



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 05:21 pm BST

PDB ID : 2XE4  
Title : Structure of Oligopeptidase B from Leishmania major  
Authors : McLuskey, K.; Paterson, N.G.; Bland, N.D.; Mottram, J.C.; Isaacs, N.W.  
Deposited on : 2010-05-11  
Resolution : 1.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

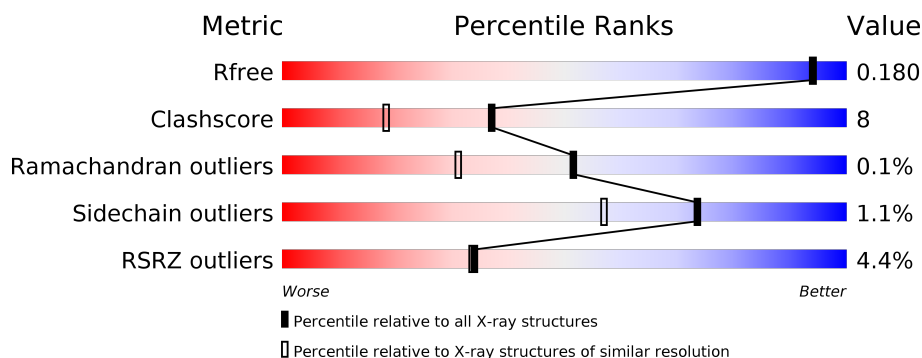
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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 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	751	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>• •</div> </div> </div>
2	B	4	<div> <div>50%</div> <div>50%</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
4	PGR	A	1767	-	X	-	-
4	PGR	A	1782	-	-	X	-
5	PGO	A	1743	X	-	-	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7215 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 OLIGOPEPTIDASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	721	Total	C	N	O	S	0	51	0
			6125	3890	1046	1148	41			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q4QHU7
A	-18	GLY	-	expression tag	UNP Q4QHU7
A	-17	SER	-	expression tag	UNP Q4QHU7
A	-16	SER	-	expression tag	UNP Q4QHU7
A	-15	HIS	-	expression tag	UNP Q4QHU7
A	-14	HIS	-	expression tag	UNP Q4QHU7
A	-13	HIS	-	expression tag	UNP Q4QHU7
A	-12	HIS	-	expression tag	UNP Q4QHU7
A	-11	HIS	-	expression tag	UNP Q4QHU7
A	-10	HIS	-	expression tag	UNP Q4QHU7
A	-9	SER	-	expression tag	UNP Q4QHU7
A	-8	SER	-	expression tag	UNP Q4QHU7
A	-7	GLY	-	expression tag	UNP Q4QHU7
A	-6	LEU	-	expression tag	UNP Q4QHU7
A	-5	VAL	-	expression tag	UNP Q4QHU7
A	-4	PRO	-	expression tag	UNP Q4QHU7
A	-3	ARG	-	expression tag	UNP Q4QHU7
A	-2	GLY	-	expression tag	UNP Q4QHU7
A	-1	SER	-	expression tag	UNP Q4QHU7
A	0	HIS	-	expression tag	UNP Q4QHU7
A	25	LEU	PHE	engineered mutation	UNP Q4QHU7

- Molecule 2 is a protein called ANTIPAIN.

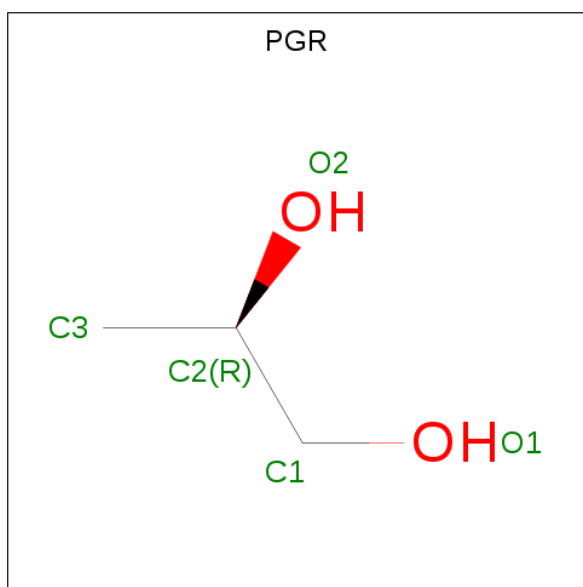
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	4	Total	C	N	O	0	0	0
			43	27	10	6			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 4 is R-1,2-PROPANEDIOL (three-letter code: PGR) (formula:  $C_3H_8O_2$ ).



