



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:33 PM GMT

PDB ID : 4TQT  
Title : Crystal structure of Dihydropyrimidinase from Brucella suis  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2014-06-12  
Resolution : 2.15 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

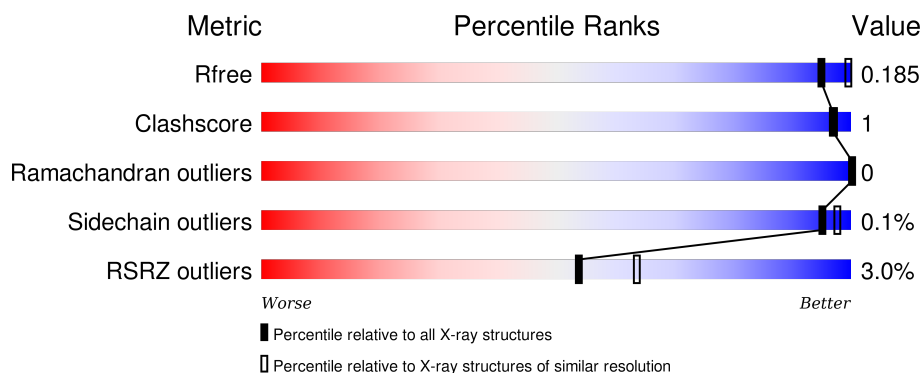
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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.



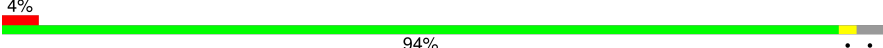
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	497	<div> <div>6%</div> <div> <div></div> <div>92%</div> <div></div> </div> <div></div> </div>
1	B	497	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div></div> </div> <div></div> </div>
1	C	497	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div></div> </div> <div></div> </div>
1	D	497	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div></div> </div> <div></div> </div>
1	E	497	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div></div> </div> <div></div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	497	

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
3	EDO	C	503	-	-	-	X
3	EDO	C	504	-	-	-	X
3	EDO	C	505	-	-	-	X
3	EDO	D	505	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23274 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 D-hydantoinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3633	2274	643	696	20			
1	B	477	Total	C	N	O	S	0	4	0
			3674	2305	649	700	20			
1	C	476	Total	C	N	O	S	0	2	0
			3628	2275	638	695	20			
1	D	481	Total	C	N	O	S	0	4	0
			3689	2314	650	705	20			
1	E	477	Total	C	N	O	S	0	4	0
			3665	2301	645	699	20			
1	F	481	Total	C	N	O	S	0	3	0
			3639	2283	637	698	21			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q8G2P0
A	-6	ALA	-	expression tag	UNP Q8G2P0
A	-5	HIS	-	expression tag	UNP Q8G2P0
A	-4	HIS	-	expression tag	UNP Q8G2P0
A	-3	HIS	-	expression tag	UNP Q8G2P0
A	-2	HIS	-	expression tag	UNP Q8G2P0
A	-1	HIS	-	expression tag	UNP Q8G2P0
A	0	HIS	-	expression tag	UNP Q8G2P0
B	-7	MET	-	expression tag	UNP Q8G2P0
B	-6	ALA	-	expression tag	UNP Q8G2P0
B	-5	HIS	-	expression tag	UNP Q8G2P0
B	-4	HIS	-	expression tag	UNP Q8G2P0
B	-3	HIS	-	expression tag	UNP Q8G2P0
B	-2	HIS	-	expression tag	UNP Q8G2P0
B	-1	HIS	-	expression tag	UNP Q8G2P0
B	0	HIS	-	expression tag	UNP Q8G2P0
C	-7	MET	-	expression tag	UNP Q8G2P0

