



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:11 PM GMT

PDB ID : 4R1L  
Title : Crystal structure of a Putative Acyl-CoA ligase (BT\_0428) from Bacteroides  
thetaiotaomicron VPI-5482 at 2.42 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2014-08-06  
Resolution : 2.42 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.

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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

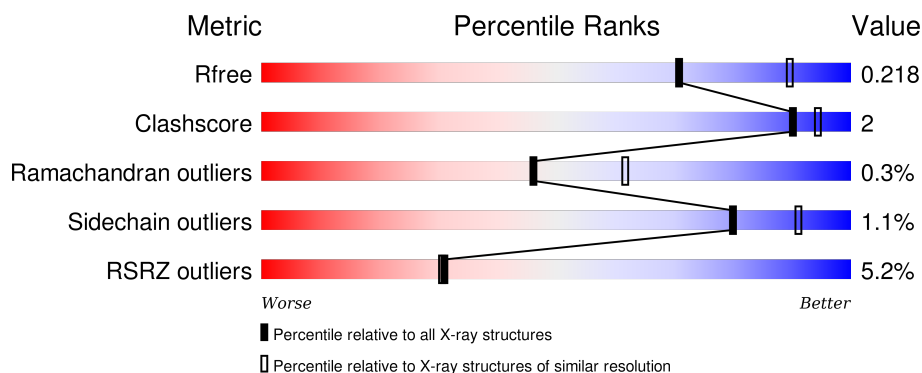
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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  $\geq 3$ , 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	436	<div> <div>2%</div> <div>94%</div> <div>5%</div> </div>
1	B	436	<div> <div>11%</div> <div>89%</div> <div>8%</div> </div>
1	C	436	<div> <div>3%</div> <div>92%</div> <div>7%</div> </div>
1	D	436	<div> <div>4%</div> <div>91%</div> <div>6%</div> </div>

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
10	PEG	D	504	-	-	-	X
5	COA	A	504[A]	-	-	-	X
5	COA	C	503[A]	-	-	-	X
7	PGE	A	508	-	-	-	X
9	EDO	A	512	-	-	-	X
9	EDO	A	514	-	-	-	X
9	EDO	A	515	-	-	-	X
9	EDO	B	505	-	-	-	X
9	EDO	C	510	-	-	-	X
9	EDO	D	506	-	-	-	X

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 14432 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 Phenylacetate-coenzyme A ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	Se	0	10	0
			3469	2187	602	659	6	15			
1	B	422	Total	C	N	O	S	Se	0	8	0
			3336	2102	578	635	6	15			
1	C	434	Total	C	N	O	S	Se	0	4	0
			3430	2165	597	647	6	15			
1	D	425	Total	C	N	O	S	Se	0	3	0
			3340	2108	578	633	6	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	LEADER SEQUENCE	UNP Q8AAN6
B	0	GLY	-	LEADER SEQUENCE	UNP Q8AAN6
C	0	GLY	-	LEADER SEQUENCE	UNP Q8AAN6
D	0	GLY	-	LEADER SEQUENCE	UNP Q8AAN6

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

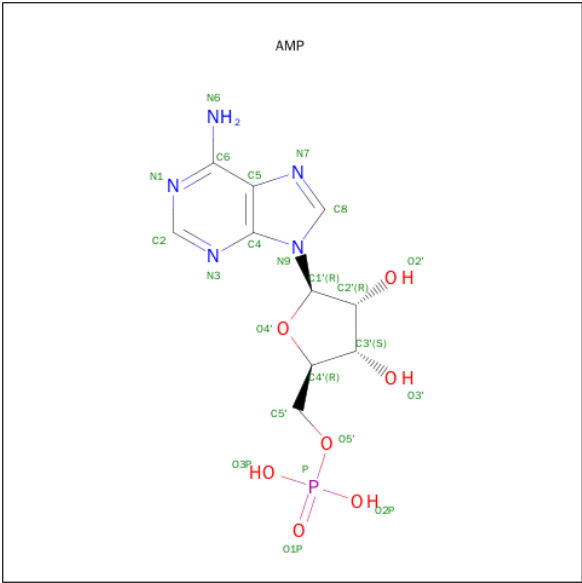
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



