



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:04 AM UTC

PDB ID : 7BBV / pdb\_00007bbv  
Title : Pectate lyase B from *Verticillium dahliae*  
Authors : Safran, J.; Habrylo, O.; Bouckaert, J.; Pau Roblot, C.; Senechal, F.; Pelloux, J.  
Deposited on : 2020-12-18  
Resolution : 1.20 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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

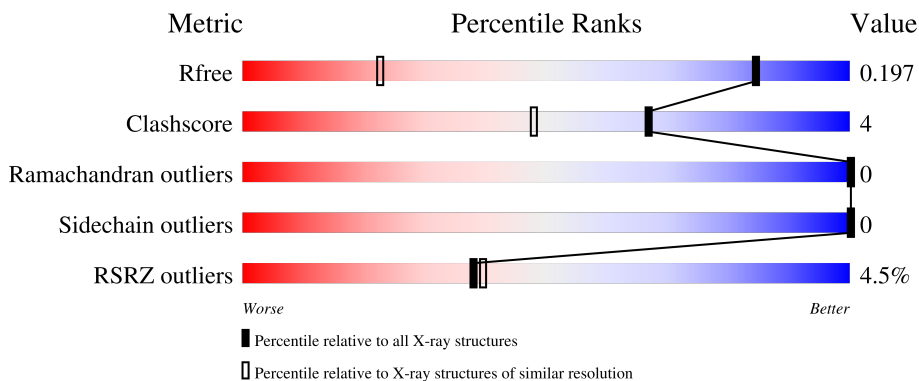
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


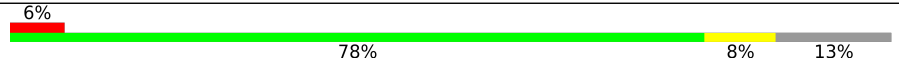
The reported resolution of this entry is 1.20 Å.

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))
$R_{free}$	180053	1216 (1.20-1.20)
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

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	343	 2% 82% 5% 13%
1	B	343	 6% 78% 8% 13%

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	PEG	B	402	-	-	X	-

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 10384 atoms, of which 4624 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 B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	298	4553	1423	2267	400	459	4	0	9	0
1	B	298	4544	1420	2262	401	457	4	0	9	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	317	ALA	-	expression tag	UNP G2X3Y1
A	318	ALA	-	expression tag	UNP G2X3Y1
A	319	ALA	-	expression tag	UNP G2X3Y1
A	320	SER	-	expression tag	UNP G2X3Y1
A	321	PHE	-	expression tag	UNP G2X3Y1
A	322	LEU	-	expression tag	UNP G2X3Y1
A	323	GLU	-	expression tag	UNP G2X3Y1
A	324	GLN	-	expression tag	UNP G2X3Y1
A	325	LYS	-	expression tag	UNP G2X3Y1
A	326	LEU	-	expression tag	UNP G2X3Y1
A	327	ILE	-	expression tag	UNP G2X3Y1
A	328	SER	-	expression tag	UNP G2X3Y1
A	329	GLU	-	expression tag	UNP G2X3Y1
A	330	GLU	-	expression tag	UNP G2X3Y1
A	331	ASP	-	expression tag	UNP G2X3Y1
A	332	LEU	-	expression tag	UNP G2X3Y1
A	333	ASN	-	expression tag	UNP G2X3Y1
A	334	SER	-	expression tag	UNP G2X3Y1
A	335	ALA	-	expression tag	UNP G2X3Y1
A	336	VAL	-	expression tag	UNP G2X3Y1
A	337	ASP	-	expression tag	UNP G2X3Y1
A	338	HIS	-	expression tag	UNP G2X3Y1
A	339	HIS	-	expression tag	UNP G2X3Y1
A	340	HIS	-	expression tag	UNP G2X3Y1
A	341	HIS	-	expression tag	UNP G2X3Y1

