



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:57 PM BST

PDB ID : 4CAK
EMDB ID: : EMD-2281
Title : Three-dimensional reconstruction of intact human integrin α IIb β 3 in a phospholipid bilayer nanodisc
Authors : Choi, W.S.; Rice, W.J.; Stokes, D.L.; Collier, B.S.
Deposited on : 2013-10-08
Resolution : 20.50 Å (reported)
Based on PDB ID : 3FCS

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

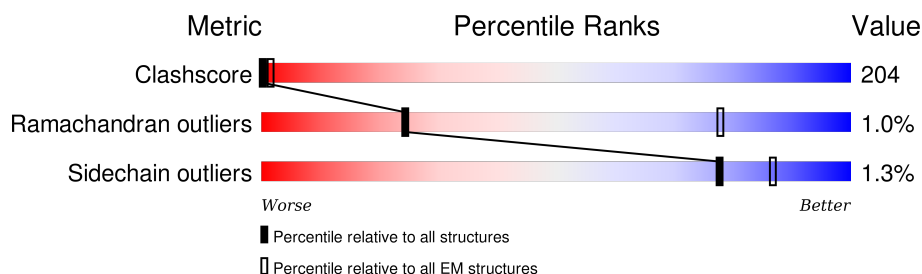
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 20.50 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	959	
2	B	690	

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	3015	X	-	-	-
3	NAG	A	3570	-	-	X	-
4	NAG	B	3452	-	-	X	-
4	NAG	B	3453	-	-	X	-
5	NAG	B	3320	-	-	X	-
5	NAG	B	3321	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BMA	B	3322	-	-	X	-
5	MAN	B	3323	-	-	X	-
6	NAG	B	3371	-	-	X	-
7	NAG	B	3560	-	-	X	-
7	MAN	B	3562	-	-	X	-
7	MAN	B	3563	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15960 atoms, of which 3296 are hydrogens and 0 are deuteriums.

In the tables below, 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						AltConf	Trace
1	A	913	Total	C	H	N	O	S	14	3
			10364	4466	3296	1236	1336	30		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	959	CYS	LEU	CONFLICT	UNP P08514

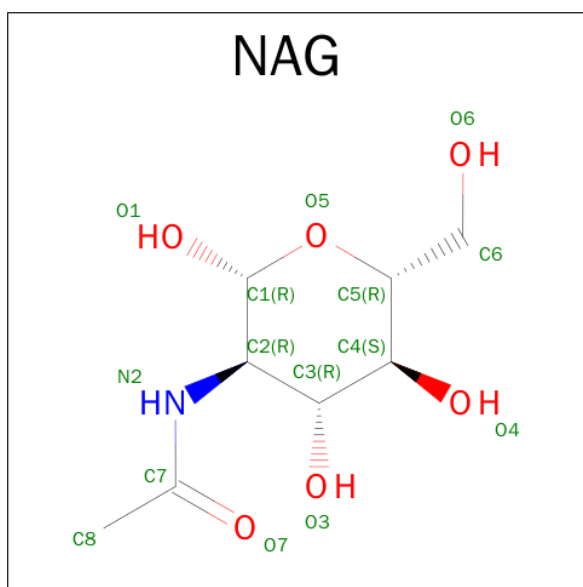
- Molecule 2 is a protein called INTEGRIN BETA-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	680	Total	C	N	O	S	19	0
			5362	3294	913	1083	72		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	688	CYS	PRO	CONFLICT	UNP P05106

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			28	16	2	10	
3	A	1	Total	C	N	O	0
			28	16	2	10	

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				AltConf
4	B	2	Total	C	N	O	0
			56	32	4	20	
4	B	2	Total	C	N	O	0
			56	32	4	20	

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				AltConf
5	B	4	Total	C	N	O	0
			50	28	2	20	

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				AltConf
6	B	3	Total	C	N	O	0
			39	22	2	15	