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	ALA	-	expression tag	UNP Q8G2P0
C	-5	HIS	-	expression tag	UNP Q8G2P0
C	-4	HIS	-	expression tag	UNP Q8G2P0
C	-3	HIS	-	expression tag	UNP Q8G2P0
C	-2	HIS	-	expression tag	UNP Q8G2P0
C	-1	HIS	-	expression tag	UNP Q8G2P0
C	0	HIS	-	expression tag	UNP Q8G2P0
D	-7	MET	-	expression tag	UNP Q8G2P0
D	-6	ALA	-	expression tag	UNP Q8G2P0
D	-5	HIS	-	expression tag	UNP Q8G2P0
D	-4	HIS	-	expression tag	UNP Q8G2P0
D	-3	HIS	-	expression tag	UNP Q8G2P0
D	-2	HIS	-	expression tag	UNP Q8G2P0
D	-1	HIS	-	expression tag	UNP Q8G2P0
D	0	HIS	-	expression tag	UNP Q8G2P0
E	-7	MET	-	expression tag	UNP Q8G2P0
E	-6	ALA	-	expression tag	UNP Q8G2P0
E	-5	HIS	-	expression tag	UNP Q8G2P0
E	-4	HIS	-	expression tag	UNP Q8G2P0
E	-3	HIS	-	expression tag	UNP Q8G2P0
E	-2	HIS	-	expression tag	UNP Q8G2P0
E	-1	HIS	-	expression tag	UNP Q8G2P0
E	0	HIS	-	expression tag	UNP Q8G2P0
F	-7	MET	-	expression tag	UNP Q8G2P0
F	-6	ALA	-	expression tag	UNP Q8G2P0
F	-5	HIS	-	expression tag	UNP Q8G2P0
F	-4	HIS	-	expression tag	UNP Q8G2P0
F	-3	HIS	-	expression tag	UNP Q8G2P0
F	-2	HIS	-	expression tag	UNP Q8G2P0
F	-1	HIS	-	expression tag	UNP Q8G2P0
F	0	HIS	-	expression tag	UNP Q8G2P0

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

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	198	Total O 198 198	0	0
4	B	244	Total O 244 244	0	0
4	C	195	Total O 195 195	0	0
4	D	208	Total O 208 208	0	0

*Continued on next page...*

*Continued from previous page...*

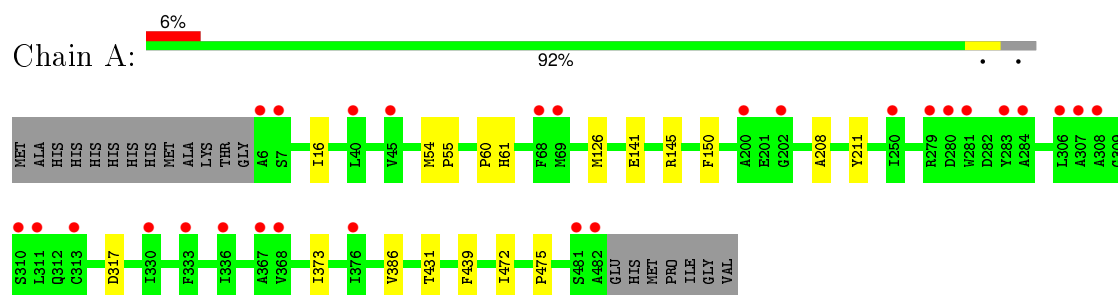
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	220	Total 220	O 220	0	0
4	F	173	Total 173	O 173	0	0



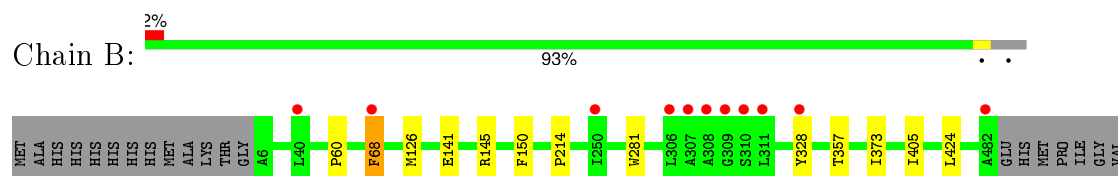
### 3 Residue-property plots [i](#)

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.

