Full wwPDB X-ray Structure Validation Report

Aug 6, 2020 – 01:29 PM BST

PDB ID	:	2VDO
Title	:	Integrin AlphaIIbBeta3 Headpiece Bound to Fibrinogen Gamma chain peptide, HHLGGAKQAGDV
Authors	:	Springer, T.A.; Zhu, J.; Xiao, T.
Deposited on	:	2007-10-10
Resolution	:	2.51 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*
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:

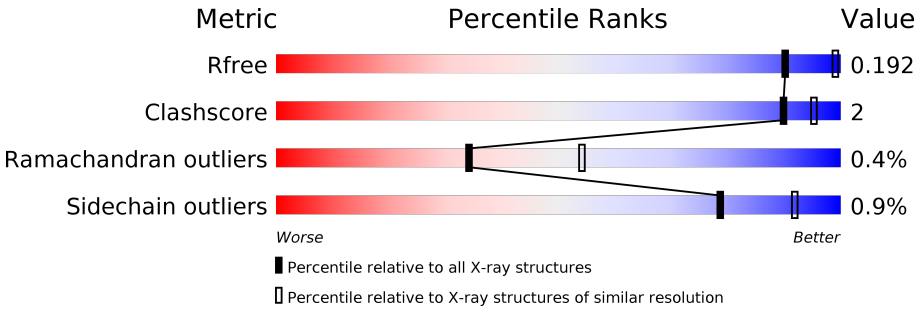
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 >=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%

Mol	Chain	Length	Quality of chain
1	A	452	96% ·
2	B	461	92% 6% ·
3	C	12	83% 17%
4	H	221	95% · ·
5	L	214	95% 5%
6	D	5	100%
7	E	7	57% 43%

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
6	MAN	D	4	X	-	-	-
6	MAN	D	5	X	-	-	-
7	MAN	E	3	X	-	-	-
7	MAN	E	5	X	-	-	-
7	MAN	E	6	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 11786 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 INTEGRIN ALPHA-IIB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	9	0
			3528	2240	615	665	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	GLY	ALA	conflict	UNP P08514

- Molecule 2 is a protein called INTEGRIN BETA-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	455	Total	C	N	O	S	0	12	0
			3577	2235	606	703	33			

- Molecule 3 is a protein called FIBRINOGEN, GAMMA POLYPEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	0	0	0
			84	50	18	16			

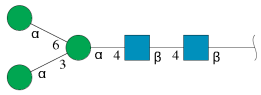
- Molecule 4 is a protein called MONOCLONAL ANTIBODY 10E5 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	219	Total	C	N	O	S	0	3	0
			1678	1064	270	338	6			

- Molecule 5 is a protein called MONOCLONAL ANTIBODY 10E5 LIGHT CHAIN.

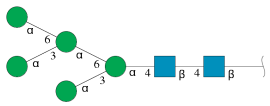
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	214	Total	C	N	O	S	0	7	0
			1671	1042	272	346	11			

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



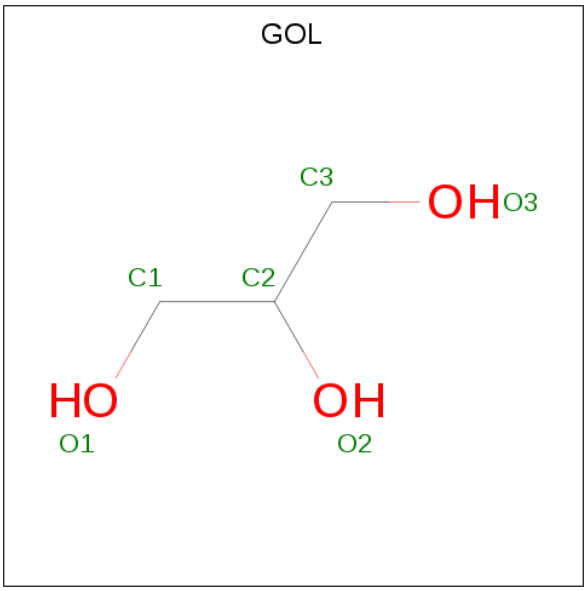
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	D	5	61	34	2	25	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	E	7	83	46	2	35	0	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