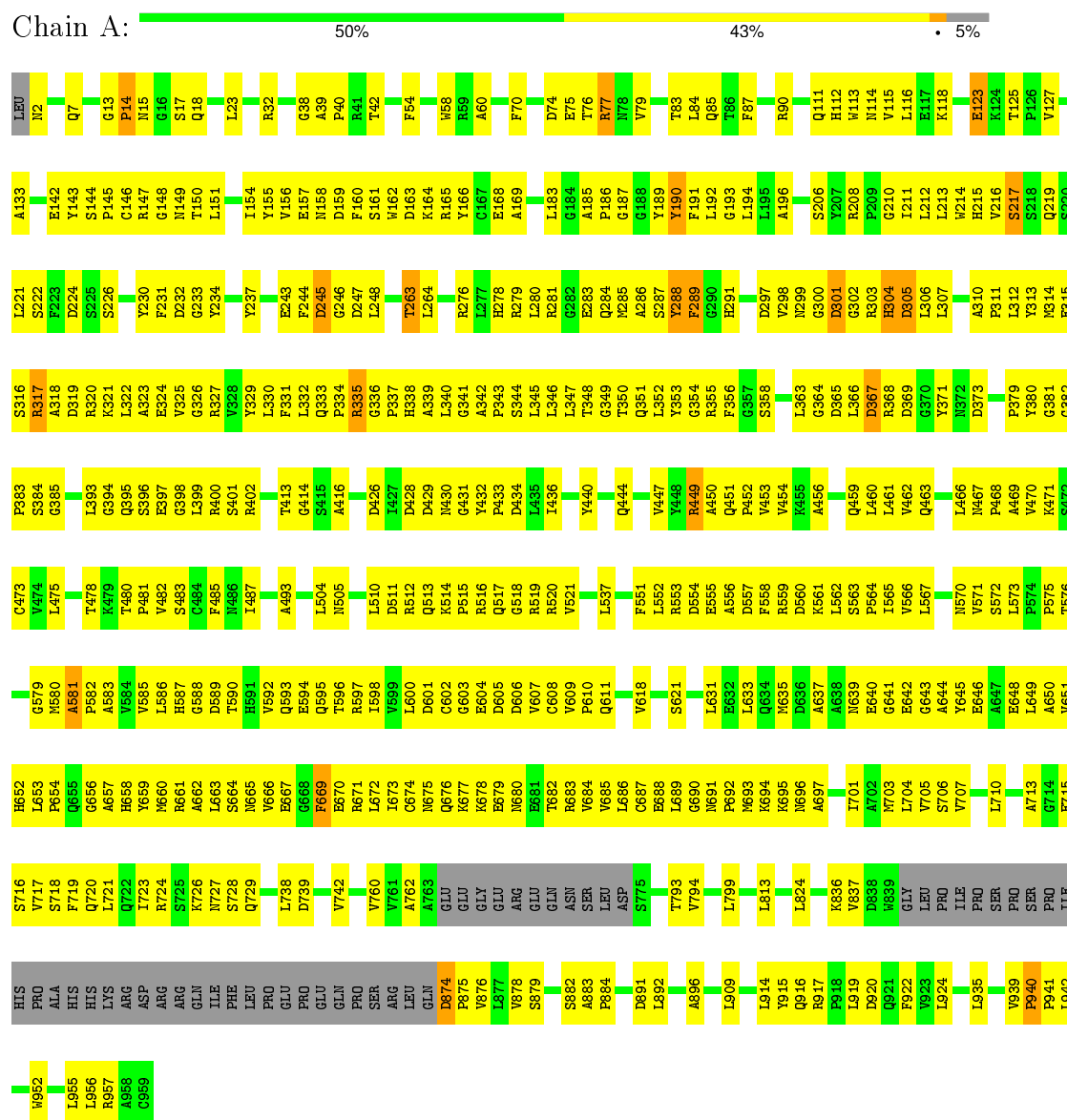
- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				AltConf
7	B	5	Total	C	N	O	0
			61	34	2	25	

