



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2016 – 11:15 AM GMT

PDB ID : 5AOV
Title : Ternary Crystal Structure of Pyrococcus furiosus Glyoxylate Hydroxypyruvate Reductase in presence of glyoxylate
Authors : Lassalle, L.; Girard, E.
Deposited on : 2015-09-12
Resolution : 1.40 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

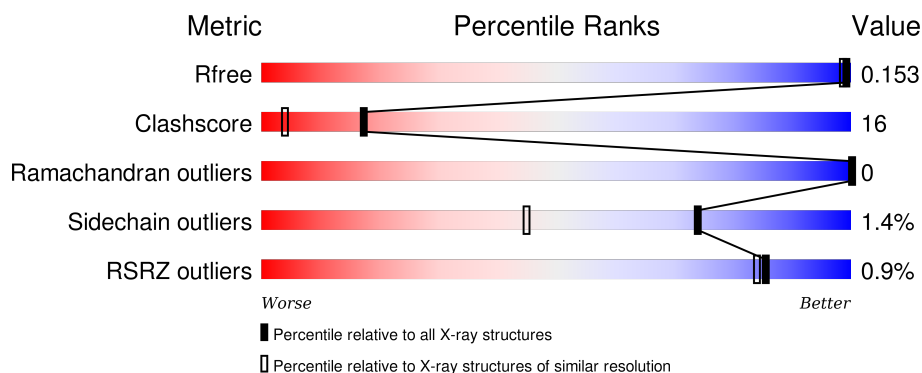
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	1199 (1.40-1.40)
Clashscore	102246	1295 (1.40-1.40)
Ramachandran outliers	100387	1259 (1.40-1.40)
Sidechain outliers	100360	1258 (1.40-1.40)
RSRZ outliers	91569	1198 (1.40-1.40)

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 $\leq 5\%$. 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	336	<div> <div></div> <div>84%</div> <div>15%</div> <div>.</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
2	NAP	A	1335[B]	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLV	A	1356	-	-	X	X
4	1PE	A	1343	-	-	X	X
4	1PE	A	1344	-	-	-	X
4	1PE	A	1346	-	-	-	X
4	1PE	A	1347	-	-	X	X
4	1PE	A	1349	-	-	X	-
4	1PE	A	1355	-	-	-	X
4	1PE	A	1359	-	-	X	X
5	EDO	A	1352	-	-	-	X
5	EDO	A	1353	-	-	-	X
6	ACY	A	1357	-	-	-	X

2 Entry composition [i](#)

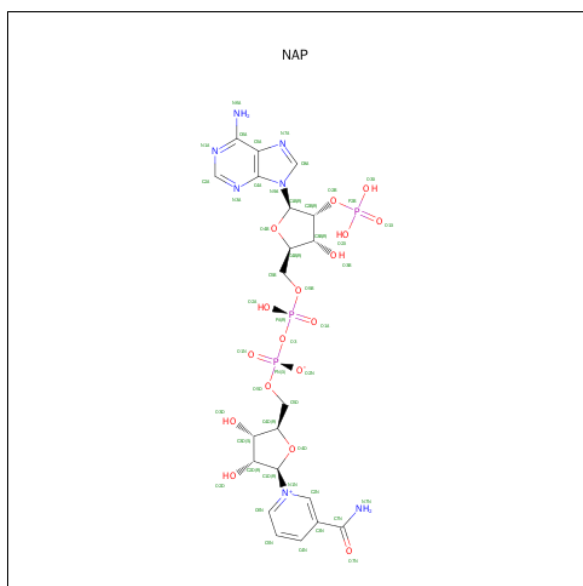
There are 7 unique types of molecules in this entry. The entry contains 6415 atoms, of which 2894 are hydrogens and 0 are deuteriums.

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 GLYOXYLATE REDUCTASE.

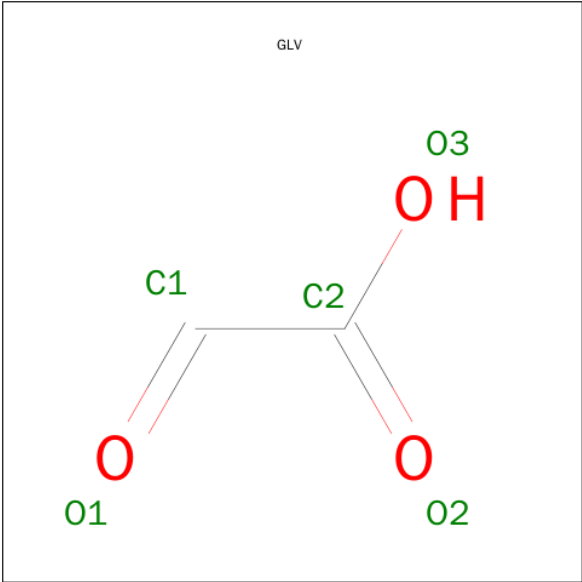
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	334	5676	1810	2858	483	517	8	0	19	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



