



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:19 AM UTC

PDB ID : 9GVN / pdb_00009gvn
Title : DEPEMOKIMAB FAB IN COMPLEX WITH INTERLEUKIN 5
Authors : Somers, D.O.
Deposited on : 2024-09-25
Resolution : 1.93 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

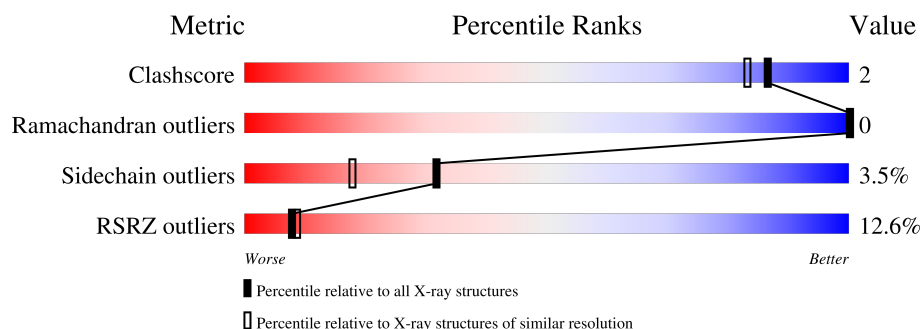
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	115	<div> <div>10%</div> <div>83%</div> <div>14%</div> <div>.</div> </div>
1	B	115	<div> <div>9%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
2	C	226	<div> <div>3%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
2	E	226	<div> <div>21%</div> <div>86%</div> <div>8%</div> <div>5%</div> </div>
3	D	220	<div> <div>3%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
3	F	220	<div> <div>25%</div> <div>94%</div> <div>5%</div> </div>
4	J	6	<div> <div>50%</div> <div>50%</div> </div>

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	GOL	D	302	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9240 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 Interleukin-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	1	0
			904	574	158	169	3			
1	B	112	Total	C	N	O	S	0	0	0
			903	574	157	169	3			

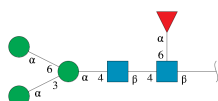
- Molecule 2 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	217	Total	C	N	O	S	0	0	0
			1618	1020	275	316	7			
2	E	214	Total	C	N	O	S	0	0	0
			1594	1005	270	312	7			

- Molecule 3 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	219	Total	C	N	O	S	0	0	0
			1678	1049	283	341	5			
3	F	219	Total	C	N	O	S	0	0	0
			1678	1049	283	341	5			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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


- Molecule 7 is water.

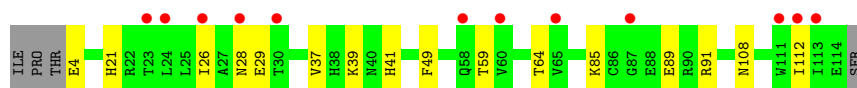
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	62	Total	O	0	0
			62	62		
7	B	100	Total	O	0	0
			100	100		
7	C	291	Total	O	0	0
			291	291		
7	D	247	Total	O	0	0
			247	247		
7	E	34	Total	O	0	0
			34	34		
7	F	38	Total	O	0	0
			38	38		

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 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.

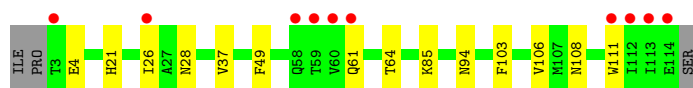
- Molecule 1: Interleukin-5

Chain A: 




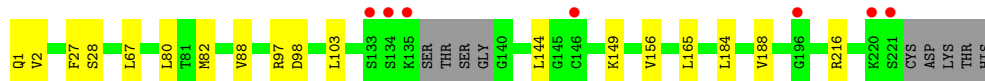
- Molecule 1: Interleukin-5

Chain B: 