3 Residue-property plots

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



• Molecule 2: INTEGRIN BETA-3



G1	V104	R204	Q272	I416	Q483	R600
I7	R105	E205	C273	K417	D484	C608
R8	R206	V207	H274	P418	E485	T609
S12	D109	Q210	N279	V419	C486	K618
C13	P111	R215	H280	Q420	S487	L625
Q14	V112	D216	E281	F421	P488	H626
C16	D113	D217	S282	K422		D627
	L117	A218	S284	D423	C501	B628
R22	L120	P219	T285	K430	L502	B629
C23	E220	P220	D288	F431	C503	T630
A24	G221	G221	Y289	D432	G504	
M25	D127	G222	S289	C433	Q505	
C26	F223	D224	A283	D434	C506	
S27	S130	A225	S284		V507	
D28	I131	L226	T285	C437	C508	
E29	M142	M227	D288	Q438	H509	
A30	R143	Q228	Y289	A439	S510	
L31	K144	A229	P290	Q440	K515	
P32	L145	T230	F299	A441	I516	
L33	L146	V231	S291	E442	T517	
G34	T146	C232	S292	P443	G518	
S35	S147	L299	L292	M444	K519	
P36	M148	D233	G293	S445	Y520	
R37	L149	E234	L294	R446	C521	
	A155	K235	M295	R447	E522	
K41	D158	L236	E358	C448	V529	
L44	P159	G237	E359	M449	R530	
R46	P160	M238	R360	Q450	Y531	
D47	V161	R239	R361	L451	K532	
M48	S162	E244	L362	G453	C536	
C49	P163	L246	L363	T454	C663	
A50	Y164	V247	L364	F455	C664	
P51	M165	F248	S369	E456	H539	
E52	Y166	T249	F370	C457	Y556	
S53	I167	D251	N371	V459	Y557	
I54	P169	A252		C460	C558	
E55	S168	K253		R461	N559	
P56	P170	T254		C462	C560	
L69	E171	H255		Q463	T561	
	A172	L256		P464	T562	
G73	L173	A257		Q465	R563	
S74	E174	Y321		W466	M568	
GLY	C184	S322		L467	L574	
ASP	L185	D259		Q470	L574	
SER	P186	G260		C471	G579	
SER	M187	P261		E472	C583	
Q79	F188	L262		C473	C588	
V80	G189	T266		S474	I589	
R93	K190	V267		E475	Q590	
P94	K191	Q267		B476	P591	
D95	H192	P268		ASP	G592	
D96	V193	M269		TVR	S593	
S97	F203	G271		ARG	Y594	
				PRO		
				GLN		

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	13	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	29000	Depositor
Image detector	TIETZ 4KX4K	Depositor

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: BMA, 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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.65	1/7233 (0.0%)	1.09	16/9839 (0.2%)
2	B	0.45	2/5447 (0.0%)	0.63	6/7341 (0.1%)
All	All	0.57	3/12680 (0.0%)	0.92	22/17180 (0.1%)

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
2	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	PRO	C-N	27.97	1.98	1.34
2	B	562[A]	THR	C-N	-20.14	0.87	1.34
2	B	562[B]	THR	C-N	-20.14	0.87	1.34

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	PRO	CA-C-N	-50.09	7.00	117.20
1	A	14	PRO	C-N-CA	-39.38	23.26	121.70
2	B	562[A]	THR	O-C-N	-24.32	83.80	122.70
2	B	562[B]	THR	O-C-N	-24.32	83.80	122.70
2	B	562[A]	THR	C-N-CA	-11.36	93.29	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	562[A]	THR	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	A	7068	3296	6699	3511	0
2	B	5362	0	4912	3094	0
3	A	28	0	23	38	0
4	B	56	0	42	75	0
5	B	50	0	40	75	0
6	B	39	0	31	17	0
7	B	61	0	44	45	0
All	All	12664	3296	11791	4980	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 204.

The worst 5 of 4980 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)
2:B:254:THR:HG21	2:B:308:PHE:CD1	1.25	1.68
1:A:351:GLN:HE21	2:B:230:THR:CG2	1.05	1.67
1:A:592:VAL:CG2	1:A:727:ASN:HA	1.17	1.65
1:A:331:PHE:CE2	1:A:661:ARG:HG3	1.17	1.65
1:A:156:VAL:CG1	1:A:190:TYR:CD1	1.77	1.65

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 PDB entries followed by that with respect to all EM entries.

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	901/959 (94%)	818 (91%)	71 (8%)	12 (1%)	15	60
2	B	669/690 (97%)	610 (91%)	55 (8%)	4 (1%)	30	74
All	All	1570/1649 (95%)	1428 (91%)	126 (8%)	16 (1%)	24	65

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	837	VAL
1	A	940	PRO
1	A	190	TYR
1	A	263	THR
1	A	581	ALA

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 PDB entries followed by that with respect to all EM entries.

