



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 03:13 PM EDT

PDB ID : 5C0E  
Title : HLA-A02 carrying YLGGPDFPTI  
Authors : Rizkallah, P.J.; Bulek, A.M.; Cole, D.K.; Sewell, A.K.  
Deposited on : 2015-06-12  
Resolution : 1.49 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

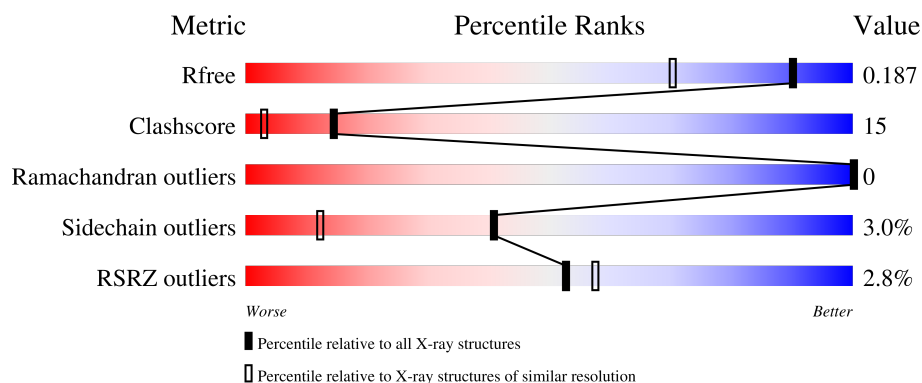
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.49 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))
$R_{free}$	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	277	<div> <div>2%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
2	B	100	<div> <div>5%</div> <div>71%</div> <div>26%</div> <div>..</div> </div>
3	C	10	<div> <div>80%</div> <div>10%</div> <div>10%</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
5	EDO	B	103	-	X	-	-
6	GOL	B	104	-	-	X	-
7	PG4	A	318	-	-	X	-
7	PG4	B	105	-	-	X	-
7	PG4	B	107	-	X	X	-
7	PG4	B	108	-	-	X	-
7	PG4	B	109	-	-	X	-
7	PG4	B	110	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3943 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	14	0
			2387	1487	442	448	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01892

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	1	0
			846	538	142	162	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Marker peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			83	57	11	15			

- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Br	0	0
			1	1		

- Molecule 5 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
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

*Continued on next page...*

Continued from previous page...

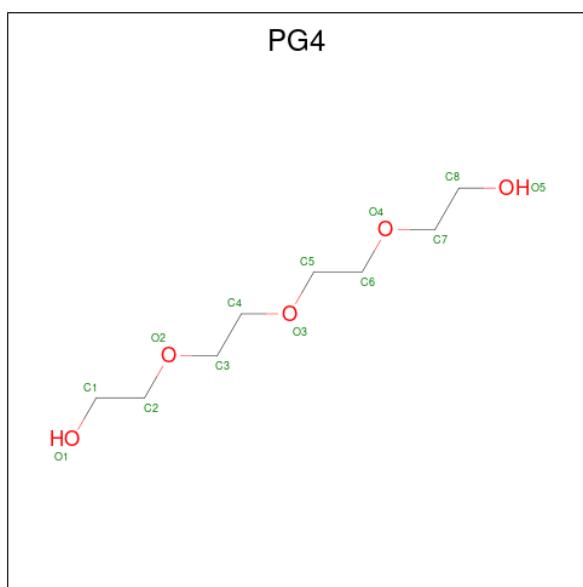
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		
7	A	1	Total	C	O	0	0
			13	8	5		
7	A	1	Total	C	O	0	0
			13	8	5		
7	A	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	285	Total	O	0	0
			285	285		

*Continued on next page...*

*Continued from previous page...*

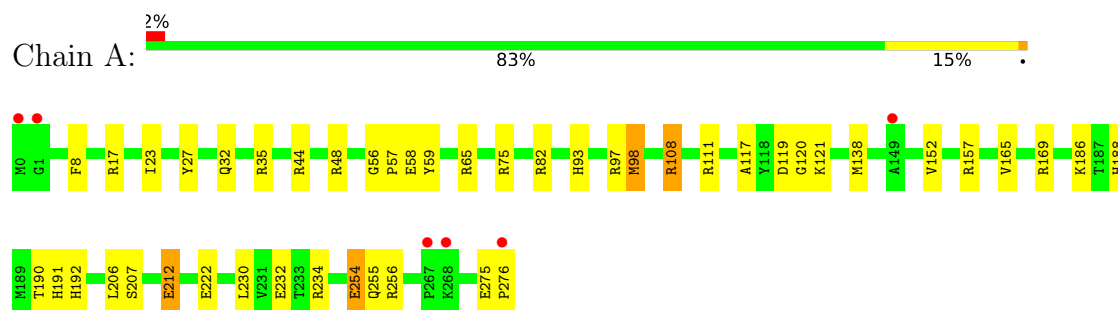
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	95	Total 95	O 95	0	0
8	C	11	Total 11	O 11	0	0