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

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

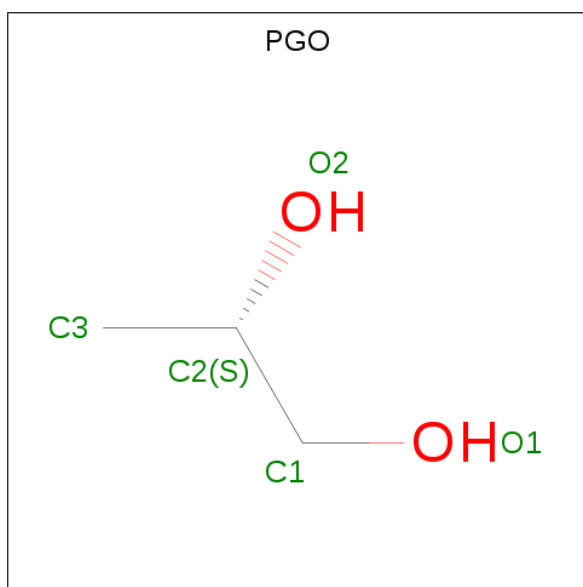
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			5	3	2		
4	A	1	Total	C	O	0	0
			5	3	2		
4	A	1	Total	C	O	0	0
			5	3	2		
4	A	1	Total	C	O	0	0
			5	3	2		
4	A	1	Total	C	O	0	0
			5	3	2		
4	A	1	Total	C	O	0	0
			5	3	2		
4	A	1	Total	C	O	0	0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

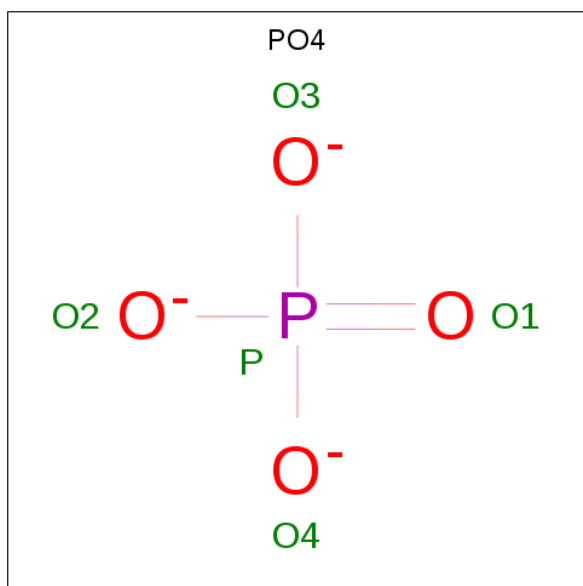
- Molecule 5 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>).





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

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	A	1	Total	O	P	0	0
			5	4	1		
6	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	Cl	0	0
			4	4		