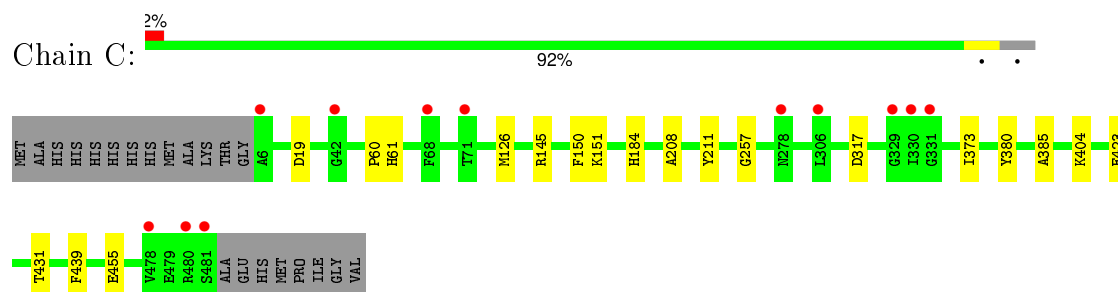
- Molecule 1: D-hydantoinase



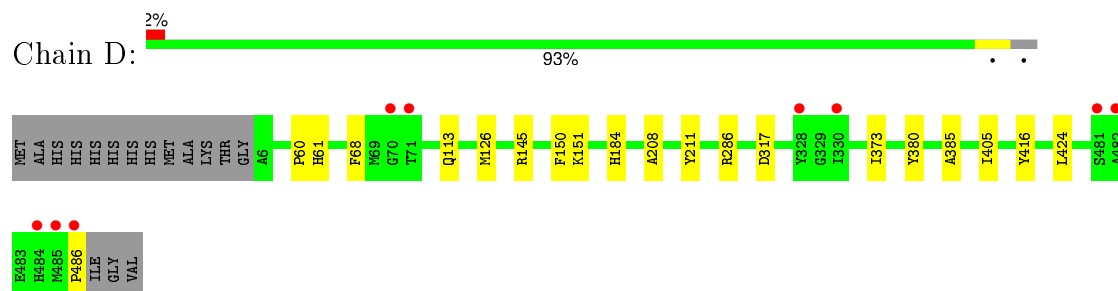
- Molecule 1: D-hydantoinase



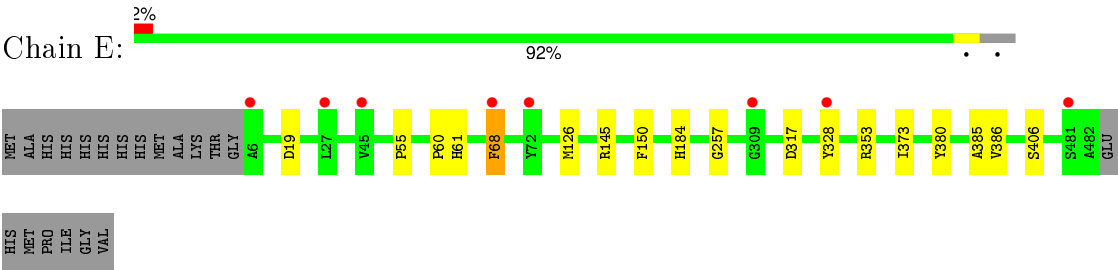
- Molecule 1: D-hydantoinase



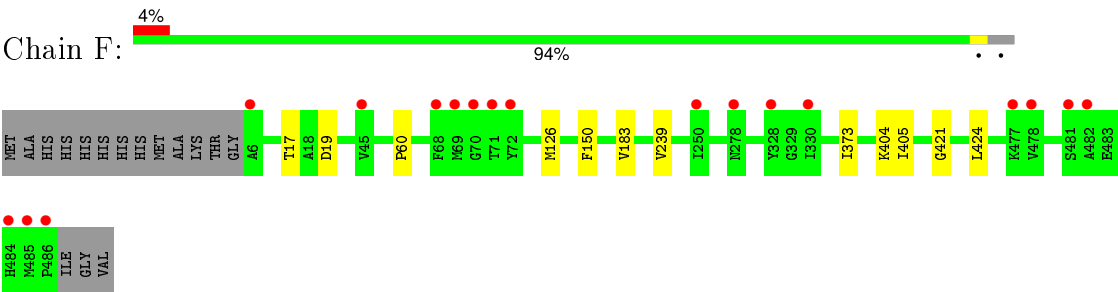
- Molecule 1: D-hydantoinase



● Molecule 1: D-hydantoinase



● Molecule 1: D-hydantoinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.69Å 88.83Å 221.24Å 90.00° 91.17° 90.00°	Depositor
Resolution (Å)	44.24 – 2.15 45.02 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.24-2.15) 99.9 (45.02-2.15)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 2.16Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, $R_{free}$	0.135 , 0.182 0.146 , 0.185	Depositor DCC
$R_{free}$ test set	8376 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.4	EDS
Estimated twinning fraction	0.010 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.011 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.013 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.016 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.012 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 165022 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	23274	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.37	0/3696	0.51	0/5013
1	B	0.40	0/3751	0.54	0/5084
1	C	0.37	0/3697	0.50	0/5013
1	D	0.38	0/3767	0.52	0/5111
1	E	0.38	0/3742	0.51	0/5073
1	F	0.34	0/3713	0.49	0/5042
All	All	0.38	0/22366	0.51	0/30336

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 [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	3633	0	3502	11	0
1	B	3674	0	3563	8	0
1	C	3628	0	3507	14	0
1	D	3689	0	3554	11	0
1	E	3665	0	3551	12	0
1	F	3639	0	3483	6	0
2	A	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	20	0	30	0	0
3	B	12	0	18	0	0
3	C	16	0	24	1	0
3	D	16	0	24	1	0
3	E	16	0	24	1	0
3	F	16	0	24	0	0
4	A	198	0	0	1	0
4	B	244	0	0	1	0
4	C	195	0	0	1	0
4	D	208	0	0	1	0
4	E	220	0	0	2	0
4	F	173	0	0	0	0
All	All	23274	0	21304	58	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 1.

