



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 09:05 pm BST

PDB ID : 3C8O  
Title : The Crystal Structure of RraA from PAO1  
Authors : Luo, M.; Niu, S.; Yin, Y.; Huang, A.; Wang, D.  
Deposited on : 2008-02-12  
Resolution : 1.90 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 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

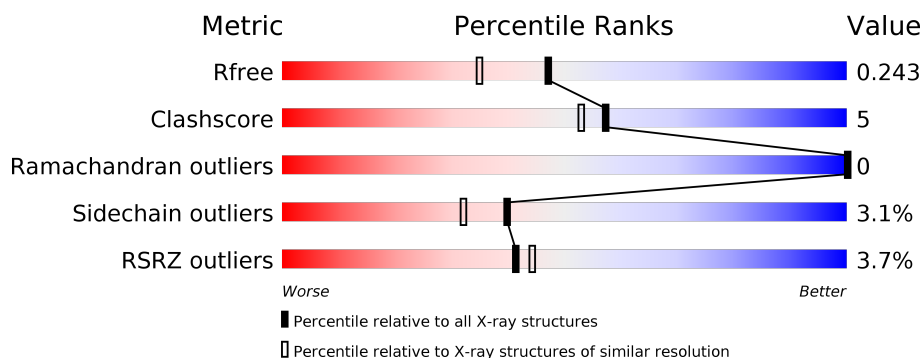
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	162	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div> </div>
1	B	162	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>10%</div> <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	EDO	A	171	-	-	-	X
2	EDO	A	179	-	-	-	X
2	EDO	A	182	-	-	-	X
2	EDO	B	175	-	-	-	X
4	PEG	A	187	-	-	X	X
4	PEG	A	188	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2855 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 Regulator of ribonuclease activity A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	18	0	0
			1204	763	204	231	6			
1	B	161	Total	C	N	O	S	11	0	0
			1212	768	205	232	7			

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

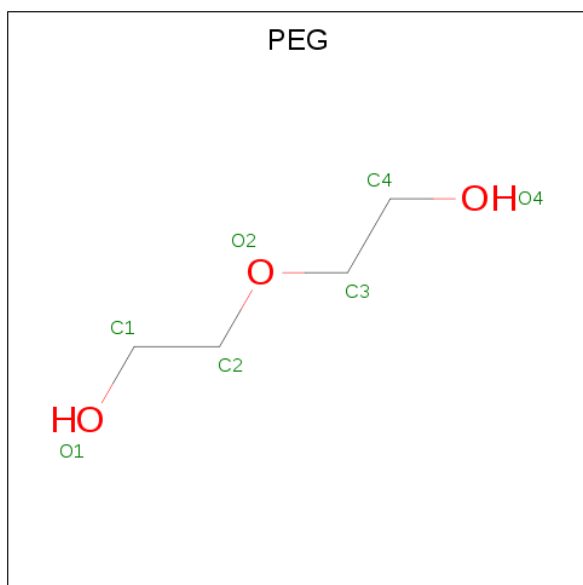
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total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

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



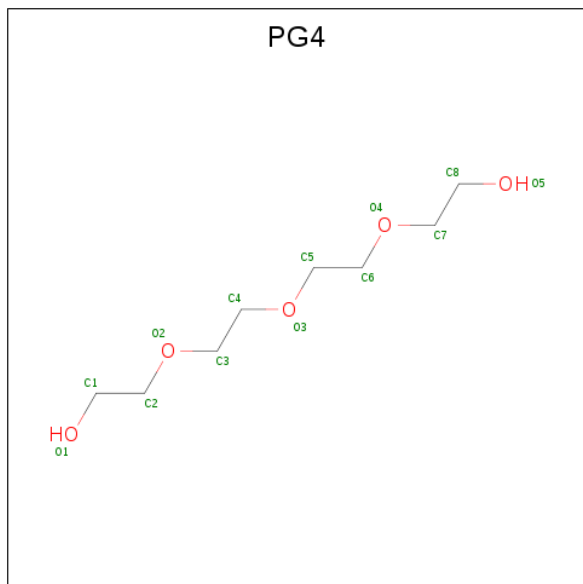
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



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
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



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




- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	74	Total 74	O 74	0	0
6	B	71	Total 71	O 71	0	0