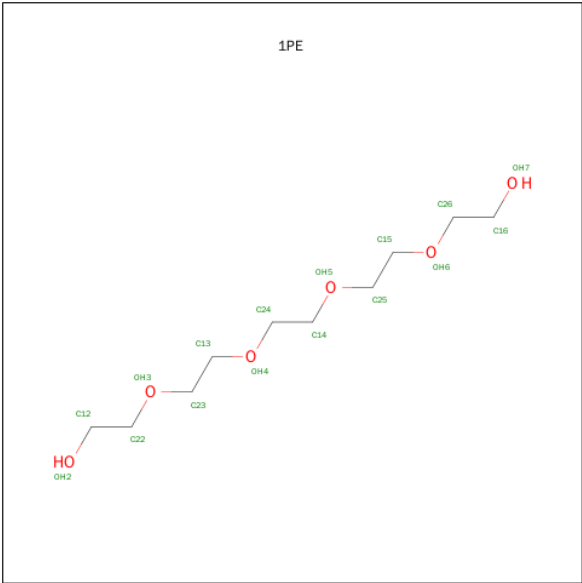
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	96	42	14	34	6	0	1

- Molecule 3 is GLYOXYLIC ACID (three-letter code: GLV) (formula: C₂H₂O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			5	2	3		
3	A	1	Total	C	O	0	0
			5	2	3		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



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

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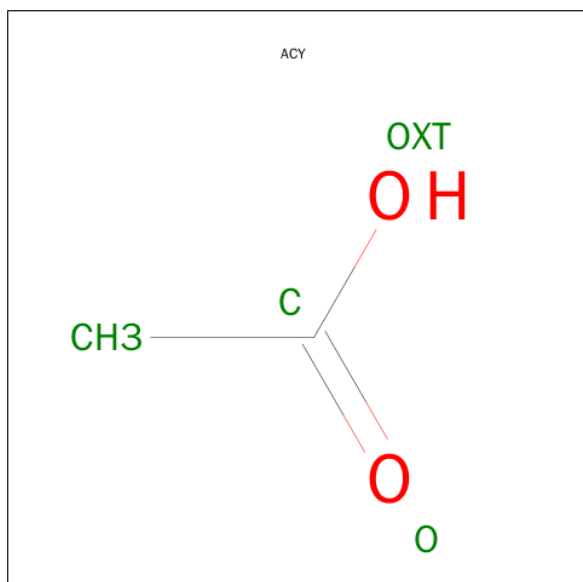
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			13	8	5		
4	A	1	Total	C	O	0	0
			16	10	6		
4	A	1	Total	C	O	0	0
			16	10	6		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			7	2	3	2		
6	A	1	Total	C	H	O	0	0
			7	2	3	2		

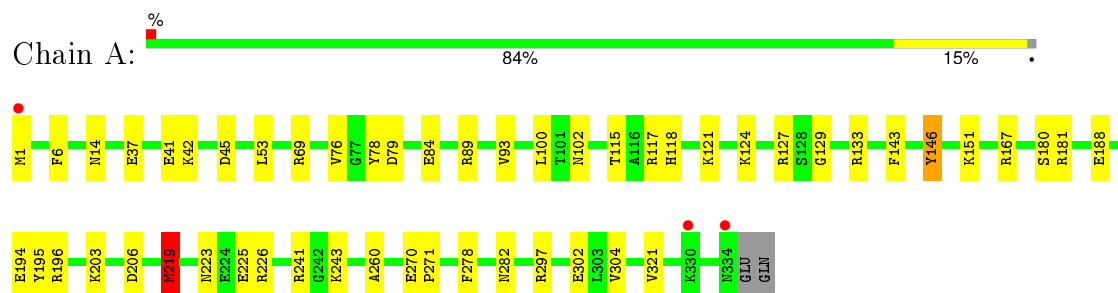
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	422	Total	O	0	0
			422	422		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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: GLYOXYLATE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	114.58Å 114.58Å 118.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.51 – 1.40 47.73 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.51-1.40) 99.4 (47.73-1.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 1.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.131 , 0.143 0.145 , 0.153	Depositor DCC
R_{free} test set	7473 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 58.5	EDS
Estimated twinning fraction	0.019 for l,-k,h 0.023 for -l,-k,-h 0.025 for -h,-l,-k 0.018 for -h,l,k 0.059 for -h,k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 148513 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	6415	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, NAP, EDO, GLV, 1PE