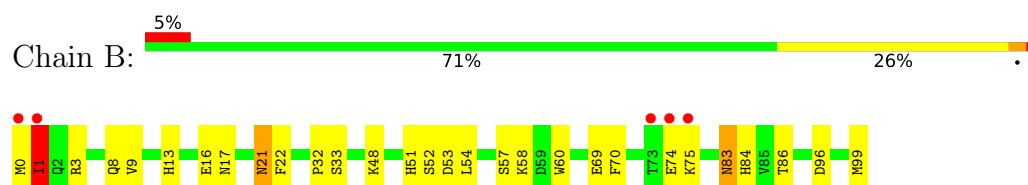
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

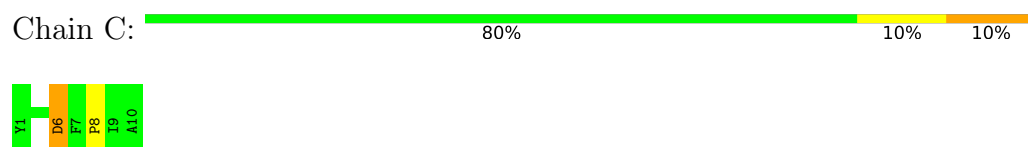
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 3: Marker peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.07Å 79.74Å 57.00Å 90.00° 115.74° 90.00°	Depositor
Resolution (Å)	31.29 – 1.49 31.29 – 1.49	Depositor EDS
% Data completeness (in resolution range)	99.0 (31.29-1.49) 99.0 (31.29-1.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 1.49Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.156 , 0.179 0.164 , 0.187	Depositor DCC
$R_{free}$ test set	3669 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.0	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 51.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3943	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, BR, GOL, PG4

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	1.02	4/2453 (0.2%)	1.20	17/3325 (0.5%)
2	B	0.95	0/869	1.03	1/1174 (0.1%)
3	C	1.35	0/87	1.60	2/117 (1.7%)
All	All	1.01	4/3409 (0.1%)	1.17	20/4616 (0.4%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	GLU	CG-CD	-5.58	1.43	1.51
1	A	254	GLU	CD-OE2	-5.05	1.20	1.25
1	A	157	ARG	CZ-NH1	5.04	1.39	1.33
1	A	27	TYR	CZ-OH	5.02	1.46	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	6	ASP	CB-CG-OD2	-11.63	107.83	118.30
1	A	157	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	A	157	ARG	NE-CZ-NH2	-9.74	115.43	120.30
1	A	75	ARG	NE-CZ-NH2	-9.69	115.46	120.30
1	A	97	ARG	NE-CZ-NH1	9.41	125.00	120.30
1	A	108[A]	ARG	NE-CZ-NH1	-8.60	116.00	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108[B]	ARG	NE-CZ-NH1	-8.60	116.00	120.30
1	A	17	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	A	111	ARG	NE-CZ-NH1	7.72	124.16	120.30
3	C	6	ASP	CB-CG-OD1	7.64	125.18	118.30
1	A	75	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	A	256	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	A	65[A]	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	65[B]	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	212	GLU	OE1-CD-OE2	6.38	130.95	123.30
2	B	1	ILE	CB-CA-C	-6.34	98.92	111.60
1	A	111	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	234	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	230	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	17	ARG	NE-CZ-NH1	5.07	122.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	GLU	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	2387	0	2242	45	0
2	B	846	0	808	43	0
3	C	83	0	74	3	0
4	A	1	0	0	0	0
5	A	56	0	83	3	0
5	B	12	0	17	0	0
6	A	12	0	16	0	0
6	B	6	0	8	4	0
6	C	6	0	8	0	0
7	A	65	0	89	21	0
7	B	78	0	106	42	0
8	A	285	0	0	12	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	95	0	0	4	0
8	C	11	0	0	2	0
All	All	3943	0	3451	108	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 15.