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


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

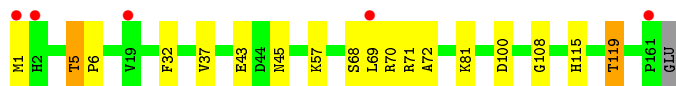
- Molecule 1: Regulator of ribonuclease activity A

Chain A: 



- Molecule 1: Regulator of ribonuclease activity A

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.68 Å 98.68 Å 180.26 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.90 49.34 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.2 (30.00-1.90) 95.0 (49.34-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 1.90 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.221 , 0.249 0.216 , 0.243	Depositor DCC
$R_{free}$ test set	2007 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.4	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 50.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2855	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.22% 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: PG4, PEG, PGE, EDO

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	0.42	1/1225 (0.1%)	0.53	0/1658
1	B	0.37	0/1233	0.52	0/1668
All	All	0.39	1/2458 (0.0%)	0.53	0/3326

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	LYS	CB-CG	-5.80	1.36	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1204	0	1199	15	0
1	B	1212	0	1211	12	0
2	A	84	0	126	3	0
2	B	80	0	120	1	0
3	A	10	0	14	0	0
3	B	30	0	42	1	0
4	A	49	0	70	7	0
4	B	28	0	40	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	13	0	18	0	0
6	A	74	0	0	0	0
6	B	71	0	0	1	0
All	All	2855	0	2840	27	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 5.

All (27) 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:B:45:ASN:H	1:B:119:THR:HG21	1.45	0.80
1:A:70:ARG:HG3	4:A:187:PEG:H22	1.70	0.73
1:A:69:LEU:H	4:A:187:PEG:H21	1.54	0.73
1:A:17:GLN:HE21	4:A:185:PEG:H21	1.55	0.71
1:A:46:SER:HB3	4:A:186:PEG:H11	1.79	0.65
1:A:2:HIS:N	2:A:165:EDO:HO1	1.98	0.60
1:B:45:ASN:N	1:B:119:THR:HG21	2.16	0.60
1:A:81:LYS:HA	2:A:170:EDO:H12	1.89	0.55
1:B:69:LEU:H	4:B:189:PEG:H42	1.72	0.54
1:A:72:ALA:HB2	1:A:115:HIS:O	2.09	0.53
1:B:100:ASP:HB2	2:B:165:EDO:H11	1.90	0.53
1:B:68:SER:HA	4:B:189:PEG:H31	1.91	0.52
1:A:17:GLN:HE21	4:A:185:PEG:C2	2.21	0.52
1:A:4:VAL:HG12	1:A:6:PRO:HD2	1.91	0.52
1:B:43:GLU:OE1	1:B:70:ARG:HD3	2.12	0.49
1:B:32:PHE:CD2	1:B:108:GLY:HA3	2.48	0.48
1:B:72:ALA:HB2	1:B:115:HIS:O	2.13	0.48
1:A:32:PHE:CD2	1:A:108:GLY:HA3	2.48	0.48
1:A:30:ASP:O	1:A:147:ASP:HA	2.14	0.47
1:A:49:LYS:HD3	2:A:164:EDO:H21	1.98	0.45
1:B:70:ARG:O	1:B:71:ARG:HD2	2.16	0.45
1:A:69:LEU:N	4:A:187:PEG:H21	2.28	0.44
1:B:119:THR:HB	6:B:215:HOH:O	2.18	0.43
1:A:42:PHE:CE1	1:A:68:SER:HB2	2.54	0.42
1:B:5:THR:HG22	1:B:6:PRO:HD3	2.02	0.42
1:A:70:ARG:HG3	4:A:187:PEG:C2	2.47	0.41
1:B:81:LYS:HA	3:B:183:PGE:H3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
1	B	159/162 (98%)	154 (97%)	5 (3%)	0	100	100
All	All	317/324 (98%)	308 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	129/131 (98%)	126 (98%)	3 (2%)	50	45
1	B	130/131 (99%)	125 (96%)	5 (4%)	33	24
All	All	259/262 (99%)	251 (97%)	8 (3%)	40	32

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	37	VAL
1	A	159	LYS
1	B	1	MET
1	B	5	THR
1	B	37	VAL
1	B	57	LYS
1	B	119	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	B	17	GLN
1	B	51	GLN