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	Na	0	0
			2	2		

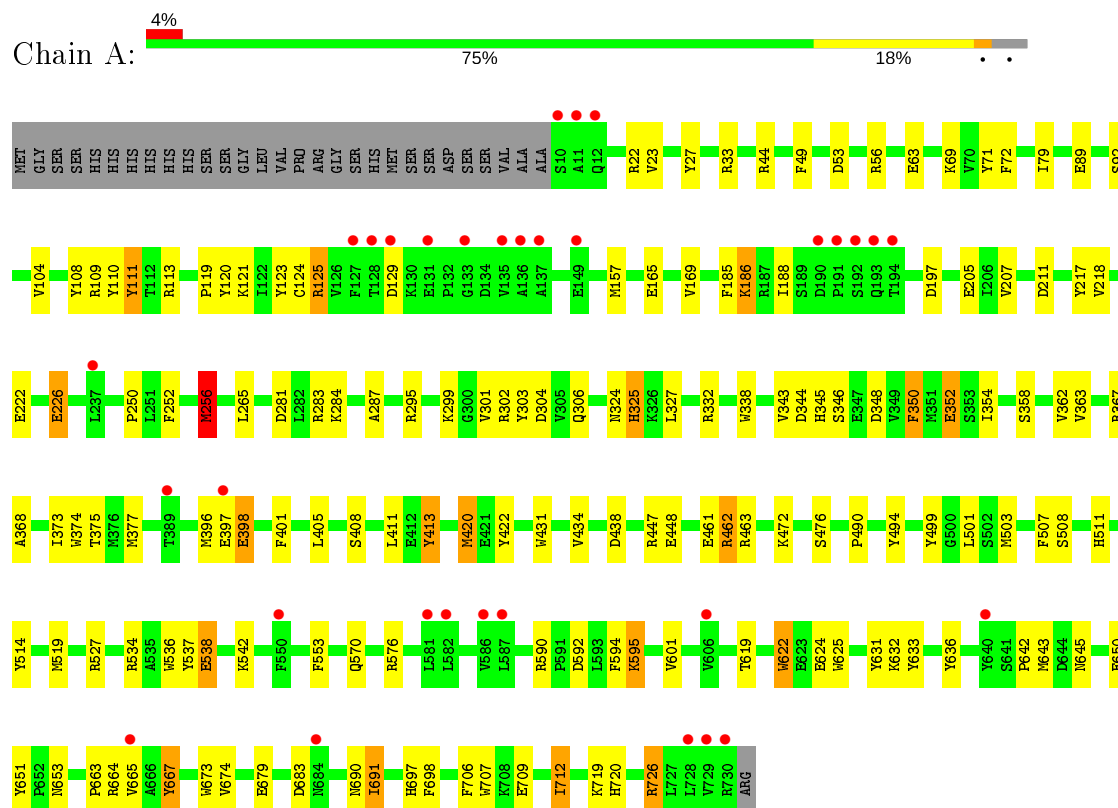
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	721	Total	O	0	0
			721	721		

### 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 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 ( $\text{RSRZ} > 2$ ). 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: OLIGOPEPTIDASE B



#### • Molecule 2: ANTIPAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.48Å 142.78Å 208.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	117.85 – 1.65 37.96 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.0 (117.85-1.65) 98.0 (37.96-1.65)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.140 , 0.178 0.142 , 0.180	Depositor DCC
$R_{free}$ test set	8321 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	7215	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: FC0, GOL, CL, NA, PO4, PGR, PGO, RGL

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	1.67	73/6332 (1.2%)	1.15	37/8586 (0.4%)
2	B	5.07	4/17 (23.5%)	11.03	3/21 (14.3%)
All	All	1.69	77/6349 (1.2%)	1.27	40/8607 (0.5%)

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	ARG	CZ-NH1	14.45	1.51	1.33
1	A	352	GLU	CG-CD	10.43	1.67	1.51
2	B	2	ARG	NE-CZ	8.91	1.44	1.33
1	A	352	GLU	CB-CG	-8.88	1.35	1.52
1	A	514	TYR	CE2-CZ	8.31	1.49	1.38

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	ARG	NE-CZ-NH2	-34.05	103.27	120.30
2	B	2	ARG	NE-CZ-NH1	31.13	135.86	120.30
2	B	2	ARG	CD-NE-CZ	19.52	150.92	123.60
1	A	576	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	A	344[A]	ASP	CB-CG-OD1	8.32	125.78	118.30

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	6125	0	5995	89	0
2	B	43	0	42	1	0
3	A	60	0	79	11	0
4	A	240	0	382	32	0
5	A	5	0	7	1	0
6	A	15	0	0	1	0
7	A	4	0	0	0	0
8	A	2	0	0	0	0
9	A	721	0	0	21	0
All	All	7215	0	6505	102	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 102 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:A:712:ILE:CD1	1:A:712:ILE:CG1	1.75	1.60
1:A:157[B]:MET:HE1	9:A:2223:HOH:O	1.56	1.06
1:A:448[B]:GLU:HG3	9:A:2471:HOH:O	1.61	1.00
1:A:448[B]:GLU:CG	9:A:2471:HOH:O	2.16	0.93
1:A:92:SER:OG	4:A:1750:PGR:H11	1.78	0.83

