Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:26 AM GMT

PDB ID	:	2QNE
Title	:	Crystal structure of putative methyltransferase (ZP_00558420.1) from Desulfitobacterium hafniense Y51 at 2.30 A resolution
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	2007-07-18
Resolution	:	2.30 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:

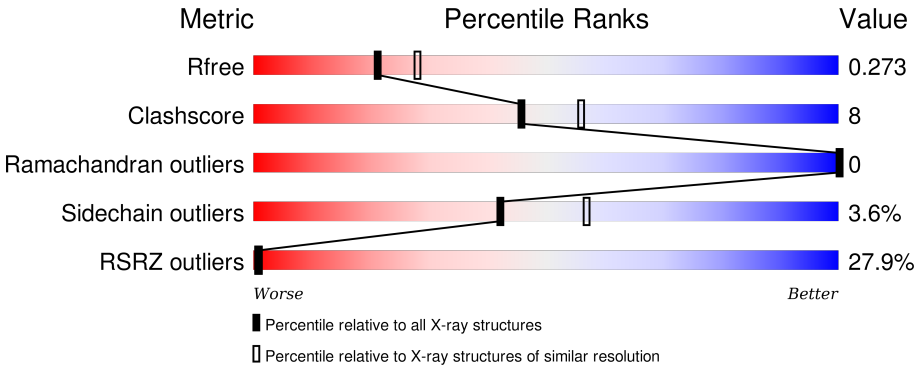
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	495	15% 83% 12%
1	B	495	37% 76% 18%

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
2	EDO	A	477	-	-	-	X
2	EDO	A	479	-	-	-	X
2	EDO	A	481	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7406 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 Putative methyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	Se	0	2	0
			3625	2302	600	701	2	20			
1	B	475	Total	C	N	O	S	Se	0	3	0
			3596	2279	598	697	2	20			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MSE	-	LEADER SEQUENCE	UNP Q24SP7
A	-17	GLY	-	LEADER SEQUENCE	UNP Q24SP7
A	-16	SER	-	LEADER SEQUENCE	UNP Q24SP7
A	-15	ASP	-	LEADER SEQUENCE	UNP Q24SP7
A	-14	LYS	-	LEADER SEQUENCE	UNP Q24SP7
A	-13	ILE	-	LEADER SEQUENCE	UNP Q24SP7
A	-12	HIS	-	LEADER SEQUENCE	UNP Q24SP7
A	-11	HIS	-	LEADER SEQUENCE	UNP Q24SP7
A	-10	HIS	-	LEADER SEQUENCE	UNP Q24SP7
A	-9	HIS	-	LEADER SEQUENCE	UNP Q24SP7
A	-8	HIS	-	LEADER SEQUENCE	UNP Q24SP7
A	-7	HIS	-	LEADER SEQUENCE	UNP Q24SP7
A	-6	GLU	-	LEADER SEQUENCE	UNP Q24SP7
A	-5	ASN	-	LEADER SEQUENCE	UNP Q24SP7
A	-4	LEU	-	LEADER SEQUENCE	UNP Q24SP7
A	-3	TYR	-	LEADER SEQUENCE	UNP Q24SP7
A	-2	PHE	-	LEADER SEQUENCE	UNP Q24SP7
A	-1	GLN	-	LEADER SEQUENCE	UNP Q24SP7
A	0	GLY	-	LEADER SEQUENCE	UNP Q24SP7
B	-18	MSE	-	LEADER SEQUENCE	UNP Q24SP7
B	-17	GLY	-	LEADER SEQUENCE	UNP Q24SP7
B	-16	SER	-	LEADER SEQUENCE	UNP Q24SP7
B	-15	ASP	-	LEADER SEQUENCE	UNP Q24SP7
B	-14	LYS	-	LEADER SEQUENCE	UNP Q24SP7
B	-13	ILE	-	LEADER SEQUENCE	UNP Q24SP7