### 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](#)

57 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	$\# Z  > 2$
4	PEG	B	188	-	6,6,6	0.43	0	5,5,5	0.31	0
4	PEG	A	191	-	6,6,6	0.43	0	5,5,5	0.30	0
4	PEG	A	187	-	6,6,6	0.43	0	5,5,5	0.43	0
4	PEG	A	185	-	6,6,6	0.42	0	5,5,5	0.36	0
2	EDO	B	176	-	3,3,3	0.47	0	2,2,2	0.32	0
2	EDO	B	172	-	3,3,3	0.47	0	2,2,2	0.36	0
2	EDO	A	164	-	3,3,3	0.52	0	2,2,2	0.36	0
2	EDO	B	182	-	3,3,3	0.49	0	2,2,2	0.33	0
2	EDO	A	169	-	3,3,3	0.47	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	A	176	-	3,3,3	0.47	0	2,2,2	0.35	0
2	EDO	B	170	-	3,3,3	0.46	0	2,2,2	0.32	0
2	EDO	A	166	-	3,3,3	0.44	0	2,2,2	0.41	0
2	EDO	B	166	-	3,3,3	0.50	0	2,2,2	0.38	0
2	EDO	A	167	-	3,3,3	0.44	0	2,2,2	0.37	0
2	EDO	B	171	-	3,3,3	0.47	0	2,2,2	0.32	0
2	EDO	A	163	-	3,3,3	0.47	0	2,2,2	0.35	0
3	PGE	B	185	-	9,9,9	0.49	0	8,8,8	0.27	0
2	EDO	B	164	-	3,3,3	0.43	0	2,2,2	0.44	0
3	PGE	A	184	-	9,9,9	0.47	0	8,8,8	0.28	0
2	EDO	A	183	-	3,3,3	0.48	0	2,2,2	0.34	0
2	EDO	B	169	-	3,3,3	0.47	0	2,2,2	0.30	0
2	EDO	B	167	-	3,3,3	0.45	0	2,2,2	0.34	0
3	PGE	B	183	-	9,9,9	0.47	0	8,8,8	0.26	0
2	EDO	A	181	-	3,3,3	0.48	0	2,2,2	0.33	0
2	EDO	A	179	-	3,3,3	0.47	0	2,2,2	0.34	0
2	EDO	A	172	-	3,3,3	0.45	0	2,2,2	0.36	0
2	EDO	B	181	-	3,3,3	0.49	0	2,2,2	0.29	0
2	EDO	A	178	-	3,3,3	0.47	0	2,2,2	0.32	0
4	PEG	A	188	-	6,6,6	0.53	0	5,5,5	0.35	0
4	PEG	A	190	-	6,6,6	0.39	0	5,5,5	0.35	0
2	EDO	A	182	-	3,3,3	0.46	0	2,2,2	0.34	0
2	EDO	B	165	-	3,3,3	0.47	0	2,2,2	0.16	0
2	EDO	B	180	-	3,3,3	0.47	0	2,2,2	0.35	0
2	EDO	A	168	-	3,3,3	0.46	0	2,2,2	0.34	0
2	EDO	B	179	-	3,3,3	0.41	0	2,2,2	0.41	0
2	EDO	A	177	-	3,3,3	0.46	0	2,2,2	0.31	0
2	EDO	B	173	-	3,3,3	0.47	0	2,2,2	0.34	0
2	EDO	A	173	-	3,3,3	0.48	0	2,2,2	0.34	0
2	EDO	B	175	-	3,3,3	0.46	0	2,2,2	0.33	0
4	PEG	B	190	-	6,6,6	0.45	0	5,5,5	0.31	0
2	EDO	A	180	-	3,3,3	0.45	0	2,2,2	0.32	0
2	EDO	A	165	-	3,3,3	0.46	0	2,2,2	0.32	0
2	EDO	B	163	-	3,3,3	0.46	0	2,2,2	0.34	0
4	PEG	B	189	-	6,6,6	0.45	0	5,5,5	0.32	0
2	EDO	A	175	-	3,3,3	0.46	0	2,2,2	0.32	0
4	PEG	A	189	-	6,6,6	0.49	0	5,5,5	0.22	0
2	EDO	B	178	-	3,3,3	0.46	0	2,2,2	0.37	0
2	EDO	A	174	-	3,3,3	0.46	0	2,2,2	0.32	0
2	EDO	A	171	-	3,3,3	0.47	0	2,2,2	0.34	0
2	EDO	A	170	-	3,3,3	0.47	0	2,2,2	0.32	0