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	770/751 (102%)	753 (98%)	16 (2%)	1 (0%)	51 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1/4 (25%)	1 (100%)	0	0	100	100
All	All	771/755 (102%)	754 (98%)	16 (2%)	1 (0%)	51	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	HIS

### 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	675/649 (104%)	666 (99%)	9 (1%)	69	50
2	B	2/2 (100%)	2 (100%)	0	100	100
All	All	677/651 (104%)	668 (99%)	9 (1%)	73	50

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256[B]	MET
1	A	691[B]	ILE
1	A	642	PRO
1	A	226	GLU
1	A	397	GLU

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 ⓘ

2 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$
2	RGL	B	4	1,2	9,10,10	2.58	3 (33%)	5,11,11	2.61	2 (40%)
2	FC0	B	1	2	11,14,15	1.47	3 (27%)	11,17,19	0.94	1 (9%)

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	RGL	B	4	1,2	-	0/8/9/9	-
2	FC0	B	1	2	-	2/7/11/12	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	RGL	O-C	6.46	1.45	1.19
2	B	4	RGL	CZ-NE	3.01	1.39	1.33
2	B	1	FC0	CB-CA	2.69	1.57	1.53
2	B	4	RGL	CG-CB	2.18	1.61	1.52
2	B	1	FC0	CA-N	2.15	1.50	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	RGL	NE-CZ-NH2	-4.95	111.99	120.70
2	B	1	FC0	O1-C1-N	-2.44	118.84	125.27
2	B	4	RGL	NH1-CZ-NH2	2.14	126.85	120.26

There are no chirality outliers.

