



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 10:54 pm BST

PDB ID : 3T9G  
Title : The crystal structure of family 3 pectate lyase from *Caldicellulosiruptor bescii*  
Authors : Alahuhta, P.M.; Lunin, V.V.  
Deposited on : 2011-08-02  
Resolution : 1.50 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

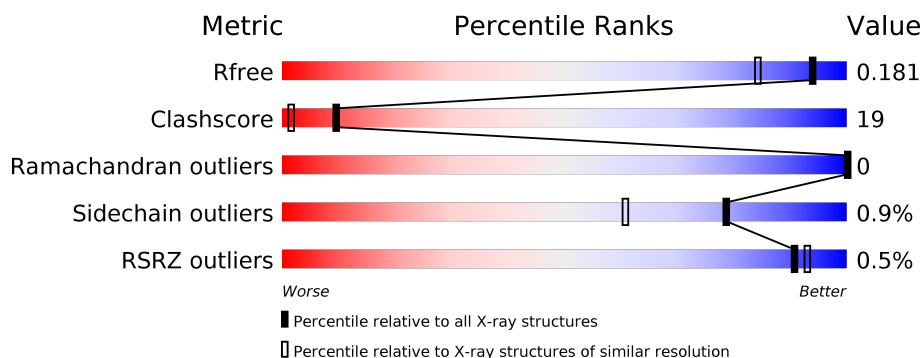
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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 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	196	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>76%</span> <span>22%</span> </div> </div>
1	B	196	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 81%, yellow 18%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>81%</span> <span>18%</span> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	PO4	B	216	-	-	X	-
10	PO4	B	217	-	-	X	-
3	MRD	A	203	-	-	X	-
3	MRD	B	206	-	-	X	-
4	MPD	A	205	-	-	X	-
6	GOL	A	208	-	-	X	-
6	GOL	B	212	-	-	X	-
8	EDO	B	208	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 3980 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 Pectate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	26	0
			1654	1047	276	325	6			
1	B	195	Total	C	N	O	S	0	21	0
			1632	1028	271	327	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	VAL	-	EXPRESSION TAG	UNP B9MKT4
A	-1	GLY	-	EXPRESSION TAG	UNP B9MKT4
A	0	THR	-	EXPRESSION TAG	UNP B9MKT4
B	-2	VAL	-	EXPRESSION TAG	UNP B9MKT4
B	-1	GLY	-	EXPRESSION TAG	UNP B9MKT4
B	0	THR	-	EXPRESSION TAG	UNP B9MKT4

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

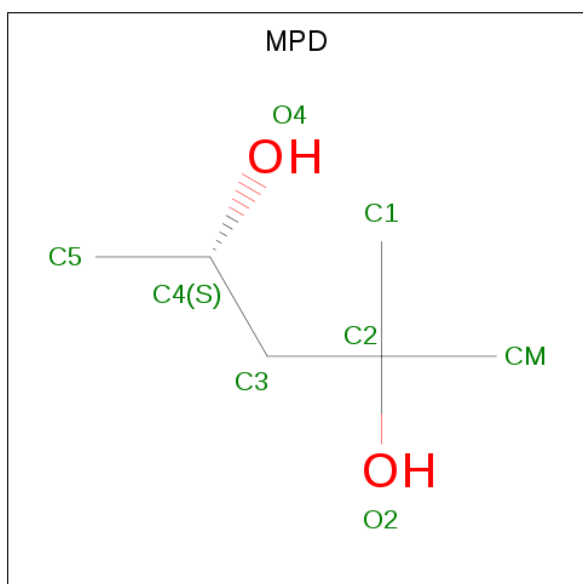
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	1
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	1
4	B	1	Total C O 8 6 2	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	3	Total Na 3 3	0	0
5	A	1	Total Na 1 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).

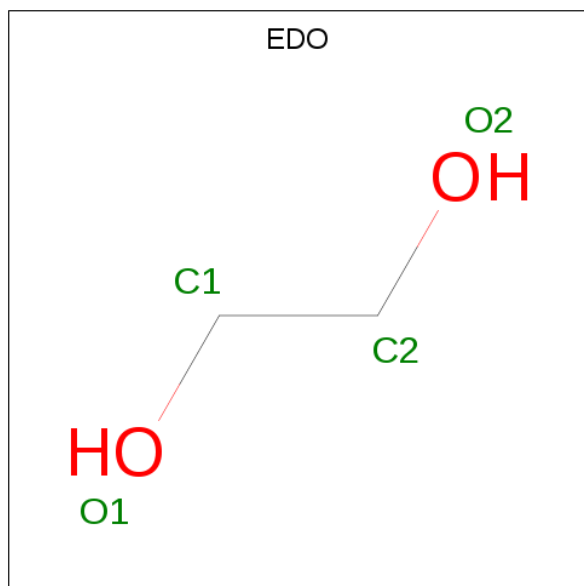


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 12 6 6	0	1
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 12 6 6	0	1