4	PEG	A	186	-	6,6,6	0.43	0	5,5,5	0.32	0
2	EDO	B	177	-	3,3,3	0.47	0	2,2,2	0.34	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PG4	B	186	-	12,12,12	0.48	0	11,11,11	0.22	0
4	PEG	B	187	-	6,6,6	0.46	0	5,5,5	0.24	0
3	PGE	B	184	-	9,9,9	0.45	0	8,8,8	0.29	0
2	EDO	B	174	-	3,3,3	0.46	0	2,2,2	0.34	0
2	EDO	B	168	-	3,3,3	0.47	0	2,2,2	0.29	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	PEG	B	188	-	-	3/4/4/4	-
4	PEG	A	191	-	-	3/4/4/4	-
4	PEG	A	187	-	-	4/4/4/4	-
4	PEG	A	185	-	-	2/4/4/4	-
2	EDO	B	176	-	-	1/1/1/1	-
2	EDO	B	172	-	-	0/1/1/1	-
2	EDO	A	164	-	-	1/1/1/1	-
2	EDO	B	182	-	-	0/1/1/1	-
2	EDO	A	169	-	-	0/1/1/1	-
2	EDO	A	176	-	-	1/1/1/1	-
2	EDO	B	170	-	-	1/1/1/1	-
2	EDO	A	166	-	-	0/1/1/1	-
2	EDO	B	166	-	-	1/1/1/1	-
2	EDO	A	167	-	-	0/1/1/1	-
2	EDO	B	171	-	-	1/1/1/1	-
2	EDO	A	163	-	-	1/1/1/1	-
3	PGE	B	185	-	-	6/7/7/7	-
2	EDO	B	164	-	-	0/1/1/1	-
3	PGE	A	184	-	-	3/7/7/7	-
2	EDO	A	183	-	-	1/1/1/1	-
2	EDO	B	169	-	-	0/1/1/1	-
2	EDO	B	167	-	-	0/1/1/1	-
3	PGE	B	183	-	-	5/7/7/7	-
2	EDO	A	181	-	-	1/1/1/1	-
2	EDO	A	179	-	-	1/1/1/1	-
2	EDO	A	172	-	-	1/1/1/1	-
2	EDO	B	181	-	-	1/1/1/1	-
2	EDO	A	178	-	-	0/1/1/1	-
4	PEG	A	188	-	-	2/4/4/4	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	190	-	-	0/4/4/4	-
2	EDO	A	182	-	-	1/1/1/1	-
2	EDO	B	165	-	-	1/1/1/1	-
2	EDO	B	180	-	-	0/1/1/1	-
2	EDO	A	168	-	-	0/1/1/1	-
2	EDO	B	179	-	-	0/1/1/1	-
2	EDO	A	177	-	-	0/1/1/1	-
2	EDO	B	173	-	-	0/1/1/1	-
2	EDO	A	173	-	-	1/1/1/1	-
2	EDO	B	175	-	-	1/1/1/1	-
4	PEG	B	190	-	-	3/4/4/4	-
2	EDO	A	180	-	-	0/1/1/1	-
2	EDO	A	165	-	-	1/1/1/1	-
2	EDO	B	163	-	-	0/1/1/1	-
4	PEG	B	189	-	-	2/4/4/4	-
2	EDO	A	175	-	-	1/1/1/1	-
4	PEG	A	189	-	-	2/4/4/4	-
2	EDO	B	178	-	-	0/1/1/1	-
2	EDO	A	174	-	-	0/1/1/1	-
2	EDO	A	171	-	-	0/1/1/1	-
2	EDO	A	170	-	-	0/1/1/1	-
4	PEG	A	186	-	-	2/4/4/4	-
2	EDO	B	177	-	-	1/1/1/1	-
5	PG4	B	186	-	-	2/10/10/10	-
4	PEG	B	187	-	-	4/4/4/4	-
3	PGE	B	184	-	-	3/7/7/7	-
2	EDO	B	174	-	-	1/1/1/1	-
2	EDO	B	168	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	184	PGE	O2-C3-C4-O3
3	B	183	PGE	O2-C3-C4-O3
3	A	184	PGE	O1-C1-C2-O2
4	B	190	PEG	O2-C3-C4-O4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	B	189	PEG	O1-C1-C2-O2
4	A	186	PEG	O2-C3-C4-O4
