



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2024 – 02:31 PM EST

PDB ID : 2VDQ
Title : Integrin AlphaIIbBeta3 Headpiece Bound to a Chimeric Fibrinogen Gamma chain peptide, HHLGGAKQRGDV
Authors : Springer, T.A.; Zhu, J.; Xiao, T.
Deposited on : 2007-10-10
Resolution : 2.59 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

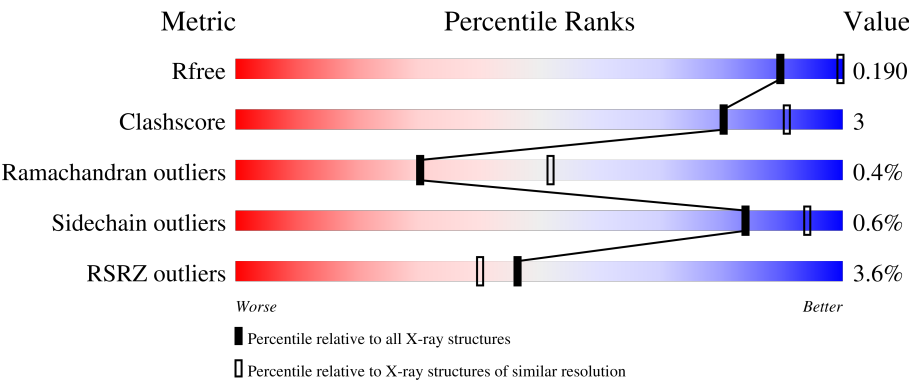
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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 ≥ 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	452	96% .
2	B	461	8% 91% 8% .
3	C	12	25% 58% 42%
4	H	221	2% 95% . .
5	L	214	93% 7%
6	D	5	60% 40%

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Mol	Chain	Length	Quality of chain
7	E	7	

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	3	X	-	-	-
7	MAN	E	3	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 12052 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	12	0
			3539	2250	616	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	9	0
			3571	2231	606	701	33			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	7	Total	C	N	O	0	0	0
			54	31	12	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	408	ARG	ALA	engineered mutation	UNP Q53Y18

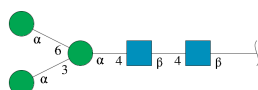
- Molecule 4 is a protein called MONOCLONAL ANTIBODY 10E5 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	219	Total	C	N	O	S	0	4	0
			1672	1060	269	337	6			

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

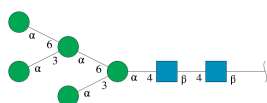
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	214	Total	C	N	O	S	0	8	0
			1679	1047	275	346	11			

- 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
6	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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
7	E	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

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

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	455	Total	O	0	0
			455	455		
12	B	335	Total	O	0	0
			335	335		
12	C	14	Total	O	0	0
			14	14		
12	H	247	Total	O	0	0
			247	247		
12	L	281	Total	O	0	0
			281	281		

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.

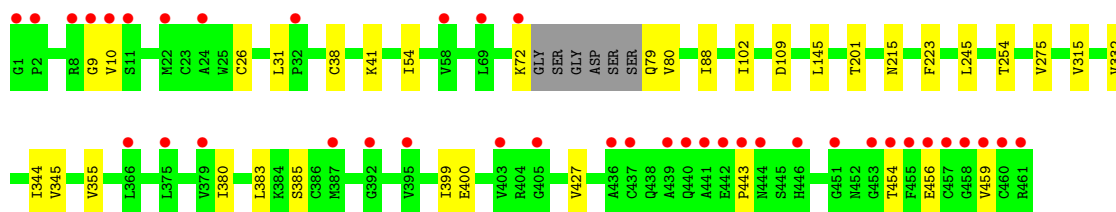
- Molecule 1: INTEGRIN ALPHA-IIB

Chain A:  96%



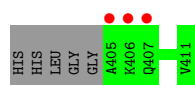
- Molecule 2: INTEGRIN BETA-3

Chain B:  8% 91% 8%



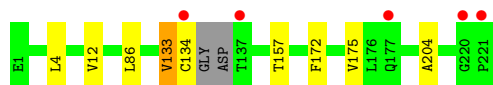
- Molecule 3: FIBRINOGEN, GAMMA POLYPEPTIDE

Chain C:  25% 58% 42%



- Molecule 4: MONOCLONAL ANTIBODY 10E5 HEAVY CHAIN

Chain H:  2% 95%



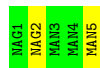
- Molecule 5: MONOCLONAL ANTIBODY 10E5 LIGHT CHAIN

