



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2024 – 03:44 am GMT

PDB ID : 6S5A
Title : CRYSTAL STRUCTURE OF FC P329G LALA WITH ANTI FC P329G FAB
Authors : Ehler, A.; Darowski, D.; Jost, C.; Stubenrauch, K.; Wessels, U.; Benz, J.; Birk, M.; Freimoser-Grundschober, A.; Bruenker, P.; Moessner, E.; Umana, P.; Kobold, S.; Klein, C.
Deposited on : 2019-07-01
Resolution : 1.72 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

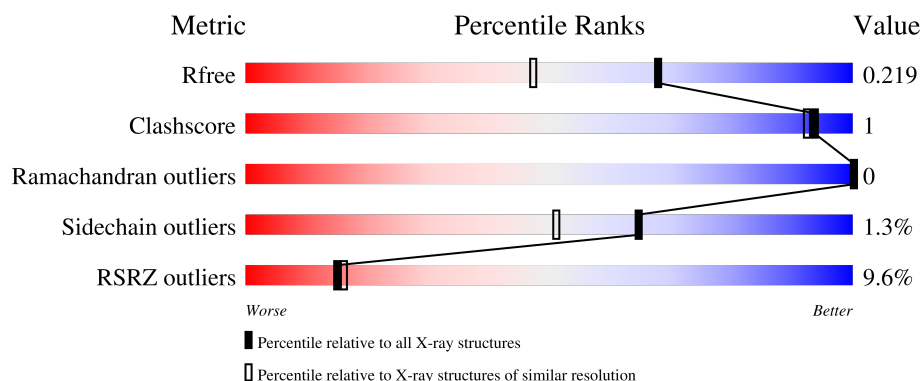
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	7106 (1.74-1.70)
Clashscore	180529	7746 (1.74-1.70)
Ramachandran outliers	177936	7654 (1.74-1.70)
Sidechain outliers	177891	7654 (1.74-1.70)
RSRZ outliers	164620	7104 (1.74-1.70)

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 $\leq 5\%$. 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	225	<div> <div>28%</div> <div> <div></div> <div>92%</div> <div>5%</div> </div> </div>
1	D	225	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>7%</div> </div> </div>
2	H	251	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>12%</div> </div> </div>
3	L	215	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> </div>
4	B	6	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	C	7	 71% 29%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7720 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 Fc P329G LALA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	3	0
			1702	1082	286	328	6			
1	D	209	Total	C	N	O	S	0	1	0
			1668	1062	281	319	6			

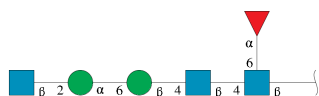
- Molecule 2 is a protein called anti P329G LALA Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	2	0
			1683	1078	275	324	6			

- Molecule 3 is a protein called anti P329G LALA Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	1	0
			1589	1001	265	319	4			

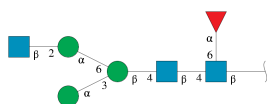
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	6	Total	C	N	O	0	0	0
			74	42	3	29			

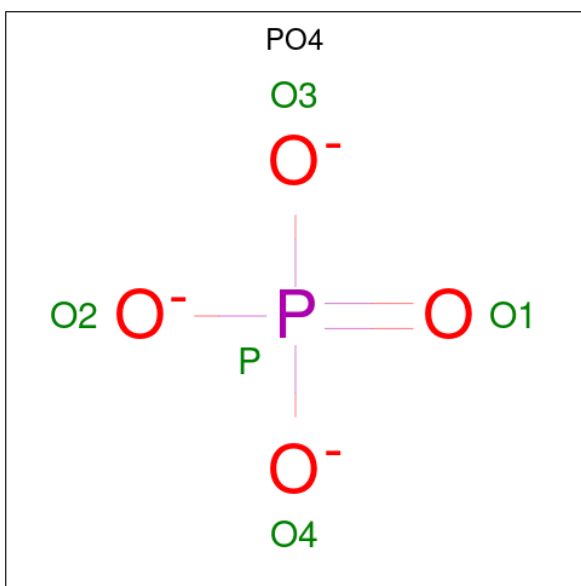
- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

oxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	7	Total	C	N	O	0	0	0
			85	48	3	34			