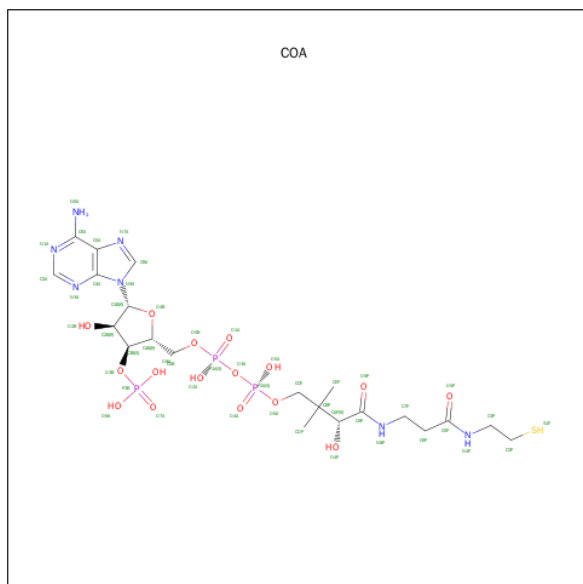
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	1
			23	10	5	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).

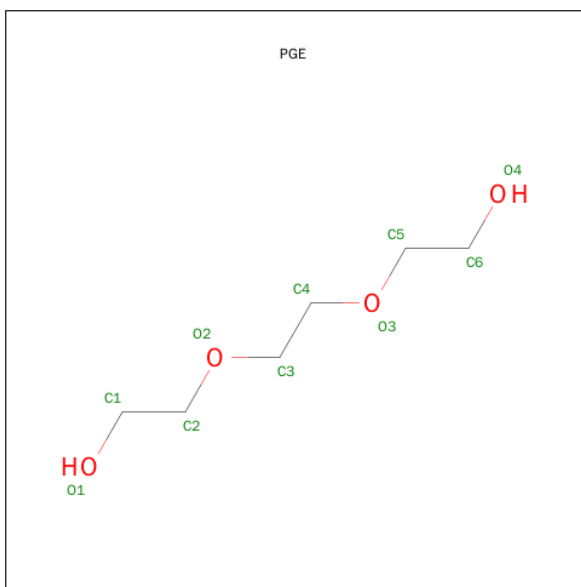


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	1
			31	10	5	13	3		
5	C	1	Total	C	N	O	P	0	1
			31	10	5	13	3		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

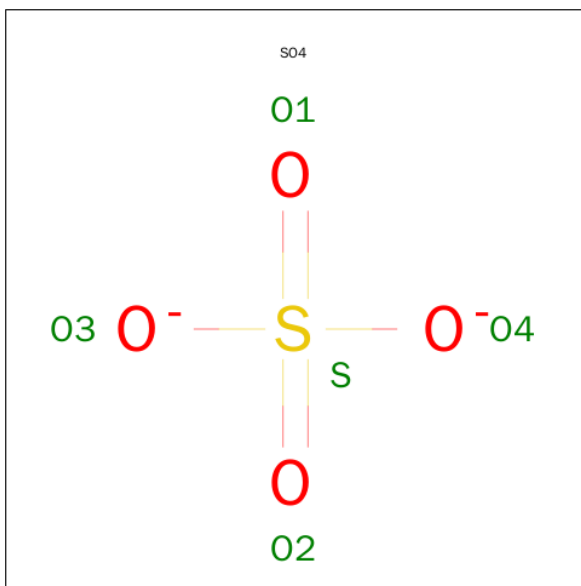
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total K 3 3	0	0
6	D	1	Total K 1 1	0	0
6	C	2	Total K 2 2	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



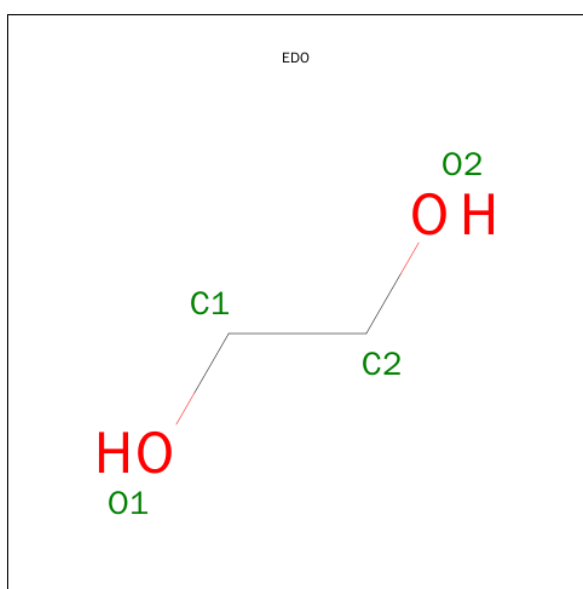
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	1
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	1
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 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
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		