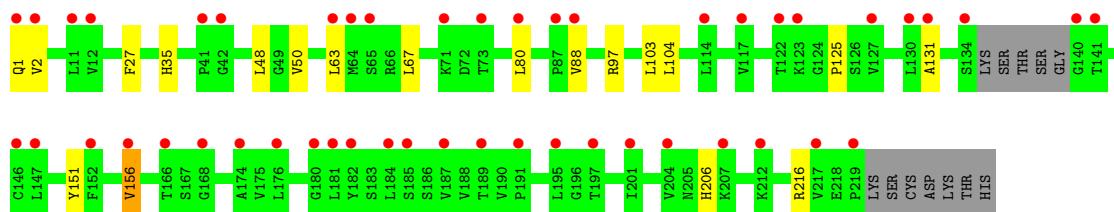
- Molecule 2: Fab heavy chain

Chain C: 

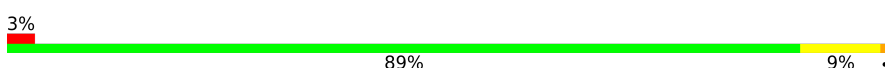


- Molecule 2: Fab heavy chain

Chain E: 



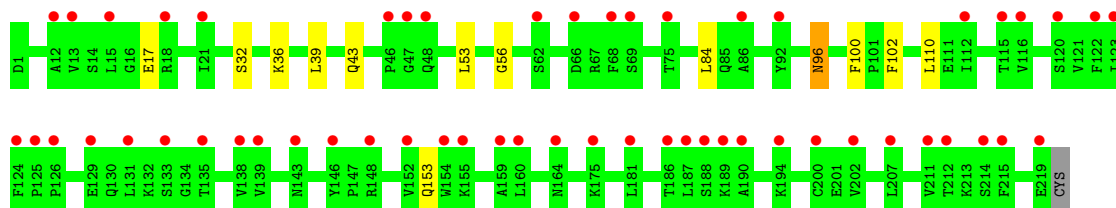
- Molecule 3: Fab light chain

Chain D: 





• Molecule 3: Fab light chain



• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.68Å 65.87Å 193.75Å 90.00° 96.62° 90.00°	Depositor
Resolution (Å)	192.46 – 1.93 192.46 – 1.93	Depositor EDS
% Data completeness (in resolution range)	55.5 (192.46-1.93) 55.5 (192.46-1.93)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.94Å)	Xtriage
Refinement program	BUSTER 2.11.8 (16-JUL-2021)	Depositor
R, R_{free}	0.183 , 0.209 0.178 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9240	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, EDO, MAN, 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	0.66	0/917	1.11	3/1237 (0.2%)
1	B	0.73	0/916	1.12	3/1236 (0.2%)
2	C	0.82	0/1656	0.99	2/2265 (0.1%)
2	E	0.56	0/1632	0.91	1/2235 (0.0%)
3	D	0.79	1/1713 (0.1%)	1.03	7/2324 (0.3%)
3	F	0.58	0/1713	0.90	4/2324 (0.2%)
All	All	0.70	1/8547 (0.0%)	0.99	20/11621 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	54	ILE	CG1-CD1	-5.46	1.30	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	PHE	CA-CB-CG	-7.53	106.27	113.80
3	D	100	PHE	CA-CB-CG	6.67	120.47	113.80
1	A	49	PHE	CA-CB-CG	-6.01	107.79	113.80
1	B	28	ASN	CA-CB-CG	5.77	118.37	112.60
1	A	28	ASN	CA-CB-CG	5.65	118.25	112.60
1	A	108	ASN	CA-CB-CG	5.63	118.23	112.60
3	D	102	PHE	CA-C-N	5.52	129.09	120.75
3	D	102	PHE	C-N-CA	5.52	129.09	120.75
2	E	131	ALA	N-CA-C	5.52	115.95	109.60
3	F	102	PHE	CA-C-N	5.44	128.43	120.71
3	F	102	PHE	C-N-CA	5.44	128.43	120.71
3	D	65	PRO	CA-C-N	5.43	128.10	120.28
3	D	65	PRO	C-N-CA	5.43	128.10	120.28
3	D	96	ASN	CA-CB-CG	5.35	117.95	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	120	SER	N-CA-C	-5.26	100.73	109.46
3	F	96	ASN	CA-CB-CG	5.21	117.81	112.60
1	B	108	ASN	CA-CB-CG	5.16	117.76	112.60
2	C	98	ASP	CB-CA-C	5.07	115.45	109.47
3	F	100	PHE	CA-CB-CG	5.06	118.86	113.80
2	C	149	LYS	N-CA-C	5.00	117.64	109.59