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	1.03	2/2909 (0.1%)	1.13	18/3925 (0.5%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	GLU	CB-CG	5.46	1.62	1.52
1	A	146	TYR	CE1-CZ	-5.05	1.31	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	ARG	NE-CZ-NH1	10.35	125.47	120.30
1	A	219	MET	CG-SD-CE	-9.50	85.00	100.20
1	A	127	ARG	NE-CZ-NH2	-9.45	115.58	120.30
1	A	241[A]	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	A	241[B]	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	A	241[A]	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	A	241[B]	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	A	226	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	45	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	45	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	A	206	ASP	CB-CG-OD2	6.92	124.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	304	VAL	CG1-CB-CG2	6.79	121.76	110.90
1	A	127	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	278	PHE	CB-CG-CD2	-5.97	116.62	120.80
1	A	206	ASP	CB-CG-OD1	-5.95	112.94	118.30
1	A	226	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	79	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ARG	Sidechain

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	2818	2858	2899	71	0
2	A	96	0	49	2	0
3	A	10	0	2	3	0
4	A	147	0	192	76	0
5	A	20	30	30	0	0
6	A	8	6	6	0	0
7	A	422	0	0	25	2
All	All	3521	2894	3178	101	2

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 16.

All (101) 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)
4:A:1359:IPE:H241	7:A:2214:HOH:O	1.34	1.25
1:A:143:PHE:H	4:A:1359:IPE:H132	1.12	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LYS:HZ2	4:A:1349:1PE:H132	1.14	1.07
4:A:1359:1PE:H242	7:A:2185:HOH:O	1.58	1.01
1:A:151:LYS:HZ2	4:A:1347:1PE:H132	1.24	1.00
1:A:203:LYS:HZ3	4:A:1348:1PE:H131	1.32	0.91
4:A:1343:1PE:H132	4:A:1343:1PE:H122	1.65	0.77
1:A:243:LYS:NZ	4:A:1349:1PE:H141	2.02	0.74
1:A:102:ASN:HD21	4:A:1346:1PE:H241	1.52	0.74
1:A:14:ASN:ND2	1:A:302[A]:GLU:HG3	2.03	0.73
4:A:1343:1PE:C13	4:A:1343:1PE:H122	2.20	0.72
4:A:1347:1PE:H131	7:A:2285:HOH:O	1.91	0.71
4:A:1343:1PE:C13	4:A:1343:1PE:C12	2.70	0.70
4:A:1343:1PE:C14	4:A:1359:1PE:OH6	2.40	0.70
1:A:118:HIS:HA	4:A:1343:1PE:H221	1.75	0.69
1:A:124[B]:LYS:HG3	7:A:2187:HOH:O	1.92	0.68
1:A:181:ARG:HH21	2:A:1335[A]:NAP:P2B	2.17	0.68
1:A:14:ASN:ND2	1:A:302[A]:GLU:CG	2.57	0.68
1:A:143:PHE:N	4:A:1359:1PE:H132	1.98	0.66
4:A:1343:1PE:H222	7:A:2186:HOH:O	1.95	0.66
3:A:1336:GLV:H1	7:A:2352:HOH:O	1.96	0.66
4:A:1359:1PE:C24	7:A:2185:HOH:O	2.27	0.66
1:A:133:ARG:HH11	4:A:1338:1PE:H131	1.61	0.64
1:A:223:ASN:HD22	4:A:1340:1PE:H121	1.63	0.64
1:A:151:LYS:NZ	4:A:1347:1PE:H141	2.13	0.64
1:A:297[B]:ARG:NH2	7:A:2351:HOH:O	2.32	0.63
4:A:1343:1PE:H141	4:A:1359:1PE:OH6	1.99	0.62
1:A:78:TYR:CZ	1:A:321[A]:VAL:HG11	2.35	0.62
1:A:118:HIS:ND1	4:A:1343:1PE:H122	2.16	0.60
4:A:1359:1PE:H152	7:A:2219:HOH:O	2.01	0.60
1:A:243:LYS:HZ2	4:A:1349:1PE:H141	1.66	0.60
1:A:146:TYR:CD1	4:A:1347:1PE:H152	2.36	0.60
1:A:151:LYS:NZ	4:A:1347:1PE:H221	2.17	0.60
4:A:1343:1PE:H142	4:A:1359:1PE:OH6	2.02	0.58