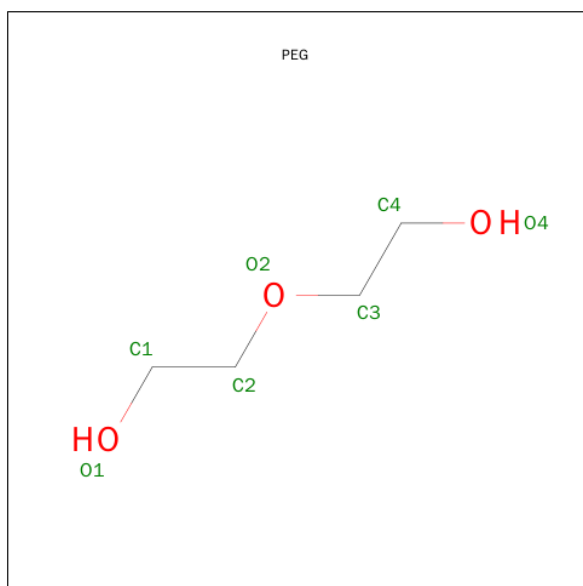
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		
9	D	1	Total	C	O	0	0
			4	2	2		
9	D	1	Total	C	O	0	0
			4	2	2		

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



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	173	Total	O	0	1
			174	174		
11	B	124	Total	O	0	0
			124	124		
11	C	114	Total	O	0	1
			115	115		

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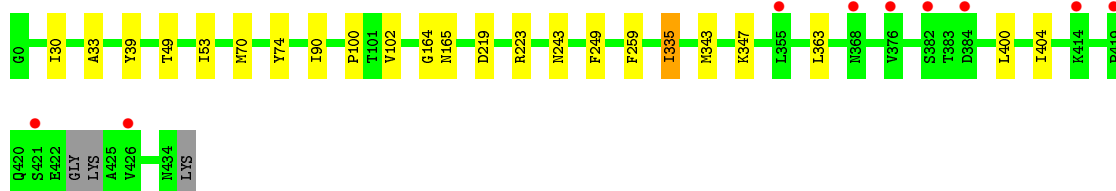
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	145	Total	O	0	0
			145	145		

### 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.

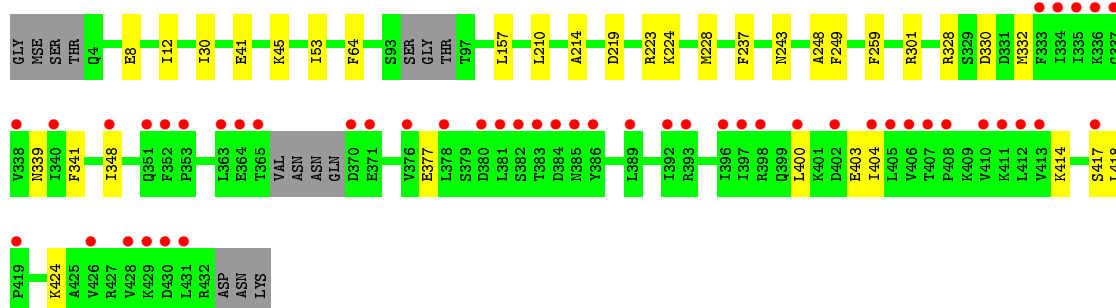
#### • Molecule 1: Phenylacetate-coenzyme A ligase

Chain A: 




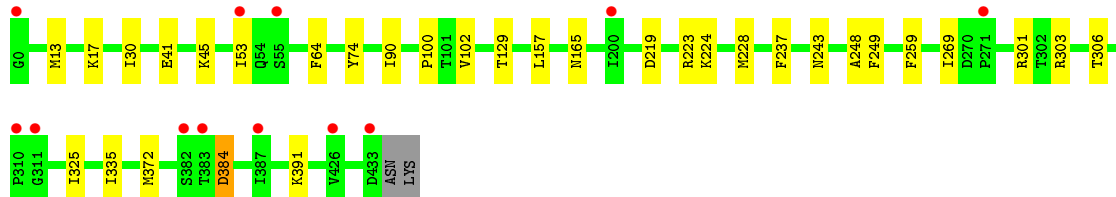
#### • Molecule 1: Phenylacetate-coenzyme A ligase

Chain B: 