Chain L:  93% 7%



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

Chain D:  60% 40%



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

Chain E:  43% 43% 14%



4 Data and refinement statistics

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)	34.63 – 2.59 34.63 – 2.59	Depositor EDS
% Data completeness (in resolution range)	92.2 (34.63-2.59) 90.7 (34.63-2.59)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.141 , 0.190 0.147 , 0.190	Depositor DCC
R_{free} test set	3207 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12052	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, MAN, GOL, CA, 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	A	0.35	0/3656	0.55	0/4980
2	B	0.33	0/3652	0.50	0/4948
3	C	0.41	0/53	0.72	0/67
4	H	0.35	0/1721	0.53	0/2357
5	L	0.37	0/1744	0.55	0/2363
All	All	0.35	0/10826	0.53	0/14715

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 [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	3539	0	3367	12	0
2	B	3571	0	3517	21	0
3	C	54	0	54	0	0
4	H	1672	0	1621	11	0
5	L	1679	0	1612	15	0
6	D	61	0	52	0	0
7	E	83	0	70	1	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	8	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	455	0	0	1	0
12	B	335	0	0	2	0
12	C	14	0	0	0	0
12	H	247	0	0	0	0
12	L	281	0	0	0	0
All	All	12052	0	10348	53	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 3.

All (53) 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:133:VAL:HG12	4:H:134:CYS:H	1.51	0.76
5:L:136:LEU:HD21	5:L:146:VAL:HG22	1.78	0.65
5:L:160[B]:LEU:HD12	5:L:161:ASN:N	2.12	0.64
2:B:88[B]:ILE:HD11	2:B:427:VAL:HG22	1.80	0.63
2:B:79:GLN:N	12:B:4037:HOH:O	2.33	0.60
1:A:270:LEU:HD23	1:A:276[A]:ARG:HA	1.85	0.59
1:A:270:LEU:HD23	1:A:276[B]:ARG:HA	1.86	0.58
2:B:443:PRO:HA	2:B:454:THR:HG22	1.86	0.56
5:L:48:ILE:HD13	5:L:54:LEU:HD12	1.88	0.55
1:A:421:LEU:CD2	1:A:437:VAL:HG22	2.37	0.54
4:H:175:VAL:HG11	5:L:160[B]:LEU:CD1	2.38	0.53
5:L:136:LEU:HD12	5:L:136:LEU:N	2.22	0.53
1:A:280:LEU:HD11	1:A:306:LEU:HD23	1.89	0.53
2:B:145:LEU:HD22	2:B:345:VAL:HG22	1.90	0.53
4:H:175:VAL:HG11	5:L:160[B]:LEU:HD11	1.90	0.53
1:A:235:TRP:CZ2	1:A:270:LEU:HD11	2.46	0.51
4:H:175:VAL:CB	5:L:160[B]:LEU:HD11	2.40	0.51
5:L:105[A]:GLU:HG3	5:L:173:TYR:OH	2.11	0.51
1:A:280:LEU:CD1	1:A:306:LEU:HD23	2.41	0.50
2:B:456:GLU:O	2:B:459:VAL:HG12	2.13	0.48
2:B:245:LEU:CD1	2:B:344:ILE:HG23	2.44	0.48
2:B:315:VAL:HG21	2:B:332:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:LYS:NZ	2:B:109:ASP:OD1	2.46	0.48
1:A:90[A]:ARG:CZ	12:A:4131:HOH:O	2.62	0.47
2:B:10:VAL:HG23	2:B:10:VAL:O	2.15	0.46
1:A:122:ALA:O	1:A:123:GLU:HB2	2.16	0.45
4:H:172:PHE:CD1	5:L:164:THR:HG23	2.51	0.45
4:H:157:THR:OG1	4:H:204:ALA:HB3	2.17	0.45
2:B:10:VAL:HG11	2:B:38:CYS:SG	2.57	0.44
4:H:175:VAL:CG1	5:L:160[B]:LEU:HD11	2.47	0.44
1:A:390:LEU:HD12	1:A:390:LEU:N	2.33	0.44
2:B:201[A]:THR:HG23	12:B:4129:HOH:O	2.18	0.44
2:B:223:PHE:CZ	2:B:254:THR:HG21	2.53	0.44
4:H:175:VAL:HB	5:L:160[B]:LEU:HD11	1.99	0.44
2:B:245:LEU:HD13	2:B:344:ILE:HD12	2.00	0.43
5:L:122:SER:O	5:L:126:THR:HG23	2.19	0.43
5:L:195:GLU:HG2	5:L:206:VAL:HG22	2.00	0.43
5:L:150:ILE:HD12	5:L:155[A]:ARG:HD3	1.99	0.42
1:A:235:TRP:HZ2	1:A:270:LEU:HD11	1.84	0.42
2:B:399:ILE:N	2:B:399:ILE:HD12	2.34	0.42
2:B:88[B]:ILE:CG1	2:B:427:VAL:HG22	2.49	0.42
2:B:26:CYS:SG	2:B:31:LEU:HD22	2.59	0.42
4:H:133:VAL:HG12	4:H:134:CYS:N	2.28	0.42
2:B:355:VAL:O	2:B:385:SER:HA	2.20	0.42
2:B:88[B]:ILE:CD1	2:B:427:VAL:HG22	2.47	0.42
2:B:41:LYS:HG3	2:B:54:ILE:HG21	2.02	0.41
5:L:105[A]:GLU:HG3	5:L:173:TYR:HH	1.85	0.41
1:A:280:LEU:CD1	1:A:306:LEU:CD2	2.99	0.41
2:B:400:GLU:HB2	7:E:1:NAG:H83	2.02	0.41
4:H:12:VAL:HG21	4:H:86:LEU:HD13	2.02	0.40
1:A:345:LEU:HD21	1:A:347:LEU:HD21	2.04	0.40
2:B:380:ILE:HG21	2:B:383:LEU:HD22	2.03	0.40
4:H:4:LEU:HD12	4:H:4:LEU:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	459/452 (102%)	447 (97%)	11 (2%)	1 (0%)	44	66
2	B	459/461 (100%)	438 (95%)	18 (4%)	3 (1%)	19	38
3	C	5/12 (42%)	5 (100%)	0	0	100	100
4	H	217/221 (98%)	212 (98%)	4 (2%)	1 (0%)	25	47
5	L	221/214 (103%)	216 (98%)	5 (2%)	0	100	100
All	All	1361/1360 (100%)	1318 (97%)	38 (3%)	5 (0%)	30	52