3	B	184	PGE	O1-C1-C2-O2
2	B	166	EDO	O1-C1-C2-O2
4	A	187	PEG	O1-C1-C2-O2
3	B	185	PGE	O1-C1-C2-O2
3	B	185	PGE	O3-C5-C6-O4
4	A	189	PEG	O2-C3-C4-O4
4	B	190	PEG	O1-C1-C2-O2
4	B	189	PEG	O2-C3-C4-O4
4	B	187	PEG	O1-C1-C2-O2
3	B	184	PGE	O3-C5-C6-O4
4	A	187	PEG	O2-C3-C4-O4
3	B	185	PGE	O2-C3-C4-O3
4	B	188	PEG	O2-C3-C4-O4
4	A	186	PEG	O1-C1-C2-O2
2	A	176	EDO	O1-C1-C2-O2
2	B	171	EDO	O1-C1-C2-O2
2	A	181	EDO	O1-C1-C2-O2
2	A	179	EDO	O1-C1-C2-O2
2	A	173	EDO	O1-C1-C2-O2
2	A	165	EDO	O1-C1-C2-O2
2	A	175	EDO	O1-C1-C2-O2
4	B	188	PEG	O1-C1-C2-O2
4	A	191	PEG	O1-C1-C2-O2
3	B	183	PGE	O1-C1-C2-O2
4	B	187	PEG	O2-C3-C4-O4
3	B	183	PGE	O3-C5-C6-O4
2	A	164	EDO	O1-C1-C2-O2
2	A	163	EDO	O1-C1-C2-O2
2	A	183	EDO	O1-C1-C2-O2
2	B	181	EDO	O1-C1-C2-O2
2	B	175	EDO	O1-C1-C2-O2
3	B	185	PGE	C4-C3-O2-C2
4	B	188	PEG	C4-C3-O2-C2
3	B	184	PGE	C3-C4-O3-C5
4	A	187	PEG	C4-C3-O2-C2
3	B	183	PGE	C4-C3-O2-C2
4	A	188	PEG	C1-C2-O2-C3
3	B	183	PGE	C6-C5-O3-C4
4	A	191	PEG	C4-C3-O2-C2
3	B	185	PGE	C3-C4-O3-C5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	B	186	PG4	C1-C2-O2-C3
4	A	191	PEG	C1-C2-O2-C3
4	A	185	PEG	C4-C3-O2-C2
4	A	189	PEG	C1-C2-O2-C3
4	A	188	PEG	O1-C1-C2-O2
4	A	187	PEG	C1-C2-O2-C3
4	B	187	PEG	C4-C3-O2-C2
2	B	170	EDO	O1-C1-C2-O2
3	B	185	PGE	C1-C2-O2-C3
4	B	187	PEG	C1-C2-O2-C3
4	B	190	PEG	C4-C3-O2-C2
2	B	177	EDO	O1-C1-C2-O2
3	A	184	PGE	O3-C5-C6-O4
4	A	185	PEG	O2-C3-C4-O4
2	B	176	EDO	O1-C1-C2-O2
2	A	172	EDO	O1-C1-C2-O2
2	A	182	EDO	O1-C1-C2-O2
2	B	174	EDO	O1-C1-C2-O2
5	B	186	PG4	O1-C1-C2-O2
2	B	165	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	187	PEG	4	0
4	A	185	PEG	2	0
2	A	164	EDO	1	0
3	B	183	PGE	1	0
2	B	165	EDO	1	0
2	A	165	EDO	1	0
4	B	189	PEG	2	0
2	A	170	EDO	1	0
4	A	186	PEG	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [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	160/162 (98%)	0.32	7 (4%) 34 37	26, 29, 33, 38	5 (3%)
1	B	161/162 (99%)	0.25	5 (3%) 49 51	26, 29, 33, 39	3 (1%)
All	All	321/324 (99%)	0.29	12 (3%) 41 44	26, 29, 33, 39	8 (2%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	4.7
1	B	2	HIS	4.1
1	A	2	HIS	3.8
1	B	161	PRO	3.1
1	A	69	LEU	3.0
1	A	161	PRO	2.8
1	A	134	GLY	2.6
1	B	19	VAL	2.6
1	B	69	LEU	2.6
1	A	112	LEU	2.3
1	A	84	LYS	2.3
1	A	19	VAL	2.3