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Cl 1 1	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



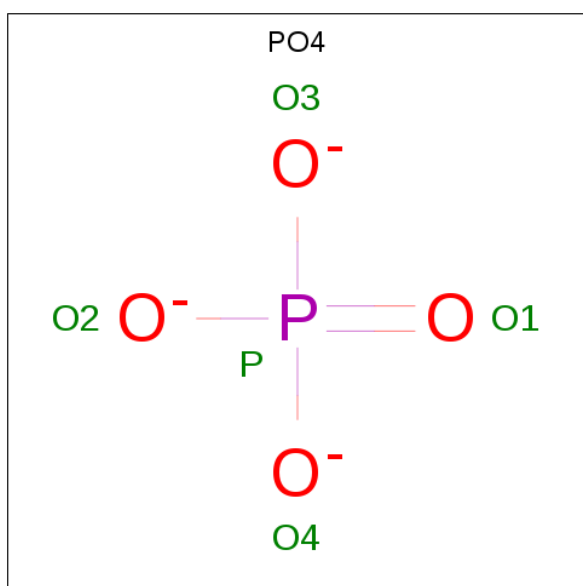
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	O	P	0	0
			5	4	1		
10	B	1	Total	O	P	0	0
			5	4	1		



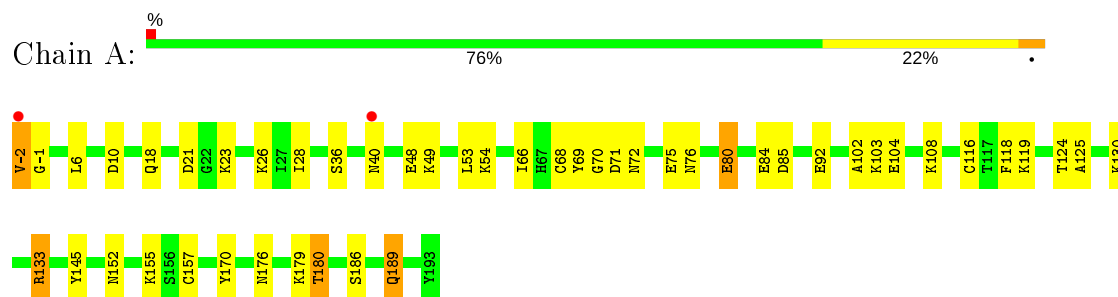
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	276	Total 293	O 293	0	17
11	B	250	Total 268	O 268	0	18

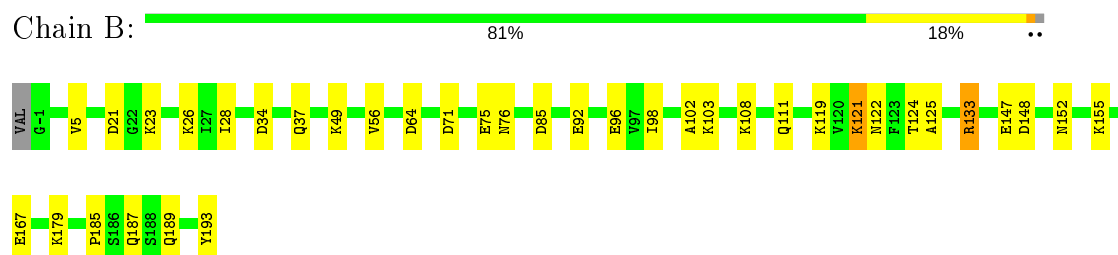
### 3 Residue-property plots [i](#)

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: Pectate lyase



#### • Molecule 1: Pectate lyase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.51Å 146.69Å 162.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.50 35.77 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (25.00-1.50) 99.4 (35.77-1.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.93 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.143 , 0.178 0.150 , 0.181	Depositor DCC
$R_{free}$ test set	3552 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.4	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3980	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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: GOL, MPD, CL, NA, CA, EDO, ACT, MRD, PO4

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	1.43	9/1715 (0.5%)	1.21	10/2319 (0.4%)
1	B	1.33	2/1680 (0.1%)	1.26	11/2270 (0.5%)
All	All	1.38	11/3395 (0.3%)	1.23	21/4589 (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