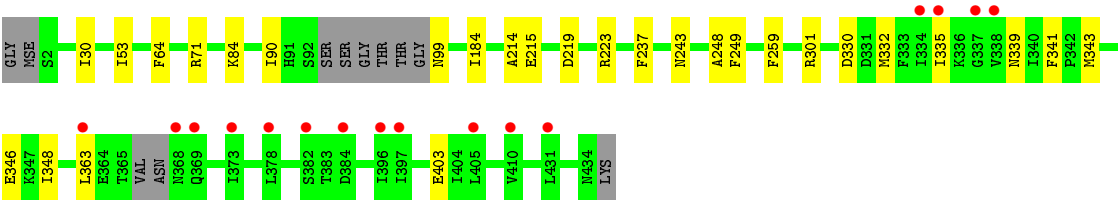
#### • Molecule 1: Phenylacetate-coenzyme A ligase

Chain C: 



#### • Molecule 1: Phenylacetate-coenzyme A ligase

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.70 Å   211.14 Å   71.86 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	48.78 – 2.42 48.78 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.78-2.42) 98.7 (48.78-2.42)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 2.42 Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.172   ,   0.213 0.180   ,   0.218	Depositor DCC
$R_{free}$ test set	3742 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.2	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 51.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 74452 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14432	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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, PGE, ADP, K, EDO, COA, SO4, AMP, PEG

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	0.52	0/3542	0.68	0/4756
1	B	0.49	0/3402	0.66	0/4573
1	C	0.48	0/3486	0.66	0/4682
1	D	0.51	0/3392	0.66	0/4562
All	All	0.50	0/13822	0.66	0/18573

