1	1:A:173:PRO:HB2	1.82	0.43
1:D:344:TRP:CD1	1:D:401:PRO:HG3	2.54	0.43
1:C:317:CYS:SG	4:C:606:NAD:C4N	3.06	0.43
1:A:275:SER:O	1:C:266:ARG:NH2	2.52	0.43
1:A:277:LEU:HD21	1:C:266:ARG:HA	1.99	0.43
1:B:86:PHE:HE1	1:B:173:PRO:HB2	1.83	0.43
1:A:266:ARG:NH2	1:C:275:SER:O	2.51	0.43
1:A:483:PHE:HE2	4:A:603:NAD:N7N	2.17	0.43
1:D:419:PHE:CE1	4:D:603:NAD:H2D	2.54	0.43
1:C:288:SER:HA	1:C:289:PRO:HD3	1.99	0.42
1:C:59:ARG:HD2	1:C:348:ASP:OD1	2.19	0.42
1:C:250:HIS:HB3	1:C:253:VAL:HG23	2.02	0.42
1:A:365:GLN:O	1:A:369:VAL:HG23	2.20	0.42
1:A:298:LEU:HA	1:A:298:LEU:HD12	1.91	0.42
1:A:254:ASP:O	1:A:279:PRO:HD2	2.20	0.41
1:D:250:HIS:HB3	1:D:253:VAL:HG23	2.02	0.41
1:B:390:CYS:HB2	1:B:391:ALA:CB	2.50	0.41
1:A:260:GLY:O	1:A:284:LEU:HA	2.20	0.41
1:D:483:PHE:HE2	4:D:603:NAD:H72N	1.69	0.41
1:D:86:PHE:HE1	1:D:173:PRO:HB2	1.85	0.41
1:B:262:THR:HA	1:B:284:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:SER:HA	1:B:127:LYS:HB2	2.03	0.41
1:A:250:HIS:HB3	1:A:253:VAL:HG23	2.02	0.40
1:B:344:TRP:CD1	1:B:401:PRO:HG3	2.56	0.40
1:B:105:ARG:HD2	1:B:105:ARG:HA	1.86	0.40
1:B:419:PHE:CE1	4:B:602:NAD:H2D	2.57	0.40

There are no symmetry-related clashes.

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	487/534 (91%)	468 (96%)	18 (4%)	1 (0%)	52	69
1	B	492/534 (92%)	470 (96%)	19 (4%)	3 (1%)	30	43
1	C	487/534 (91%)	468 (96%)	16 (3%)	3 (1%)	30	43
1	D	487/534 (91%)	470 (96%)	16 (3%)	1 (0%)	52	69
All	All	1953/2136 (91%)	1876 (96%)	69 (4%)	8 (0%)	39	56

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	391	ALA
1	B	395	LYS
1	C	391	ALA
1	C	396	GLY
1	A	444	GLY
1	D	444	GLY
1	B	444	GLY
1	C	361	VAL

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	381/415 (92%)	360 (94%)	21 (6%)	27	42
1	B	383/415 (92%)	362 (94%)	21 (6%)	27	42
1	C	381/415 (92%)	362 (95%)	19 (5%)	30	48
1	D	381/415 (92%)	362 (95%)	19 (5%)	30	48
All	All	1526/1660 (92%)	1446 (95%)	80 (5%)	29	45

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	29	ASP
1	A	66	SER
1	A	77	LEU
1	A	105	ARG
1	A	136	ASP
1	A	145	ARG
1	A	171	ARG
1	A	192	VAL
1	A	198	LEU
1	A	207	LYS
1	A	211	GLN
1	A	219	LEU
1	A	295	ASP
1	A	298	LEU
1	A	313	LYS
1	A	318	VAL
1	A	361	VAL
1	A	390	CYS
1	A	395	LYS
1	A	449	VAL
1	B	26	LEU
1	B	29	ASP
1	B	34	ARG