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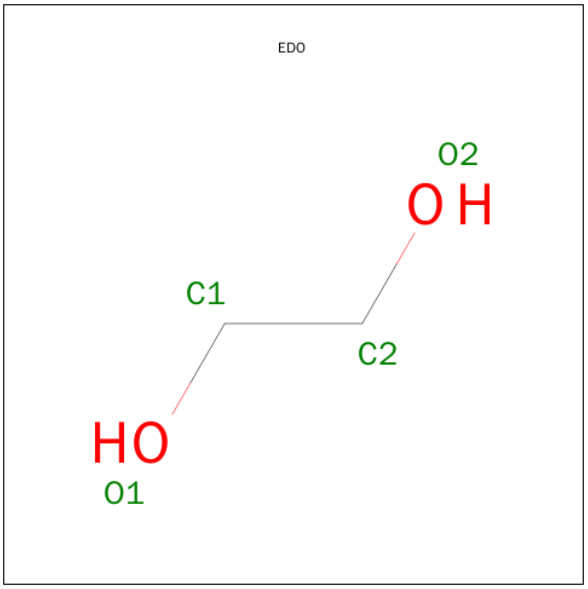
Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	LEADER SEQUENCE	UNP Q24SP7
B	-11	HIS	-	LEADER SEQUENCE	UNP Q24SP7
B	-10	HIS	-	LEADER SEQUENCE	UNP Q24SP7
B	-9	HIS	-	LEADER SEQUENCE	UNP Q24SP7
B	-8	HIS	-	LEADER SEQUENCE	UNP Q24SP7
B	-7	HIS	-	LEADER SEQUENCE	UNP Q24SP7
B	-6	GLU	-	LEADER SEQUENCE	UNP Q24SP7
B	-5	ASN	-	LEADER SEQUENCE	UNP Q24SP7
B	-4	LEU	-	LEADER SEQUENCE	UNP Q24SP7
B	-3	TYR	-	LEADER SEQUENCE	UNP Q24SP7
B	-2	PHE	-	LEADER SEQUENCE	UNP Q24SP7
B	-1	GLN	-	LEADER SEQUENCE	UNP Q24SP7
B	0	GLY	-	LEADER SEQUENCE	UNP Q24SP7

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



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

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

- Molecule 3 is water.

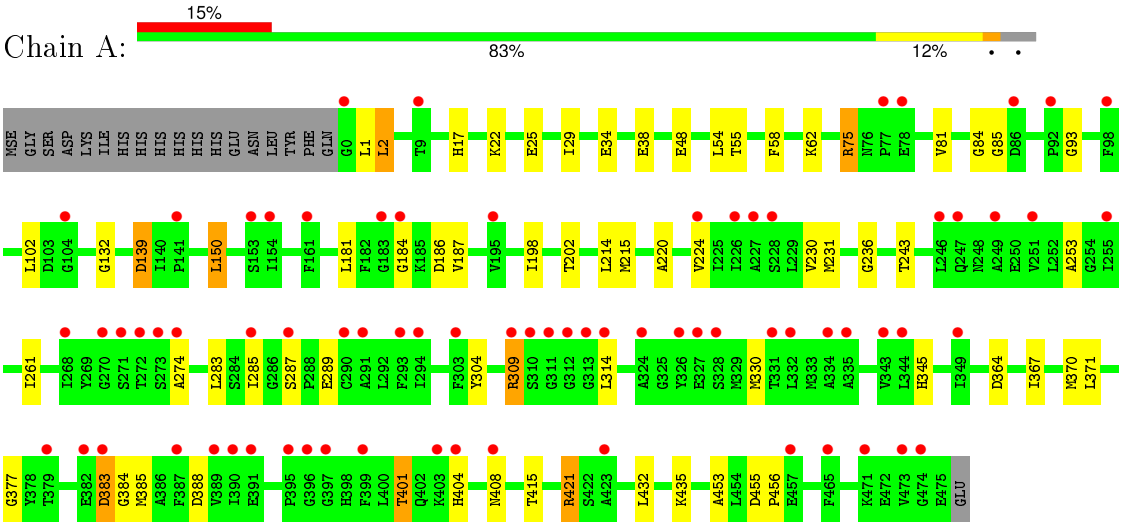
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	120	Total O 120 120	0	0
3	B	25	Total O 25 25	0	0

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.