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	3469	0	3476	13	0
1	B	3336	0	3279	17	0
1	C	3430	0	3431	16	0
1	D	3340	0	3283	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	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	12	0	0
3	D	27	0	12	0	0
4	A	23	0	12	0	0
4	C	23	0	12	0	0
5	A	31	0	11	1	0
5	C	31	0	11	0	0
6	A	3	0	0	0	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
7	A	10	0	14	1	0
8	A	15	0	0	0	0
8	B	5	0	0	0	0
8	C	10	0	0	0	0
8	D	5	0	0	0	0
9	A	16	0	24	2	0
9	B	12	0	18	1	0
9	C	12	0	18	3	0
9	D	8	0	12	0	0
10	D	7	0	10	2	0
11	A	174	0	0	1	0
11	B	124	0	0	1	0
11	C	115	0	0	1	0
11	D	145	0	0	1	0
All	All	14432	0	13647	63	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 (63) 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:332[A]:MSE:HE2	1:D:339:ASN:HB3	1.69	0.74
1:B:332[A]:MSE:HE2	1:B:339:ASN:HB3	1.72	0.71
1:A:219:ASP:O	1:A:223:ARG:HG2	1.93	0.67
1:A:90:ILE:HG23	1:A:102:VAL:HG13	1.76	0.67
9:C:510:EDO:H11	11:C:647:HOH:O	1.95	0.66
1:A:30:ILE:HD13	1:A:53:ILE:HG13	1.77	0.66
1:D:30:ILE:HD13	1:D:53:ILE:HG13	1.77	0.65
1:C:303:ARG:HH11	9:C:510:EDO:H12	1.62	0.64
1:B:30:ILE:HD13	1:B:53:ILE:HG13	1.81	0.62
1:C:30:ILE:HD13	1:C:53:ILE:HG13	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:LYS:O	1:B:228:MSE:HG3	2.03	0.59
1:B:214:ALA:HB1	1:B:424:LYS:HE2	1.85	0.58
1:D:348:ILE:HD11	1:D:403:GLU:CB	2.32	0.58
10:D:504:PEG:H11	11:D:737:HOH:O	2.05	0.56
1:B:400:LEU:O	1:B:404:ILE:HG12	2.08	0.54
1:B:414:LYS:HB3	1:B:417:SER:OG	2.08	0.53
1:D:343:MSE:HE1	1:D:346:GLU:OE1	2.09	0.52
1:C:237:PHE:HB3	1:C:248:ALA:HB3	1.92	0.52
1:C:90:ILE:HG23	1:C:102:VAL:HG13	1.92	0.52
1:A:49:THR:HA	9:A:512:EDO:H21	1.90	0.52
1:D:71:ARG:HD3	1:D:99:ASN:HB2	1.91	0.51
1:A:70:MSE:O	9:A:514:EDO:H11	2.12	0.50
1:B:237:PHE:HB3	1:B:248:ALA:HB3	1.93	0.50
1:C:219:ASP:O	1:C:223:ARG:HG2	2.12	0.49
1:D:30:ILE:CD1	1:D:53:ILE:HG13	2.41	0.49
9:B:505:EDO:H11	11:B:653:HOH:O	2.12	0.49
1:D:335:ILE:HD13	1:D:363:LEU:HD22	1.94	0.49
1:A:30:ILE:CD1	1:A:53:ILE:HG13	2.42	0.49
1:D:332[A]:MSE:HE3	1:D:341:PHE:CE2	2.49	0.48
1:A:74:TYR:CE1	1:A:100:PRO:HD2	2.49	0.48
1:C:74:TYR:CE1	1:C:100:PRO:HD2	2.48	0.48
1:B:377:GLU:HG3	1:B:418:LEU:HD12	1.94	0.48
1:D:237:PHE:HB3	1:D:248:ALA:HB3	1.95	0.47
1:C:41:GLU:HG3	1:C:45:LYS:HE2	1.97	0.47
1:C:13:MSE:HG3	1:C:17:LYS:HE3	1.97	0.47
1:A:164:GLY:HA2	5:A:504[A]:COA:H1B	1.96	0.46
1:B:219:ASP:O	1:B:223:ARG:HG2	2.15	0.46
1:B:30:ILE:CD1	1:B:53:ILE:HG13	2.44	0.46
1:B:332[A]:MSE:HE3	1:B:341:PHE:CE2	2.50	0.46
1:D:64:PHE:HB3	1:D:301:ARG:HG3	1.98	0.45
1:C:335:ILE:HD13	1:C:372:MSE:HB2	1.98	0.45
1:C:30:ILE:CD1	1:C:53:ILE:HG13	2.43	0.45
1:D:219:ASP:O	1:D:223:ARG:HG2	2.16	0.45
1:B:8:GLU:O	1:B:12:ILE:HG12	2.16	0.45
1:A:90:ILE:HD11	1:B:157:LEU:HD21	1.98	0.45
1:B:41:GLU:OE2	1:B:45:LYS:HE2	2.16	0.45
1:C:64:PHE:HB3	1:C:301:ARG:HG3	1.98	0.44
1:A:400:LEU:O	1:A:404:ILE:HG12	2.17	0.44
1:A:33:ALA:O	1:A:39:TYR:HB2	2.17	0.43
1:B:348:ILE:HD11	1:B:403:GLU:HB3	2.00	0.43
1:B:64:PHE:HB3	1:B:301:ARG:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:ALA:HB2	10:D:504:PEG:H12	2.00	0.43
7:A:508:PGE:H6	11:A:772:HOH:O	2.19	0.42
1:C:224:LYS:O	1:C:228:MSE:HG3	2.19	0.42
1:D:184:ILE:HD12	1:D:215:GLU:OE2	2.20	0.41
1:C:129:THR:HB	1:D:84:LYS:HE2	2.02	0.41
1:C:306:THR:HB	1:C:325:ILE:HD13	2.03	0.41
1:D:348:ILE:HD11	1:D:403:GLU:HB3	2.01	0.41
1:C:303:ARG:NH1	9:C:510:EDO:H12	2.34	0.41
1:A:343[B]:MSE:HG3	1:A:347:LYS:HE3	2.03	0.41
1:A:335:ILE:HD13	1:A:363:LEU:HD22	2.02	0.41
1:C:157:LEU:HD21	1:D:90:ILE:HD11	2.02	0.41
1:B:328:ARG:HD3	1:B:330:ASP:OD2	2.21	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	439/436 (101%)	420 (96%)	18 (4%)	1 (0%)	52	69
1	B	423/436 (97%)	408 (96%)	14 (3%)	1 (0%)	52	69
1	C	436/436 (100%)	419 (96%)	15 (3%)	2 (0%)	34	47
1	D	422/436 (97%)	406 (96%)	15 (4%)	1 (0%)	52	69
All	All	1720/1744 (99%)	1653 (96%)	62 (4%)	5 (0%)	46	62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ASN
1	B	243	ASN
1	C	243	ASN

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Mol	Chain	Res	Type
1	D	243	ASN
1	C	384	ASP

### 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	382/370 (103%)	378 (99%)	4 (1%)	82	92
1	B	360/370 (97%)	357 (99%)	3 (1%)	86	94
1	C	373/370 (101%)	367 (98%)	6 (2%)	70	85
1	D	358/370 (97%)	355 (99%)	3 (1%)	86	94
All	All	1473/1480 (100%)	1457 (99%)	16 (1%)	80	91

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	A	249	PHE
1	A	259	PHE
1	A	335	ILE
1	B	210	LEU
1	B	249	PHE
1	B	259	PHE
1	C	165	ASN
1	C	249	PHE
1	C	259	PHE
1	C	269	ILE
1	C	384	ASP
1	C	391	LYS
1	D	249	PHE
1	D	259	PHE
1	D	330	ASP