1:A:203:LYS:NZ	4:A:1348:1PE:H131	2.14	0.58
1:A:118:HIS:CE1	4:A:1343:1PE:H142	2.39	0.58
4:A:1339:1PE:H121	7:A:2401:HOH:O	2.04	0.57
1:A:133:ARG:HG2	4:A:1338:1PE:H121	1.85	0.57
4:A:1349:1PE:H122	7:A:2416:HOH:O	2.04	0.56
1:A:14:ASN:HD21	1:A:302[A]:GLU:HG3	1.70	0.56
1:A:243:LYS:NZ	4:A:1349:1PE:H121	2.21	0.55
1:A:146:TYR:HD1	4:A:1347:1PE:H152	1.71	0.55
1:A:118:HIS:ND1	4:A:1343:1PE:C12	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1349:1PE:H132	4:A:1349:1PE:H121	1.88	0.55
1:A:243:LYS:HZ3	4:A:1349:1PE:H141	1.70	0.54
1:A:203:LYS:HZ3	4:A:1348:1PE:H222	1.73	0.54
1:A:282:ASN:HA	4:A:1343:1PE:H131	1.90	0.54
4:A:1346:1PE:H231	7:A:2412:HOH:O	2.07	0.53
1:A:93:VAL:O	1:A:321[B]:VAL:HG22	2.07	0.53
4:A:1344:1PE:H242	7:A:2194:HOH:O	2.08	0.53
4:A:1349:1PE:H121	4:A:1349:1PE:C13	2.39	0.53
4:A:1345:1PE:H241	7:A:2410:HOH:O	2.08	0.53
1:A:151:LYS:HZ2	4:A:1347:1PE:H141	1.75	0.52
1:A:41[B]:GLU:HG2	7:A:2082:HOH:O	2.09	0.52
1:A:14:ASN:HD22	1:A:302[A]:GLU:CG	2.23	0.51
4:A:1346:1PE:H131	7:A:2413:HOH:O	2.11	0.51
1:A:203:LYS:NZ	4:A:1348:1PE:H222	2.25	0.51
1:A:194:GLU:CD	1:A:196:ARG:HH12	2.15	0.50
4:A:1343:1PE:C12	7:A:2189:HOH:O	2.59	0.50
1:A:151:LYS:NZ	4:A:1347:1PE:H132	2.10	0.50
1:A:194:GLU:HG2	1:A:196:ARG:NH1	2.26	0.49
1:A:6:PHE:CE1	1:A:42:LYS:HD3	2.46	0.49
1:A:37[B]:GLU:O	1:A:41[B]:GLU:HG3	2.14	0.48
1:A:243:LYS:NZ	4:A:1349:1PE:H132	2.03	0.48
1:A:133:ARG:NH1	4:A:1338:1PE:H131	2.27	0.47
3:A:1356:GLV:H1	7:A:2095:HOH:O	2.15	0.47
1:A:121:LYS:CE	4:A:1343:1PE:OH2	2.63	0.47
1:A:219:MET:HE1	4:A:1349:1PE:H241	1.96	0.46
1:A:53:LEU:H	3:A:1356:GLV:C1	2.28	0.46
1:A:118:HIS:ND1	4:A:1343:1PE:H221	2.30	0.46
1:A:118:HIS:CE1	4:A:1359:1PE:H151	2.50	0.46
1:A:84:GLU:OE1	7:A:2149:HOH:O	2.21	0.46
1:A:118:HIS:HE1	4:A:1343:1PE:H142	1.81	0.45
1:A:225:GLU:HG3	7:A:2300:HOH:O	2.15	0.45
1:A:282:ASN:HA	4:A:1343:1PE:H232	1.98	0.45
1:A:69:ARG:HD3	7:A:2127:HOH:O	2.16	0.45
1:A:219:MET:CE	4:A:1349:1PE:H142	2.46	0.45
1:A:118:HIS:CE1	4:A:1343:1PE:H132	2.52	0.44
1:A:203:LYS:HZ3	4:A:1348:1PE:C13	2.16	0.44
1:A:129:GLY:HA3	4:A:1338:1PE:H132	1.99	0.44
4:A:1345:1PE:H121	4:A:1345:1PE:H231	1.79	0.44
1:A:219:MET:HE3	4:A:1349:1PE:H142	1.99	0.44
4:A:1359:1PE:H141	7:A:2185:HOH:O	2.18	0.44
1:A:260:ALA:O	4:A:1343:1PE:H241	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLU:HA	1:A:271:PRO:C	2.38	0.43
1:A:118:HIS:ND1	4:A:1343:1PE:C22	2.82	0.43
1:A:76:VAL:CG1	2:A:1335[A]:NAP:H6N	2.48	0.43
1:A:195:TYR:CE1	4:A:1341:1PE:H132	2.54	0.43
4:A:1343:1PE:C22	7:A:2186:HOH:O	2.62	0.42
1:A:102:ASN:ND2	4:A:1346:1PE:H241	2.26	0.41
1:A:124[B]:LYS:HE3	7:A:2187:HOH:O	2.20	0.41
1:A:151:LYS:HZ1	4:A:1347:1PE:H141	1.86	0.41
4:A:1349:1PE:H141	4:A:1349:1PE:H132	1.90	0.41
1:A:194:GLU:OE1	1:A:196:ARG:NH2	2.53	0.41
1:A:223:ASN:HB3	4:A:1340:1PE:H121	2.02	0.41
1:A:133:ARG:NH1	4:A:1338:1PE:C13	2.83	0.41
1:A:124[B]:LYS:HE2	7:A:2192:HOH:O	2.21	0.40
4:A:1349:1PE:H122	4:A:1349:1PE:H231	1.88	0.40
1:A:115:THR:O	4:A:1343:1PE:H231	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2059:HOH:O	7:A:2251:HOH:O[3_645]	1.94	0.26
7:A:2220:HOH:O	7:A:2354:HOH:O[6_765]	1.97	0.23