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	P	0	0
			5	4	1		
6	L	1	Total	O	P	0	0
			5	4	1		
6	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		
7	L	1	Total	C	O	0	0
			6	3	3		

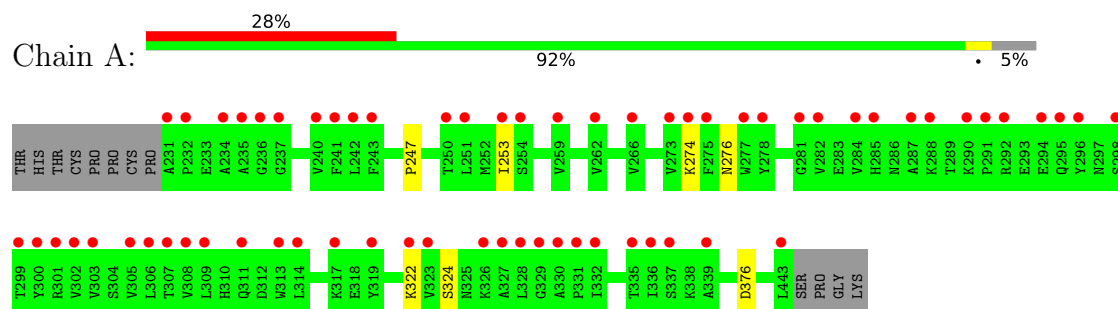
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	126	Total	O	0	0
			126	126		
8	D	260	Total	O	0	0
			260	260		
8	H	265	Total	O	0	0
			265	265		
8	L	235	Total	O	0	0
			235	235		

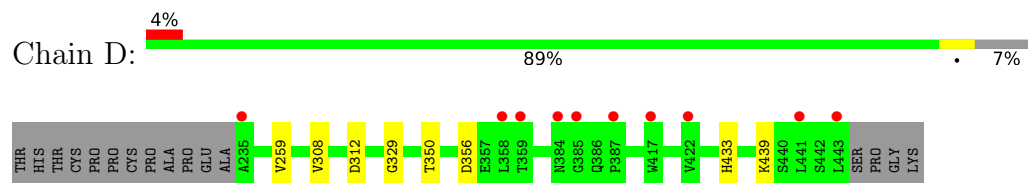
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