All (2) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	B	1	FC0	CA-CB-CG-CD2
2	B	1	FC0	CA-CB-CG-CD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	FC0	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 68 ligands modelled in this entry, 6 are monoatomic - leaving 62 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	$\# Z  > 2$
4	PGR	A	1770	-	3,4,4	0.76	0	1,4,4	0.09	0
4	PGR	A	1786	-	3,4,4	0.61	0	1,4,4	1.15	0
4	PGR	A	1787	-	3,4,4	1.88	1 (33%)	1,4,4	0.39	0
4	PGR	A	1757	-	3,4,4	0.99	0	1,4,4	0.34	0
4	PGR	A	1761	-	3,4,4	1.69	1 (33%)	1,4,4	0.04	0
3	GOL	A	1733	-	5,5,5	0.49	0	5,5,5	1.60	1 (20%)
3	GOL	A	1736	-	5,5,5	0.68	0	5,5,5	0.81	0
3	GOL	A	1737	-	5,5,5	0.37	0	5,5,5	0.50	0
3	GOL	A	1739	-	5,5,5	0.51	0	5,5,5	0.96	0
4	PGR	A	1762	-	3,4,4	0.33	0	1,4,4	0.10	0
3	GOL	A	1741	-	5,5,5	1.14	0	5,5,5	1.87	2 (40%)
6	PO4	A	1791	-	4,4,4	2.60	1 (25%)	6,6,6	1.76	2 (33%)
6	PO4	A	1792	-	4,4,4	1.22	0	6,6,6	0.69	0
4	PGR	A	1789	-	3,4,4	1.03	0	1,4,4	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PGR	A	1782	-	3,4,4	0.94	0	1,4,4	0.79	0
4	PGR	A	1754	-	3,4,4	0.70	0	1,4,4	0.01	0
4	PGR	A	1764	-	3,4,4	0.99	0	1,4,4	0.57	0
4	PGR	A	1759	-	3,4,4	0.69	0	1,4,4	0.24	0
4	PGR	A	1768	-	3,4,4	0.62	0	1,4,4	0.66	0
4	PGR	A	1742	-	3,4,4	1.34	0	1,4,4	0.90	0
4	PGR	A	1765	-	3,4,4	0.81	0	1,4,4	1.95	0
4	PGR	A	1783	-	3,4,4	1.96	1 (33%)	1,4,4	0.01	0
4	PGR	A	1752	-	3,4,4	0.43	0	1,4,4	0.11	0
4	PGR	A	1745	-	3,4,4	0.81	0	1,4,4	0.75	0
4	PGR	A	1769	-	3,4,4	0.59	0	1,4,4	0.59	0
4	PGR	A	1766	-	3,4,4	1.08	0	1,4,4	0.51	0
4	PGR	A	1744	-	3,4,4	0.74	0	1,4,4	0.98	0
4	PGR	A	1774	-	3,4,4	1.25	0	1,4,4	1.52	0
4	PGR	A	1771	-	3,4,4	1.76	1 (33%)	1,4,4	2.41	1 (100%)
4	PGR	A	1785	-	3,4,4	0.98	0	1,4,4	0.12	0
4	PGR	A	1788	-	3,4,4	0.44	0	1,4,4	1.06	0
4	PGR	A	1781	-	3,4,4	0.94	0	1,4,4	1.78	0
4	PGR	A	1784	-	3,4,4	1.51	1 (33%)	1,4,4	0.44	0
4	PGR	A	1749	-	3,4,4	1.09	0	1,4,4	1.02	0
3	GOL	A	1732	-	5,5,5	1.59	1 (20%)	5,5,5	1.39	1 (20%)
4	PGR	A	1746	-	3,4,4	2.09	1 (33%)	1,4,4	0.11	0
4	PGR	A	1748	-	3,4,4	0.42	0	1,4,4	0.80	0
4	PGR	A	1773	-	3,4,4	0.70	0	1,4,4	0.46	0
4	PGR	A	1772	-	3,4,4	0.32	0	1,4,4	0.69	0
5	PGO	A	1743	-	3,4,4	0.66	0	1,4,4	3.56	1 (100%)
4	PGR	A	1777	-	3,4,4	1.29	1 (33%)	1,4,4	0.31	0
4	PGR	A	1755	-	3,4,4	1.55	1 (33%)	1,4,4	0.09	0
3	GOL	A	1734	-	5,5,5	0.59	0	5,5,5	1.03	0
4	PGR	A	1747	-	3,4,4	1.10	0	1,4,4	2.34	1 (100%)
4	PGR	A	1778	-	3,4,4	0.84	0	1,4,4	0.75	0
4	PGR	A	1763	-	3,4,4	1.41	0	1,4,4	2.03	1 (100%)
3	GOL	A	1740	-	5,5,5	0.63	0	5,5,5	1.10	0
4	PGR	A	1775	-	3,4,4	0.54	0	1,4,4	1.25	0
4	PGR	A	1776	-	3,4,4	1.56	1 (33%)	1,4,4	0.69	0