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	904	0	928	6	0
1	B	903	0	929	6	0
2	C	1618	0	1620	6	0
2	E	1594	0	1589	9	0
3	D	1678	0	1630	10	0
3	F	1678	0	1630	4	0
4	J	71	0	61	0	0
5	B	4	0	6	0	0
6	C	6	0	8	0	0
6	D	12	0	16	4	0
7	A	62	0	0	0	0
7	B	100	0	0	0	0
7	C	291	0	0	0	0
7	D	247	0	0	0	0
7	E	34	0	0	0	0
7	F	38	0	0	0	0
All	All	9240	0	8417	35	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 (35) 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)
3:D:172:GLN:HB2	6:D:302:GOL:H2	1.58	0.83
3:F:43:GLN:HB2	3:F:53:LEU:HD11	1.64	0.79
2:C:67:LEU:HD21	2:C:82:MET:HE2	1.68	0.75
3:D:179:TYR:OH	6:D:302:GOL:H32	1.93	0.67
2:C:103:LEU:HD11	3:D:36:LYS:HG2	1.77	0.66
3:D:86:ALA:HA	3:D:112:ILE:CD1	2.26	0.65
1:A:21:HIS:CD2	1:A:64:THR:HG21	2.33	0.63
3:D:169:VAL:HG22	3:D:181:LEU:HD12	1.81	0.61
2:E:156:VAL:HG23	2:E:206:HIS:HD2	1.67	0.60
1:A:37:VAL:HG22	1:B:85:LYS:HB3	1.84	0.58
2:E:67:LEU:HD11	2:E:80:LEU:HD11	1.88	0.56
1:B:21:HIS:CD2	1:B:64:THR:HG21	2.42	0.55
2:E:125:PRO:HB3	2:E:151:TYR:HB3	1.92	0.51
2:E:103:LEU:HD13	3:F:56:GLY:HA3	1.94	0.49
2:C:67:LEU:HD22	2:C:80:LEU:HD11	1.96	0.48
1:A:85:LYS:HB3	1:B:37:VAL:HG22	1.95	0.48
1:A:89:GLU:OE1	1:A:91:ARG:NH1	2.48	0.47
3:D:43:GLN:HB2	3:D:53:LEU:HD11	1.96	0.47
3:D:111:GLU:HB2	6:D:302:GOL:O3	2.15	0.47
2:C:2:VAL:HG13	2:C:27:PHE:CD1	2.50	0.46
3:F:84:LEU:HD11	3:F:110:LEU:HD21	1.97	0.46
3:D:18:ARG:HD2	3:D:80:THR:HG23	1.97	0.46
3:D:109:LYS:HE2	6:D:302:GOL:H12	1.97	0.46
1:B:21:HIS:CG	1:B:64:THR:HG21	2.51	0.45
2:E:63:LEU:HD13	2:E:67:LEU:HD13	1.98	0.45
1:B:106:VAL:HG12	1:B:111:TRP:CD1	2.52	0.45
2:C:165:LEU:HD21	2:C:188:VAL:HG21	1.99	0.45
2:E:48:LEU:HD22	2:E:63:LEU:HD11	1.99	0.44
1:A:39:LYS:HB2	1:A:112:ILE:HD13	1.99	0.44
2:C:67:LEU:CD2	2:C:82:MET:HE2	2.43	0.44
2:E:103:LEU:HD11	3:F:36:LYS:HG2	2.01	0.43
3:D:18:ARG:HD2	3:D:80:THR:CG2	2.50	0.42
1:A:41:HIS:HB3	1:B:103:PHE:HD1	1.84	0.42
2:E:35:HIS:CD2	2:E:50:VAL:HG23	2.55	0.41
2:E:2:VAL:HG13	2:E:27:PHE:CD1	2.55	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	110/115 (96%)	108 (98%)	2 (2%)	0	100	100
1	B	110/115 (96%)	107 (97%)	3 (3%)	0	100	100
2	C	213/226 (94%)	209 (98%)	4 (2%)	0	100	100
2	E	210/226 (93%)	205 (98%)	5 (2%)	0	100	100
3	D	217/220 (99%)	212 (98%)	5 (2%)	0	100	100
3	F	217/220 (99%)	210 (97%)	7 (3%)	0	100	100
All	All	1077/1122 (96%)	1051 (98%)	26 (2%)	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	102/105 (97%)	98 (96%)	4 (4%)	28	15
1	B	102/105 (97%)	98 (96%)	4 (4%)	28	15
2	C	188/196 (96%)	180 (96%)	8 (4%)	26	13
2	E	185/196 (94%)	179 (97%)	6 (3%)	34	20
3	D	191/192 (100%)	184 (96%)	7 (4%)	30	16
3	F	191/192 (100%)	186 (97%)	5 (3%)	40	28
All	All	959/986 (97%)	925 (96%)	34 (4%)	32	18