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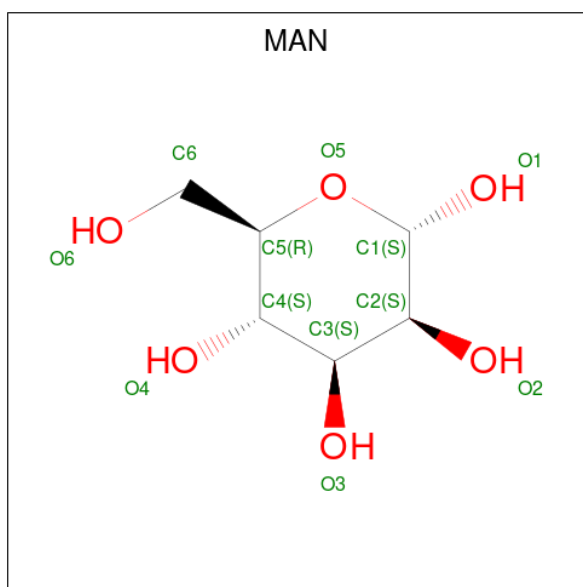
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Chain	Residue	Modelled	Actual	Comment	Reference
A	342	HIS	-	expression tag	UNP G2X3Y1
A	343	HIS	-	expression tag	UNP G2X3Y1
B	317	ALA	-	expression tag	UNP G2X3Y1
B	318	ALA	-	expression tag	UNP G2X3Y1
B	319	ALA	-	expression tag	UNP G2X3Y1
B	320	SER	-	expression tag	UNP G2X3Y1
B	321	PHE	-	expression tag	UNP G2X3Y1
B	322	LEU	-	expression tag	UNP G2X3Y1
B	323	GLU	-	expression tag	UNP G2X3Y1
B	324	GLN	-	expression tag	UNP G2X3Y1
B	325	LYS	-	expression tag	UNP G2X3Y1
B	326	LEU	-	expression tag	UNP G2X3Y1
B	327	ILE	-	expression tag	UNP G2X3Y1
B	328	SER	-	expression tag	UNP G2X3Y1
B	329	GLU	-	expression tag	UNP G2X3Y1
B	330	GLU	-	expression tag	UNP G2X3Y1
B	331	ASP	-	expression tag	UNP G2X3Y1
B	332	LEU	-	expression tag	UNP G2X3Y1
B	333	ASN	-	expression tag	UNP G2X3Y1
B	334	SER	-	expression tag	UNP G2X3Y1
B	335	ALA	-	expression tag	UNP G2X3Y1
B	336	VAL	-	expression tag	UNP G2X3Y1
B	337	ASP	-	expression tag	UNP G2X3Y1
B	338	HIS	-	expression tag	UNP G2X3Y1
B	339	HIS	-	expression tag	UNP G2X3Y1
B	340	HIS	-	expression tag	UNP G2X3Y1
B	341	HIS	-	expression tag	UNP G2X3Y1
B	342	HIS	-	expression tag	UNP G2X3Y1
B	343	HIS	-	expression tag	UNP G2X3Y1

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	17	6	6	5	0	0
3	A	1	17	6	6	5	0	0
3	A	1	19	6	8	5	0	0
3	A	1	19	6	8	5	0	0
3	A	1	19	6	8	5	0	0
3	A	1	17	6	6	5	0	0
3	B	1	17	6	6	5	0	0
3	B	1	19	6	8	5	0	0
3	B	1	19	6	8	5	0	0
3	B	1	17	6	6	5	0	0
3	B	1	19	6	8	5	0	0
3	B	1	18	6	7	5	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	B	1	17	4	10	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	543	543	543	0	0
5	B	508	508	508	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.89Å 59.69Å 93.87Å 90.00° 96.35° 90.00°	Depositor
Resolution (Å)	60.52 – 1.20 60.52 – 1.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (60.52-1.20) 99.3 (60.52-1.20)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.96 (at 1.20Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.172 , 0.196 0.173 , 0.197	Depositor DCC
$R_{free}$ test set	10378 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtrriage
Anisotropy	0.120	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 51.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	10384	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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: MAN, CA, PEG

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	0.67	0/2349	0.81	0/3174
1	B	0.73	3/2346 (0.1%)	0.82	0/3171
All	All	0.70	3/4695 (0.1%)	0.81	0/6345

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	290	ILE	CA-C	-6.19	1.48	1.53
1	B	186	ALA	C-O	-5.33	1.17	1.24
1	B	104	LYS	C-N	-5.28	1.26	1.33

There are no bond angle outliers.