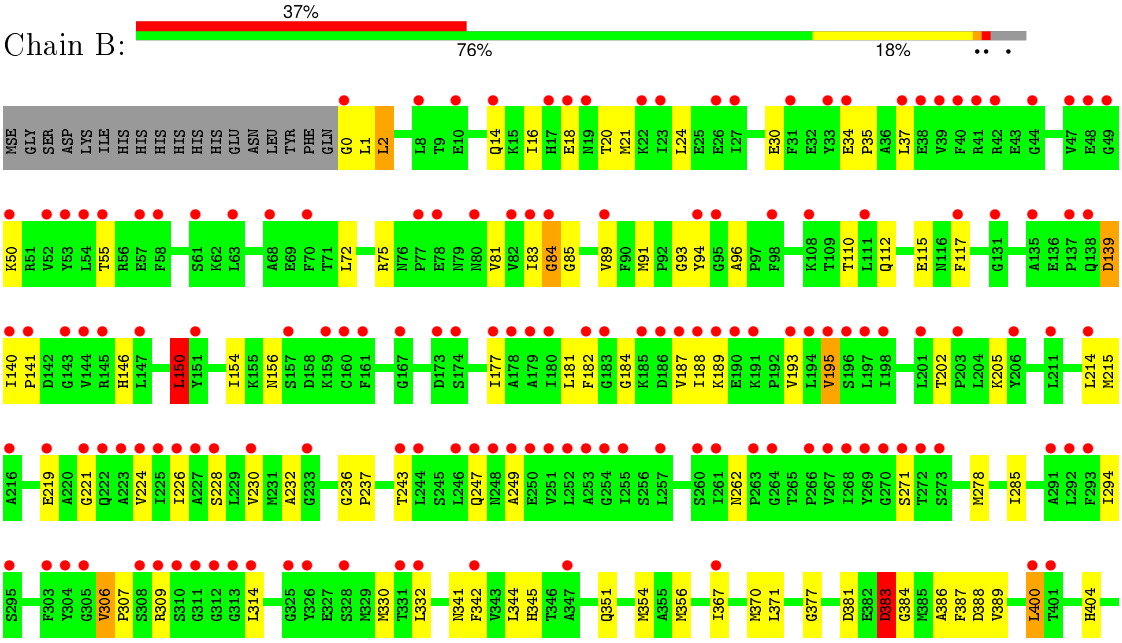
- Molecule 1: Putative methyltransferase

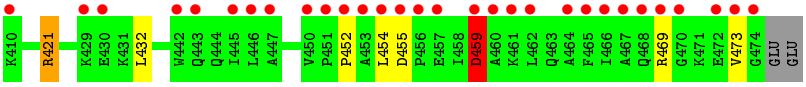
Chain A:



- Molecule 1: Putative methyltransferase

Chain B:




K410
R421
K429
E430
K431
L432
W442
Q443
Q444
L445
L446
A447
V450
P451
P452
A453
L454
D455
P456
E457
I458
D459
A460
K461
L462
Q463
A464
F465
I466
A467
Q468
R469
G470
K471
E472
V473
G474
GLU
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	123.86Å 123.86Å 122.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.75 – 2.30 28.92 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.75-2.30) 99.7 (28.92-2.48)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.158 , 0.204 0.256 , 0.273	Depositor DCC
R_{free} test set	1934 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	49.1	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 64.5	EDS
Estimated twinning fraction	0.065 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 38697 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7406	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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: EDO

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	0.80	1/3676 (0.0%)	0.87	9/4939 (0.2%)
1	B	0.71	4/3648 (0.1%)	0.78	7/4908 (0.1%)
All	All	0.76	5/7324 (0.1%)	0.82	16/9847 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	5
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	GLN	CD-NE2	10.56	1.59	1.32
1	B	181	LEU	C-O	10.03	1.42	1.23
1	B	459	ASP	CG-OD2	8.67	1.45	1.25
1	A	139	ASP	CB-CG	-5.61	1.40	1.51
1	B	459	ASP	CG-OD1	5.06	1.36	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	112	GLN	OE1-CD-NE2	-15.58	86.06	121.90
1	B	112	GLN	CG-CD-NE2	13.68	149.54	116.70
1	A	75	ARG	NE-CZ-NH2	-12.04	114.28	120.30
1	A	75	ARG	NE-CZ-NH1	10.91	125.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	421	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	A	421	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	A	421	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	A	139	ASP	CB-CG-OD1	-7.13	111.89	118.30
1	A	150	LEU	CA-CB-CG	6.78	130.89	115.30
1	B	150	LEU	CA-CB-CG	6.38	129.98	115.30
1	A	220	ALA	C-N-CA	-5.90	109.92	122.30
1	B	459	ASP	CB-CG-OD1	-5.79	113.08	118.30
1	A	84	GLY	C-N-CA	-5.68	110.37	122.30
1	B	84	GLY	N-CA-C	5.19	126.08	113.10
1	B	383	ASP	N-CA-C	5.09	124.73	111.00
1	A	1	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	85	GLY	Peptide
1	B	383	ASP	Peptide
1	B	459	ASP	Sidechain
1	B	55	THR	Mainchain
1	B	83	ILE	Peptide
1	B	85	GLY	Peptide

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	3625	0	3544	47	0
1	B	3596	0	3466	76	0
2	A	28	0	42	3	0
2	B	12	0	18	1	0
3	A	120	0	0	2	0
3	B	25	0	0	1	0
All	All	7406	0	7070	111	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 8.