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

### 5.3.3 RNA ⓘ

There are no RNA 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 ⓘ

Of 38 ligands modelled in this entry, 10 are monoatomic - leaving 28 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	ADP	A	502[A]	6	22,29,29	0.62	0	27,45,45	0.80	1 (3%)
4	AMP	A	503[B]	6	20,25,25	0.67	0	22,38,38	0.64	0
5	COA	A	504[A]	-	26,33,50	0.74	0	33,52,75	1.77	6 (18%)
7	PGE	A	508	-	9,9,9	0.21	0	8,8,8	0.21	0
8	SO4	A	509[B]	-	4,4,4	0.20	0	6,6,6	0.09	0
8	SO4	A	510	-	4,4,4	0.49	0	6,6,6	0.31	0
8	SO4	A	511	-	4,4,4	0.16	0	6,6,6	0.11	0
9	EDO	A	512	-	3,3,3	0.60	0	2,2,2	0.15	0
9	EDO	A	513	-	3,3,3	0.58	0	2,2,2	0.40	0
9	EDO	A	514	-	3,3,3	0.41	0	2,2,2	0.36	0
9	EDO	A	515	-	3,3,3	0.81	0	2,2,2	0.24	0
3	ADP	B	502	-	22,29,29	0.62	0	27,45,45	0.65	1 (3%)
8	SO4	B	503	-	4,4,4	0.08	0	6,6,6	0.21	0
9	EDO	B	504	-	3,3,3	0.54	0	2,2,2	0.43	0
9	EDO	B	505	-	3,3,3	0.65	0	2,2,2	0.26	0
9	EDO	B	506	-	3,3,3	0.74	0	2,2,2	0.05	0
4	AMP	C	502	6	20,25,25	0.58	0	22,38,38	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	COA	C	503[A]	-	26,33,50	0.75	1 (3%)	33,52,75	1.61	5 (15%)
8	SO4	C	506[B]	-	4,4,4	0.17	0	6,6,6	0.09	0
8	SO4	C	507	-	4,4,4	0.19	0	6,6,6	0.12	0
9	EDO	C	508	-	3,3,3	0.56	0	2,2,2	0.55	0
9	EDO	C	509	-	3,3,3	0.65	0	2,2,2	0.39	0
9	EDO	C	510	-	3,3,3	0.65	0	2,2,2	0.35	0
3	ADP	D	502	-	22,29,29	0.57	0	27,45,45	0.76	1 (3%)
10	PEG	D	504	-	6,6,6	0.27	0	5,5,5	0.29	0
8	SO4	D	505	-	4,4,4	0.32	0	6,6,6	0.22	0
9	EDO	D	506	-	3,3,3	0.69	0	2,2,2	0.22	0
9	EDO	D	507	-	3,3,3	0.67	0	2,2,2	0.37	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	ADP	A	502[A]	6	-	0/12/32/32	0/3/3/3
4	AMP	A	503[B]	6	-	0/6/26/26	0/3/3/3
5	COA	A	504[A]	-	-	0/17/37/64	0/3/3/3
7	PGE	A	508	-	-	0/7/7/7	0/0/0/0
8	SO4	A	509[B]	-	-	0/0/0/0	0/0/0/0
8	SO4	A	510	-	-	0/0/0/0	0/0/0/0
8	SO4	A	511	-	-	0/0/0/0	0/0/0/0
9	EDO	A	512	-	-	0/1/1/1	0/0/0/0
9	EDO	A	513	-	-	0/1/1/1	0/0/0/0
9	EDO	A	514	-	-	0/1/1/1	0/0/0/0
9	EDO	A	515	-	-	0/1/1/1	0/0/0/0
3	ADP	B	502	-	-	0/12/32/32	0/3/3/3
8	SO4	B	503	-	-	0/0/0/0	0/0/0/0
9	EDO	B	504	-	-	0/1/1/1	0/0/0/0
9	EDO	B	505	-	-	0/1/1/1	0/0/0/0
9	EDO	B	506	-	-	0/1/1/1	0/0/0/0
4	AMP	C	502	6	-	0/6/26/26	0/3/3/3
5	COA	C	503[A]	-	-	0/17/37/64	0/3/3/3
8	SO4	C	506[B]	-	-	0/0/0/0	0/0/0/0
8	SO4	C	507	-	-	0/0/0/0	0/0/0/0
9	EDO	C	508	-	-	0/1/1/1	0/0/0/0
9	EDO	C	509	-	-	0/1/1/1	0/0/0/0
9	EDO	C	510	-	-	0/1/1/1	0/0/0/0
3	ADP	D	502	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PEG	D	504	-	-	0/4/4/4	0/0/0/0