All (108) 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)
2:B:9:VAL:O	7:B:110:PG4:H81	1.30	1.22
7:A:318:PG4:H61	8:C:207:HOH:O	1.47	1.13
2:B:9:VAL:O	7:B:110:PG4:C8	2.18	0.91
2:B:99:MET:HB2	7:B:110:PG4:H71	1.55	0.86
2:B:21:ASN:HD22	2:B:22:PHE:H	1.21	0.86
1:A:186:LYS:HD2	7:B:105:PG4:H62	1.58	0.85
1:A:23:ILE:HD13	7:B:107:PG4:H81	1.66	0.77
2:B:99:MET:HB2	7:B:110:PG4:C7	2.15	0.76
2:B:16:GLU:OE1	7:B:109:PG4:H72	1.87	0.73
1:A:206:LEU:CD1	7:B:108:PG4:H51	2.17	0.73
2:B:48:LYS:O	2:B:48:LYS:HG3	1.93	0.68
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.76	0.68
1:A:8:PHE:HE2	7:B:106:PG4:H61	1.59	0.68
1:A:255:GLN:NE2	8:A:401:HOH:O	2.10	0.67
2:B:13:HIS:H	2:B:21:ASN:HD21	1.41	0.67
7:B:109:PG4:H82	8:B:276:HOH:O	1.96	0.66
8:A:530:HOH:O	7:B:107:PG4:H61	1.94	0.66
1:A:206:LEU:HD11	7:B:108:PG4:H51	1.77	0.66
7:A:319:PG4:H71	8:A:547:HOH:O	1.96	0.66
1:A:232[B]:GLU:OE2	8:A:402:HOH:O	2.13	0.65
1:A:186:LYS:CD	7:B:105:PG4:H62	2.26	0.65
2:B:54:LEU:H	7:B:107:PG4:H82	1.61	0.65
2:B:57:SER:O	7:B:106:PG4:H62	1.98	0.64
2:B:69[B]:GLU:H	2:B:69[B]:GLU:CD	2.01	0.64
1:A:188:HIS:HD2	8:A:561:HOH:O	1.80	0.64
2:B:33:SER:O	7:B:107:PG4:H32	1.98	0.64
1:A:58:GLU:HB3	7:A:318:PG4:H32	1.80	0.63
2:B:99:MET:C	7:B:110:PG4:H82	2.17	0.63
1:A:138:MET:HG2	7:A:320:PG4:H12	1.80	0.63
1:A:56:GLY:HA3	7:A:318:PG4:H21	1.82	0.62
7:B:105:PG4:H51	7:B:109:PG4:H12	1.81	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:319:PG4:H11	8:A:474:HOH:O	2.01	0.61
1:A:44:ARG:HE	7:A:322:PG4:H52	1.66	0.61
1:A:165[B]:VAL:CG1	1:A:169:ARG:NH2	2.64	0.60
2:B:17:ASN:HB3	6:B:104:GOL:C1	2.31	0.60
7:B:107:PG4:H62	7:B:107:PG4:H21	1.84	0.60
1:A:93:HIS:HE1	8:A:455:HOH:O	1.83	0.60
1:A:206:LEU:HD11	7:B:108:PG4:C5	2.32	0.60
2:B:99:MET:OXT	7:B:108:PG4:H11	2.02	0.59
1:A:32:GLN:H	7:A:319:PG4:C8	2.16	0.58
7:B:110:PG4:C8	7:B:110:PG4:H41	2.33	0.58
2:B:99:MET:O	7:B:110:PG4:H32	2.04	0.58
2:B:84:HIS:HD2	2:B:86:THR:OG1	1.87	0.58
2:B:22:PHE:CE2	2:B:69[A]:GLU:HG2	2.39	0.58
2:B:96:ASP:O	7:B:110:PG4:H72	2.04	0.57
1:A:35[B]:ARG:NE	1:A:48[B]:ARG:NH1	2.51	0.57
1:A:206:LEU:HD13	7:B:108:PG4:H51	1.85	0.57
1:A:59:TYR:HA	7:A:318:PG4:H51	1.87	0.56
7:B:105:PG4:H42	7:B:109:PG4:H41	1.87	0.56
7:A:322:PG4:H31	7:A:322:PG4:O1	2.06	0.55
1:A:191:HIS:HD2	8:A:654:HOH:O	1.89	0.55
1:A:58:GLU:HG2	7:A:318:PG4:H62	1.89	0.54
2:B:17:ASN:HB3	6:B:104:GOL:H12	1.89	0.53
1:A:119:ASP:O	2:B:1:ILE:HD11	2.09	0.53
2:B:74:GLU:HB2	6:B:104:GOL:O1	2.08	0.53
7:A:319:PG4:C1	8:A:474:HOH:O	2.56	0.53
2:B:17:ASN:HB3	6:B:104:GOL:H11	1.90	0.52
1:A:35[A]:ARG:NH2	8:A:404:HOH:O	2.30	0.52