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	26	ILE
1	A	29	GLU
1	A	59	THR
1	B	4	GLU
1	B	26	ILE
1	B	61	GLN
1	B	94	ASN
2	C	1	GLN
2	C	28	SER
2	C	88	VAL
2	C	97	ARG
2	C	144	LEU
2	C	156	VAL
2	C	184	LEU
2	C	216	ARG
3	D	18	ARG
3	D	36	LYS
3	D	39	LEU
3	D	96	ASN
3	D	113	LYS
3	D	187	LEU
3	D	211	VAL
2	E	1	GLN
2	E	88	VAL
2	E	97	ARG
2	E	104	LEU
2	E	156	VAL
2	E	216	ARG
3	F	17	GLU
3	F	32	SER
3	F	39	LEU
3	F	96	ASN
3	F	153	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	40	ASN
1	A	41	HIS

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Mol	Chain	Res	Type
1	A	95	GLN
1	B	41	HIS
1	B	61	GLN
1	B	82	GLN
2	E	39	GLN
2	E	177	GLN
3	F	44	GLN
3	F	48	GLN
3	F	85	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 ⓘ

6 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	J	1	1,4	14,14,15	0.31	0	17,19,21	0.68	0
4	NAG	J	2	4	14,14,15	0.29	0	17,19,21	0.68	0
4	MAN	J	3	4	11,11,12	0.45	0	15,15,17	1.68	2 (13%)
4	MAN	J	4	4	11,11,12	0.31	0	15,15,17	0.89	1 (6%)
4	MAN	J	5	4	11,11,12	0.22	0	15,15,17	0.96	1 (6%)
4	FUC	J	6	4	10,10,11	0.32	0	14,14,16	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
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	MAN	J	3	4	-	0/2/19/22	1/1/1/1
4	MAN	J	4	4	-	0/2/19/22	0/1/1/1
4	MAN	J	5	4	-	0/2/19/22	0/1/1/1
4	FUC	J	6	4	-	-	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	3	MAN	C1-O5-C5	5.06	118.97	112.19
4	J	5	MAN	C1-O5-C5	3.31	116.62	112.19
4	J	3	MAN	C1-C2-C3	3.10	114.16	109.64
4	J	4	MAN	C1-O5-C5	2.96	116.16	112.19

There are no chirality outliers.