All (111) 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:B:454:LEU:HD23	1:B:459:ASP:HB3	1.49	0.93
1:A:330[A]:MSE:HE3	1:B:371:LEU:HD23	1.59	0.82
1:A:370:MSE:HE2	1:B:330[A]:MSE:SE	2.30	0.81
1:A:330[B]:MSE:SE	1:B:370:MSE:HE2	2.32	0.80
1:B:454:LEU:CD2	1:B:459:ASP:HB3	2.14	0.77
1:B:84:GLY:HA2	1:B:341:ASN:ND2	2.03	0.73
1:A:330[A]:MSE:HE3	1:B:371:LEU:CD2	2.19	0.72
1:A:421:ARG:HD2	3:B:497:HOH:O	1.88	0.72
3:A:568:HOH:O	1:B:421:ARG:HD2	1.89	0.72
1:B:75:ARG:NH1	1:B:154:ILE:O	2.22	0.71
1:A:385:MSE:HE1	1:B:16:ILE:HD13	1.75	0.69
1:A:330[A]:MSE:CE	1:B:371:LEU:HD23	2.27	0.65
1:A:214:LEU:C	1:A:214:LEU:HD23	2.17	0.65
1:B:0:GLY:O	1:B:1:LEU:HD22	1.98	0.63
1:B:35:PRO:CB	1:B:215:MSE:HE1	2.29	0.63
1:B:146:HIS:O	1:B:150:LEU:HD22	1.98	0.63
1:A:383:ASP:N	1:A:384:GLY:HA3	2.13	0.63
1:B:232:ALA:HA	1:B:243:THR:HG21	1.82	0.62
1:B:81:VAL:HG13	1:B:89:VAL:HG11	1.82	0.62
1:A:330[B]:MSE:HE1	1:B:370:MSE:CE	2.29	0.62
1:B:224:VAL:HG23	1:B:226:ILE:HD11	1.81	0.62
1:B:214:LEU:HD23	1:B:214:LEU:C	2.20	0.61
1:A:184:GLY:O	1:A:187:VAL:HG12	2.02	0.60
1:B:14:GLN:O	1:B:18:GLU:HG2	2.02	0.59
1:B:20:THR:HG22	1:B:21:MSE:HE2	1.86	0.58
1:B:383:ASP:O	1:B:404:HIS:NE2	2.31	0.58
1:A:75:ARG:HD3	3:A:583:HOH:O	2.04	0.58
1:A:371:LEU:HD23	1:B:330[B]:MSE:HE3	1.85	0.58
1:A:93:GLY:HA2	1:A:345:HIS:HA	1.85	0.58
1:B:306:VAL:HG22	1:B:307:PRO:HD2	1.86	0.57
1:B:150:LEU:CD2	1:B:177:ILE:HD13	2.35	0.57
1:A:214:LEU:O	1:A:214:LEU:HD23	2.05	0.57
1:B:81:VAL:CG1	1:B:89:VAL:HG11	2.35	0.57
1:B:93:GLY:HA2	1:B:345:HIS:HA	1.88	0.56
1:B:224:VAL:HG23	1:B:226:ILE:CD1	2.36	0.56
1:A:2:LEU:HD13	1:A:377:GLY:HA3	1.88	0.55
1:B:35:PRO:HB3	1:B:215:MSE:HE1	1.89	0.55
1:A:330[B]:MSE:CE	1:B:370:MSE:CE	2.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:GLY:HA2	1:B:341:ASN:CG	2.28	0.54
1:A:17:HIS:HD2	1:A:304:TYR:OH	1.90	0.54
1:B:224:VAL:CG2	1:B:226:ILE:HD11	2.38	0.53
1:B:214:LEU:HD23	1:B:214:LEU:O	2.10	0.52
1:B:94:TYR:HB2	1:B:344:LEU:HD11	1.91	0.52
1:A:75:ARG:HG2	1:A:181:LEU:HD11	1.91	0.52
1:B:237:PRO:O	1:B:243:THR:HG23	2.10	0.51
1:A:230:VAL:CG1	1:A:243:THR:HG23	2.40	0.51
1:B:454:LEU:O	1:B:455:ASP:C	2.48	0.51
1:B:110:THR:HB	1:B:139:ASP:OD2	2.10	0.51
1:B:184:GLY:O	1:B:187:VAL:CG1	2.60	0.50
1:B:72:LEU:HD13	1:B:195:VAL:HG22	1.93	0.50
1:B:34:GLU:HB3	1:B:35:PRO:HD3	1.93	0.50
1:A:198:ILE:HD13	1:A:224:VAL:HB	1.93	0.50
1:A:231:MSE:HG2	1:A:283:LEU:HD13	1.93	0.50
1:A:75:ARG:NH2	1:A:453:ALA:O	2.45	0.49
1:A:309:ARG:HH22	2:A:478:EDO:H21	1.77	0.49
1:B:72:LEU:CD1	1:B:195:VAL:HG22	2.43	0.48
1:A:22:LYS:HG2	1:B:387:PHE:CE1	2.47	0.48
1:B:351:GLN:O	1:B:354:MSE:HB2	2.13	0.48
1:B:2:LEU:HD13	1:B:377:GLY:HA3	1.95	0.48