1:A:120:GLY:HA3	2:B:1:ILE:HD11	1.91	0.51
7:B:105:PG4:C2	7:B:109:PG4:H52	2.40	0.51
1:A:222:GLU:HG3	5:A:305:EDO:H12	1.94	0.49
7:B:110:PG4:H82	7:B:110:PG4:H41	1.93	0.49
7:B:110:PG4:H21	8:B:216:HOH:O	2.13	0.49
1:A:82:ARG:HD2	8:A:615:HOH:O	2.12	0.49
1:A:191:HIS:HE1	1:A:254:GLU:OE1	1.95	0.49
5:A:311:EDO:O2	7:A:322:PG4:H42	2.12	0.49
2:B:54:LEU:H	7:B:107:PG4:H71	1.77	0.49
3:C:8:PRO:HG2	8:C:210:HOH:O	2.13	0.48
1:A:32:GLN:HB2	7:A:319:PG4:H81	1.94	0.48
2:B:83:ASN:HD22	2:B:84:HIS:H	1.60	0.48
2:B:32:PRO:O	2:B:84:HIS:HE1	1.97	0.48
2:B:21:ASN:HD22	2:B:22:PHE:N	2.02	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:PHE:CE2	7:B:106:PG4:H61	2.44	0.47
2:B:96:ASP:HB3	7:B:110:PG4:H72	1.96	0.47
1:A:35[A]:ARG:HE	2:B:53:ASP:CG	2.18	0.47
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.49	0.47
2:B:8:GLN:OE1	7:B:110:PG4:H31	2.15	0.46
7:B:105:PG4:O2	7:B:109:PG4:H52	2.15	0.46
2:B:51:HIS:HD2	2:B:52:SER:O	1.99	0.46
2:B:69[B]:GLU:CD	2:B:69[B]:GLU:N	2.68	0.46
1:A:121[B]:LYS:HB3	1:A:121[B]:LYS:HE2	1.73	0.46
7:A:319:PG4:H42	7:A:319:PG4:H62	1.67	0.45
1:A:98:MET:O	1:A:98:MET:HE3	2.16	0.45
1:A:59:TYR:HB2	7:A:318:PG4:H41	1.99	0.45
1:A:165[B]:VAL:HG11	1:A:169:ARG:NH2	2.32	0.45
2:B:1:ILE:HD13	2:B:3:ARG:HH11	1.82	0.45
1:A:58:GLU:HB3	7:A:318:PG4:H12	1.98	0.44
1:A:152:VAL:HG21	3:C:8:PRO:HG3	2.00	0.44
2:B:54:LEU:H	7:B:107:PG4:C8	2.30	0.44
7:B:105:PG4:O3	7:B:109:PG4:H42	2.18	0.44
2:B:99:MET:OXT	7:B:108:PG4:C1	2.65	0.44
2:B:1:ILE:HA	8:B:281:HOH:O	2.18	0.44
1:A:108[A]:ARG:HH11	1:A:108[A]:ARG:HD2	1.59	0.43
1:A:121[A]:LYS:HD3	2:B:1:ILE:HG12	1.99	0.43
1:A:255:GLN:H	1:A:255:GLN:CD	2.21	0.43
8:A:505:HOH:O	3:C:6:ASP:HA	2.19	0.43
2:B:58:LYS:N	7:B:106:PG4:H52	2.34	0.43
1:A:57:PRO:HA	7:A:322:PG4:H72	2.01	0.42
2:B:48:LYS:O	2:B:48:LYS:CG	2.57	0.42
1:A:44:ARG:HE	7:A:322:PG4:C5	2.31	0.42
5:A:310:EDO:O2	7:A:320:PG4:H51	2.20	0.42
2:B:22:PHE:CE2	2:B:69[A]:GLU:CG	3.01	0.42
7:B:110:PG4:C7	7:B:110:PG4:H41	2.50	0.42
2:B:96:ASP:H	7:B:110:PG4:H72	1.83	0.42
1:A:190:THR:OG1	1:A:192:HIS:HE1	2.02	0.41
7:B:108:PG4:C8	8:B:249:HOH:O	2.67	0.41
7:A:320:PG4:C6	7:A:320:PG4:O5	2.69	0.40
7:B:108:PG4:H22	7:B:108:PG4:H41	1.81	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	289/277 (104%)	286 (99%)	3 (1%)	0	100	100
2	B	99/100 (99%)	98 (99%)	1 (1%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
All	All	396/387 (102%)	392 (99%)	4 (1%)	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	247/233 (106%)	243 (98%)	4 (2%)	62	36
2	B	96/95 (101%)	90 (94%)	6 (6%)	18	2
3	C	8/8 (100%)	8 (100%)	0	100	100
All	All	351/336 (104%)	341 (97%)	10 (3%)	41	14