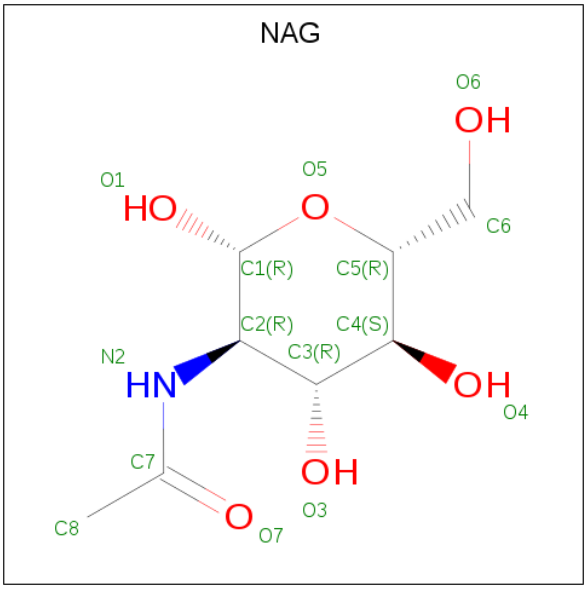


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	2	Total Ca 2 2	0	0
9	A	4	Total Ca 4 4	0	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C N O 14 8 1 5	0	0
10	A	1	Total C N O 14 8 1 5	0	0
10	B	1	Total C N O 14 8 1 5	0	0

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total Mg 1 1	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	393	Total O 393 393	0	0
12	B	208	Total O 208 208	0	0
12	C	14	Total O 14 14	0	0
12	H	205	Total O 205 205	0	0
12	L	223	Total O 223 223	0	0

3 Residue-property plots (i)

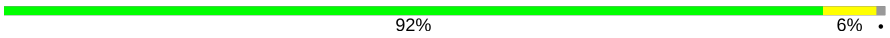
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

- Molecule 1: INTEGRIN ALPHA-IIB

Chain A:

- Molecule 2: INTEGRIN BETA-3

Chain B:

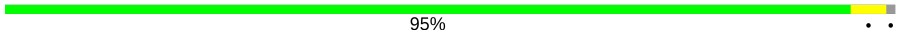


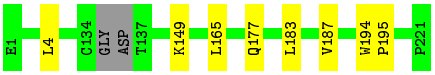
- Molecule 3: FIBRINOGEN, GAMMA POLYPEPTIDE

Chain C:

- Molecule 4: MONOCLONAL ANTIBODY 10E5 HEAVY CHAIN

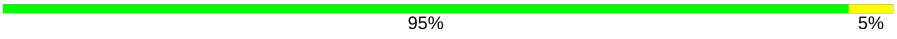
Chain H:





- Molecule 5: MONOCLONAL ANTIBODY 10E5 LIGHT CHAIN

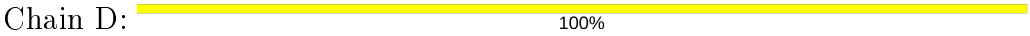
Chain L:



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

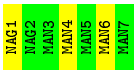
nose

Chain D:



• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	148.33Å 148.33Å 176.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.13 – 2.51 46.10 – 2.51	Depositor EDS
% Data completeness (in resolution range)	97.3 (46.13-2.51) 97.0 (46.10-2.51)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.83 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.148 , 0.190 0.152 , 0.192	Depositor DCC
R_{free} test set	3807 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	47.2	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11786	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, MG, CA, NAG, MAN

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	0.35	0/3640	0.55	0/4957
2	B	0.33	0/3661	0.49	0/4960
3	C	0.41	0/85	0.56	0/111
4	H	0.33	0/1730	0.52	0/2369
5	L	0.36	0/1733	0.55	0/2349
All	All	0.34	0/10849	0.53	0/14746

There are no bond length outliers.

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	3528	0	3374	10	0
2	B	3577	0	3512	13	0
3	C	84	0	77	0	0
4	H	1678	0	1637	9	0
5	L	1671	0	1599	12	0
6	D	61	0	52	0	0
7	E	83	0	70	0	0
8	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	6	0	7	0	0
9	A	4	0	0	0	0
9	B	2	0	0	0	0
10	A	28	0	26	0	0
10	B	14	0	13	0	0
11	B	1	0	0	0	0
12	A	393	0	0	0	0
12	B	208	0	0	0	0
12	C	14	0	0	0	0
12	H	205	0	0	0	0
12	L	223	0	0	1	0
All	All	11786	0	10375	39	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 2.