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Mol	Chain	Res	Type
1	B	66	SER
1	B	77	LEU
1	B	105	ARG
1	B	136	ASP
1	B	145	ARG
1	B	192	VAL
1	B	198	LEU
1	B	207	LYS
1	B	211	GLN
1	B	219	LEU
1	B	294	ASP
1	B	313	LYS
1	B	318	VAL
1	B	342	ARG
1	B	385	THR
1	B	405	THR
1	B	427	LYS
1	B	449	VAL
1	C	27	LEU
1	C	29	ASP
1	C	34	ARG
1	C	66	SER
1	C	77	LEU
1	C	171	ARG
1	C	192	VAL
1	C	198	LEU
1	C	207	LYS
1	C	211	GLN
1	C	219	LEU
1	C	298	LEU
1	C	313	LYS
1	C	318	VAL
1	C	385	THR
1	C	390	CYS
1	C	408	LYS
1	C	426	MET
1	C	449	VAL
1	D	29	ASP
1	D	66	SER
1	D	101	ARG
1	D	116	GLU
1	D	127	LYS

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Mol	Chain	Res	Type
1	D	136	ASP
1	D	145	ARG
1	D	157	GLU
1	D	192	VAL
1	D	198	LEU
1	D	207	LYS
1	D	298	LEU
1	D	313	LYS
1	D	318	VAL
1	D	385	THR
1	D	415	LYS
1	D	426	MET
1	D	449	VAL
1	D	468	VAL

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	41	ASN
1	A	211	GLN
1	A	360	GLN
1	B	211	GLN
1	C	211	GLN
1	C	221	GLN
1	D	41	ASN
1	D	221	GLN
1	D	365	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 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	PEG	A	602	-	6,6,6	0.17	0	5,5,5	0.05	0
4	NAD	A	603	-	38,48,48	0.58	0	47,73,73	0.70	1 (2%)
5	EDO	A	604	-	3,3,3	0.68	0	2,2,2	0.37	0
5	EDO	A	605	-	3,3,3	0.58	0	2,2,2	0.49	0
5	EDO	A	606	-	3,3,3	0.66	0	2,2,2	0.40	0
4	NAD	B	602	-	38,48,48	0.56	0	47,73,73	0.66	0
5	EDO	C	602	-	3,3,3	0.60	0	2,2,2	0.20	0
5	EDO	C	603	-	3,3,3	0.56	0	2,2,2	0.50	0
5	EDO	C	604	-	3,3,3	0.67	0	2,2,2	0.32	0
5	EDO	C	605	-	3,3,3	0.58	0	2,2,2	0.42	0
4	NAD	C	606	-	38,48,48	0.58	0	47,73,73	0.77	0
5	EDO	D	602	-	3,3,3	0.61	0	2,2,2	0.37	0
4	NAD	D	603	-	38,48,48	0.58	0	47,73,73	0.70	1 (2%)