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	MET
1	A	207	SER
1	A	212	GLU
1	A	276	PRO
2	B	0	MET

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	B	1	ILE
2	B	21	ASN
2	B	70	PHE
2	B	75	LYS
2	B	83	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	93	HIS
1	A	188	HIS
1	A	191	HIS
1	A	192	HIS
2	B	21	ASN
2	B	24	ASN
2	B	51	HIS
2	B	83	ASN
2	B	84	HIS

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 1 is monoatomic - leaving 32 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
7	PG4	A	319	-	12,12,12	0.80	0	11,11,11	1.25	1 (9%)
7	PG4	B	107	-	12,12,12	1.42	2 (16%)	11,11,11	2.05	5 (45%)
5	EDO	A	312	-	3,3,3	1.85	1 (33%)	2,2,2	0.43	0
7	PG4	A	321	-	12,12,12	0.95	0	11,11,11	1.82	3 (27%)
7	PG4	B	110	-	12,12,12	0.97	0	11,11,11	2.09	5 (45%)
5	EDO	A	315	-	3,3,3	1.02	0	2,2,2	0.50	0
5	EDO	A	310	-	3,3,3	0.83	0	2,2,2	0.25	0
6	GOL	B	104	-	5,5,5	0.40	0	5,5,5	1.61	2 (40%)
5	EDO	B	101	-	3,3,3	0.47	0	2,2,2	0.44	0
5	EDO	A	302	-	3,3,3	0.61	0	2,2,2	1.18	0
5	EDO	A	307	-	3,3,3	0.24	0	2,2,2	0.91	0
5	EDO	B	102	-	3,3,3	0.31	0	2,2,2	0.49	0
7	PG4	A	320	-	12,12,12	1.22	1 (8%)	11,11,11	1.34	1 (9%)
5	EDO	A	314	-	3,3,3	0.56	0	2,2,2	0.26	0
7	PG4	B	105	-	12,12,12	0.41	0	11,11,11	0.61	0
5	EDO	A	304	-	3,3,3	0.42	0	2,2,2	0.44	0
7	PG4	A	318	-	12,12,12	1.18	0	11,11,11	1.45	3 (27%)
5	EDO	A	311	-	3,3,3	0.41	0	2,2,2	0.60	0
5	EDO	A	309	-	3,3,3	0.73	0	2,2,2	0.18	0
7	PG4	B	109	-	12,12,12	0.70	0	11,11,11	0.86	0
5	EDO	A	308	-	3,3,3	0.76	0	2,2,2	0.02	0
6	GOL	A	316	-	5,5,5	0.69	0	5,5,5	0.96	0
5	EDO	A	306	-	3,3,3	0.37	0	2,2,2	0.75	0
5	EDO	B	103	-	3,3,3	2.99	1 (33%)	2,2,2	2.24	1 (50%)
7	PG4	B	108	-	12,12,12	0.79	0	11,11,11	1.97	5 (45%)
6	GOL	C	101	-	5,5,5	0.44	0	5,5,5	2.34	3 (60%)
5	EDO	A	313	-	3,3,3	0.68	0	2,2,2	0.32	0
6	GOL	A	317	-	5,5,5	0.73	0	5,5,5	0.82	0
7	PG4	B	106	-	12,12,12	0.79	0	11,11,11	0.99	0
5	EDO	A	305	-	3,3,3	0.57	0	2,2,2	0.34	0
7	PG4	A	322	-	12,12,12	0.88	0	11,11,11	0.77	0
5	EDO	A	303	-	3,3,3	0.71	0	2,2,2	0.65	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
7	PG4	A	319	-	-	6/10/10/10	-
7	PG4	B	107	-	-	7/10/10/10	-
5	EDO	A	312	-	-	0/1/1/1	-
7	PG4	A	321	-	-	6/10/10/10	-
7	PG4	B	110	-	-	8/10/10/10	-
5	EDO	A	315	-	-	1/1/1/1	-
5	EDO	A	310	-	-	0/1/1/1	-
6	GOL	B	104	-	-	2/4/4/4	-
5	EDO	B	101	-	-	0/1/1/1	-
5	EDO	A	302	-	-	1/1/1/1	-
5	EDO	A	307	-	-	1/1/1/1	-
5	EDO	B	102	-	-	1/1/1/1	-
7	PG4	A	320	-	-	5/10/10/10	-
5	EDO	A	314	-	-	1/1/1/1	-
7	PG4	B	105	-	-	3/10/10/10	-
5	EDO	A	304	-	-	1/1/1/1	-
7	PG4	A	318	-	-	7/10/10/10	-
5	EDO	A	311	-	-	1/1/1/1	-
5	EDO	A	309	-	-	1/1/1/1	-
7	PG4	B	109	-	-	7/10/10/10	-
5	EDO	A	308	-	-	0/1/1/1	-
6	GOL	A	316	-	-	1/4/4/4	-
5	EDO	A	306	-	-	0/1/1/1	-
5	EDO	B	103	-	-	1/1/1/1	-
7	PG4	B	108	-	-	8/10/10/10	-
6	GOL	C	101	-	-	2/4/4/4	-
5	EDO	A	313	-	-	0/1/1/1	-
6	GOL	A	317	-	-	2/4/4/4	-
7	PG4	B	106	-	-	6/10/10/10	-
5	EDO	A	305	-	-	1/1/1/1	-
7	PG4	A	322	-	-	5/10/10/10	-
5	EDO	A	303	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	103	EDO	O1-C1	-5.04	1.16	1.42
5	A	312	EDO	O1-C1	-2.95	1.26	1.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	320	PG4	O2-C2	-2.93	1.29	1.42
7	B	107	PG4	O4-C7	2.25	1.51	1.42
7	B	107	PG4	O5-C8	2.02	1.52	1.42