1:A:330[A]:MSE:SE	1:B:370:MSE:HE2	2.64	0.48
1:B:140:ILE:HG23	1:B:141:PRO:HD2	1.94	0.48
1:A:102:LEU:CD1	1:A:435:LYS:HG3	2.44	0.48
1:B:75:ARG:NH2	1:B:452:PRO:HB2	2.29	0.47
1:A:102:LEU:HD11	1:A:435:LYS:HG2	1.95	0.47
1:B:91:MSE:HE1	1:B:342:PHE:CZ	2.49	0.47
1:B:294:ILE:HG12	2:B:479:EDO:H21	1.96	0.47
1:B:226:ILE:N	1:B:226:ILE:HD12	2.29	0.47
1:B:182:PHE:CD1	1:B:193:VAL:HG21	2.49	0.46
1:A:230:VAL:CG1	1:A:236:GLY:HA3	2.46	0.46
1:A:102:LEU:CD1	1:A:435:LYS:CG	2.94	0.46
1:B:30:GLU:HB2	1:B:205:LYS:HG2	1.97	0.46
1:A:132:GLY:HA2	2:A:477:EDO:H22	1.98	0.46
1:B:332:LEU:HD23	1:B:367:ILE:HG13	1.98	0.45
1:A:274:ALA:HB3	1:A:283:LEU:HD11	1.99	0.45
1:B:381:ASP:O	1:B:384:GLY:HA3	2.17	0.45
1:B:96:ALA:HB3	1:B:356:MSE:HG2	2.00	0.44
1:B:202:THR:HG21	1:B:230:VAL:HG22	1.99	0.44
1:B:37:LEU:HD11	1:B:50:LYS:HA	1.98	0.44
1:A:364:ASP:HA	1:A:367:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LEU:HD13	1:B:195:VAL:CG2	2.48	0.44
1:B:187:VAL:HG13	1:B:188:ILE:HG23	2.00	0.44
1:B:2:LEU:HD13	1:B:377:GLY:CA	2.48	0.43
1:A:285:ILE:HD12	1:A:314:LEU:HB3	1.99	0.43
1:B:189:LYS:HA	1:B:221:GLY:HA3	1.99	0.43
1:B:232:ALA:CA	1:B:243:THR:HG21	2.48	0.43
1:A:401:THR:O	1:A:401:THR:HG23	2.18	0.43
1:A:287:SER:HB2	1:A:289:GLU:OE1	2.19	0.43
1:B:230:VAL:CG1	1:B:236:GLY:HA3	2.49	0.43
1:A:370:MSE:CE	1:B:330[A]:MSE:HE1	2.49	0.43
1:A:455:ASP:HA	1:A:456:PRO:HD3	1.91	0.43
1:B:115:GLU:HG3	1:B:156:ASN:ND2	2.35	0.42
1:B:35:PRO:HB2	1:B:215:MSE:HE1	2.02	0.42
1:A:202:THR:HG21	1:A:230:VAL:HG22	2.00	0.42
2:A:479:EDO:H12	1:B:400:LEU:HD12	2.02	0.42
1:B:469:ARG:HH12	1:B:473:VAL:HG23	1.85	0.42
1:B:306:VAL:HG22	1:B:307:PRO:CD	2.47	0.41
1:A:214:LEU:C	1:A:214:LEU:CD2	2.87	0.41
1:A:54:LEU:HD22	1:A:58:PHE:CE2	2.55	0.41
1:A:29:ILE:HD12	1:A:253:ALA:CB	2.50	0.41
1:B:386:ALA:HB1	1:B:389:VAL:CG1	2.50	0.41
1:B:285:ILE:HD12	1:B:314:LEU:HD22	2.03	0.41
1:B:24:LEU:HD21	1:B:249:ALA:O	2.20	0.41
1:A:34:GLU:O	1:A:38[B]:GLU:HG3	2.21	0.41
1:A:215:MSE:HG2	1:A:261:ILE:CD1	2.51	0.41
1:A:25:GLU:HG2	1:A:55:THR:HA	2.03	0.40
1:B:247:GLN:NE2	1:B:271:SER:OG	2.54	0.40
1:A:383:ASP:O	1:A:404:HIS:NE2	2.53	0.40
1:B:214:LEU:CD2	1:B:214:LEU:C	2.87	0.40
1:A:102:LEU:HD12	1:A:435:LYS:HG3	2.04	0.40
1:B:117:PHE:CE1	1:B:356:MSE:HE3	2.57	0.40
1:B:262:ASN:C	1:B:262:ASN:OD1	2.59	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	476/495 (96%)	463 (97%)	13 (3%)	0	100	100
1	B	476/495 (96%)	459 (96%)	17 (4%)	0	100	100
All	All	952/990 (96%)	922 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	372/385 (97%)	358 (96%)	14 (4%)	40	54
1	B	364/385 (94%)	352 (97%)	12 (3%)	45	61
All	All	736/770 (96%)	710 (96%)	26 (4%)	42	58