All (58) 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:E:60:PRO:HB3	1:E:373:ILE:HG12	1.74	0.68
1:E:19:ASP:OD2	4:E:815:HOH:O	2.13	0.66
1:D:60:PRO:HB3	1:D:373:ILE:HG12	1.80	0.63
1:F:60:PRO:HB3	1:F:373:ILE:HG12	1.82	0.60
1:C:404:LYS:NZ	1:C:423:GLU:OE2	2.30	0.59
1:C:60:PRO:HB3	1:C:373:ILE:HG12	1.83	0.59
1:D:113:GLN:NE2	4:D:601:HOH:O	2.35	0.58
1:B:60:PRO:HB3	1:B:373:ILE:HG12	1.84	0.58
1:F:17:THR:OG1	1:F:19[A]:ASP:OD1	2.23	0.57
1:B:68:PHE:HZ	1:B:328:TYR:HD2	1.51	0.57
1:A:60:PRO:HB3	1:A:373:ILE:HG12	1.85	0.56
1:B:281:TRP:HB3	1:D:486:PRO:HD3	1.86	0.56
1:D:380:TYR:CE1	1:D:385:ALA:HB2	2.42	0.55
1:C:257:GLY:O	3:C:505:EDO:H12	2.09	0.53
1:C:151:KCX:OQ1	1:C:184:HIS:HB2	2.10	0.52
1:E:257:GLY:O	3:E:505:EDO:H12	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ARG:HD3	4:A:605:HOH:O	2.12	0.49
1:D:405:ILE:HD11	1:D:424:LEU:HD11	1.95	0.48
1:C:380:TYR:CE1	1:C:385:ALA:HB2	2.49	0.48
1:F:405:ILE:HD11	1:F:424:LEU:HD11	1.95	0.48
1:C:257:GLY:HA3	3:D:502:EDO:H22	1.95	0.48
1:C:455:GLU:OE1	1:E:406:SER:OG	2.26	0.48
1:B:214:PRO:HB2	4:B:643:HOH:O	2.14	0.48
1:A:141:GLU:O	1:A:145:ARG:HG3	2.13	0.48
1:D:126:MET:O	1:D:150:PHE:HA	2.14	0.47
1:E:380:TYR:CE1	1:E:385:ALA:HB2	2.49	0.47
1:E:68:PHE:HZ	1:E:328:TYR:HD2	1.62	0.47
1:D:151:KCX:OQ1	1:D:184:HIS:HB2	2.15	0.47
1:B:141:GLU:O	1:B:145[A]:ARG:HG2	2.15	0.47
1:E:61:HIS:CD2	1:E:317:ASP:HA	2.50	0.47
1:C:19:ASP:OD2	4:C:672:HOH:O	2.21	0.47
1:B:405:ILE:HD11	1:B:424:LEU:HD11	1.98	0.46
1:C:208:ALA:HA	1:C:211:TYR:CD2	2.51	0.46
1:F:404:LYS:HE3	1:F:421:GLY:HA2	1.97	0.45
1:A:431:THR:HB	1:A:439:PHE:HB3	1.98	0.45
1:D:286:ARG:HG2	1:D:416:TYR:CZ	2.52	0.45
1:C:61:HIS:CD2	1:C:317:ASP:HA	2.52	0.45
1:E:126:MET:O	1:E:150:PHE:HA	2.16	0.45
1:A:55:PRO:HG3	1:A:386:VAL:HG23	1.99	0.45
1:D:61:HIS:CD2	1:D:317:ASP:HA	2.51	0.45
1:C:431:THR:HB	1:C:439:PHE:HB3	1.99	0.44
1:A:61:HIS:CD2	1:A:317:ASP:HA	2.53	0.44