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	107	PG4	C3-O2-C2	3.64	129.05	113.29
7	B	110	PG4	O3-C4-C3	3.57	126.51	110.39
7	A	321	PG4	O2-C2-C1	3.48	125.36	110.07
7	A	320	PG4	O4-C6-C5	3.32	125.36	110.39
6	C	101	GOL	O3-C3-C2	-3.27	94.53	110.20
7	A	321	PG4	C7-O4-C6	3.16	126.99	113.29
7	B	110	PG4	C3-O2-C2	2.87	125.71	113.29
5	B	103	EDO	O1-C1-C2	2.86	132.46	111.91
6	C	101	GOL	O2-C2-C3	-2.85	96.59	109.12
6	C	101	GOL	C3-C2-C1	2.83	122.72	111.70
7	B	108	PG4	C5-O3-C4	2.81	125.48	113.29
7	B	107	PG4	O2-C2-C1	-2.78	97.87	110.07
7	B	107	PG4	O3-C4-C3	2.70	122.58	110.39
7	B	108	PG4	O2-C2-C1	2.66	121.77	110.07
7	A	321	PG4	O1-C1-C2	2.65	127.17	111.81
7	A	319	PG4	C7-O4-C6	2.62	124.64	113.29
7	B	108	PG4	O3-C5-C6	2.56	121.95	110.39
7	B	110	PG4	O3-C5-C6	2.56	121.95	110.39
7	B	110	PG4	O4-C6-C5	2.50	121.64	110.39
7	B	107	PG4	O3-C5-C6	2.47	121.53	110.39
7	A	318	PG4	O2-C3-C4	2.42	121.30	110.39
7	B	108	PG4	C3-O2-C2	-2.28	103.39	113.29
7	B	108	PG4	O4-C6-C5	-2.24	100.31	110.39
6	B	104	GOL	O1-C1-C2	2.23	120.90	110.20
6	B	104	GOL	C3-C2-C1	-2.17	103.28	111.70
7	B	107	PG4	O5-C8-C7	2.15	124.25	111.81
7	B	110	PG4	O4-C7-C8	2.14	119.48	110.07
7	A	318	PG4	C7-O4-C6	2.09	122.36	113.29
7	A	318	PG4	O4-C7-C8	2.03	119.00	110.07