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	48	GLU
1	A	62	LYS
1	A	81	VAL
1	A	139	ASP
1	A	150	LEU
1	A	186	ASP
1	A	309	ARG
1	A	383	ASP
1	A	388	ASP
1	A	401	THR
1	A	408	ASN
1	A	415	THR
1	A	432	LEU

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Mol	Chain	Res	Type
1	B	2	LEU
1	B	139	ASP
1	B	150	LEU
1	B	195	VAL
1	B	219	GLU
1	B	228	SER
1	B	278	MSE
1	B	306	VAL
1	B	309	ARG
1	B	388	ASP
1	B	400	LEU
1	B	432	LEU

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	17	HIS
1	A	148	GLN
1	A	247	GLN
1	B	17	HIS
1	B	45	GLN
1	B	156	ASN
1	B	247	GLN
1	B	443	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)

10 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	EDO	A	477	-	3,3,3	0.81	0	2,2,2	0.95	0
2	EDO	A	478	-	3,3,3	1.05	0	2,2,2	0.21	0
2	EDO	A	479	-	3,3,3	0.55	0	2,2,2	0.27	0
2	EDO	A	480	-	3,3,3	0.32	0	2,2,2	0.89	0
2	EDO	A	481	-	3,3,3	0.94	0	2,2,2	0.70	0
2	EDO	A	482	-	3,3,3	0.59	0	2,2,2	0.14	0
2	EDO	A	483	-	3,3,3	0.53	0	2,2,2	0.44	0
2	EDO	B	477	-	3,3,3	0.59	0	2,2,2	0.17	0
2	EDO	B	478	-	3,3,3	0.67	0	2,2,2	0.38	0
2	EDO	B	479	-	3,3,3	0.51	0	2,2,2	0.41	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
2	EDO	A	477	-	-	0/1/1/1	0/0/0/0
2	EDO	A	478	-	-	0/1/1/1	0/0/0/0
2	EDO	A	479	-	-	0/1/1/1	0/0/0/0
2	EDO	A	480	-	-	0/1/1/1	0/0/0/0
2	EDO	A	481	-	-	0/1/1/1	0/0/0/0
2	EDO	A	482	-	-	0/1/1/1	0/0/0/0
2	EDO	A	483	-	-	0/1/1/1	0/0/0/0
2	EDO	B	477	-	-	0/1/1/1	0/0/0/0
2	EDO	B	478	-	-	0/1/1/1	0/0/0/0
2	EDO	B	479	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	477	EDO	1	0
2	A	478	EDO	1	0
2	A	479	EDO	1	0
2	B	479	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, 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	457/495 (92%)	0.96	74 (16%)	3 4	49, 57, 69, 91	0
1	B	456/495 (92%)	1.85	181 (39%)	0 0	48, 57, 68, 89	0
All	All	913/990 (92%)	1.40	255 (27%)	1 1	48, 57, 68, 91	0