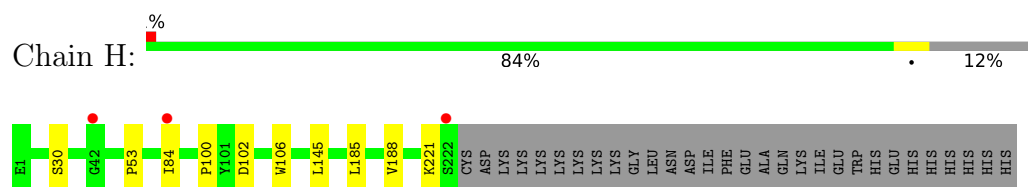
- Molecule 1: Fc P329G LALA



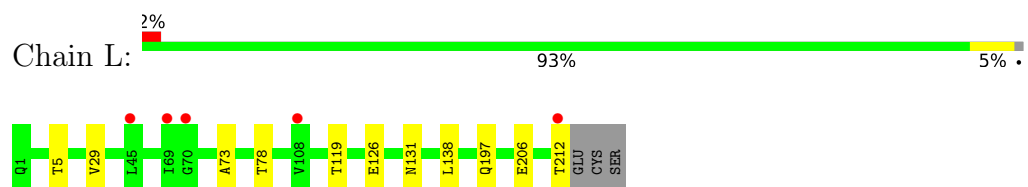
- Molecule 1: Fc P329G LALA



- Molecule 2: anti P329G LALA Fab heavy chain



- Molecule 3: anti P329G LALA Fab light chain



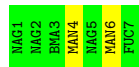
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 5: 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 C:  71% 29%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.02Å 135.54Å 137.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.63 – 1.72 68.63 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.9 (68.63-1.72) 99.9 (68.63-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.72Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.196 , 0.226 0.194 , 0.219	Depositor DCC
R_{free} test set	7250 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7720	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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: PO4, BMA, GOL, MAN, NAG, FUC

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	0.45	0/1757	0.61	0/2393
1	D	0.50	0/1716	0.63	0/2337
2	H	0.58	0/1734	0.67	0/2364
3	L	0.55	0/1631	0.67	0/2232
All	All	0.52	0/6838	0.64	0/9326

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	1702	0	1670	3	0
1	D	1668	0	1638	4	0
2	H	1683	0	1670	6	0
3	L	1589	0	1553	7	0
4	B	74	0	64	0	0
5	C	85	0	73	0	0
6	D	5	0	0	0	0
6	L	10	0	0	0	0
7	D	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	6	0	8	0	0
7	L	6	0	8	1	0
8	A	126	0	0	0	0
8	D	260	0	0	0	0
8	H	265	0	0	0	0
8	L	235	0	0	2	0
All	All	7720	0	6692	17	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 1.

All (17) 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:D:312:ASP:OD2	7:D:509:GOL:H32	1.87	0.74
3:L:197:GLN:HG2	3:L:206:GLU:HG3	1.78	0.65
3:L:126[A]:GLU:HG2	8:L:447:HOH:O	2.03	0.58
1:A:274:LYS:HB3	1:A:324:SER:HB2	1.89	0.54
1:D:329:GLY:HA3	2:H:100:PRO:HB2	1.89	0.53
1:A:276:ASN:HB2	1:A:322:LYS:HB3	1.91	0.51
2:H:188[B]:VAL:HG21	3:L:138:LEU:HD12	1.95	0.48
2:H:100:PRO:HB3	2:H:106:TRP:HA	1.97	0.46
3:L:119:THR:OG1	7:L:303:GOL:H2	2.16	0.44
1:D:259[A]:VAL:HG23	1:D:308:VAL:HG11	2.00	0.43
3:L:78:THR:HG23	8:L:414:HOH:O	2.16	0.43
2:H:188[B]:VAL:HG21	3:L:138:LEU:CD1	2.49	0.42
1:A:247:PRO:HG3	1:A:376:ASP:HB3	2.02	0.42
2:H:30:SER:O	2:H:53:PRO:HB3	2.20	0.41
2:H:185:LEU:HD12	2:H:185:LEU:C	2.41	0.41
3:L:29:VAL:HG11	3:L:73:ALA:HB2	2.03	0.41
1:D:350:THR:HG23	1:D:439:LYS:HB3	2.03	0.41

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	214/225 (95%)	211 (99%)	3 (1%)	0	100	100
1	D	208/225 (92%)	204 (98%)	4 (2%)	0	100	100
2	H	221/251 (88%)	216 (98%)	5 (2%)	0	100	100
3	L	211/215 (98%)	201 (95%)	10 (5%)	0	100	100
All	All	854/916 (93%)	832 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	197/205 (96%)	196 (100%)	1 (0%)	86	82
1	D	193/205 (94%)	191 (99%)	2 (1%)	73	63
2	H	189/215 (88%)	185 (98%)	4 (2%)	48	31
3	L	175/177 (99%)	172 (98%)	3 (2%)	56	40
All	All	754/802 (94%)	744 (99%)	10 (1%)	65	51

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	ILE
1	D	356	ASP
1	D	433	HIS
2	H	84	ILE
2	H	102	ASP
2	H	145	LEU
2	H	221	LYS
3	L	5	THR
3	L	131	ASN
3	L	212	THR