8	SO4	D	505	-	-	0/0/0/0	0/0/0/0
9	EDO	D	506	-	-	0/1/1/1	0/0/0/0
9	EDO	D	507	-	-	0/1/1/1	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	503[A]	COA	P2A-O6A	2.25	1.62	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504[A]	COA	O6A-P2A-O5A	-2.67	97.21	107.38
5	C	503[A]	COA	O6A-P2A-O5A	-2.36	98.38	107.38
5	A	504[A]	COA	P1A-O3A-P2A	-2.27	125.06	132.67
3	A	502[A]	ADP	O5'-PA-O1A	2.15	117.98	109.62
3	B	502	ADP	O5'-PA-O1A	2.19	118.11	109.62
3	D	502	ADP	O5'-PA-O1A	2.35	118.76	109.62
5	C	503[A]	COA	O5A-P2A-O4A	2.78	119.54	110.58
5	C	503[A]	COA	O6A-P2A-O3A	3.05	118.91	105.09
5	A	504[A]	COA	O6A-P2A-O3A	3.47	120.83	105.09
5	A	504[A]	COA	O5A-P2A-O4A	3.78	122.75	110.58
5	C	503[A]	COA	O3B-P3B-O7A	3.78	116.56	107.11
5	A	504[A]	COA	O3B-P3B-O7A	4.15	117.47	107.11
5	C	503[A]	COA	O3A-P1A-O5B	5.38	117.20	102.94
5	A	504[A]	COA	O3A-P1A-O5B	5.46	117.42	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	504[A]	COA	1	0
7	A	508	PGE	1	0
9	A	512	EDO	1	0
9	A	514	EDO	1	0
9	B	505	EDO	1	0
9	C	510	EDO	3	0
10	D	504	PEG	2	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	418/436 (95%)	-0.23	9 (2%) 65 64	23, 45, 81, 124	0
1	B	408/436 (93%)	0.30	49 (12%) 6 5	28, 54, 107, 128	0
1	C	419/436 (96%)	-0.09	12 (2%) 55 54	29, 56, 96, 119	0
1	D	411/436 (94%)	-0.09	16 (3%) 43 43	27, 48, 94, 122	0
All	All	1656/1744 (94%)	-0.03	86 (5%) 31 30	23, 51, 97, 128	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	400	LEU	7.0
1	C	382	SER	6.9
1	B	410	VAL	5.2
1	B	396	ILE	5.0
1	B	405	LEU	4.9
1	D	338	VAL	4.8
1	B	378	LEU	4.8
1	A	421	SER	4.6
1	B	333	PHE	4.6
1	B	389	LEU	4.5
1	B	404	ILE	4.3
1	B	340	ILE	4.2
1	B	370	ASP	4.0
1	B	411	LYS	3.9
1	C	0	GLY	3.8
1	B	380	ASP	3.8
1	C	53	ILE	3.7
1	B	371	GLU	3.7
1	D	363	LEU	3.6
1	A	426	VAL	3.5
1	D	373	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	408	PRO	3.5
1	A	419	PRO	3.5
1	B	386	TYR	3.4
1	B	407	THR	3.4
1	D	405	LEU	3.4
1	D	334	ILE	3.4
1	B	376	VAL	3.3
1	B	406	VAL	3.2
1	D	368	ASN	3.2
1	B	363	LEU	3.2
1	D	431	LEU	3.1
1	A	368	ASN	3.1
1	B	426	VAL	3.1
1	B	430	ASP	3.1
1	B	402	ASP	3.1
1	C	271	PRO	3.0
1	B	337	GLY	3.0
1	D	335	ILE	3.0
1	B	392	ILE	2.9
1	B	382	SER	2.9
1	C	433	ASP	2.9
1	A	355	LEU	2.9
1	B	381	LEU	2.9
1	B	384	ASP	2.8
1	B	348	ILE	2.8
1	B	417	SER	2.8
1	B	364	GLU	2.8
1	D	382	SER	2.8
1	C	383	THR	2.7
1	B	334	ILE	2.7
1	B	335	ILE	2.6
1	B	398	ARG	2.6
1	C	55	SER	2.6
1	B	365	THR	2.6
1	C	200	ILE	2.6
1	B	351[A]	GLN	2.5
1	B	383	THR	2.5