All (255) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	466	ILE	9.1
1	B	37	LEU	7.5
1	B	182	PHE	7.2
1	B	473	VAL	7.0
1	B	137	PRO	6.8
1	A	391	GLU	6.5
1	B	221	GLY	6.2
1	B	147	LEU	6.1
1	B	183	GLY	6.1
1	B	464	ALA	6.0
1	B	38	GLU	6.0
1	B	140	ILE	5.7
1	B	144	VAL	5.7
1	B	53	TYR	5.7
1	B	457	GLU	5.6
1	B	453	ALA	5.5
1	B	468	GLN	5.5
1	B	450	VAL	5.5
1	B	452	PRO	5.4
1	B	190	GLU	5.3
1	A	473	VAL	5.2
1	B	179	ALA	5.1
1	A	328	SER	5.0
1	B	167	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	143	GLY	4.9
1	B	462	LEU	4.8
1	B	255	ILE	4.8
1	A	0	GLY	4.8
1	B	252	LEU	4.8
1	B	233	GLY	4.7
1	B	271	SER	4.7
1	B	33	TYR	4.7
1	A	474	GLY	4.7
1	A	404	HIS	4.7
1	B	447	ALA	4.6
1	B	186	ASP	4.6
1	B	454	LEU	4.6
1	B	225	ILE	4.4
1	B	460	ALA	4.3
1	B	270	GLY	4.3
1	B	455	ASP	4.3
1	B	145	ARG	4.2
1	B	95	GLY	4.2
1	B	14	GLN	4.1
1	B	42	ARG	4.1
1	B	470	GLY	4.1
1	B	55	THR	4.1
1	B	269	TYR	4.1
1	B	251	VAL	4.1
1	A	387	PHE	4.0
1	B	195	VAL	4.0
1	B	244	LEU	4.0
1	B	474	GLY	4.0
1	A	290	CYS	4.0
1	B	467	ALA	4.0
1	B	226	ILE	4.0
1	B	41	ARG	3.9
1	A	314	LEU	3.9
1	B	267	VAL	3.9
1	B	0	GLY	3.9
1	B	188	ILE	3.9
1	B	445	ILE	3.9
1	A	331	THR	3.9
1	B	261	ILE	3.9
1	B	310	SER	3.8
1	B	263	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	201	LEU	3.8
1	B	224	VAL	3.8
1	B	291	ALA	3.7
1	B	77	PRO	3.7
1	B	18	GLU	3.7
1	B	219	GLU	3.7
1	B	472	GLU	3.6
1	B	151	TYR	3.6
1	A	332	LEU	3.6
1	B	49	GLY	3.6
1	A	344	LEU	3.6
1	A	273	SER	3.6
1	B	268	ILE	3.5
1	A	310	SER	3.5
1	A	383	ASP	3.5
1	B	50	LYS	3.5
1	B	138	GLN	3.5
1	B	227	ALA	3.5
1	B	44	GLY	3.5
1	A	324	ALA	3.5
1	A	86	ASP	3.5
1	B	191	LYS	3.4
1	B	47	VAL	3.4
1	B	443	GLN	3.4
1	B	293	PHE	3.3
1	B	58	PHE	3.3
1	A	270	GLY	3.3
1	B	111	LEU	3.3
1	B	185	LYS	3.3
1	A	228	SER	3.2
1	A	271	SER	3.2
1	B	135	ALA	3.2
1	A	311	GLY	3.2
1	B	254	GLY	3.2
1	B	197	LEU	3.1
1	B	82	VAL	3.1
1	B	247	GLN	3.1
1	B	211	LEU	3.1
1	B	228	SER	3.1
1	B	40	PHE	3.1
1	B	68	ALA	3.0
1	B	63	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	27	ILE	3.0
1	B	429	LYS	3.0
1	B	161	PHE	3.0
1	A	285	ILE	3.0
1	A	395	PRO	3.0
1	B	456	PRO	3.0
1	B	311	GLY	2.9
1	B	70	PHE	2.9
1	A	272	THR	2.9
1	B	173	ASP	2.9
1	A	249	ALA	2.9
1	B	61	SER	2.9
1	B	160	CYS	2.9
1	A	349	ILE	2.9
1	B	117	PHE	2.9
1	A	408	ASN	2.9
1	B	187	VAL	2.9
1	B	48	GLU	2.9
1	A	78	GLU	2.8
1	A	141	PRO	2.8
1	A	303	PHE	2.8
1	A	326	TYR	2.8
1	B	295	SER	2.8
1	B	328	SER	2.8
1	A	226	ILE	2.8
1	B	332	LEU	2.8
1	A	471	LYS	2.8
1	A	9	THR	2.8
1	B	26	GLU	2.8
1	B	305	GLY	2.7
1	B	326	TYR	2.7
1	B	442	TRP	2.7
1	B	250	GLU	2.7
1	B	22	LYS	2.7
1	B	10	GLU	2.7
1	B	248	ASN	2.7
1	A	184	GLY	2.7