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	2286	2267	2253	12	0
1	B	2282	2262	2245	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	66	42	60	0	0
3	B	66	43	60	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	7	10	10	7	0
5	A	543	0	0	4	4
5	B	508	0	0	5	4
All	All	5760	4624	4628	35	4

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 4.

All (35) 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:122:ASP:OD2	4:B:402:PEG:H42	1.65	0.94
1:B:121:GLY:HA3	4:B:402:PEG:H12	1.54	0.88
1:B:76:LYS:HG3	4:B:402:PEG:H11	1.70	0.72
1:B:99:TYR:CD1	4:B:402:PEG:H31	2.26	0.70
1:B:147:LYS:O	1:B:175:LYS:HE2	1.96	0.65
1:A:190:LYS:NZ	5:A:502:HOH:O	2.30	0.60
1:B:262:GLU:OE1	5:B:501:HOH:O	2.16	0.60
1:B:89:LYS:HD2	5:B:600:HOH:O	2.02	0.59
1:B:70:LYS:HE3	1:B:94:VAL:HG21	1.84	0.58
1:A:236:MET:SD	1:A:260[B]:SER:OG	2.66	0.54
1:B:99:TYR:HD1	4:B:402:PEG:H31	1.73	0.54
1:A:110:ASN:HA	1:A:136:HIS:O	2.12	0.49
1:B:236:MET:SD	1:B:260[A]:SER:OG	2.70	0.49
1:B:62:LYS:HE2	5:B:763:HOH:O	2.13	0.48
1:A:243:GLU:HA	1:A:269:GLY:O	2.13	0.48
1:B:84:THR:HG22	1:B:86:ILE:HG13	1.95	0.48
1:A:92[B]:GLU:HG3	1:A:93:LEU:N	2.29	0.48
1:A:136:HIS:HA	1:A:167:ASN:O	2.15	0.47
1:B:267[A]:THR:HG23	5:B:891:HOH:O	2.15	0.47
1:A:86:ILE:HG12	1:A:109:ARG:HB3	1.98	0.46
1:B:110:ASN:HA	1:B:136:HIS:O	2.15	0.45
1:B:243:GLU:HA	1:B:269:GLY:O	2.16	0.44
1:A:263:LYS:NZ	5:A:517:HOH:O	2.48	0.44
1:A:109:ARG:HA	1:A:135:ASP:O	2.18	0.44
1:B:173:HIS:O	1:B:205:VAL:HA	2.19	0.43
1:B:136:HIS:HA	1:B:167:ASN:O	2.18	0.43
1:B:89:LYS:HD2	1:B:89:LYS:HA	1.94	0.43
1:B:122:ASP:OD2	4:B:402:PEG:C4	2.51	0.43
1:A:130:LYS:NZ	5:A:518:HOH:O	2.49	0.42
1:A:259:ASP:OD1	5:A:501:HOH:O	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LYS:HA	1:B:130:LYS:O	2.20	0.42
1:B:99:TYR:HA	4:B:402:PEG:H22	2.02	0.41
1:B:288:SER:HB3	5:B:581:HOH:O	2.21	0.40
1:A:86:ILE:HA	1:A:109:ARG:O	2.22	0.40
1:B:187:LYS:HA	1:B:187:LYS:HD2	1.93	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:910:HOH:O	5:B:942:HOH:O[2_454]	2.11	0.09
5:A:899:HOH:O	5:B:669:HOH:O[1_655]	2.14	0.06
5:A:1010:HOH:O	5:B:962:HOH:O[2_455]	2.18	0.02
5:A:742:HOH:O	5:B:886:HOH:O[2_455]	2.19	0.01