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	351/336 (104%)	342 (97%)	9 (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	301/284 (106%)	297 (99%)	4 (1%)	76	48

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	100	LEU
1	A	180	SER
1	A	219	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN

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](#)

26 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	NAP	A	1335[A]	-	45,52,52	3.21	12 (26%)	55,80,80	2.55	17 (30%)
2	NAP	A	1335[B]	-	45,52,52	2.89	12 (26%)	55,80,80	2.56	15 (27%)
3	GLV	A	1336	-	1,4,4	0.74	0	0,4,4	0.00	-
4	1PE	A	1337	-	6,6,15	0.41	0	5,5,14	0.80	0
4	1PE	A	1338	-	6,6,15	0.69	0	5,5,14	1.74	1 (20%)
4	1PE	A	1339	-	6,6,15	0.84	0	5,5,14	1.88	2 (40%)
4	1PE	A	1340	-	6,6,15	0.78	0	5,5,14	1.66	2 (40%)
4	1PE	A	1341	-	6,6,15	0.66	0	5,5,14	1.87	2 (40%)
4	1PE	A	1342	-	6,6,15	0.78	0	5,5,14	1.92	2 (40%)
4	1PE	A	1343	-	9,9,15	0.98	0	8,8,14	1.65	2 (25%)
4	1PE	A	1344	-	9,9,15	0.52	0	8,8,14	2.39	4 (50%)
4	1PE	A	1345	-	9,9,15	0.55	0	8,8,14	2.30	4 (50%)
4	1PE	A	1346	-	9,9,15	0.62	0	8,8,14	1.90	3 (37%)
4	1PE	A	1347	-	12,12,15	0.91	0	11,11,14	1.48	3 (27%)
4	1PE	A	1348	-	15,15,15	0.83	0	14,14,14	1.76	4 (28%)
4	1PE	A	1349	-	15,15,15	0.83	0	14,14,14	1.85	5 (35%)
5	EDO	A	1350	-	3,3,3	0.51	0	2,2,2	0.23	0
5	EDO	A	1351	-	3,3,3	0.56	0	2,2,2	0.16	0
5	EDO	A	1352	-	3,3,3	0.54	0	2,2,2	0.48	0
5	EDO	A	1353	-	3,3,3	0.54	0	2,2,2	0.36	0
5	EDO	A	1354	-	3,3,3	0.59	0	2,2,2	0.16	0
4	1PE	A	1355	-	6,6,15	0.80	0	5,5,14	1.51	0
3	GLV	A	1356	-	1,4,4	0.05	0	0,4,4	0.00	-
6	ACY	A	1357	-	0,3,3	0.00	-	0,3,3	0.00	-
6	ACY	A	1358	-	0,3,3	0.00	-	0,3,3	0.00	-
4	1PE	A	1359	-	12,12,15	0.71	0	11,11,14	2.67	6 (54%)