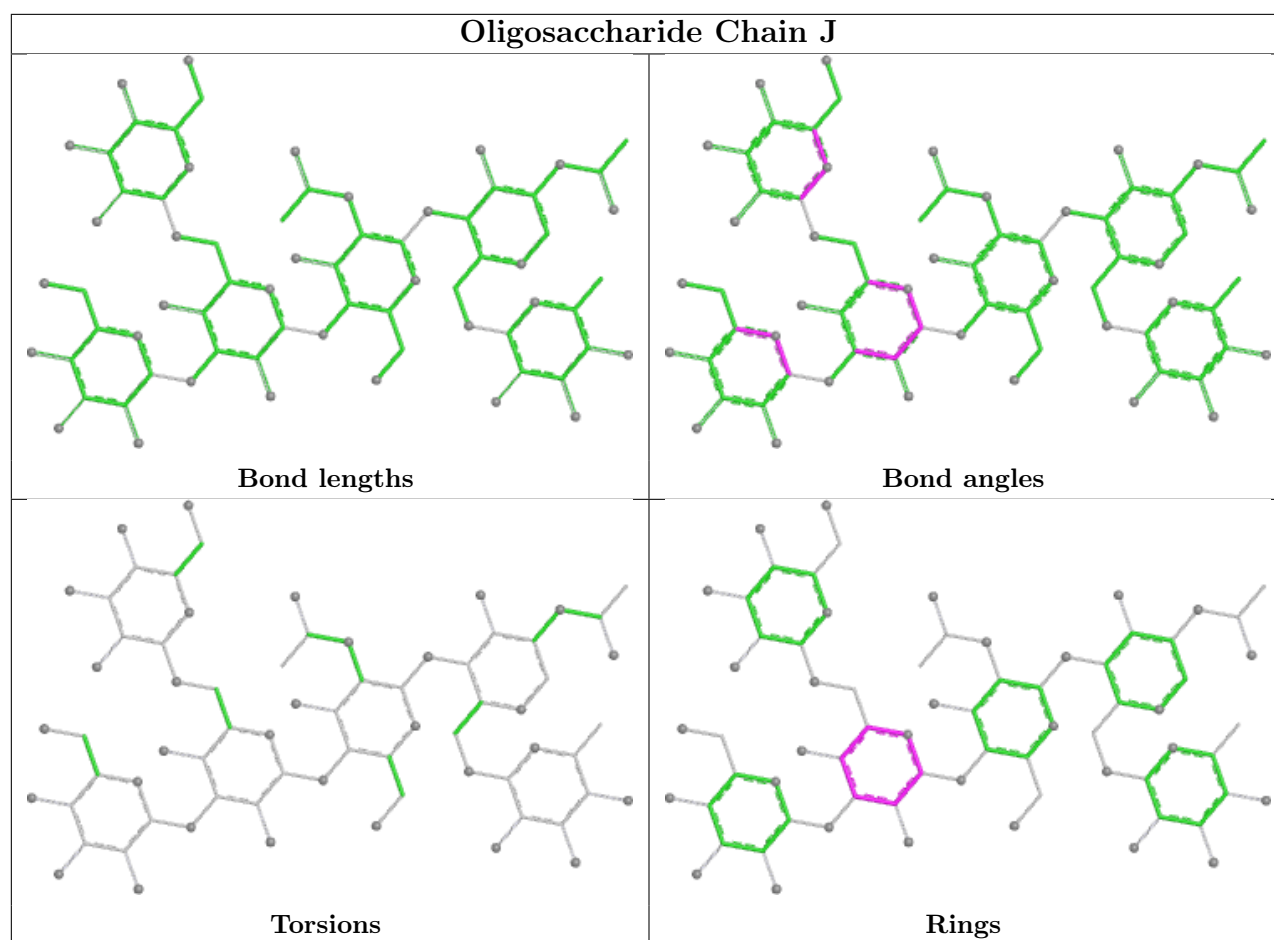
There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	3	MAN	C1-C2-C3-C4-C5-O5

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](#)

4 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	$\# Z > 2$
5	EDO	B	201	-	3,3,3	0.57	0	2,2,2	0.19	0
6	GOL	D	302	-	5,5,5	0.08	0	5,5,5	0.51	0
6	GOL	C	301	-	5,5,5	0.28	0	5,5,5	0.53	0
6	GOL	D	301	-	5,5,5	0.35	0	5,5,5	0.75	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
5	EDO	B	201	-	-	0/1/1/1	-
6	GOL	D	302	-	-	2/4/4/4	-
6	GOL	C	301	-	-	3/4/4/4	-
6	GOL	D	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	301	GOL	O1-C1-C2-C3
6	D	301	GOL	O1-C1-C2-C3
6	D	301	GOL	C1-C2-C3-O3
6	D	302	GOL	C1-C2-C3-O3
6	C	301	GOL	O1-C1-C2-O2
6	D	301	GOL	O1-C1-C2-O2
6	D	301	GOL	O2-C2-C3-O3
6	D	302	GOL	O2-C2-C3-O3
6	C	301	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	302	GOL	4	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.