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	GLU	CD-OE1	11.23	1.38	1.25
1	A	49	LYS	CD-CE	7.39	1.69	1.51
1	B	56[A]	VAL	CB-CG1	6.53	1.66	1.52
1	B	56[B]	VAL	CB-CG1	6.53	1.66	1.52
1	A	189	GLN	CD-OE1	6.22	1.37	1.24

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64	ASP	CB-CG-OD2	-11.13	108.28	118.30
1	B	21	ASP	CB-CG-OD1	10.59	127.83	118.30
1	B	133	ARG	NE-CZ-NH2	10.24	125.42	120.30
1	A	10	ASP	CB-CG-OD1	9.75	127.07	118.30
1	A	133	ARG	NE-CZ-NH2	-6.99	116.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40[B]	ASN	Peptide

## 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	1654	0	1665	49	0
1	B	1632	0	1624	62	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	16	0	28	10	0
3	B	16	0	28	12	0
4	A	16	0	28	12	0
4	B	16	0	28	1	0
5	A	1	0	0	1	0
5	B	3	0	0	0	0
6	A	18	0	24	6	0
6	B	18	0	24	5	0
7	B	1	0	0	0	0
8	B	8	0	12	12	0
9	B	8	0	6	1	0
10	B	10	0	0	4	0
11	A	293	0	0	18	0
11	B	268	0	0	34	0
All	All	3980	0	3467	135	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 19.

The worst 5 of 135 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)
3:A:203:MRD:H1C3	3:A:203:MRD:C5	1.52	1.37
3:A:203:MRD:H5C2	3:A:203:MRD:C1	1.54	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92[A]:GLU:OE1	11:B:528[A]:HOH:O	1.61	1.18
4:A:205:MPD:HM1	11:A:436:HOH:O	1.46	1.16
1:B:152[A]:ASN:ND2	11:B:535:HOH:O	1.77	1.15

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	219/196 (112%)	210 (96%)	9 (4%)	0	100	100
1	B	215/196 (110%)	199 (93%)	16 (7%)	0	100	100
All	All	434/392 (111%)	409 (94%)	25 (6%)	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	190/166 (114%)	186 (98%)	4 (2%)	53	23
1	B	186/166 (112%)	183 (98%)	3 (2%)	62	36
All	All	376/332 (113%)	369 (98%)	7 (2%)	78	27

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180[B]	THR
1	B	121[C]	LYS
1	B	121[A]	LYS
1	A	-2[B]	VAL
1	B	121[B]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	B	189	GLN
1	B	18	GLN
1	A	152	ASN
1	B	137	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](#)

Of 27 ligands modelled in this entry, 7 are monoatomic - leaving 20 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
9	ACT	B	215	-	1,3,3	2.12	1 (100%)	0,3,3	0.00	-
6	GOL	A	207[A]	-	5,5,5	0.61	0	5,5,5	0.70	0
6	GOL	A	207[B]	-	5,5,5	0.41	0	5,5,5	0.65	0
3	MRD	A	202	-	7,7,7	0.60	0	9,10,10	1.26	2 (22%)
4	MPD	A	204	-	7,7,7	0.51	0	9,10,10	0.81	0
9	ACT	B	214	-	1,3,3	2.22	1 (100%)	0,3,3	0.00	-
10	PO4	B	216	-	4,4,4	1.05	0	6,6,6	0.82	0
4	MPD	B	204[B]	-	7,7,7	0.28	0	9,10,10	0.27	0
3	MRD	B	203[A]	-	7,7,7	0.70	0	9,10,10	0.64	0
6	GOL	A	208	-	5,5,5	0.43	0	5,5,5	0.23	0
8	EDO	B	208	-	3,3,3	0.44	0	2,2,2	0.48	0
4	MPD	A	205	-	7,7,7	0.86	0	9,10,10	2.09	5 (55%)
10	PO4	B	217	-	4,4,4	0.62	0	6,6,6	1.09	0
8	EDO	B	207	-	3,3,3	0.62	0	2,2,2	0.23	0
6	GOL	B	213[A]	-	5,5,5	0.42	0	5,5,5	0.41	0
4	MPD	B	205	-	7,7,7	0.49	0	9,10,10	0.81	0
6	GOL	B	212	-	5,5,5	0.37	0	5,5,5	0.40	0
6	GOL	B	213[B]	-	5,5,5	0.46	0	5,5,5	0.39	0
3	MRD	A	203	-	7,7,7	0.57	0	9,10,10	1.15	1 (11%)
3	MRD	B	206	-	7,7,7	0.56	0	9,10,10	2.40	3 (33%)