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	NAP	A	1335[A]	-	-	0/27/67/67	0/5/5/5
2	NAP	A	1335[B]	-	1/1/12/12	0/27/67/67	0/5/5/5
3	GLV	A	1336	-	-	0/0/2/2	0/0/0/0
4	1PE	A	1337	-	-	0/4/4/13	0/0/0/0
4	1PE	A	1338	-	-	0/4/4/13	0/0/0/0
4	1PE	A	1339	-	-	0/4/4/13	0/0/0/0
4	1PE	A	1340	-	-	0/4/4/13	0/0/0/0
4	1PE	A	1341	-	-	0/4/4/13	0/0/0/0
4	1PE	A	1342	-	-	0/4/4/13	0/0/0/0
4	1PE	A	1343	-	-	0/7/7/13	0/0/0/0
4	1PE	A	1344	-	-	0/7/7/13	0/0/0/0
4	1PE	A	1345	-	-	0/7/7/13	0/0/0/0
4	1PE	A	1346	-	-	0/7/7/13	0/0/0/0
4	1PE	A	1347	-	-	0/10/10/13	0/0/0/0
4	1PE	A	1348	-	-	0/13/13/13	0/0/0/0
4	1PE	A	1349	-	-	0/13/13/13	0/0/0/0
5	EDO	A	1350	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1351	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1352	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1353	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1354	-	-	0/1/1/1	0/0/0/0
4	1PE	A	1355	-	-	0/4/4/13	0/0/0/0
3	GLV	A	1356	-	-	0/0/2/2	0/0/0/0
6	ACY	A	1357	-	-	0/0/0/0	0/0/0/0
6	ACY	A	1358	-	-	0/0/0/0	0/0/0/0
4	1PE	A	1359	-	-	0/10/10/13	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1335[A]	NAP	C2D-C1D	-11.22	1.35	1.53
2	A	1335[B]	NAP	C2D-C1D	-8.69	1.39	1.53
2	A	1335[A]	NAP	C2B-C1B	-7.64	1.32	1.53
2	A	1335[B]	NAP	C2B-C1B	-6.00	1.36	1.53
2	A	1335[A]	NAP	C3B-C4B	-5.77	1.37	1.53
2	A	1335[B]	NAP	C3B-C4B	-5.10	1.39	1.53
2	A	1335[B]	NAP	O4D-C4D	-4.83	1.34	1.45
2	A	1335[A]	NAP	O4D-C4D	-3.35	1.37	1.45
2	A	1335[B]	NAP	P2B-O2X	-2.47	1.46	1.54
2	A	1335[A]	NAP	C5N-C4N	2.23	1.43	1.38
2	A	1335[A]	NAP	C4N-C3N	2.52	1.43	1.39
2	A	1335[A]	NAP	O2D-C2D	2.58	1.49	1.43
2	A	1335[B]	NAP	O4B-C4B	2.76	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1335[A]	NAP	O4B-C4B	3.27	1.52	1.45
2	A	1335[B]	NAP	C4N-C3N	3.70	1.45	1.39
2	A	1335[A]	NAP	C7N-N7N	4.13	1.41	1.33
2	A	1335[B]	NAP	C5N-C4N	4.14	1.47	1.38
2	A	1335[B]	NAP	C7N-N7N	4.19	1.41	1.33
2	A	1335[A]	NAP	C3B-C2B	4.54	1.63	1.53
2	A	1335[B]	NAP	C3B-C2B	4.56	1.63	1.53
2	A	1335[B]	NAP	O4B-C1B	4.82	1.48	1.41
2	A	1335[A]	NAP	O4B-C1B	5.03	1.48	1.41
2	A	1335[B]	NAP	O4D-C1D	9.11	1.54	1.41
2	A	1335[A]	NAP	O4D-C1D	10.97	1.56	1.41