1	B	325	GLY	2.7
1	B	292	LEU	2.7
1	A	390	ILE	2.7
1	B	303	PHE	2.7
1	A	183	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	206	TYR	2.7
1	B	34	GLU	2.7
1	B	461	LYS	2.7
1	B	31	PHE	2.6
1	B	141	PRO	2.6
1	B	78	GLU	2.6
1	A	343	VAL	2.6
1	B	249	ALA	2.6
1	A	293	PHE	2.6
1	B	272	THR	2.6
1	A	246	LEU	2.6
1	A	313	GLY	2.6
1	B	193	VAL	2.6
1	B	198	ILE	2.6
1	B	253	ALA	2.6
1	B	446	LEU	2.6
1	B	180	ILE	2.6
1	A	327	GLU	2.5
1	B	203	PRO	2.5
1	A	274	ALA	2.5
1	B	223	ALA	2.5
1	B	8	LEU	2.5
1	B	430	GLU	2.5
1	A	104	GLY	2.5
1	B	469	ARG	2.5
1	A	195	VAL	2.5
1	B	52	VAL	2.5
1	B	410	LYS	2.5
1	A	309	ARG	2.5
1	B	257	LEU	2.5
1	A	251	VAL	2.5
1	A	396	GLY	2.5
1	B	131	GLY	2.5
1	B	177	ILE	2.5
1	A	335	ALA	2.5
1	B	108	LYS	2.4
1	B	178	ALA	2.4
1	B	273	SER	2.4
1	B	246	LEU	2.4
1	B	157	SER	2.4
1	B	308	SER	2.4
1	B	194	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	224	VAL	2.4
1	B	312	GLY	2.4
1	A	92	PRO	2.4
1	A	161	PHE	2.4
1	B	347	ALA	2.4
1	B	309	ARG	2.4
1	A	227	ALA	2.3
1	A	153	SER	2.3
1	A	379	THR	2.3
1	B	342	PHE	2.3
1	B	83	ILE	2.3
1	A	403	LYS	2.3
1	A	154	ILE	2.3
1	A	312	GLY	2.3
1	B	465	PHE	2.3
1	B	80	ASN	2.3
1	B	266	PRO	2.3
1	A	268	ILE	2.3
1	B	17	HIS	2.3
1	B	196	SER	2.3
1	B	400	LEU	2.3
1	A	98	PHE	2.2
1	A	399	PHE	2.2
1	A	247	GLN	2.2
1	A	77	PRO	2.2
1	B	57	GLU	2.2
1	B	260	SER	2.2
1	B	19	ASN	2.2
1	B	159	LYS	2.2
1	A	389	VAL	2.2
1	B	264	GLY	2.2
1	B	331	THR	2.2
1	A	334	ALA	2.2
1	A	255	ILE	2.2
1	B	367	ILE	2.2
1	B	39	VAL	2.2
1	A	382	GLU	2.2
1	B	401	THR	2.2
1	B	89	VAL	2.1
1	B	304	TYR	2.1
1	B	54	LEU	2.1
1	A	423	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	23	ILE	2.1
1	B	243	THR	2.1
1	A	294	ILE	2.1
1	B	214	LEU	2.1
1	B	189	LYS	2.1
1	B	216	ALA	2.1
1	B	313	GLY	2.1
1	A	457	GLU	2.1
1	B	314	LEU	2.1
1	B	174	SER	2.1
1	A	397	GLY	2.0
1	B	84	GLY	2.0
1	B	459	ASP	2.0
1	B	230	VAL	2.0
1	A	465	PHE	2.0
1	B	98	PHE	2.0
1	A	291	ALA	2.0
1	B	94	TYR	2.0
1	A	287	SER	2.0
1	B	222	GLN	2.0
1	B	451	PRO	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
2	EDO	A	481	4/4	0.91	0.38	5.52	44,53,59,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	EDO	A	479	4/4	0.91	0.33	3.88	60,69,71,72	0
2	EDO	A	477	4/4	0.87	0.30	2.21	56,58,63,68	0
2	EDO	A	478	4/4	0.84	0.27	0.47	38,46,48,57	0
2	EDO	B	479	4/4	0.89	0.27	-0.35	63,65,65,68	0
2	EDO	B	477	4/4	0.92	0.17	-1.41	65,65,73,81	0
2	EDO	A	480	4/4	0.81	0.41	-	72,76,77,81	0
2	EDO	B	478	4/4	0.74	0.21	-	76,77,79,84	0
2	EDO	A	482	4/4	0.80	0.33	-	70,72,73,82	0
2	EDO	A	483	4/4	0.66	0.20	-	55,71,74,75	0

6.5 Other polymers (i)

There are no such residues in this entry.