1:A:208:ALA:HA	1:A:211:TYR:CD2	2.53	0.44
1:F:126:MET:O	1:F:150:PHE:HA	2.17	0.43
1:E:55:PRO:HG3	1:E:386:VAL:HG23	2.00	0.43
1:E:145[B]:ARG:NH1	4:E:747:HOH:O	2.43	0.43
1:B:126:MET:O	1:B:150:PHE:HA	2.18	0.43
1:A:126:MET:O	1:A:150:PHE:HA	2.19	0.42
1:A:475:PRO:HB2	1:C:211:TYR:CD2	2.56	0.41
1:E:184:HIS:C	1:E:184:HIS:CD2	2.94	0.41
1:C:126:MET:O	1:C:150:PHE:HA	2.21	0.40
1:A:472:ILE:CD1	1:B:357:THR:HA	2.51	0.40
1:E:353:ARG:HD3	1:E:353:ARG:HA	1.86	0.40
1:D:208:ALA:HA	1:D:211:TYR:CD2	2.57	0.40
1:F:183:VAL:O	1:F:239:VAL:HG22	2.21	0.40
1:A:16:ILE:HB	1:A:54:MET:HG2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	474/497 (95%)	460 (97%)	14 (3%)	0	100	100
1	B	478/497 (96%)	464 (97%)	14 (3%)	0	100	100
1	C	475/497 (96%)	460 (97%)	15 (3%)	0	100	100
1	D	482/497 (97%)	467 (97%)	15 (3%)	0	100	100
1	E	478/497 (96%)	463 (97%)	15 (3%)	0	100	100
1	F	481/497 (97%)	466 (97%)	15 (3%)	0	100	100
All	All	2868/2982 (96%)	2780 (97%)	88 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/398 (93%)	370 (100%)	0	100	100
1	B	377/398 (95%)	376 (100%)	1 (0%)	94	97
1	C	371/398 (93%)	371 (100%)	0	100	100
1	D	376/398 (94%)	375 (100%)	1 (0%)	94	97
1	E	376/398 (94%)	375 (100%)	1 (0%)	94	97
1	F	368/398 (92%)	368 (100%)	0	100	100
All	All	2238/2388 (94%)	2235 (100%)	3 (0%)	95	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	68	PHE
1	D	68	PHE
1	E	68	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	338	ASN
1	D	277	HIS
1	D	338	ASN
1	E	277	HIS
1	E	338	ASN
1	F	338	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	KCX	A	151	1,2	7,11,12	0.90	0	7,12,14	1.80	2 (28%)
1	KCX	B	151	1,2	7,11,12	0.93	0	7,12,14	1.69	1 (14%)
1	KCX	C	151	1,2	7,11,12	0.85	0	7,12,14	2.04	1 (14%)
1	KCX	D	151	1,2	7,11,12	0.85	0	7,12,14	1.97	2 (28%)
1	KCX	E	151	1,2	7,11,12	0.90	0	7,12,14	1.91	2 (28%)
1	KCX	F	151	1,2	7,11,12	0.84	0	7,12,14	2.28	1 (14%)