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	104	GOL	C1-C2-C3-O3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	C	101	GOL	O1-C1-C2-C3
7	A	320	PG4	C4-C3-O2-C2
7	A	322	PG4	C1-C2-O2-C3
7	B	107	PG4	C3-C4-O3-C5
7	B	110	PG4	C4-C3-O2-C2
7	A	319	PG4	C6-C5-O3-C4
7	A	321	PG4	C5-C6-O4-C7
7	A	319	PG4	O3-C5-C6-O4
7	A	321	PG4	O3-C5-C6-O4
7	A	320	PG4	O2-C3-C4-O3
7	A	318	PG4	O2-C3-C4-O3
7	A	322	PG4	O3-C5-C6-O4
7	B	108	PG4	O3-C5-C6-O4
7	B	110	PG4	O4-C7-C8-O5
7	B	105	PG4	O2-C3-C4-O3
7	B	109	PG4	O2-C3-C4-O3
7	A	321	PG4	O2-C3-C4-O3
7	A	322	PG4	O2-C3-C4-O3
7	B	107	PG4	O3-C5-C6-O4
7	A	320	PG4	O3-C5-C6-O4
7	A	319	PG4	O4-C7-C8-O5
7	B	106	PG4	O1-C1-C2-O2
7	B	107	PG4	O4-C7-C8-O5
7	B	108	PG4	O1-C1-C2-O2
7	B	109	PG4	O4-C7-C8-O5
7	B	110	PG4	O1-C1-C2-O2
7	B	107	PG4	O2-C3-C4-O3
6	A	316	GOL	O1-C1-C2-C3
6	A	317	GOL	C1-C2-C3-O3
7	B	106	PG4	O2-C3-C4-O3
6	B	104	GOL	O2-C2-C3-O3
6	C	101	GOL	O1-C1-C2-O2
7	A	318	PG4	O4-C7-C8-O5
5	A	307	EDO	O1-C1-C2-O2
7	B	108	PG4	C3-C4-O3-C5
7	B	110	PG4	O3-C5-C6-O4
7	A	321	PG4	O4-C7-C8-O5
7	A	320	PG4	O1-C1-C2-O2
7	A	322	PG4	O4-C7-C8-O5
7	B	110	PG4	O2-C3-C4-O3
7	B	108	PG4	C4-C3-O2-C2
7	B	108	PG4	O4-C7-C8-O5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	A	309	EDO	O1-C1-C2-O2
5	A	311	EDO	O1-C1-C2-O2
7	B	107	PG4	O1-C1-C2-O2
7	B	108	PG4	C5-C6-O4-C7
7	B	109	PG4	C8-C7-O4-C6
7	B	109	PG4	C1-C2-O2-C3
7	B	109	PG4	C3-C4-O3-C5
7	B	110	PG4	C8-C7-O4-C6
7	A	318	PG4	C4-C3-O2-C2
7	B	106	PG4	C5-C6-O4-C7
7	B	106	PG4	O3-C5-C6-O4
7	B	108	PG4	C8-C7-O4-C6
7	A	318	PG4	O1-C1-C2-O2
7	A	321	PG4	C4-C3-O2-C2
7	A	320	PG4	C5-C6-O4-C7
7	A	319	PG4	O1-C1-C2-O2
7	B	105	PG4	O4-C7-C8-O5
7	B	109	PG4	C4-C3-O2-C2
5	B	102	EDO	O1-C1-C2-O2
5	B	103	EDO	O1-C1-C2-O2
7	A	322	PG4	C8-C7-O4-C6
7	B	107	PG4	C8-C7-O4-C6
7	B	107	PG4	C4-C3-O2-C2
7	A	318	PG4	O3-C5-C6-O4
7	B	105	PG4	C5-C6-O4-C7
7	B	110	PG4	C1-C2-O2-C3
5	A	305	EDO	O1-C1-C2-O2
5	A	314	EDO	O1-C1-C2-O2
5	A	315	EDO	O1-C1-C2-O2
7	A	319	PG4	O2-C3-C4-O3
7	B	110	PG4	C3-C4-O3-C5
7	B	109	PG4	O1-C1-C2-O2
7	B	108	PG4	O2-C3-C4-O3
5	A	304	EDO	O1-C1-C2-O2
7	B	106	PG4	C6-C5-O3-C4
7	A	318	PG4	C5-C6-O4-C7
6	A	317	GOL	O2-C2-C3-O3
7	A	321	PG4	C1-C2-O2-C3
7	A	318	PG4	C6-C5-O3-C4
7	B	106	PG4	C1-C2-O2-C3
5	A	302	EDO	O1-C1-C2-O2
7	A	319	PG4	C5-C6-O4-C7

There are no ring outliers.