4	PGR	A	1779	-	3,4,4	0.61	0	1,4,4	0.43	0
4	PGR	A	1751	-	3,4,4	2.00	1 (33%)	1,4,4	0.74	0
4	PGR	A	1750	-	3,4,4	1.25	0	1,4,4	1.37	0
4	PGR	A	1780	-	3,4,4	0.44	0	1,4,4	1.39	0
4	PGR	A	1790	-	3,4,4	1.19	0	1,4,4	2.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	PO4	A	1793	-	4,4,4	1.60	1 (25%)	6,6,6	1.09	1 (16%)
4	PGR	A	1767	-	3,4,4	1.38	1 (33%)	1,4,4	2.74	1 (100%)
3	GOL	A	1738	-	5,5,5	0.77	0	5,5,5	0.60	0
3	GOL	A	1735	-	5,5,5	0.78	0	5,5,5	1.89	1 (20%)
4	PGR	A	1756	-	3,4,4	0.53	0	1,4,4	0.24	0
4	PGR	A	1758	-	3,4,4	0.95	0	1,4,4	0.86	0
4	PGR	A	1760	-	3,4,4	1.43	0	1,4,4	1.11	0
4	PGR	A	1753	-	3,4,4	1.07	0	1,4,4	0.13	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
4	PGR	A	1770	-	-	2/2/2/2	-
4	PGR	A	1786	-	-	0/2/2/2	-
4	PGR	A	1787	-	-	1/2/2/2	-
4	PGR	A	1757	-	-	2/2/2/2	-
4	PGR	A	1761	-	-	0/2/2/2	-
3	GOL	A	1733	-	-	4/4/4/4	-
3	GOL	A	1736	-	-	3/4/4/4	-
3	GOL	A	1737	-	-	2/4/4/4	-
3	GOL	A	1739	-	-	4/4/4/4	-
4	PGR	A	1762	-	-	2/2/2/2	-
3	GOL	A	1741	-	-	3/4/4/4	-
4	PGR	A	1789	-	-	1/2/2/2	-
4	PGR	A	1782	-	-	2/2/2/2	-
4	PGR	A	1754	-	-	2/2/2/2	-
4	PGR	A	1764	-	-	2/2/2/2	-
4	PGR	A	1759	-	-	2/2/2/2	-
4	PGR	A	1768	-	-	2/2/2/2	-
4	PGR	A	1742	-	-	2/2/2/2	-
4	PGR	A	1765	-	-	0/2/2/2	-
4	PGR	A	1783	-	-	2/2/2/2	-
4	PGR	A	1752	-	-	0/2/2/2	-
4	PGR	A	1745	-	-	0/2/2/2	-
4	PGR	A	1769	-	-	1/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGR	A	1766	-	-	2/2/2/2	-
4	PGR	A	1744	-	-	0/2/2/2	-
4	PGR	A	1774	-	-	2/2/2/2	-
4	PGR	A	1771	-	-	0/2/2/2	-
4	PGR	A	1785	-	-	2/2/2/2	-
4	PGR	A	1788	-	-	2/2/2/2	-
4	PGR	A	1781	-	-	2/2/2/2	-
5	PGO	A	1743	-	1/1/1/1	1/2/2/2	-
4	PGR	A	1749	-	-	2/2/2/2	-
3	GOL	A	1732	-	-	2/4/4/4	-
4	PGR	A	1746	-	-	2/2/2/2	-
4	PGR	A	1748	-	-	0/2/2/2	-
4	PGR	A	1773	-	-	1/2/2/2	-
4	PGR	A	1772	-	-	1/2/2/2	-
4	PGR	A	1784	-	-	1/2/2/2	-
4	PGR	A	1777	-	-	2/2/2/2	-
4	PGR	A	1755	-	-	0/2/2/2	-
3	GOL	A	1734	-	-	4/4/4/4	-
4	PGR	A	1747	-	-	2/2/2/2	-
4	PGR	A	1778	-	-	1/2/2/2	-
4	PGR	A	1763	-	-	1/2/2/2	-
3	GOL	A	1740	-	-	4/4/4/4	-
4	PGR	A	1775	-	-	0/2/2/2	-
4	PGR	A	1776	-	-	0/2/2/2	-
4	PGR	A	1779	-	-	2/2/2/2	-
4	PGR	A	1751	-	-	1/2/2/2	-
4	PGR	A	1750	-	-	1/2/2/2	-
4	PGR	A	1780	-	-	0/2/2/2	-
4	PGR	A	1790	-	-	2/2/2/2	-
4	PGR	A	1767	-	-	2/2/2/2	-
3	GOL	A	1738	-	-	2/4/4/4	-
3	GOL	A	1735	-	-	4/4/4/4	-
4	PGR	A	1756	-	-	0/2/2/2	-
4	PGR	A	1758	-	-	0/2/2/2	-
4	PGR	A	1760	-	-	1/2/2/2	-
4	PGR	A	1753	-	-	1/2/2/2	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1791	PO4	P-O4	-4.94	1.39	1.54
4	A	1746	PGR	O1-C1	3.57	1.57	1.42
4	A	1751	PGR	O2-C2	3.02	1.56	1.43
4	A	1771	PGR	O2-C2	2.99	1.56	1.43
4	A	1787	PGR	O1-C1	2.80	1.54	1.42