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1335[B]	NAP	N3A-C2A-N1A	-10.07	120.96	128.87
2	A	1335[A]	NAP	N3A-C2A-N1A	-9.87	121.11	128.87
2	A	1335[B]	NAP	C2D-C3D-C4D	-7.87	86.54	102.64
2	A	1335[A]	NAP	C4B-O4B-C1B	-7.35	101.86	109.64
2	A	1335[A]	NAP	C1B-N9A-C4A	-5.67	120.48	126.81
2	A	1335[B]	NAP	O4D-C1D-N1N	-5.09	102.61	108.10
2	A	1335[A]	NAP	O2X-P2B-O1X	-4.35	96.42	110.63
2	A	1335[B]	NAP	C5N-C4N-C3N	-4.15	115.40	120.35
2	A	1335[A]	NAP	C2D-C3D-C4D	-3.73	95.00	102.64
2	A	1335[B]	NAP	C1B-N9A-C4A	-3.53	122.87	126.81
2	A	1335[A]	NAP	C3N-C7N-N7N	-3.18	114.23	117.82
2	A	1335[B]	NAP	C4B-O4B-C1B	-2.94	106.53	109.64
2	A	1335[A]	NAP	C2B-C1B-N9A	-2.67	105.84	113.48
2	A	1335[A]	NAP	C3N-C2N-N1N	-2.63	117.34	120.34
2	A	1335[B]	NAP	O5B-C5B-C4B	-2.15	101.35	109.09
2	A	1335[A]	NAP	O3X-P2B-O1X	-2.06	103.91	110.63
2	A	1335[B]	NAP	O2B-P2B-O1X	-2.06	102.57	107.48
2	A	1335[B]	NAP	O3X-P2B-O1X	-2.00	104.09	110.63
4	A	1348	1PE	OH5-C25-C15	2.04	119.45	110.40
4	A	1359	1PE	OH6-C15-C25	2.07	124.80	112.18
4	A	1344	1PE	OH3-C23-C13	2.07	119.61	110.40
2	A	1335[A]	NAP	O4B-C4B-C3B	2.08	109.39	105.16
4	A	1346	1PE	OH3-C22-C12	2.11	119.07	110.25
2	A	1335[B]	NAP	O2X-P2B-O1X	2.14	117.62	110.63
4	A	1349	1PE	OH3-C23-C13	2.15	119.93	110.40
4	A	1340	1PE	OH3-C22-C12	2.17	119.31	110.25
2	A	1335[A]	NAP	C2A-N1A-C6A	2.21	122.70	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1335[B]	NAP	C2A-N1A-C6A	2.22	122.72	118.77
4	A	1339	1PE	OH3-C23-C13	2.22	119.52	110.25
4	A	1349	1PE	OH6-C26-C16	2.23	119.58	110.25
4	A	1338	1PE	OH3-C23-C13	2.24	119.60	110.25
4	A	1341	1PE	OH3-C23-C13	2.29	119.80	110.25
4	A	1344	1PE	C23-OH3-C22	2.29	123.11	113.31
4	A	1346	1PE	OH4-C13-C23	2.30	120.60	110.40
4	A	1347	1PE	OH3-C23-C13	2.30	120.61	110.40
4	A	1359	1PE	OH3-C23-C13	2.33	120.72	110.40
4	A	1342	1PE	OH3-C23-C13	2.37	120.16	110.25
2	A	1335[A]	NAP	C2N-C3N-C4N	2.41	121.00	118.27
4	A	1348	1PE	OH6-C26-C16	2.41	120.32	110.25
4	A	1340	1PE	OH3-C23-C13	2.41	120.34	110.25
4	A	1347	1PE	OH3-C22-C12	2.42	120.38	110.25
4	A	1341	1PE	OH3-C22-C12	2.52	120.80	110.25
4	A	1339	1PE	OH3-C22-C12	2.59	121.07	110.25
4	A	1343	1PE	OH3-C22-C12	2.59	121.08	110.25
4	A	1348	1PE	OH6-C15-C25	2.59	121.90	110.40
2	A	1335[A]	NAP	P2B-O2B-C2B	2.63	128.30	121.56
4	A	1347	1PE	OH4-C13-C23	2.64	122.09	110.40
2	A	1335[A]	NAP	N6A-C6A-N1A	2.69	123.03	118.52
4	A	1345	1PE	OH4-C13-C23	2.73	122.53	110.40
4	A	1359	1PE	OH4-C13-C23	2.83	122.95	110.40
4	A	1346	1PE	OH3-C23-C13	2.83	122.98	110.40
4	A	1345	1PE	OH4-C24-C14	2.83	122.10	110.25
4	A	1349	1PE	OH5-C25-C15	2.94	123.43	110.40
4	A	1349	1PE	OH6-C15-C25	2.99	123.64	110.40
4	A	1348	1PE	OH3-C22-C12	3.05	123.00	110.25
4	A	1343	1PE	OH3-C23-C13	3.08	124.06	110.40
4	A	1344	1PE	OH4-C24-C14	3.14	123.36	110.25
4	A	1345	1PE	OH3-C22-C12	3.19	123.57	110.25
2	A	1335[B]	NAP	C2N-C3N-C4N	3.20	121.90	118.27
4	A	1345	1PE	OH3-C23-C13	3.20	124.60	110.40
2	A	1335[A]	NAP	O3X-P2B-O2B	3.22	116.24	106.62
4	A	1342	1PE	OH3-C22-C12	3.26	123.87	110.25
2	A	1335[A]	NAP	O3X-P2B-O2X	3.48	120.23	107.44
4	A	1349	1PE	OH5-C14-C24	3.50	125.92	110.40
4	A	1359	1PE	OH5-C25-C15	3.66	125.56	110.25
2	A	1335[B]	NAP	P2B-O2B-C2B	3.80	131.30	121.56
4	A	1359	1PE	C23-OH3-C22	3.86	129.81	113.31
2	A	1335[B]	NAP	O2D-C2D-C1D	3.90	123.82	111.61
4	A	1344	1PE	OH3-C22-C12	4.06	127.23	110.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1359	1PE	OH4-C24-C14	4.79	131.63	110.40
2	A	1335[A]	NAP	C2D-C1D-N1N	5.65	124.61	113.53
2	A	1335[B]	NAP	C2D-C1D-N1N	5.74	124.78	113.53