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
1	KCX	A	151	1,2	-	0/6/10/12	0/0/0/0
1	KCX	B	151	1,2	-	0/6/10/12	0/0/0/0
1	KCX	C	151	1,2	-	0/6/10/12	0/0/0/0
1	KCX	D	151	1,2	-	0/6/10/12	0/0/0/0
1	KCX	E	151	1,2	-	0/6/10/12	0/0/0/0
1	KCX	F	151	1,2	-	0/6/10/12	0/0/0/0

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	151	KCX	CE-NZ-CX	-5.08	117.74	123.49
1	C	151	KCX	CE-NZ-CX	-4.35	118.56	123.49
1	E	151	KCX	CE-NZ-CX	-4.21	118.72	123.49
1	D	151	KCX	CE-NZ-CX	-3.79	119.20	123.49
1	A	151	KCX	CE-NZ-CX	-3.51	119.52	123.49
1	B	151	KCX	CE-NZ-CX	-2.52	120.64	123.49
1	A	151	KCX	O-C-CA	-2.26	119.59	125.49
1	E	151	KCX	O-C-CA	-2.09	120.06	125.49
1	D	151	KCX	O-C-CA	-2.07	120.09	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	151	KCX	1	0
1	D	151	KCX	1	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	EDO	A	503	-	3,3,3	0.45	0	2,2,2	0.45	0
3	EDO	A	504	-	3,3,3	0.48	0	2,2,2	0.73	0
3	EDO	A	505	-	3,3,3	0.46	0	2,2,2	0.62	0
3	EDO	A	506	-	3,3,3	0.45	0	2,2,2	0.35	0
3	EDO	A	507	-	3,3,3	0.50	0	2,2,2	0.41	0
3	EDO	B	502	-	3,3,3	0.47	0	2,2,2	0.31	0
3	EDO	B	503	-	3,3,3	0.50	0	2,2,2	0.59	0
3	EDO	B	504	-	3,3,3	0.35	0	2,2,2	1.05	0
3	EDO	C	502	-	3,3,3	0.56	0	2,2,2	0.15	0
3	EDO	C	503	-	3,3,3	0.47	0	2,2,2	0.66	0
3	EDO	C	504	-	3,3,3	0.41	0	2,2,2	0.98	0
3	EDO	C	505	-	3,3,3	0.49	0	2,2,2	0.44	0
3	EDO	D	502	-	3,3,3	0.50	0	2,2,2	0.36	0
3	EDO	D	503	-	3,3,3	0.52	0	2,2,2	0.66	0
3	EDO	D	504	-	3,3,3	0.40	0	2,2,2	0.67	0
3	EDO	D	505	-	3,3,3	0.41	0	2,2,2	0.47	0
3	EDO	E	502	-	3,3,3	0.47	0	2,2,2	0.39	0
3	EDO	E	503	-	3,3,3	0.44	0	2,2,2	0.77	0
3	EDO	E	504	-	3,3,3	0.37	0	2,2,2	1.04	0
3	EDO	E	505	-	3,3,3	0.55	0	2,2,2	0.35	0
3	EDO	F	502	-	3,3,3	0.47	0	2,2,2	0.33	0
3	EDO	F	503	-	3,3,3	0.44	0	2,2,2	0.77	0
3	EDO	F	504	-	3,3,3	0.51	0	2,2,2	0.63	0
3	EDO	F	505	-	3,3,3	0.42	0	2,2,2	0.45	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	EDO	A	503	-	-	0/1/1/1	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	504	-	-	0/1/1/1	0/0/0/0
3	EDO	A	505	-	-	0/1/1/1	0/0/0/0
3	EDO	A	506	-	-	0/1/1/1	0/0/0/0
3	EDO	A	507	-	-	0/1/1/1	0/0/0/0
3	EDO	B	502	-	-	0/1/1/1	0/0/0/0
3	EDO	B	503	-	-	0/1/1/1	0/0/0/0
3	EDO	B	504	-	-	0/1/1/1	0/0/0/0
3	EDO	C	502	-	-	0/1/1/1	0/0/0/0
3	EDO	C	503	-	-	0/1/1/1	0/0/0/0
3	EDO	C	504	-	-	0/1/1/1	0/0/0/0