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	9	GLY
4	H	133	VAL
2	B	80	VAL
2	B	275	VAL

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	A	369/360 (102%)	364 (99%)	5 (1%)	62	82
2	B	413/409 (101%)	411 (100%)	2 (0%)	86	95
3	C	5/8 (62%)	5 (100%)	0	100	100
4	H	191/190 (100%)	191 (100%)	0	100	100
5	L	197/188 (105%)	197 (100%)	0	100	100
All	All	1175/1155 (102%)	1168 (99%)	7 (1%)	84	94

All (7) 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
1	A	319	ASP
2	B	102	ILE
2	B	215	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	316	ASN
2	B	428	GLN
2	B	438	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	0.56	0	17,19,21	0.85	0
6	NAG	D	2	6	14,14,15	0.73	0	17,19,21	1.12	2 (11%)
6	MAN	D	3	6	11,11,12	0.59	0	15,15,17	0.70	0
6	MAN	D	4	6	11,11,12	0.53	0	15,15,17	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	D	5	6	11,11,12	0.67	0	15,15,17	1.27	2 (13%)
7	NAG	E	1	2,7	14,14,15	0.70	0	17,19,21	0.92	1 (5%)
7	NAG	E	2	7	14,14,15	0.53	0	17,19,21	0.94	0
7	MAN	E	3	7	11,11,12	0.55	0	15,15,17	0.76	0
7	MAN	E	4	7	11,11,12	0.54	0	15,15,17	1.21	1 (6%)
7	MAN	E	5	7	11,11,12	0.52	0	15,15,17	0.91	1 (6%)
7	MAN	E	6	7	11,11,12	0.56	0	15,15,17	0.84	1 (6%)
7	MAN	E	7	7	11,11,12	0.58	0	15,15,17	0.74	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	-	0/6/23/26	0/1/1/1
6	MAN	D	3	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	D	4	6	-	0/2/19/22	0/1/1/1
6	MAN	D	5	6	-	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	-	0/2/19/22	0/1/1/1
7	MAN	E	5	7	-	0/2/19/22	0/1/1/1
7	MAN	E	6	7	-	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 (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	4	MAN	C1-O5-C5	3.95	117.48	112.19
6	D	5	MAN	C1-C2-C3	3.50	114.73	109.64
7	E	5	MAN	C1-O5-C5	2.68	115.78	112.19
6	D	2	NAG	C4-C3-C2	2.49	114.67	111.02
6	D	5	MAN	C1-O5-C5	2.27	115.23	112.19
7	E	1	NAG	O5-C1-C2	-2.24	107.82	111.29
7	E	6	MAN	C1-O5-C5	2.20	115.13	112.19
6	D	2	NAG	C1-C2-N2	-2.09	107.13	110.43