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1335[B]	NAP	C2D

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1335[A]	NAP	2	0
3	A	1336	GLV	1	0
4	A	1338	1PE	5	0
4	A	1339	1PE	1	0
4	A	1340	1PE	2	0
4	A	1341	1PE	1	0
4	A	1343	1PE	24	0
4	A	1344	1PE	1	0
4	A	1345	1PE	2	0
4	A	1346	1PE	4	0
4	A	1347	1PE	9	0
4	A	1348	1PE	5	0
4	A	1349	1PE	14	0
3	A	1356	GLV	2	0
4	A	1359	1PE	11	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/336 (99%)	-0.48	3 (0%) 85 84	16, 23, 40, 78	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	ASN	5.3
1	A	1	MET	5.1
1	A	330	LYS	2.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	GLV	A	1356	5/5	0.93	0.31	40.49	19,21,36,50	5
4	1PE	A	1359	13/16	0.76	0.28	18.92	20,39,58,64	13

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	EDO	A	1353	4/4	0.84	0.35	12.05	47,70,87,95	0
4	1PE	A	1343	10/16	0.85	0.19	8.86	28,47,68,73	0
4	1PE	A	1346	10/16	0.85	0.15	6.02	37,71,78,82	0
4	1PE	A	1347	13/16	0.93	0.11	5.50	30,46,66,87	0
4	1PE	A	1344	10/16	0.72	0.23	5.40	39,63,69,70	0
5	EDO	A	1352	4/4	0.75	0.25	2.43	66,79,92,92	0
4	1PE	A	1355	7/16	0.78	0.19	2.40	75,78,87,99	0
6	ACY	A	1357	4/4	0.87	0.12	2.28	25,31,33,37	0
4	1PE	A	1349	16/16	0.93	0.11	1.48	30,48,82,87	0
6	ACY	A	1358	4/4	0.93	0.09	1.25	30,36,44,53	0
4	1PE	A	1341	7/16	0.83	0.09	1.11	64,69,75,79	0
2	NAP	A	1335[B]	48/48	0.98	0.09	1.04	14,17,22,26	48
2	NAP	A	1335[A]	48/48	0.98	0.09	0.84	13,18,29,31	48
4	1PE	A	1337	7/16	0.94	0.07	0.81	31,33,44,52	0
5	EDO	A	1354	4/4	0.74	0.24	0.79	68,82,95,114	0
4	1PE	A	1345	10/16	0.84	0.10	0.66	38,47,67,73	0
4	1PE	A	1342	7/16	0.94	0.08	-0.30	41,51,77,81	0
3	GLV	A	1336	5/5	0.98	0.06	-0.72	15,24,26,29	0
5	EDO	A	1350	4/4	0.91	0.09	-	49,60,72,83	0
4	1PE	A	1339	7/16	0.95	0.09	-	49,56,77,88	0
5	EDO	A	1351	4/4	0.70	0.16	-	59,71,78,79	0
4	1PE	A	1340	7/16	0.89	0.18	-	46,55,78,82	0
4	1PE	A	1348	16/16	0.87	0.15	-	34,53,75,77	0
4	1PE	A	1338	7/16	0.90	0.10	-	52,58,78,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.