3	EDO	C	505	-	-	0/1/1/1	0/0/0/0
3	EDO	D	502	-	-	0/1/1/1	0/0/0/0
3	EDO	D	503	-	-	0/1/1/1	0/0/0/0
3	EDO	D	504	-	-	0/1/1/1	0/0/0/0
3	EDO	D	505	-	-	0/1/1/1	0/0/0/0
3	EDO	E	502	-	-	0/1/1/1	0/0/0/0
3	EDO	E	503	-	-	0/1/1/1	0/0/0/0
3	EDO	E	504	-	-	0/1/1/1	0/0/0/0
3	EDO	E	505	-	-	0/1/1/1	0/0/0/0
3	EDO	F	502	-	-	0/1/1/1	0/0/0/0
3	EDO	F	503	-	-	0/1/1/1	0/0/0/0
3	EDO	F	504	-	-	0/1/1/1	0/0/0/0
3	EDO	F	505	-	-	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	505	EDO	1	0
3	D	502	EDO	1	0
3	E	505	EDO	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	476/497 (95%)	0.09	28 (5%)	26 36	23, 39, 58, 83	0
1	B	476/497 (95%)	-0.21	11 (2%)	64 72	21, 33, 54, 93	0
1	C	475/497 (95%)	-0.01	12 (2%)	61 69	22, 38, 58, 91	0
1	D	480/497 (96%)	-0.28	9 (1%)	70 78	22, 36, 59, 88	0
1	E	476/497 (95%)	-0.23	8 (1%)	73 80	21, 35, 56, 89	0
1	F	480/497 (96%)	0.06	18 (3%)	44 54	25, 43, 66, 103	0
All	All	2863/2982 (96%)	-0.10	86 (3%)	54 64	21, 37, 59, 103	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	6	ALA	5.3
1	A	482	ALA	5.1
1	F	485	MET	4.8
1	A	6	ALA	4.8
1	E	68	PHE	4.7
1	F	484	HIS	4.6
1	B	482	ALA	4.5
1	F	71	THR	4.2
1	C	478	VAL	4.0
1	E	328	TYR	4.0
1	D	482	ALA	3.9
1	B	68	PHE	3.8
1	A	69	MET	3.7
1	F	486	PRO	3.7
1	D	484	HIS	3.6
1	C	6	ALA	3.5
1	A	281	TRP	3.4
1	F	70	GLY	3.3
1	B	328	TYR	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	481	SER	3.3
1	D	486	PRO	3.3
1	A	330	ILE	3.2
1	A	40	LEU	3.2
1	D	328	TYR	3.1
1	F	478	VAL	3.1
1	F	481	SER	3.1
1	A	202	GLY	3.0
1	A	250	ILE	3.0
1	A	68	PHE	3.0
1	C	68	PHE	3.0
1	A	311	LEU	2.9
1	F	482	ALA	2.8
1	D	485	MET	2.8
1	A	306	LEU	2.8
1	A	368	VAL	2.7
1	F	72	TYR	2.7
1	A	376	ILE	2.7
1	C	42	GLY	2.7
1	A	284	ALA	2.6
1	A	308	ALA	2.6
1	A	45	VAL	2.6
1	E	481	SER	2.5
1	C	329	GLY	2.5
1	A	279	ARG	2.5
1	C	71	THR	2.5
1	D	70	GLY	2.5
1	B	307	ALA	2.5
1	F	330	ILE	2.5
1	A	307	ALA	2.5
1	A	481	SER	2.5
1	F	477	LYS	2.5
1	E	45	VAL	2.4
1	A	310	SER	2.4
1	B	40	LEU	2.3
1	E	309	GLY	2.3
1	B	306	LEU	2.3
1	A	200	ALA	2.3
1	C	330	ILE	2.3
1	B	250	ILE	2.3
1	D	481	SER	2.2
1	F	68	PHE	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	71	THR	2.2
1	A	336	ILE	2.2
1	F	69	MET	2.2
1	F	250	ILE	2.2
1	F	45	VAL	2.2
1	B	309	GLY	2.2
1	C	306	LEU	2.2
1	E	6	ALA	2.2
1	C	278	ASN	2.2
1	A	283	TYR	2.1
1	C	480	ARG	2.1
1	B	311	LEU	2.1
1	F	328	TYR	2.1
