wwPDB X-ray Structure Validation Summary Report (i)

Aug 7, 2020 – 12:06 PM BST

PDB ID	:	1PPG
Title	:	The refined 2.3 angstroms crystal structure of human leukocyte elastase in a complex with a valine chloromethyl ketone inhibitor
Authors	:	Bode, W.; Wei, A-Z.
Deposited on	:	1991-10-24
Resolution	:	2.30 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

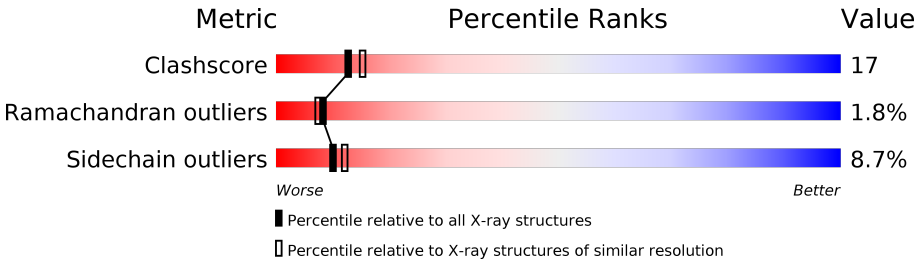
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	218	52% 33% 12% .
2	I	6	17% 83%
3	A	8	38% 63%
4	B	8	88% 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
3	NAG	A	5	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NDG	B	5	X	-	-	-
4	GLC	B	6	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2053 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.

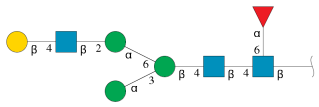
- Molecule 1 is a protein called HUMAN LEUKOCYTE ELASTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	218	Total	C	N	O	S	43	0	0
			1636	1026	316	283	11			

- Molecule 2 is a protein called MEO-SUCCINYL-ALA-ALA-PRO-VAL CHLOROMETHYLKETONE.

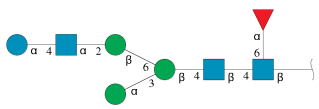
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	6	Total	C	N	O	0	0	1
			33	22	4	7			

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	8	Total	C	N	O	60	0	0
			96	54	3	39			

- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	8	Total	C	N	O	72	0	0
			96	54	3	39			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	189	Total	O	29	0
			189	189		
5	I	3	Total	O	1	0
			3	3		

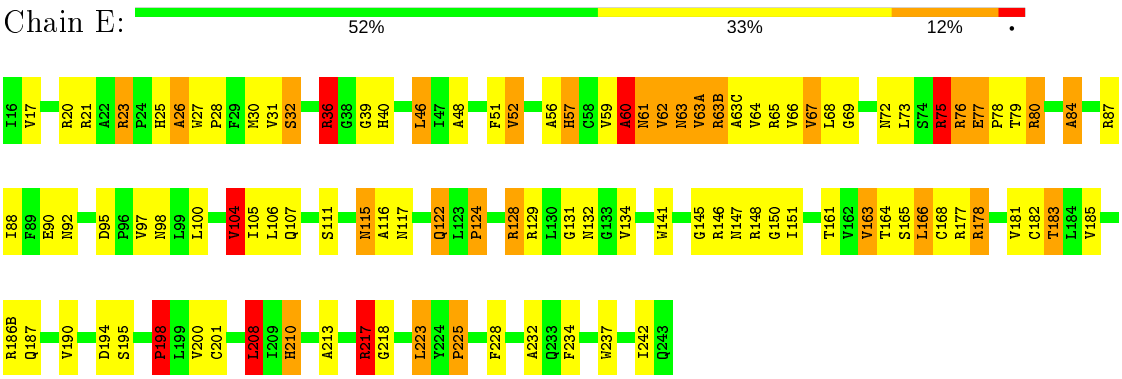
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

• Molecule 1: HUMAN LEUKOCYTE ELASTASE

Chain E:



• Molecule 2: MEO-SUCCINYL-ALA-ALA-PRO-VAL CHLOROMETHYLKETONE

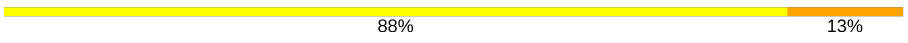
Chain I:

• Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:

• Molecule 4: alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:




NAG1
NAG2
BMA3
BMA4
NDG5
GLC6
MAN7
FUC8

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	74.20Å 74.20Å 70.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.145 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2053	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: VAI, BMA, 0QE, GLC, NDG, GAL, FUC, MAN, HMB, NAG

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	E	1.35	9/1666 (0.5%)	1.81	37/2263 (1.6%)
2	I	1.24	0/17	1.27	0/23
All	All	1.35	9/1683 (0.5%)	1.81	37/2286 (1.6%)

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	E	0	24
2	I	1	0
All	All	1	24

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	141	TRP	NE1-CE2	-7.82	1.27	1.37
1	E	237	TRP	NE1-CE2	-6.85	1.28	1.37
1	E	75	ARG	NE-CZ	6.25	1.41	1.33
1	E	76	ARG	CZ-NH1	5.95	1.40	1.33
1	E	27	TRP	NE1-CE2	-5.91	1.29	1.37

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	217	ARG	NE-CZ-NH1	11.60	126.10	120.30
1	E	23	ARG	NE-CZ-NH1	-10.33	115.14	120.30
1	E	177	ARG	NE-CZ-NH2	-9.85	115.37	120.30
1	E	217	ARG	NH1-CZ-NH2	-8.41	110.15	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	194	ASP	CB-CG-OD2	7.70	125.23	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	I	1	HMB	CG

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	26	ALA	Mainchain
1	E	28	PRO	Mainchain
1	E	46	LEU	Mainchain
1	E	52	VAL	Mainchain
1	E	60	ALA	Mainchain

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	E	1636	0	1650	54	26
2	I	33	0	33	8	0
3	A	96	0	82	0	30
4	B	96	0	81	1	0
5	E	189	0	0	3	9
5	I	3	0	0	0	0
All	All	2053	0	1846	55	34

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 17.

The worst 5 of 55 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:E:195:SER:OG	2:I:6:0QE:C1	1.78	1.28
1:E:218:GLY:H	2:I:1:HMB:HB1	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:ILE:HG22	1:E:106:LEU:HD22	1.56	0.87
1:E:195:SER:CB	2:I:6:0QE:C1	2.55	0.85
1:E:105:ILE:HG13	5:E:1239:HOH:O	1.85	0.77

The worst 5 of 34 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)
1:E:97:VAL:CB	3:A:5:NAG:C5[4_564]	0.32	1.88
1:E:97:VAL:CA	3:A:5:NAG:C6[4_564]	0.62	1.58
3:A:4:MAN:C3	5:E:1234:HOH:O[4_565]	0.74	1.46
1:E:97:VAL:CG1	3:A:5:NAG:O5[4_564]	0.86	1.34
1:E:97:VAL:CG2	3:A:5:NAG:C4[4_564]	0.89	1.31

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	E	216/218 (99%)	201 (93%)	11 (5%)	4 (2%)	8 7
2	I	3/6 (50%)	3 (100%)	0	0	100 100
All	All	219/224 (98%)	204 (93%)	11 (5%)	4 (2%)	8 7

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	36	ARG
1	E	146	ARG
1	E	213	ALA
1	E	124	PRO

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	E	172/172 (100%)	157 (91%)	15 (9%)	10 12
2	I	1/1 (100%)	1 (100%)	0	100 100
All	All	173/173 (100%)	158 (91%)	15 (9%)	10 12

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	104	VAL
1	E	115	ASN
1	E	200	VAL
1	E	92	ASN
1	E	166	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	132	ASN
1	E	210	HIS
1	E	135	GLN
1	E	115	ASN
1	E	156	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

1 non-standard protein/DNA/RNA residue is 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	VAI	I	5	1,2	6,6,7	0.75	0	4,7,9	0.50	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
2	VAI	I	5	1,2	-	1/6/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	5	VAI	O-C-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	5	VAI	1	0