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	389	ASN
1	D	347	GLN
1	D	419	GLN
3	L	39	GLN
3	L	131	ASN

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 ⓘ

13 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	$\# Z > 2$
4	NAG	B	1	4,1	14,14,15	0.33	0	17,19,21	0.65	1 (5%)
4	NAG	B	2	4	14,14,15	0.30	0	17,19,21	0.49	0
4	BMA	B	3	4	11,11,12	0.34	0	15,15,17	0.64	0
4	MAN	B	4	4	11,11,12	0.39	0	15,15,17	0.75	1 (6%)
4	NAG	B	5	4	14,14,15	0.31	0	17,19,21	0.80	1 (5%)
4	FUC	B	6	4	10,10,11	0.40	0	14,14,16	0.76	0
5	NAG	C	1	5,1	14,14,15	0.34	0	17,19,21	0.74	0
5	NAG	C	2	5	14,14,15	0.34	0	17,19,21	0.54	0
5	BMA	C	3	5	11,11,12	0.37	0	15,15,17	0.56	0
5	MAN	C	4	5	11,11,12	0.33	0	15,15,17	0.74	1 (6%)
5	NAG	C	5	5	14,14,15	0.29	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	C	6	5	11,11,12	0.38	0	15,15,17	0.76	1 (6%)
5	FUC	C	7	5	10,10,11	0.40	0	14,14,16	0.71	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	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
4	BMA	B	3	4	-	0/2/19/22	0/1/1/1
4	MAN	B	4	4	-	0/2/19/22	0/1/1/1
4	NAG	B	5	4	-	0/6/23/26	0/1/1/1
4	FUC	B	6	4	-	-	0/1/1/1
5	NAG	C	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
5	BMA	C	3	5	-	0/2/19/22	0/1/1/1
5	MAN	C	4	5	-	0/2/19/22	0/1/1/1
5	NAG	C	5	5	-	0/6/23/26	0/1/1/1
5	MAN	C	6	5	-	2/2/19/22	0/1/1/1
5	FUC	C	7	5	-	-	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	5	NAG	C1-O5-C5	2.51	115.59	112.19
5	C	4	MAN	C1-O5-C5	2.50	115.58	112.19
5	C	6	MAN	C1-O5-C5	2.20	115.18	112.19
4	B	1	NAG	C1-O5-C5	2.19	115.16	112.19
4	B	4	MAN	C1-O5-C5	2.14	115.10	112.19

There are no chirality outliers.