## 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	305/343 (89%)	291 (95%)	14 (5%)	0	100	100
1	B	305/343 (89%)	290 (95%)	15 (5%)	0	100	100
All	All	610/686 (89%)	581 (95%)	29 (5%)	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	254/283 (90%)	254 (100%)	0	100	100
1	B	254/283 (90%)	254 (100%)	0	100	100
All	All	508/566 (90%)	508 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	206	ASN
1	A	300	ASN
1	B	101	ASN
1	B	300	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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$
3	MAN	B	406	1	11,11,12	0.26	0	15,15,17	0.52	0
4	PEG	B	402	-	6,6,6	0.39	0	5,5,5	0.28	0
3	MAN	B	407	1	11,11,12	1.30	2 (18%)	15,15,17	1.00	1 (6%)
3	MAN	A	405	1	11,11,12	0.26	0	15,15,17	0.51	0
3	MAN	A	402	1	11,11,12	1.17	1 (9%)	15,15,17	1.74	4 (26%)
3	MAN	A	407	1	11,11,12	1.35	1 (9%)	15,15,17	2.14	6 (40%)
3	MAN	A	406	1	11,11,12	0.26	0	15,15,17	0.53	0
3	MAN	B	404	1	11,11,12	0.25	0	15,15,17	0.50	0
3	MAN	B	405	1	11,11,12	1.16	1 (9%)	15,15,17	1.02	1 (6%)
3	MAN	B	403	1	11,11,12	0.26	0	15,15,17	0.51	0
3	MAN	A	403	1	11,11,12	1.65	2 (18%)	15,15,17	0.96	1 (6%)
3	MAN	A	404	1	11,11,12	0.26	0	15,15,17	0.52	0
3	MAN	B	408	1	11,11,12	0.98	0	15,15,17	2.38	5 (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
3	MAN	B	406	1	-	2/2/19/22	0/1/1/1
4	PEG	B	402	-	-	3/4/4/4	-
3	MAN	B	407	1	-	0/2/19/22	0/1/1/1
3	MAN	A	405	1	-	1/2/19/22	0/1/1/1
3	MAN	A	402	1	-	0/2/19/22	0/1/1/1
3	MAN	A	407	1	-	0/2/19/22	0/1/1/1
3	MAN	A	406	1	-	0/2/19/22	0/1/1/1
3	MAN	B	404	1	-	0/2/19/22	0/1/1/1
3	MAN	B	405	1	-	0/2/19/22	0/1/1/1
3	MAN	B	403	1	-	0/2/19/22	0/1/1/1
3	MAN	A	403	1	-	1/2/19/22	0/1/1/1
3	MAN	A	404	1	-	2/2/19/22	0/1/1/1
3	MAN	B	408	1	-	2/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	405	MAN	O5-C1	-3.32	1.38	1.43
3	A	403	MAN	O5-C1	-3.25	1.38	1.43
3	A	407	MAN	O5-C1	-3.06	1.38	1.43
3	B	407	MAN	C2-C3	3.01	1.57	1.52
3	A	403	MAN	O5-C5	-2.92	1.37	1.43
3	B	407	MAN	O5-C5	2.42	1.48	1.43
3	A	402	MAN	O5-C1	-2.06	1.40	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	408	MAN	O5-C5-C6	5.60	118.56	107.66
3	A	407	MAN	C1-O5-C5	-3.96	106.87	112.19
3	B	408	MAN	O2-C2-C3	-3.83	102.21	110.15
3	A	402	MAN	O5-C1-C2	-3.65	102.09	110.79
3	A	402	MAN	O2-C2-C1	3.47	117.17	109.22
3	A	407	MAN	O2-C2-C1	3.45	117.12	109.22
3	B	408	MAN	O5-C1-C2	-3.30	102.92	110.79
3	A	407	MAN	O5-C5-C6	3.14	113.78	107.66
3	A	407	MAN	O5-C1-C2	-3.11	103.36	110.79
3	A	407	MAN	O2-C2-C3	-2.91	104.13	110.15
3	B	408	MAN	C1-O5-C5	-2.90	108.31	112.19
3	A	403	MAN	O2-C2-C1	2.68	115.36	109.22
3	A	402	MAN	C1-C2-C3	-2.59	105.87	109.64
3	B	408	MAN	C6-C5-C4	-2.53	106.82	113.02
3	B	405	MAN	O2-C2-C3	-2.48	105.01	110.15
3	A	402	MAN	O5-C5-C6	2.27	112.08	107.66
3	A	407	MAN	C6-C5-C4	-2.12	107.82	113.02
3	B	407	MAN	O2-C2-C3	-2.06	105.88	110.15