14 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	319	PG4	6	0
7	B	107	PG4	7	0
7	B	110	PG4	14	0
5	A	310	EDO	1	0
6	B	104	GOL	4	0
7	A	320	PG4	3	0
7	B	105	PG4	7	0
7	A	318	PG4	7	0
5	A	311	EDO	1	0
7	B	109	PG4	7	0
7	B	108	PG4	8	0
7	B	106	PG4	4	0
5	A	305	EDO	1	0
7	A	322	PG4	5	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, 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	277/277 (100%)	-0.12	6 (2%) 62 67	8, 14, 27, 76	0
2	B	100/100 (100%)	0.05	5 (5%) 28 31	10, 20, 39, 53	0
3	C	10/10 (100%)	-0.43	0 100 100	11, 16, 22, 22	0
All	All	387/387 (100%)	-0.08	11 (2%) 53 57	8, 15, 33, 76	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	MET	11.4
2	B	1	ILE	6.9
2	B	75	LYS	4.2
1	A	1	GLY	3.3
1	A	276	PRO	3.2
2	B	0	MET	2.8
2	B	74	GLU	2.8
1	A	267	PRO	2.4
1	A	149	ALA	2.4
2	B	73	THR	2.2
1	A	268	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 monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	A	314	4/4	0.69	0.17	45,52,53,55	0
5	EDO	A	309	4/4	0.71	0.28	30,39,40,41	0
5	EDO	A	308	4/4	0.72	0.14	49,49,49,51	0
6	GOL	A	317	6/6	0.72	0.16	38,45,46,53	0
7	PG4	A	322	13/13	0.75	0.29	31,41,52,54	0
7	PG4	B	107	13/13	0.76	0.20	19,24,37,38	0
5	EDO	A	310	4/4	0.77	0.18	34,36,37,38	0
5	EDO	A	313	4/4	0.79	0.17	38,44,47,49	0
7	PG4	A	319	13/13	0.80	0.23	26,38,44,44	0
7	PG4	B	106	13/13	0.82	0.22	24,40,55,57	0
6	GOL	C	101	6/6	0.82	0.22	31,39,41,44	0
7	PG4	B	105	13/13	0.83	0.18	26,46,50,53	0
7	PG4	A	321	13/13	0.83	0.22	26,39,60,63	0
7	PG4	A	320	13/13	0.83	0.29	7,16,22,24	13
7	PG4	B	110	13/13	0.83	0.26	19,30,41,42	0
5	EDO	A	305	4/4	0.84	0.24	27,36,37,39	0
7	PG4	B	108	13/13	0.84	0.19	17,28,36,38	0
5	EDO	A	302	4/4	0.84	0.15	26,27,29,42	0
7	PG4	B	109	13/13	0.85	0.21	21,31,37,38	0
5	EDO	A	311	4/4	0.85	0.20	41,44,49,53	0
5	EDO	B	102	4/4	0.88	0.24	34,37,38,46	0
7	PG4	A	318	13/13	0.88	0.20	22,31,38,40	0
5	EDO	A	307	4/4	0.88	0.18	32,36,36,39	0
5	EDO	A	306	4/4	0.89	0.12	25,27,28,30	0
6	GOL	A	316	6/6	0.89	0.28	21,37,44,47	0
5	EDO	A	315	4/4	0.89	0.12	16,20,21,26	0
5	EDO	A	312	4/4	0.91	0.23	12,18,30,40	0
6	GOL	B	104	6/6	0.91	0.33	31,35,43,46	0
5	EDO	B	101	4/4	0.92	0.22	33,35,35,37	0
5	EDO	B	103	4/4	0.93	0.23	9,12,22,34	0
5	EDO	A	303	4/4	0.93	0.11	21,22,22,22	0
5	EDO	A	304	4/4	0.95	0.16	26,29,30,37	0
4	BR	A	301	1/1	1.00	0.03	10,10,10,10	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.