All (2) chirality outliers are listed below:

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

All (6) torsion outliers are listed below:

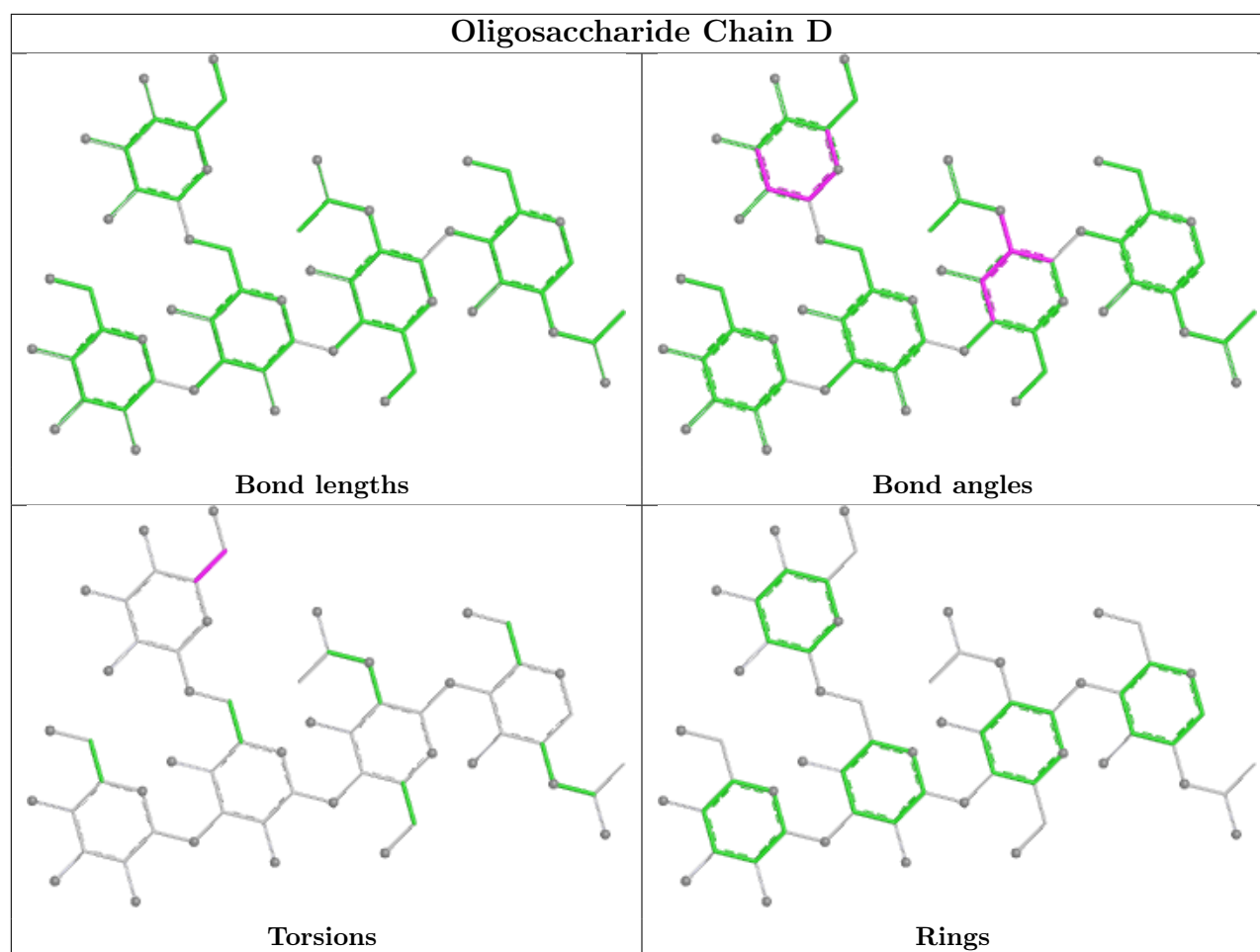
Mol	Chain	Res	Type	Atoms
7	E	2	NAG	O5-C5-C6-O6
7	E	6	MAN	O5-C5-C6-O6
7	E	2	NAG	C4-C5-C6-O6
7	E	6	MAN	C4-C5-C6-O6
6	D	5	MAN	O5-C5-C6-O6
6	D	5	MAN	C4-C5-C6-O6