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	408	MAN	O5-C5-C6-O6
3	B	408	MAN	C4-C5-C6-O6
3	B	406	MAN	C4-C5-C6-O6
4	B	402	PEG	O1-C1-C2-O2
4	B	402	PEG	O2-C3-C4-O4
3	B	406	MAN	O5-C5-C6-O6
3	A	405	MAN	O5-C5-C6-O6
3	A	404	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	403	MAN	C4-C5-C6-O6
3	A	404	MAN	O5-C5-C6-O6
4	B	402	PEG	C1-C2-O2-C3

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	402	PEG	7	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

### 6.1 Protein, DNA and RNA chains

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	298/343 (86%)	0.13	7 (2%) 61 61	15, 28, 48, 83	9 (3%)
1	B	298/343 (86%)	0.46	20 (6%) 24 25	12, 30, 55, 87	9 (3%)
All	All	596/686 (86%)	0.30	27 (4%) 38 39	12, 29, 52, 87	18 (3%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	316	PHE	5.6
1	A	316	PHE	4.6
1	B	19	ALA	4.3
1	A	19	ALA	3.6
1	B	315	GLY	3.4
1	A	315	GLY	3.0
1	B	286	GLY	2.8
1	B	287	SER	2.6
1	B	289	ASN	2.6
1	B	55	LYS	2.4
1	B	284	THR	2.3
1	B	50	LEU	2.3
1	B	149	TYR	2.3
1	B	53	PHE	2.3
1	B	74	GLY	2.3
1	A	307	TYR	2.3
1	B	86	ILE	2.2
1	B	288	SER	2.2
1	A	22	THR	2.2
1	A	184	SER	2.2
1	B	144	LYS	2.1
1	A	148	ASP	2.1
1	B	75	ALA	2.1
1	B	71	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	72	SER	2.0
1	B	119	SER	2.0
1	B	94	VAL	2.0

## 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 oligosaccharides 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
3	MAN	A	406	11/12	0.69	0.19	50,58,72,87	19
3	MAN	B	406	11/12	0.76	0.15	52,59,72,74	17
3	MAN	A	405	11/12	0.80	0.14	40,54,68,75	0
3	MAN	B	408	11/12	0.80	0.13	46,57,71,84	18
3	MAN	A	404	11/12	0.84	0.13	39,49,62,62	0
4	PEG	B	402	7/7	0.85	0.16	27,40,46,48	17
3	MAN	B	404	11/12	0.87	0.12	44,55,68,72	0
3	MAN	B	403	11/12	0.87	0.13	34,46,59,69	0
3	MAN	A	402	11/12	0.93	0.10	32,41,55,65	0
3	MAN	B	407	11/12	0.93	0.10	28,34,66,79	0
3	MAN	A	407	11/12	0.94	0.09	29,35,50,50	0
3	MAN	A	403	11/12	0.95	0.08	29,34,52,59	0
3	MAN	B	405	11/12	0.95	0.09	28,39,61,61	0
2	CA	B	401	1/1	0.98	0.05	32,32,32,32	1
2	CA	A	401	1/1	0.99	0.03	22,22,22,22	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.