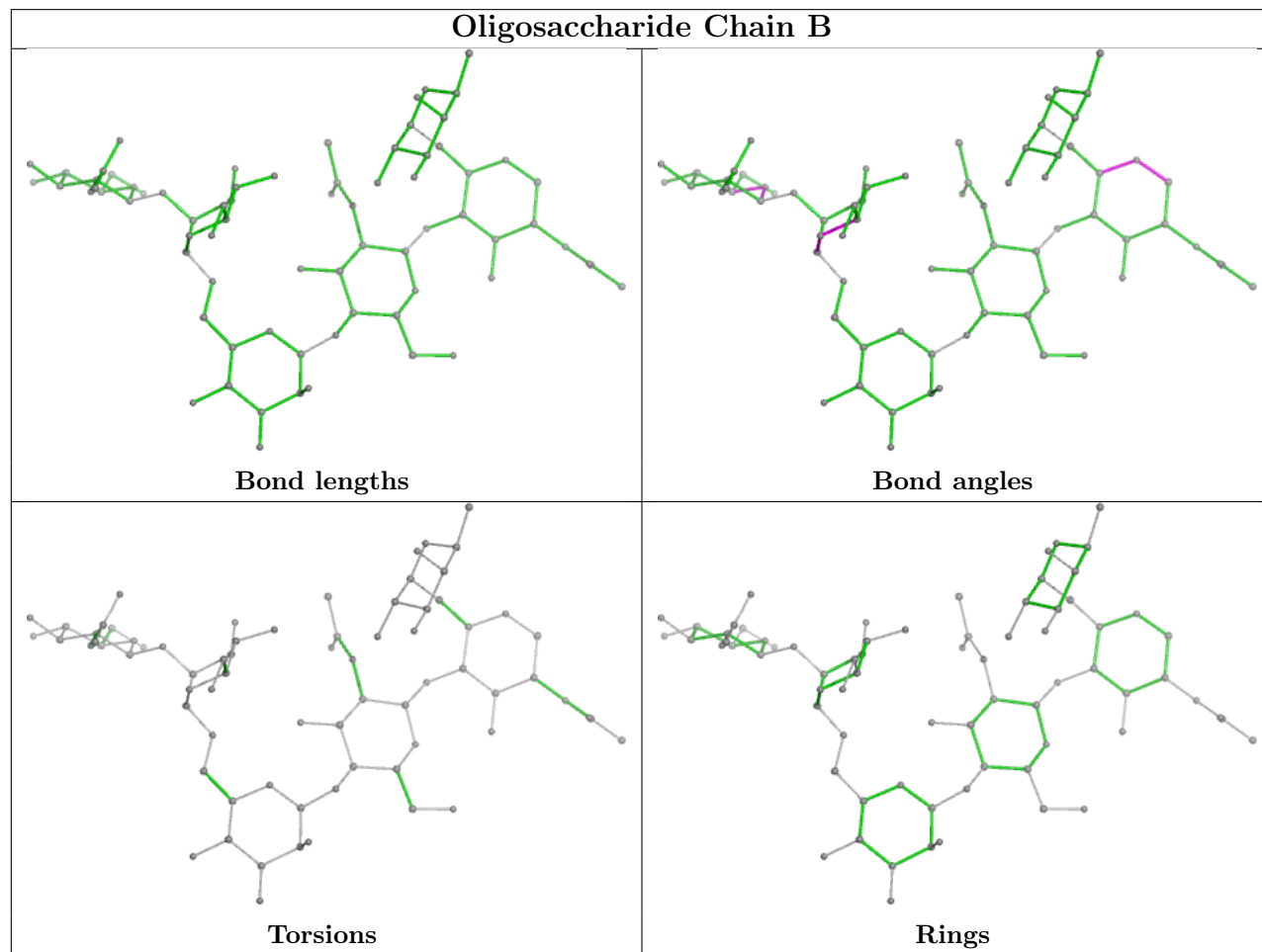
All (2) torsion outliers are listed below:

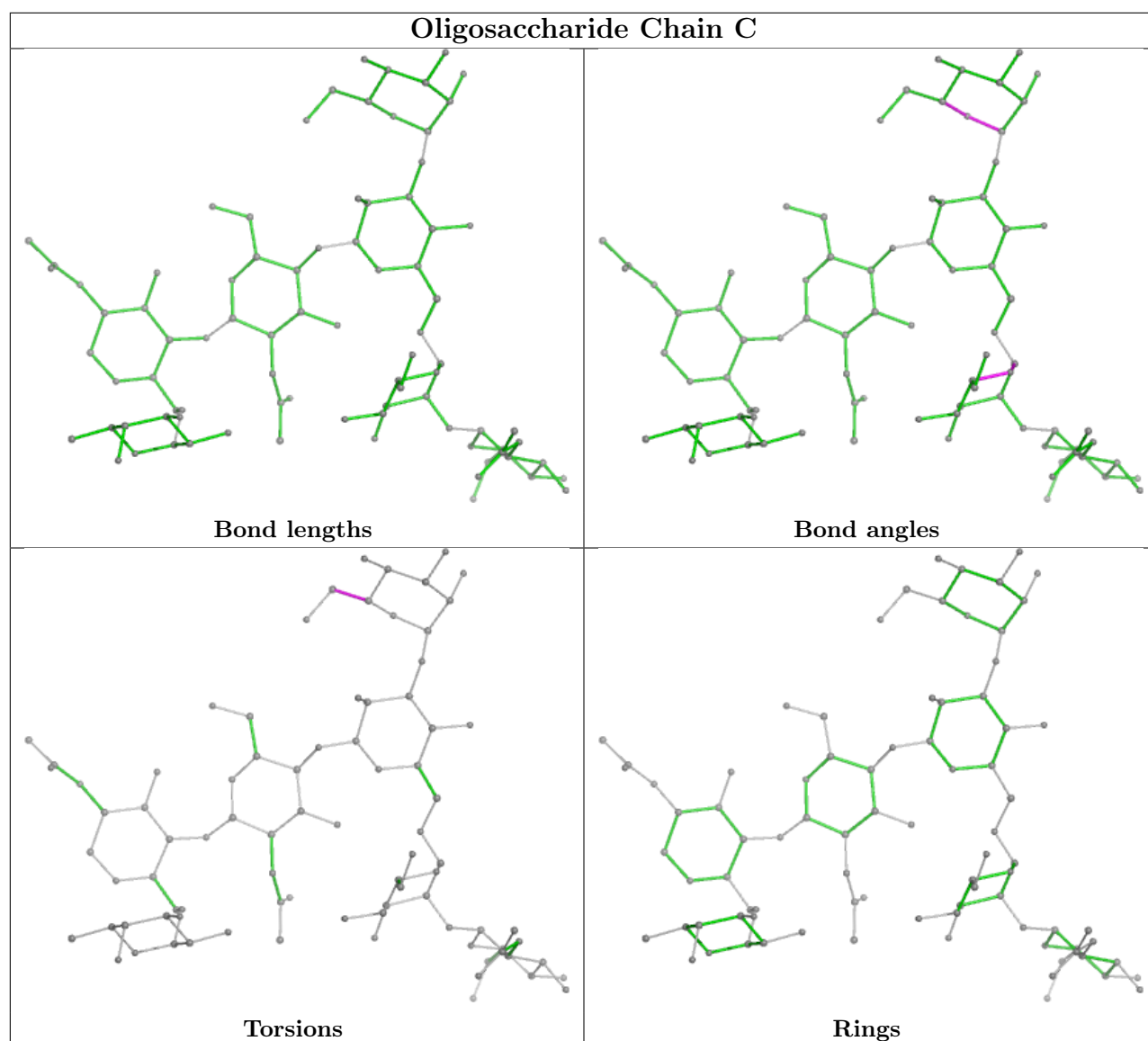
Mol	Chain	Res	Type	Atoms
5	C	6	MAN	C4-C5-C6-O6
5	C	6	MAN	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