1	C	331	GLY	2.1
1	D	330	ILE	2.1
1	A	313	CYS	2.1
1	A	367	ALA	2.1
1	A	280	ASP	2.1
1	B	308	ALA	2.1
1	B	310	SER	2.1
1	F	278	ASN	2.1
1	A	333	PHE	2.1
1	E	27	LEU	2.0
1	E	72	TYR	2.0
1	A	7	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	KCX	C	151	12/13	0.97	0.09	-	29,33,43,48	0
1	KCX	A	151	12/13	0.98	0.09	-	27,33,36,42	0
1	KCX	E	151	12/13	0.96	0.07	-	22,28,33,38	0
1	KCX	D	151	12/13	0.97	0.08	-	24,28,40,44	0
1	KCX	B	151	12/13	0.96	0.08	-	25,29,36,42	0
1	KCX	F	151	12/13	0.94	0.09	-	31,35,45,54	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	EDO	C	503	4/4	0.94	0.24	3.88	35,41,41,41	0
3	EDO	D	505	4/4	0.94	0.24	3.01	44,45,46,53	0
3	EDO	C	504	4/4	0.96	0.23	2.32	44,47,47,47	0
3	EDO	C	505	4/4	0.89	0.19	2.07	35,43,45,58	0
3	EDO	A	506	4/4	0.92	0.22	1.77	32,34,40,53	0
3	EDO	C	502	4/4	0.96	0.18	1.76	36,44,44,45	0
3	EDO	D	502	4/4	0.95	0.17	1.56	40,46,49,51	0
3	EDO	F	505	4/4	0.93	0.17	1.50	40,45,45,55	0
3	EDO	F	504	4/4	0.94	0.15	1.49	43,49,51,52	0
3	EDO	A	507	4/4	0.90	0.21	1.29	39,46,49,51	0
3	EDO	E	504	4/4	0.99	0.16	1.27	42,43,45,51	0
3	EDO	E	505	4/4	0.87	0.18	1.25	36,38,41,50	0
3	EDO	D	504	4/4	0.99	0.13	1.19	39,40,44,50	0
3	EDO	B	504	4/4	0.96	0.15	1.12	39,41,43,46	0
3	EDO	A	505	4/4	0.98	0.18	0.99	37,37,39,43	0
3	EDO	A	503	4/4	0.96	0.18	0.83	37,44,50,50	0
3	EDO	F	502	4/4	0.90	0.16	0.69	43,49,49,49	0
3	EDO	E	502	4/4	0.95	0.15	0.68	44,50,50,53	0
3	EDO	B	502	4/4	0.97	0.16	0.45	32,42,47,48	0
2	ZN	C	501	1/1	0.98	0.06	-1.65	53,53,53,53	0
2	ZN	A	502	1/1	0.99	0.07	-1.89	50,50,50,50	0
2	ZN	B	501	1/1	0.99	0.06	-2.11	48,48,48,48	0
2	ZN	D	501	1/1	0.99	0.04	-2.34	50,50,50,50	0
2	ZN	E	501	1/1	0.99	0.05	-2.36	51,51,51,51	0
2	ZN	F	501	1/1	0.99	0.04	-2.46	56,56,56,56	0
2	ZN	F	500	1/1	0.98	0.04	-	53,53,53,53	0
3	EDO	B	503	4/4	0.89	0.33	-	38,39,45,47	0
2	ZN	C	500	1/1	0.99	0.07	-	51,51,51,51	0
3	EDO	F	503	4/4	0.97	0.19	-	36,41,41,44	0
2	ZN	A	501	1/1	0.99	0.06	-	47,47,47,47	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	D	503	4/4	0.94	0.20	-	42,43,44,45	0
3	EDO	A	504	4/4	0.95	0.33	-	36,40,41,43	0
2	ZN	D	500	1/1	0.97	0.06	-	46,46,46,46	0
2	ZN	B	500	1/1	1.00	0.06	-	44,44,44,44	0
2	ZN	E	500	1/1	0.99	0.06	-	45,45,45,45	0
3	EDO	E	503	4/4	0.95	0.22	-	40,41,46,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.