### 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 ⓘ

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	EDO	A	179	4/4	0.05	0.70	67,67,67,67	0
3	PGE	A	184	10/10	0.31	0.29	47,49,49,49	0
4	PEG	A	188	7/7	0.32	0.80	52,53,54,54	0
4	PEG	B	189	7/7	0.45	0.38	33,34,35,35	0
2	EDO	B	177	4/4	0.48	0.20	53,53,53,53	0
4	PEG	A	187	7/7	0.51	0.44	39,39,40,41	0
2	EDO	B	181	4/4	0.58	0.38	43,43,43,43	0
4	PEG	A	189	7/7	0.61	0.23	28,29,31,31	0
3	PGE	B	185	10/10	0.62	0.23	49,49,50,50	0
2	EDO	A	182	4/4	0.63	0.42	39,39,39,39	0
2	EDO	A	174	4/4	0.65	0.14	48,48,48,48	0
2	EDO	B	178	4/4	0.65	0.14	49,49,49,49	0
2	EDO	B	165	4/4	0.66	0.39	29,29,29,29	0
2	EDO	B	173	4/4	0.67	0.20	42,42,42,42	0
2	EDO	A	176	4/4	0.69	0.32	51,51,51,51	0
2	EDO	A	173	4/4	0.69	0.19	50,50,50,50	0
2	EDO	B	169	4/4	0.69	0.15	44,44,44,44	0
2	EDO	B	174	4/4	0.69	0.31	48,49,49,49	0
2	EDO	B	168	4/4	0.69	0.14	49,49,49,49	0
2	EDO	B	175	4/4	0.70	0.60	50,50,50,51	0
2	EDO	A	183	4/4	0.70	0.18	45,45,45,45	0
4	PEG	A	186	7/7	0.71	0.24	48,48,48,48	0
2	EDO	B	171	4/4	0.72	0.18	41,42,42,42	0
2	EDO	B	179	4/4	0.72	0.29	37,37,37,38	0
2	EDO	B	180	4/4	0.73	0.23	32,32,33,33	0
2	EDO	A	172	4/4	0.73	0.19	45,45,45,45	0
2	EDO	B	172	4/4	0.73	0.23	52,52,53,53	0
4	PEG	A	191	7/7	0.73	0.28	48,48,48,48	0
4	PEG	B	190	7/7	0.74	0.24	45,45,45,45	0
4	PEG	B	187	7/7	0.74	0.15	29,31,32,33	0
2	EDO	B	182	4/4	0.74	0.32	56,56,56,56	0
2	EDO	B	170	4/4	0.74	0.25	43,43,43,43	0
2	EDO	A	169	4/4	0.75	0.30	50,50,50,50	0
3	PGE	B	184	10/10	0.75	0.24	41,43,44,44	0
2	EDO	A	178	4/4	0.76	0.16	45,45,45,45	0
2	EDO	A	166	4/4	0.76	0.26	34,34,34,34	0
3	PGE	B	183	10/10	0.77	0.21	41,42,42,42	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	B	164	4/4	0.78	0.22	30,30,30,30	0
2	EDO	A	171	4/4	0.79	0.48	37,38,38,38	0
5	PG4	B	186	13/13	0.79	0.20	27,28,30,31	0
2	EDO	A	164	4/4	0.80	0.27	42,42,42,43	0
2	EDO	B	176	4/4	0.80	0.24	44,45,45,45	0
2	EDO	A	181	4/4	0.81	0.16	42,42,42,42	0
2	EDO	B	167	4/4	0.82	0.14	46,46,46,47	0
2	EDO	A	163	4/4	0.82	0.57	30,30,30,30	0
2	EDO	A	168	4/4	0.84	0.23	45,45,45,45	0
2	EDO	A	175	4/4	0.85	0.27	42,42,42,42	0
2	EDO	A	165	4/4	0.85	0.20	47,47,47,47	0
2	EDO	A	167	4/4	0.85	0.27	37,37,38,38	0
4	PEG	B	188	7/7	0.86	0.37	40,40,40,40	0
4	PEG	A	185	7/7	0.86	0.18	38,38,39,39	0
2	EDO	B	166	4/4	0.86	0.20	47,47,47,47	0
2	EDO	B	163	4/4	0.88	0.30	44,44,44,44	0
2	EDO	A	170	4/4	0.88	0.27	42,42,42,42	0
2	EDO	A	180	4/4	0.88	0.17	41,41,41,41	0
2	EDO	A	177	4/4	0.91	0.58	40,40,40,40	0
4	PEG	A	190	7/7	0.93	0.19	23,23,24,24	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.