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	PEG	A	602	-	-	0/4/4/4	0/0/0/0
4	NAD	A	603	-	-	0/22/62/62	0/5/5/5
5	EDO	A	604	-	-	0/1/1/1	0/0/0/0
5	EDO	A	605	-	-	0/1/1/1	0/0/0/0
5	EDO	A	606	-	-	0/1/1/1	0/0/0/0
4	NAD	B	602	-	-	0/22/62/62	0/5/5/5
5	EDO	C	602	-	-	0/1/1/1	0/0/0/0
5	EDO	C	603	-	-	0/1/1/1	0/0/0/0
5	EDO	C	604	-	-	0/1/1/1	0/0/0/0
5	EDO	C	605	-	-	0/1/1/1	0/0/0/0
4	NAD	C	606	-	-	0/22/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	D	602	-	-	0/1/1/1	0/0/0/0
4	NAD	D	603	-	-	0/22/62/62	0/5/5/5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	603	NAD	O4D-C1D-N1N	2.05	110.38	108.13
4	A	603	NAD	C4D-O4D-C1D	2.26	112.20	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	PEG	1	0
4	A	603	NAD	5	0
4	B	602	NAD	1	0
4	C	606	NAD	1	0
4	D	603	NAD	2	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, 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	491/534 (91%)	-0.16	5 (1%)	84	83	53, 70, 97, 124	0
1	B	494/534 (92%)	0.03	16 (3%)	51	51	58, 80, 110, 131	0
1	C	491/534 (91%)	-0.08	5 (1%)	84	83	56, 78, 102, 132	0
1	D	491/534 (91%)	0.34	37 (7%)	17	17	59, 95, 131, 156	0
All	All	1967/2136 (92%)	0.03	63 (3%)	51	51	53, 80, 118, 156	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	391	ALA	6.0
1	A	392	PRO	5.0
1	B	26	LEU	4.5
1	C	391	ALA	4.4
1	D	387	GLY	4.3
1	B	393	GLU	4.3
1	D	35	PHE	4.3
1	D	34	ARG	4.2
1	B	28	PHE	4.1
1	B	354	ARG	4.0
1	B	391	ALA	3.9
1	C	354	ARG	3.9
1	D	381	ALA	3.8
1	D	27	LEU	3.6
1	D	36	THR	3.6
1	D	28	PHE	3.6
1	B	27	LEU	3.6
1	D	30	VAL	3.6
1	C	353	PRO	3.4
1	D	390	CYS	3.3
1	D	351	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	282	LEU	3.2
1	D	281	TYR	3.2
1	D	48	VAL	3.2
1	D	384	LEU	3.0
1	D	218	TYR	3.0
1	B	353	PRO	3.0
1	D	491	PHE	2.8
1	D	280	VAL	2.7
1	B	429	LYS	2.7
1	D	342	ARG	2.7
1	B	73	GLU	2.7
1	C	387	GLY	2.7
1	C	345	VAL	2.6
1	D	382	THR	2.6
1	B	154	ILE	2.6
1	D	333	PHE	2.5
1	D	217	LEU	2.5
1	A	390	CYS	2.5
1	D	338	ALA	2.5
1	D	31	PRO	2.4
1	D	243	ALA	2.4
1	B	501	ASP	2.4
1	D	302	VAL	2.4
1	D	301	ALA	2.4
1	D	408	LYS	2.3
1	B	280	VAL	2.3
1	B	281	TYR	2.3
1	D	181	ILE	2.3
1	B	408	LYS	2.3
1	D	26	LEU	2.3
1	D	498	HIS	2.3
1	B	492	GLY	2.2
1	D	500	LEU	2.2
1	D	392	PRO	2.2
1	B	157	GLU	2.2
1	D	502	LYS	2.2
1	D	501	ASP	2.2
1	A	354	ARG	2.1
1	D	499	ALA	2.1
1	D	494	ASP	2.1
1	D	317	CYS	2.0
1	A	496	GLY	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, 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	LLDF	B-factors(Å^2)	Q<0.9
5	EDO	C	602	4/4	0.94	0.35	10.97	82,83,83,85	0
5	EDO	C	603	4/4	0.77	0.46	10.27	108,109,109,109	0
5	EDO	A	604	4/4	0.81	0.55	10.01	82,83,85,86	0
5	EDO	A	606	4/4	0.89	0.25	3.30	104,105,105,106	0
5	EDO	D	602	4/4	0.87	0.22	2.07	92,97,100,100	0
5	EDO	A	605	4/4	0.89	0.17	1.43	100,101,101,102	0
3	PEG	A	602	7/7	0.72	0.22	1.27	102,103,107,108	0
2	NA	B	601	1/1	0.78	0.13	-0.30	84,84,84,84	0
4	NAD	A	603	44/44	0.96	0.12	-0.58	66,73,82,86	0
4	NAD	D	603	44/44	0.94	0.14	-0.59	94,105,116,121	0
4	NAD	B	602	44/44	0.97	0.12	-0.62	76,85,89,93	0
4	NAD	C	606	44/44	0.97	0.14	-0.67	63,71,81,84	0
2	NA	D	601	1/1	0.71	0.09	-1.00	104,104,104,104	0
2	NA	C	601	1/1	0.85	0.09	-1.34	84,84,84,84	0
2	NA	A	601	1/1	0.96	0.07	-1.73	79,79,79,79	0
5	EDO	C	605	4/4	0.91	0.41	-	91,93,95,97	0
5	EDO	C	604	4/4	0.69	0.20	-	88,90,92,93	0

6.5 Other polymers (i)

There are no such residues in this entry.