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1735	GOL	O1-C1-C2	-3.61	92.91	110.20
5	A	1743	PGO	O2-C2-C3	3.56	124.78	109.38
3	A	1741	GOL	O2-C2-C3	3.05	122.54	109.12
3	A	1733	GOL	O2-C2-C1	2.97	122.20	109.12
6	A	1791	PO4	O3-P-O2	-2.86	98.77	107.97

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1743	PGO	C2

5 of 89 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1770	PGR	O1-C1-C2-C3
4	A	1770	PGR	O1-C1-C2-O2
4	A	1787	PGR	O1-C1-C2-C3
4	A	1757	PGR	O1-C1-C2-C3
4	A	1757	PGR	O1-C1-C2-O2

There are no ring outliers.

27 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1770	PGR	1	0
3	A	1741	GOL	3	0
6	A	1791	PO4	1	0
4	A	1782	PGR	5	0
4	A	1764	PGR	1	0
4	A	1768	PGR	1	0
4	A	1752	PGR	3	0
4	A	1781	PGR	1	0
4	A	1784	PGR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1749	PGR	2	0
3	A	1732	GOL	1	0
4	A	1746	PGR	1	0
5	A	1743	PGO	1	0
4	A	1777	PGR	1	0
3	A	1734	GOL	1	0
4	A	1747	PGR	1	0
4	A	1778	PGR	1	0
3	A	1740	GOL	3	0
4	A	1750	PGR	2	0
4	A	1780	PGR	1	0
4	A	1767	PGR	3	0
3	A	1738	GOL	2	0
3	A	1735	GOL	1	0
4	A	1756	PGR	3	0
4	A	1758	PGR	1	0
4	A	1760	PGR	1	0
4	A	1753	PGR	2	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	721/751 (96%)	0.03	32 (4%) 34 34	28, 36, 53, 79	0
2	B	2/4 (50%)	0.31	0 100 100	38, 38, 38, 49	0
All	All	723/755 (95%)	0.03	32 (4%) 34 34	28, 36, 53, 79	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	SER	5.6
1	A	135	VAL	5.6
1	A	136	ALA	4.9
1	A	137	ALA	4.3
1	A	10	SER	3.9

### 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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
2	FC0	B	1	14/15	0.88	0.15	62,84,89,89	0
2	RGL	B	4	11/11	0.97	0.14	28,31,33,36	0