1	A	384	ASP	2.5
1	C	311	GLY	2.5
1	B	393	ARG	2.4
1	B	428	VAL	2.4
1	B	429	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	376	VAL	2.4
1	D	337	GLY	2.4
1	B	419	PRO	2.4
1	B	413	VAL	2.4
1	D	397	ILE	2.4
1	C	387	ILE	2.4
1	B	412	LEU	2.3
1	A	414	LYS	2.3
1	C	310	PRO	2.3
1	B	431	LEU	2.3
1	D	369	GLN	2.3
1	C	426	VAL	2.2
1	A	382	SER	2.2
1	B	385	ASN	2.2
1	B	397	ILE	2.2
1	B	336	LYS	2.2
1	D	378	LEU	2.1
1	B	338	VAL	2.1
1	D	396	ILE	2.1
1	D	384	ASP	2.1
1	B	352	PHE	2.0
1	D	410	VAL	2.0
1	B	353	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<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( $\text{\AA}^2$ )	Q<0.9
9	EDO	A	512	4/4	0.91	0.35	13.64	59,59,59,60	0
7	PGE	A	508	10/10	0.90	0.36	9.89	64,75,78,78	0
10	PEG	D	504	7/7	0.79	0.34	6.58	63,65,73,74	0
5	COA	C	503[A]	31/48	0.93	0.29	5.21	23,35,42,43	31
9	EDO	A	515	4/4	0.96	0.17	4.84	31,36,38,41	0
9	EDO	A	514	4/4	0.95	0.24	4.42	61,61,62,63	0
9	EDO	B	505	4/4	0.89	0.29	3.46	55,55,58,60	0
5	COA	A	504[A]	31/48	0.91	0.25	3.06	37,45,59,61	31
9	EDO	C	510	4/4	0.88	0.21	2.98	58,59,59,60	0
9	EDO	D	506	4/4	0.82	0.18	2.93	76,78,78,78	0
9	EDO	B	504	4/4	0.81	0.18	1.81	74,74,74,76	0
3	ADP	A	502[A]	27/27	0.97	0.15	0.90	38,52,55,55	27
8	SO4	C	506[B]	5/5	0.98	0.14	0.77	126,126,126,126	5
8	SO4	B	503	5/5	0.95	0.15	0.68	43,43,44,45	5
8	SO4	C	507	5/5	0.90	0.19	0.15	49,50,51,52	5
8	SO4	D	505	5/5	0.97	0.14	0.07	78,79,80,81	0
4	AMP	A	503[B]	23/23	0.98	0.13	0.04	13,21,24,25	23
3	ADP	B	502	27/27	0.95	0.14	-0.08	41,54,85,86	0
4	AMP	C	502	23/23	0.93	0.14	-0.17	37,45,53,61	0
8	SO4	A	510	5/5	0.99	0.12	-0.19	53,54,58,60	0
6	K	A	507	1/1	0.97	0.14	-0.21	43,43,43,43	0
3	ADP	D	502	27/27	0.95	0.14	-0.41	31,43,80,83	0
8	SO4	A	509[B]	5/5	0.97	0.09	-0.82	102,102,102,102	5
2	ZN	A	501	1/1	0.99	0.10	-0.86	47,47,47,47	0
2	ZN	C	501	1/1	0.97	0.07	-1.55	65,65,65,65	0
6	K	C	505	1/1	0.97	0.07	-2.03	42,42,42,42	0
6	K	D	503	1/1	0.98	0.05	-3.37	37,37,37,37	0
6	K	A	506	1/1	0.99	0.05	-3.59	32,32,32,32	0
2	ZN	B	501	1/1	0.96	0.09	-3.96	48,48,48,48	0
2	ZN	D	501	1/1	0.99	0.06	-4.61	47,47,47,47	0
9	EDO	A	513	4/4	0.90	0.26	-	69,70,71,74	0
6	K	C	504	1/1	0.99	0.07	-	45,45,45,45	0
9	EDO	C	509	4/4	0.89	0.27	-	63,65,66,68	0
9	EDO	D	507	4/4	0.91	0.15	-	50,51,51,52	0
9	EDO	B	506	4/4	0.70	0.25	-	59,62,63,64	0
8	SO4	A	511	5/5	0.88	0.17	-	53,53,56,58	5
9	EDO	C	508	4/4	0.85	0.20	-	68,68,68,68	0
6	K	A	505	1/1	0.99	0.06	-	40,40,40,40	0

## 6.5 Other polymers

There are no such residues in this entry.