All (39) 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)
4:H:177[B]:GLN:OE1	5:L:160[B]:LEU:HD11	1.09	1.23
4:H:177[B]:GLN:OE1	5:L:160[B]:LEU:CD1	1.97	1.12
2:B:88[B]:ILE:HD11	2:B:427:VAL:HG22	1.78	0.66
1:A:235:TRP:CZ2	1:A:270:LEU:HD11	2.33	0.64
4:H:177[B]:GLN:CD	5:L:160[B]:LEU:HD21	2.21	0.60
5:L:136:LEU:HD12	5:L:136:LEU:N	2.21	0.54
4:H:177[B]:GLN:OE1	5:L:160[B]:LEU:CG	2.55	0.54
2:B:230:THR:HG23	2:B:304:ILE:HD12	1.89	0.53
2:B:308:PHE:CE2	2:B:328:THR:HG21	2.44	0.53
5:L:48:ILE:HD13	5:L:54:LEU:HD12	1.91	0.53
1:A:235:TRP:HZ2	1:A:270:LEU:HD11	1.72	0.53
2:B:399:ILE:N	2:B:399:ILE:HD12	2.25	0.52
5:L:48:ILE:CD1	5:L:54:LEU:HD12	2.40	0.51
5:L:105[B]:GLU:HG3	5:L:173:TYR:OH	2.11	0.51
1:A:394:GLY:HA2	1:A:399:LEU:HD23	1.92	0.50
2:B:245:LEU:HD23	2:B:305:ASN:HB2	1.92	0.50
4:H:165:LEU:CD2	4:H:187:VAL:HG21	2.41	0.49
1:A:270:LEU:HD23	1:A:276[A]:ARG:HA	1.95	0.49
1:A:122:ALA:O	1:A:123:GLU:HB2	2.12	0.48
5:L:122:SER:O	5:L:126:THR:HG23	2.13	0.48
1:A:270:LEU:HD23	1:A:276[B]:ARG:HA	1.95	0.48
2:B:90:LEU:HD11	2:B:100:PHE:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:165:LEU:HD21	4:H:187:VAL:HG21	1.97	0.46
5:L:45:MET:HE3	12:L:4065:HOH:O	2.15	0.45
2:B:366:LEU:HD11	2:B:429:VAL:HG21	1.99	0.45
2:B:223:PHE:CZ	2:B:254:THR:HG21	2.53	0.43
1:A:122:ALA:O	1:A:123:GLU:CB	2.67	0.42
1:A:388:GLN:NE2	1:A:406:VAL:HG11	2.34	0.42
2:B:72:LYS:NZ	2:B:109:ASP:OD1	2.52	0.42
1:A:427:ILE:HG22	1:A:434:ASP:OD1	2.20	0.42
4:H:177[B]:GLN:NE2	5:L:160[B]:LEU:HD21	2.34	0.42
2:B:15:GLN:O	2:B:19:VAL:HG23	2.20	0.41
2:B:176:PRO:HB2	2:B:214:ARG:HB3	2.03	0.41
4:H:4:LEU:N	4:H:4:LEU:HD12	2.35	0.41
2:B:88[B]:ILE:CD1	2:B:427:VAL:HG22	2.49	0.41
4:H:194:TRP:CG	4:H:195:PRO:HA	2.55	0.41
2:B:362:LEU:HD12	2:B:363:PRO:HD2	2.03	0.40
5:L:4:MET:HE2	5:L:90:GLN:HB3	2.03	0.40
1:A:297:ASP:O	1:A:372:ASN:HB2	2.22	0.40

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	458/452 (101%)	446 (97%)	11 (2%)	1 (0%)	47 68
2	B	460/461 (100%)	438 (95%)	19 (4%)	3 (1%)	22 39
3	C	10/12 (83%)	6 (60%)	3 (30%)	1 (10%)	0 0
4	H	218/221 (99%)	214 (98%)	4 (2%)	0	100 100
5	L	220/214 (103%)	215 (98%)	5 (2%)	0	100 100
All	All	1366/1360 (100%)	1319 (97%)	42 (3%)	5 (0%)	34 54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	9[A]	GLY
2	B	80	VAL
3	C	402	LEU
2	B	10	VAL

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	368/360 (102%)	364 (99%)	4 (1%)	73 89
2	B	414/409 (101%)	410 (99%)	4 (1%)	76 90
3	C	7/7 (100%)	6 (86%)	1 (14%)	3 6
4	H	192/190 (101%)	190 (99%)	2 (1%)	76 90
5	L	196/188 (104%)	196 (100%)	0	100 100
All	All	1177/1154 (102%)	1166 (99%)	11 (1%)	78 92

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	166	TYR
1	A	190	TYR
1	A	288	TYR
2	B	215	ASN
2	B	387[A]	MET
2	B	387[B]	MET
2	B	396	SER
3	C	401	HIS
4	H	149	LYS
4	H	183	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	388	GLN
2	B	316	ASN
2	B	342	GLN
2	B	428	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