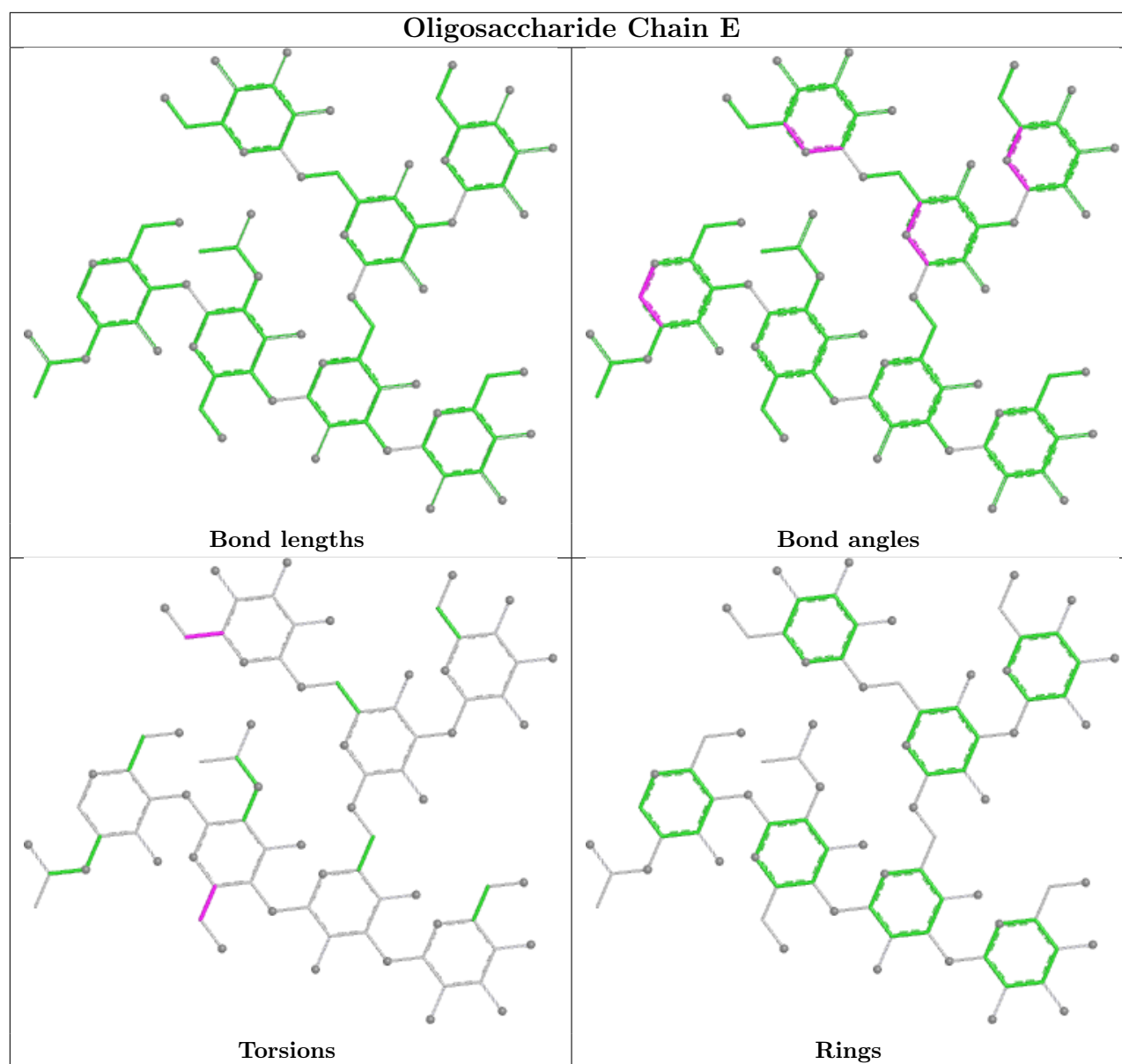
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