### 6.3 Carbohydrates [i](#)

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. 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
4	PGR	A	1753	5/5	0.54	0.27	63,67,69,72	0
4	PGR	A	1786	5/5	0.57	0.29	87,87,89,89	0
4	PGR	A	1773	5/5	0.66	0.31	86,91,93,94	0
4	PGR	A	1784	5/5	0.67	0.29	49,52,55,57	5
4	PGR	A	1789	5/5	0.69	0.23	67,69,73,75	5
4	PGR	A	1770	5/5	0.69	0.34	63,69,70,71	5
3	GOL	A	1739	6/6	0.72	0.19	57,69,71,72	6
4	PGR	A	1751	5/5	0.74	0.18	54,55,58,61	0
4	PGR	A	1787	5/5	0.74	0.19	65,73,78,79	0
4	PGR	A	1748	5/5	0.78	0.25	85,88,91,93	0
4	PGR	A	1790	5/5	0.78	0.23	69,76,77,78	0
4	PGR	A	1760	5/5	0.78	0.27	71,75,81,83	0
4	PGR	A	1759	5/5	0.78	0.22	89,90,92,92	0
4	PGR	A	1779	5/5	0.79	0.25	78,86,92,93	0
4	PGR	A	1771	5/5	0.80	0.14	43,46,51,53	5
4	PGR	A	1785	5/5	0.81	0.29	67,67,70,73	5
4	PGR	A	1778	5/5	0.81	0.35	73,75,78,78	0
4	PGR	A	1780	5/5	0.81	0.25	67,70,71,72	5
3	GOL	A	1737	6/6	0.83	0.20	68,70,73,73	6
4	PGR	A	1767	5/5	0.84	0.21	67,71,76,76	0
4	PGR	A	1782	5/5	0.84	0.27	48,61,67,70	4
3	GOL	A	1740	6/6	0.84	0.45	46,48,53,54	6
4	PGR	A	1750	5/5	0.85	0.14	68,74,75,75	0
4	PGR	A	1788	5/5	0.85	0.20	63,70,73,73	5
3	GOL	A	1736	6/6	0.85	0.18	71,82,85,89	0
4	PGR	A	1763	5/5	0.86	0.24	67,77,80,82	0
4	PGR	A	1769	5/5	0.86	0.32	59,69,70,70	4
4	PGR	A	1764	5/5	0.86	0.15	48,54,60,61	0
4	PGR	A	1768	5/5	0.86	0.17	81,84,85,86	0
4	PGR	A	1783	5/5	0.86	0.12	61,62,66,66	0
4	PGR	A	1754	5/5	0.87	0.18	87,88,89,90	0
3	GOL	A	1735	6/6	0.87	0.16	64,74,78,78	0
3	GOL	A	1741	6/6	0.88	0.12	42,48,52,56	6
4	PGR	A	1755	5/5	0.88	0.26	51,59,61,64	0
4	PGR	A	1757	5/5	0.89	0.12	52,59,64,67	0
3	GOL	A	1732	6/6	0.89	0.10	44,46,49,50	0
6	PO4	A	1792	5/5	0.89	0.18	74,75,76,77	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PGR	A	1744	5/5	0.89	0.12	47,48,51,53	0
4	PGR	A	1781	5/5	0.89	0.09	70,70,72,73	0
3	GOL	A	1734	6/6	0.89	0.13	50,67,70,70	0
3	GOL	A	1733	6/6	0.90	0.15	75,81,82,84	0
4	PGR	A	1766	5/5	0.90	0.23	60,73,75,79	0
4	PGR	A	1749	5/5	0.90	0.12	53,59,62,62	0
4	PGR	A	1745	5/5	0.90	0.10	51,55,60,65	0
3	GOL	A	1738	6/6	0.92	0.20	46,49,53,64	5
4	PGR	A	1742	5/5	0.92	0.15	41,41,46,50	0
4	PGR	A	1761	5/5	0.93	0.11	55,58,64,71	0
4	PGR	A	1765	5/5	0.93	0.15	35,53,58,58	0
4	PGR	A	1772	5/5	0.93	0.33	79,82,83,85	0
4	PGR	A	1777	5/5	0.94	0.17	56,59,62,63	0
4	PGR	A	1774	5/5	0.94	0.23	41,56,67,69	0
4	PGR	A	1758	5/5	0.94	0.22	77,78,80,81	0
6	PO4	A	1793	5/5	0.94	0.24	53,53,56,58	5
4	PGR	A	1776	5/5	0.94	0.13	41,52,58,65	0
4	PGR	A	1746	5/5	0.95	0.16	34,43,56,61	0
4	PGR	A	1756	5/5	0.95	0.07	54,58,63,63	0
4	PGR	A	1747	5/5	0.95	0.07	44,57,61,61	0
4	PGR	A	1775	5/5	0.95	0.08	42,53,61,65	0
4	PGR	A	1752	5/5	0.95	0.18	54,60,65,71	0
4	PGR	A	1762	5/5	0.96	0.20	69,70,71,72	0
7	CL	A	1799	1/1	0.97	0.04	66,66,66,66	0
6	PO4	A	1791	5/5	0.97	0.17	47,50,56,58	5
5	PGO	A	1743	5/5	0.98	0.14	30,34,41,43	0
8	NA	A	1795	1/1	0.99	0.05	47,47,47,47	0
8	NA	A	1797	1/1	0.99	0.17	34,34,34,34	0
7	CL	A	1796	1/1	1.00	0.04	46,46,46,46	0
7	CL	A	1798	1/1	1.00	0.13	42,42,42,42	0
7	CL	A	1794	1/1	1.00	0.09	45,45,45,45	0

## 6.5 Other polymers

There are no such residues in this entry.