12 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	$\#\|Z\| > 2$
6	NAG	D	1	2,6	14,14,15	0.60	0	17,19,21	0.83	1 (5%)
6	NAG	D	2	6	14,14,15	0.70	0	17,19,21	0.98	1 (5%)
6	MAN	D	3	6	11,11,12	0.72	0	15,15,17	2.22	4 (26%)
6	MAN	D	4	6	11,11,12	0.69	0	15,15,17	0.80	1 (6%)
6	MAN	D	5	6	11,11,12	0.62	0	15,15,17	0.92	1 (6%)
7	NAG	E	1	2,7	14,14,15	0.66	0	17,19,21	0.87	1 (5%)
7	NAG	E	2	7	14,14,15	0.53	0	17,19,21	0.82	0
7	MAN	E	3	7	11,11,12	0.64	0	15,15,17	0.82	0
7	MAN	E	4	7	11,11,12	0.60	0	15,15,17	1.87	4 (26%)
7	MAN	E	5	7	11,11,12	0.58	0	15,15,17	0.90	0
7	MAN	E	6	7	11,11,12	0.71	0	15,15,17	1.35	3 (20%)
7	MAN	E	7	7	11,11,12	0.64	0	15,15,17	0.70	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
6	NAG	D	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	D	2	6	-	1/6/23/26	0/1/1/1
6	MAN	D	3	6	-	2/2/19/22	0/1/1/1
6	MAN	D	4	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	D	5	6	1/1/4/5	2/2/19/22	0/1/1/1
7	NAG	E	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	E	2	7	-	2/6/23/26	0/1/1/1
7	MAN	E	3	7	1/1/4/5	0/2/19/22	0/1/1/1
7	MAN	E	4	7	-	1/2/19/22	0/1/1/1
7	MAN	E	5	7	1/1/4/5	0/2/19/22	0/1/1/1
7	MAN	E	6	7	1/1/4/5	2/2/19/22	0/1/1/1
7	MAN	E	7	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	E	4	MAN	O3-C3-C2	5.14	119.83	109.99
6	D	3	MAN	O5-C5-C6	4.56	114.35	107.20
6	D	3	MAN	C1-C2-C3	4.50	115.20	109.67
6	D	3	MAN	C1-O5-C5	4.09	117.73	112.19
7	E	6	MAN	C3-C4-C5	2.86	115.34	110.24
7	E	6	MAN	O5-C1-C2	-2.79	106.46	110.77
7	E	4	MAN	C1-O5-C5	2.56	115.66	112.19
7	E	4	MAN	O5-C5-C6	2.42	111.00	107.20
6	D	3	MAN	C2-C3-C4	2.35	114.95	110.89
6	D	4	MAN	O5-C1-C2	-2.28	107.25	110.77
7	E	6	MAN	C1-C2-C3	-2.27	106.88	109.67
6	D	2	NAG	C4-C3-C2	2.26	114.33	111.02
7	E	4	MAN	C2-C3-C4	-2.24	107.02	110.89
6	D	5	MAN	O5-C1-C2	-2.24	107.32	110.77
7	E	1	NAG	O5-C1-C2	-2.10	107.97	111.29
6	D	1	NAG	O5-C1-C2	-2.03	108.08	111.29

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	E	6	MAN	C1

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Mol	Chain	Res	Type	Atom
7	E	5	MAN	C1
6	D	4	MAN	C1
7	E	3	MAN	C1
6	D	5	MAN	C1

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	3	MAN	C4-C5-C6-O6
6	D	3	MAN	O5-C5-C6-O6
6	D	5	MAN	O5-C5-C6-O6
7	E	6	MAN	C4-C5-C6-O6
6	D	5	MAN	C4-C5-C6-O6
7	E	6	MAN	O5-C5-C6-O6
7	E	2	NAG	O5-C5-C6-O6
7	E	2	NAG	C4-C5-C6-O6
7	E	4	MAN	C4-C5-C6-O6
6	D	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
10	NAG	A	3015	-	14,14,15	0.47	0	17,19,21	0.68	0
10	NAG	A	3249	-	14,14,15	0.50	0	17,19,21	0.70	0
8	GOL	B	1462	9	5,5,5	0.40	0	5,5,5	0.27	0
10	NAG	B	3099	2	14,14,15	0.43	0	17,19,21	1.05	1 (5%)
8	GOL	A	1453	-	5,5,5	0.47	0	5,5,5	0.10	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
10	NAG	A	3015	-	-	0/6/23/26	0/1/1/1
10	NAG	A	3249	-	-	0/6/23/26	0/1/1/1
8	GOL	B	1462	9	-	0/4/4/4	-
10	NAG	B	3099	2	-	2/6/23/26	0/1/1/1
8	GOL	A	1453	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	3099	NAG	O5-C1-C2	-2.64	107.11	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	3099	NAG	O5-C5-C6-O6
10	B	3099	NAG	C4-C5-C6-O6
8	A	1453	GOL	O1-C1-C2-C3
8	A	1453	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.