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	767/799 (96%)	755 (98%)	12 (2%)	70	88
2	B	620/612 (101%)	614 (99%)	6 (1%)	82	92
All	All	1387/1411 (98%)	1369 (99%)	18 (1%)	78	89

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	444	GLN
1	A	597	ARG
2	B	423	ASP
1	A	304	HIS
1	A	367	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	517	GLN
1	A	676	GLN
2	B	303	ASN
1	A	451	GLN
2	B	408	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 ⓘ

16 carbohydrates 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	NAG	B	3099	2,4	14,14,15	0.59	0	15,19,21	1.10	1 (6%)
4	NAG	B	3100	4	14,14,15	0.57	0	15,19,21	0.89	1 (6%)
5	NAG	B	3320	2,5	14,14,15	0.48	0	15,19,21	0.65	0
5	NAG	B	3321	5	14,14,15	0.53	0	15,19,21	0.55	0
5	BMA	B	3322	5	11,11,12	0.59	0	15,15,17	0.66	0
5	MAN	B	3323	5	11,11,12	0.49	0	15,15,17	2.45	3 (20%)
6	NAG	B	3371	2,6	14,14,15	0.62	0	15,19,21	0.61	0
6	NAG	B	3372	6	14,14,15	0.49	0	15,19,21	0.70	0
6	BMA	B	3373	6	11,11,12	0.62	0	15,15,17	0.58	0
4	NAG	B	3452	2,4	14,14,15	0.64	0	15,19,21	0.85	1 (6%)
4	NAG	B	3453	4	14,14,15	0.51	0	15,19,21	0.59	0
7	NAG	B	3559	2,7	14,14,15	0.60	0	15,19,21	0.77	0
7	NAG	B	3560	7	14,14,15	0.46	0	15,19,21	0.97	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BMA	B	3561	7	11,11,12	0.55	0	15,15,17	0.85	0
7	MAN	B	3562	7	11,11,12	0.55	0	15,15,17	0.68	0
7	MAN	B	3563	7	11,11,12	0.60	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
4	NAG	B	3099	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	3100	4	-	0/6/23/26	0/1/1/1
5	NAG	B	3320	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	3321	5	-	0/6/23/26	0/1/1/1
5	BMA	B	3322	5	-	0/2/19/22	0/1/1/1
5	MAN	B	3323	5	-	0/2/19/22	0/1/1/1
6	NAG	B	3371	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	3372	6	-	0/6/23/26	0/1/1/1
6	BMA	B	3373	6	-	0/2/19/22	0/1/1/1
4	NAG	B	3452	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	3453	4	-	0/6/23/26	0/1/1/1
7	NAG	B	3559	2,7	-	0/6/23/26	0/1/1/1
7	NAG	B	3560	7	-	0/6/23/26	0/1/1/1
7	BMA	B	3561	7	-	0/2/19/22	0/1/1/1
7	MAN	B	3562	7	-	0/2/19/22	0/1/1/1
7	MAN	B	3563	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3452	NAG	O5-C5-C4	-2.27	106.37	110.13
7	B	3560	NAG	C4-C3-C2	-2.05	108.16	111.34
4	B	3100	NAG	C4-C3-C2	2.02	114.47	111.34
4	B	3099	NAG	C4-C3-C2	3.07	116.11	111.34
5	B	3323	MAN	O5-C1-C2	3.93	117.17	110.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 211 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	3099	NAG	1	0
5	B	3320	NAG	42	0
5	B	3321	NAG	11	0
5	B	3322	BMA	10	0
5	B	3323	MAN	12	0
6	B	3371	NAG	15	0
6	B	3372	NAG	2	0
4	B	3452	NAG	37	0
4	B	3453	NAG	37	0
7	B	3559	NAG	3	0
7	B	3560	NAG	9	0
7	B	3561	BMA	5	0
7	B	3562	MAN	23	0
7	B	3563	MAN	6	0

5.6 Ligand geometry ⓘ

2 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	$\# Z > 2$
3	NAG	A	3015	1	14,14,15	0.47	0	15,19,21	0.56	0
3	NAG	A	3570	1	14,14,15	0.64	0	15,19,21	1.45	1 (6%)

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	3015	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	3570	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	3570	NAG	C1-O5-C5	5.03	119.53	112.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	3015	NAG	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3570	NAG	38	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.