6 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	$\# Z > 2$
6	PO4	D	508	-	4,4,4	2.51	2 (50%)	6,6,6	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PO4	L	302	-	4,4,4	2.50	1 (25%)	6,6,6	0.79	0
7	GOL	H	301	-	5,5,5	0.14	0	5,5,5	0.20	0
7	GOL	D	509	-	5,5,5	0.16	0	5,5,5	0.25	0
7	GOL	L	303	-	5,5,5	0.03	0	5,5,5	0.43	0
6	PO4	L	301	-	4,4,4	1.82	0	6,6,6	1.02	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
7	GOL	L	303	-	-	4/4/4/4	-
7	GOL	H	301	-	-	0/4/4/4	-
7	GOL	D	509	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	302	PO4	P-O1	4.18	1.60	1.50
6	D	508	PO4	P-O1	4.13	1.60	1.50
6	D	508	PO4	P-O4	2.01	1.60	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	303	GOL	C1-C2-C3-O3
7	L	303	GOL	O2-C2-C3-O3
7	L	303	GOL	O1-C1-C2-O2
7	L	303	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	509	GOL	1	0
7	L	303	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	213/225 (94%)	1.23	64 (30%) 1 1	21, 65, 107, 120	3 (1%)
1	D	209/225 (92%)	0.41	10 (4%) 36 40	18, 40, 71, 88	1 (0%)
2	H	221/251 (88%)	-0.01	3 (1%) 73 77	20, 35, 55, 102	2 (0%)
3	L	212/215 (98%)	0.32	5 (2%) 59 63	23, 42, 62, 86	1 (0%)
All	All	855/916 (93%)	0.48	82 (9%) 15 16	18, 40, 94, 120	7 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	TYR	5.5
1	A	336	ILE	5.4
1	A	328	LEU	5.1
2	H	222	SER	5.1
1	A	231	ALA	4.4
1	D	443	LEU	4.2
1	A	235	ALA	4.1
1	D	235	ALA	4.1
3	L	212	THR	4.0
1	A	234	ALA	3.9
2	H	42	GLY	3.8
1	A	266	VAL	3.8
1	A	232	PRO	3.8
1	A	290	LYS	3.8
1	A	305	VAL	3.7
1	A	332	ILE	3.7
1	A	314	LEU	3.7
1	A	329	GLY	3.7
1	A	291	PRO	3.6
3	L	69	ILE	3.6
1	A	275	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	306	LEU	3.3
1	A	323	VAL	3.3
1	A	277	TRP	3.3
1	A	253	ILE	3.3
1	A	236	GLY	3.2
1	A	287	ALA	3.2
1	A	322	LYS	3.2
1	A	309	LEU	3.1
1	D	441	LEU	3.0
1	D	422	VAL	3.0
1	A	335	THR	3.0
1	A	294	GLU	3.0
1	A	303	VAL	3.0
1	A	326	LYS	2.9
1	D	359	THR	2.9
1	A	317	LYS	2.9
1	D	358	LEU	2.9
1	A	295	GLN	2.9
1	A	330	ALA	2.9
1	A	331	PRO	2.9
1	A	278	TYR	2.8
1	A	243	PHE	2.8
3	L	45	LEU	2.8
1	A	313	TRP	2.8
1	A	282	VAL	2.8
1	A	300	TYR	2.8
1	A	288	LYS	2.8
1	A	299	THR	2.7
1	A	339	ALA	2.7
1	A	262	VAL	2.7
1	A	237	GLY	2.7
1	A	319	TYR	2.7
1	D	387	PRO	2.6
1	A	284	VAL	2.5
1	A	308	VAL	2.5
1	A	337	SER	2.5
1	D	384	ASN	2.5
2	H	84	ILE	2.5
1	A	254	SER	2.5
1	A	327	ALA	2.4
1	A	298	SER	2.4
1	D	385	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	307	THR	2.4
1	A	273	VAL	2.4
1	A	302	VAL	2.4
1	A	274	LYS	2.3
1	A	259	VAL	2.3
1	A	443	LEU	2.3
1	A	301	ARG	2.3
1	D	417	TRP	2.3
1	A	285	HIS	2.2
1	A	292	ARG	2.2
1	A	242	LEU	2.2
1	A	311	GLN	2.1
1	A	251	LEU	2.1
1	A	240	VAL	2.1
3	L	108	VAL	2.1
1	A	241	PHE	2.1
3	L	70	GLY	2.0
1	A	250	THR	2.0
1	A	281	GLY	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(\AA^2)	Q<0.9
6	PO4	D	508	5/5	0.82	0.16	65,72,73,73	0
7	GOL	D	509	6/6	0.83	0.20	62,65,69,70	0
7	GOL	L	303	6/6	0.84	0.16	45,52,58,60	0
6	PO4	L	302	5/5	0.89	0.13	52,61,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	GOL	H	301	6/6	0.93	0.10	49,51,51,52	0
6	PO4	L	301	5/5	0.95	0.09	48,54,57,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.