5.5 Carbohydrates (i)

16 monosaccharides 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	$\#\|Z\|>2$
3	NAG	A	1	1,3	14,14,15	1.00	0	17,19,21	2.57	8 (47%)
3	NAG	A	2	3	14,14,15	0.75	0	17,19,21	1.43	2 (11%)
3	BMA	A	3	3	11,11,12	0.84	1 (9%)	15,15,17	1.85	2 (13%)
3	MAN	A	4	3	11,11,12	0.43	0	15,15,17	1.96	1 (6%)
3	NAG	A	5	3	14,14,15	0.65	0	17,19,21	1.42	1 (5%)
3	GAL	A	6	3	11,11,12	0.58	0	15,15,17	1.44	1 (6%)
3	MAN	A	7	3	11,11,12	0.56	0	15,15,17	1.70	1 (6%)
3	FUC	A	8	3	10,10,11	1.25	1 (10%)	14,14,16	1.79	4 (28%)
4	NAG	B	1	1,4	14,14,15	1.59	5 (35%)	17,19,21	2.04	5 (29%)
4	NAG	B	2	4	14,14,15	0.95	0	17,19,21	1.72	3 (17%)
4	BMA	B	3	4	11,11,12	0.80	0	15,15,17	1.93	5 (33%)
4	BMA	B	4	4	11,11,12	0.65	0	15,15,17	1.68	4 (26%)
4	NDG	B	5	4	14,14,15	0.87	1 (7%)	17,19,21	2.96	8 (47%)
4	GLC	B	6	4	11,11,12	0.67	0	15,15,17	1.93	3 (20%)
4	MAN	B	7	4	11,11,12	0.58	0	15,15,17	2.09	2 (13%)
4	FUC	B	8	4	10,10,11	1.34	1 (10%)	14,14,16	2.05	5 (35%)

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	NAG	A	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2	3	-	0/6/23/26	0/1/1/1
3	BMA	A	3	3	-	0/2/19/22	0/1/1/1
3	MAN	A	4	3	-	0/2/19/22	0/1/1/1
3	NAG	A	5	3	-	0/6/23/26	0/1/1/1
3	GAL	A	6	3	-	1/2/19/22	0/1/1/1
3	MAN	A	7	3	-	0/2/19/22	0/1/1/1
3	FUC	A	8	3	-	-	0/1/1/1
4	NAG	B	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	4/6/23/26	0/1/1/1
4	BMA	B	3	4	-	2/2/19/22	0/1/1/1
4	BMA	B	4	4	-	0/2/19/22	0/1/1/1
4	NDG	B	5	4	1/1/5/7	5/6/23/26	0/1/1/1
4	GLC	B	6	4	1/1/4/5	1/2/19/22	0/1/1/1
4	MAN	B	7	4	-	0/2/19/22	1/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUC	B	8	4	-	-	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	NAG	C3-C2	2.52	1.57	1.52
4	B	1	NAG	C4-C3	2.43	1.58	1.52
3	A	3	BMA	C1-C2	2.32	1.57	1.52
4	B	1	NAG	O3-C3	2.32	1.48	1.43
4	B	1	NAG	C8-C7	2.28	1.55	1.50

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	7	MAN	C1-O5-C5	7.11	121.82	112.19
3	A	4	MAN	C1-O5-C5	6.70	121.27	112.19
4	B	6	GLC	C1-O5-C5	6.34	120.78	112.19
4	B	5	NDG	C1-O5-C5	6.29	120.71	112.19
3	A	7	MAN	C1-O5-C5	5.95	120.26	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	6	GLC	C3
4	B	5	NDG	C3

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2	NAG	O5-C5-C6-O6
4	B	3	BMA	O5-C5-C6-O6
4	B	2	NAG	C4-C5-C6-O6
4	B	2	NAG	C8-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	7	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	8	FUC	1	0
3	A	4	MAN	0	5
3	A	3	BMA	0	1
3	A	6	GAL	0	2
3	A	5	NAG	0	20
3	A	7	MAN	0	2

5.6 Ligand geometry (i)

There are no ligands in this entry.

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.