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
8	GOL	A	1453	-	5,5,5	0.43	0	5,5,5	0.14	0
8	GOL	B	1462	9	5,5,5	0.35	0	5,5,5	0.41	0
10	NAG	A	3015	1	14,14,15	0.48	0	17,19,21	0.80	1 (5%)
10	NAG	B	3099	2	14,14,15	0.45	0	17,19,21	0.84	1 (5%)
10	NAG	A	3249	1	14,14,15	0.55	0	17,19,21	0.96	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
8	GOL	A	1453	-	-	0/4/4/4	-
8	GOL	B	1462	9	-	0/4/4/4	-
10	NAG	A	3015	1	-	0/6/23/26	0/1/1/1
10	NAG	B	3099	2	-	2/6/23/26	0/1/1/1
10	NAG	A	3249	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	3099	NAG	O5-C1-C2	-2.06	108.11	111.29
10	A	3015	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (2) 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

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 ⓘ

Warning: The R factor obtained from EDS is 0.2262, which does not match the depositor's R factor of 0.141. Please interpret the results in this section carefully.

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, 95th 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 ²)	Q<0.9
1	A	452/452 (100%)	0.07	2 (0%) 89 86	21, 46, 61, 87	12 (2%)
2	B	455/461 (98%)	0.65	39 (8%) 18 15	21, 56, 93, 106	8 (1%)
3	C	7/12 (58%)	1.82	3 (42%) 1 1	39, 48, 108, 111	0
4	H	219/221 (99%)	0.07	5 (2%) 61 55	28, 46, 73, 105	4 (1%)
5	L	214/214 (100%)	-0.03	0 100 100	20, 43, 57, 92	8 (3%)
All	All	1347/1360 (99%)	0.26	49 (3%) 46 40	20, 48, 85, 111	32 (2%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	457	CYS	5.0
2	B	72	LYS	4.4
1	A	1	LEU	4.4
2	B	461	ARG	4.3
2	B	456	GLU	4.1
4	H	221	PRO	4.1
2	B	1	GLY	3.9
2	B	458	GLY	3.8
3	C	406	LYS	3.8
2	B	10	VAL	3.8
2	B	437	CYS	3.4
2	B	453	GLY	3.4
2	B	441	ALA	3.4
2	B	436	ALA	3.3
2	B	442	GLU	3.3
3	C	405	ALA	3.3
2	B	11	SER	3.1
2	B	366	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	407	GLN	2.9
2	B	379	VAL	2.9
2	B	444	ASN	2.8
2	B	439	ALA	2.8
2	B	405	GLY	2.7
2	B	24	ALA	2.7
2	B	443	PRO	2.7
2	B	455	PHE	2.7
4	H	134	CYS	2.7
2	B	459	VAL	2.6
4	H	177[A]	GLN	2.5
2	B	9	GLY	2.5
2	B	454	THR	2.4
2	B	395	VAL	2.3
2	B	446	HIS	2.3
2	B	2	PRO	2.3
2	B	403	VAL	2.3
2	B	392	GLY	2.3
2	B	387[A]	MET	2.3
4	H	137	THR	2.3
2	B	451	GLY	2.2
2	B	22	MET	2.2
2	B	58	VAL	2.2
1	A	326	GLY	2.1
2	B	8	ARG	2.1
2	B	460	CYS	2.1
4	H	220	GLY	2.1
2	B	32	PRO	2.1
2	B	69	LEU	2.0
2	B	375	LEU	2.0
2	B	440	GLN	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](#)

SUGAR-RSR INFOmissingINFO

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, 95th 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 ²)	Q<0.9
10	NAG	A	3249	14/15	0.17	0.22	98,102,104,105	14
10	NAG	A	3015	14/15	0.51	0.21	90,95,97,97	14
10	NAG	B	3099	14/15	0.62	0.17	99,105,111,112	0
8	GOL	A	1453	6/6	0.90	0.16	58,64,68,72	0
8	GOL	B	1462	6/6	0.92	0.16	54,55,57,58	0
11	MG	B	2001	1/1	0.98	0.13	23,23,23,23	0
9	CA	B	2002	1/1	0.99	0.15	35,35,35,35	0
9	CA	B	2003	1/1	0.99	0.18	34,34,34,34	0
9	CA	A	2004	1/1	0.99	0.12	58,58,58,58	0
9	CA	A	2005	1/1	0.99	0.15	49,49,49,49	0
9	CA	A	2006	1/1	0.99	0.11	64,64,64,64	0
9	CA	A	2007	1/1	0.99	0.11	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.