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
6	GOL	A	207[A]	-	-	2/4/4/4	-
6	GOL	A	207[B]	-	-	2/4/4/4	-
4	MPD	A	204	-	-	1/5/5/5	-
3	MRD	A	202	-	-	0/5/5/5	-
4	MPD	B	205	-	-	0/5/5/5	-
4	MPD	B	204[B]	-	-	0/5/5/5	-
3	MRD	B	203[A]	-	-	0/5/5/5	-
6	GOL	A	208	-	-	2/4/4/4	-
8	EDO	B	208	-	-	1/1/1/1	-
4	MPD	A	205	-	-	1/5/5/5	-
8	EDO	B	207	-	-	1/1/1/1	-
6	GOL	B	213[A]	-	-	2/4/4/4	-
6	GOL	B	212	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	213[B]	-	-	2/4/4/4	-
3	MRD	A	203	-	-	3/5/5/5	-
3	MRD	B	206	-	-	1/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	214	ACT	CH3-C	2.22	1.51	1.48
9	B	215	ACT	CH3-C	2.12	1.51	1.48

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	206	MRD	CM-C2-C1	5.59	122.22	110.57
4	A	205	MPD	CM-C2-C1	-3.43	103.43	110.57
4	A	205	MPD	C1-C2-C3	3.38	125.71	109.96
3	B	206	MRD	O2-C2-C3	3.10	121.44	109.80
3	B	206	MRD	O2-C2-C1	-2.57	99.83	108.08

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	205	MPD	C2-C3-C4-C5
6	A	208	GOL	O1-C1-C2-O2
6	A	208	GOL	O1-C1-C2-C3
6	B	213[B]	GOL	C1-C2-C3-O3
3	A	203	MRD	C2-C3-C4-C5

There are no ring outliers.

11 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	215	ACT	1	0
6	A	207[A]	GOL	2	0
10	B	216	PO4	2	0
4	B	204[B]	MPD	1	0
6	A	208	GOL	4	0
8	B	208	EDO	12	0
4	A	205	MPD	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	217	PO4	2	0
6	B	212	GOL	5	0
3	A	203	MRD	10	0
3	B	206	MRD	12	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	196/196 (100%)	-0.64	2 (1%) 82 85	6, 11, 20, 32	3 (1%)
1	B	195/196 (99%)	-0.66	0 100 100	6, 11, 19, 30	1 (0%)
All	All	391/392 (99%)	-0.65	2 (0%) 91 93	6, 11, 20, 32	4 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-2[A]	VAL	4.6
1	A	40[A]	ASN	4.4

### 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. 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
8	EDO	B	207	4/4	0.69	0.12	39,42,42,46	0
9	ACT	B	215	4/4	0.70	0.17	31,32,32,35	4
6	GOL	A	208	6/6	0.71	0.25	31,32,33,35	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	B	213[A]	6/6	0.71	0.17	54,55,56,57	6
6	GOL	B	213[B]	6/6	0.71	0.17	30,32,33,34	6
8	EDO	B	208	4/4	0.76	0.14	28,28,31,31	4
6	GOL	B	212	6/6	0.78	0.18	22,31,36,38	6
10	PO4	B	217	5/5	0.80	0.17	49,50,55,56	5
10	PO4	B	216	5/5	0.87	0.12	35,38,41,45	5
3	MRD	B	203[A]	8/8	0.87	0.13	12,17,22,23	8
3	MRD	A	203	8/8	0.87	0.14	23,25,30,30	8
3	MRD	B	206	8/8	0.89	0.12	24,28,32,32	8
9	ACT	B	214	4/4	0.89	0.12	52,53,53,53	0
4	MPD	A	205	8/8	0.91	0.11	15,20,25,26	8
4	MPD	B	205	8/8	0.91	0.09	17,24,27,29	0
4	MPD	A	204	8/8	0.91	0.11	16,23,26,26	8
4	MPD	B	204[B]	8/8	0.91	0.15	61,61,62,62	8
6	GOL	A	207[B]	6/6	0.92	0.14	20,23,25,27	6
6	GOL	A	207[A]	6/6	0.92	0.14	18,23,26,29	6
3	MRD	A	202	8/8	0.94	0.09	21,25,28,28	0
5	NA	B	211	1/1	0.98	0.11	22,22,22,22	0
5	NA	B	209	1/1	0.98	0.08	9,9,9,9	1
5	NA	A	206	1/1	0.98	0.08	15,15,15,15	1
7	CL	B	202	1/1	0.99	0.06	12,12,12,12	0
5	NA	B	210	1/1	0.99	0.04	25,25,25,25	0
2	CA	A	201	1/1	1.00	0.04	10,10,10,10	0
2	CA	B	201	1/1	1.00	0.03	7,7,7,7	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.