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	111/115 (96%)	0.86	12 (10%)	11 12	20, 64, 98, 107	1 (0%)
1	B	112/115 (97%)	0.67	10 (8%)	15 17	31, 49, 79, 89	0
2	C	217/226 (96%)	0.02	7 (3%)	50 56	23, 36, 65, 79	0
2	E	214/226 (94%)	1.36	48 (22%)	2 1	63, 102, 135, 142	0
3	D	219/220 (99%)	0.14	6 (2%)	56 63	26, 42, 62, 77	0
3	F	219/220 (99%)	1.49	55 (25%)	1 1	59, 106, 135, 145	0
All	All	1092/1122 (97%)	0.75	138 (12%)	8 9	20, 62, 129, 145	1 (0%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	THR	6.1
1	B	60	VAL	5.7
3	F	47	GLY	4.8
2	C	135	LYS	4.3
3	F	124	PHE	4.2
2	E	219	PRO	4.2
3	F	200	CYS	4.1
2	E	65	SER	3.9
2	E	201	ILE	3.9
1	B	59	THR	3.8
2	C	134	SER	3.7
2	E	146	CYS	3.6
1	A	112	ILE	3.6
3	F	219	GLU	3.6
2	E	63	LEU	3.6
3	F	116	VAL	3.5
3	F	164	ASN	3.4
3	F	112	ILE	3.3
3	F	154	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	111	TRP	3.3
2	C	221	SER	3.2
3	F	212	THR	3.2
2	E	41	PRO	3.2
3	F	152	VAL	3.1
2	C	133	SER	3.1
2	E	134	SER	3.1
3	F	15	LEU	3.1
3	F	13	VAL	3.1
1	A	26	ILE	3.0
2	E	141	THR	3.0
3	F	139	VAL	3.0
3	F	115	THR	2.9
3	F	135	THR	2.9
3	F	86	ALA	2.9
1	B	61	GLN	2.9
2	E	176	LEU	2.9
3	F	155	LYS	2.9
2	E	181	LEU	2.9
2	E	73	THR	2.9
3	D	218	GLY	2.9
3	F	138	VAL	2.9
3	F	48	GLN	2.8
3	F	68	PHE	2.8
3	F	122	PHE	2.8
1	B	111	TRP	2.8
1	A	87	GLY	2.8
3	F	148	ARG	2.8
3	F	160	LEU	2.8
2	E	131	ALA	2.7
2	E	114	LEU	2.7
2	E	87	PRO	2.7
1	A	113	ILE	2.7
2	E	212	LYS	2.7
2	E	2	VAL	2.7
2	E	12	VAL	2.7
1	A	30	THR	2.7
1	A	58	GLN	2.6
2	E	1	GLN	2.6
3	F	129	GLU	2.6
2	E	189	THR	2.6
3	D	200	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	11	LEU	2.6
3	F	123	ILE	2.6
2	E	182	TYR	2.6
3	F	125	PRO	2.6
2	E	187	VAL	2.6
3	F	190	ALA	2.6
3	F	211	VAL	2.6
3	F	215	PHE	2.5
3	F	187	LEU	2.5
2	E	140	GLY	2.5
2	C	196	GLY	2.5
1	A	23	THR	2.5
1	B	113	ILE	2.5
3	F	62	SER	2.5
3	F	146	TYR	2.4
2	E	147	LEU	2.4
1	B	26	ILE	2.4
2	E	122	THR	2.4
2	E	191	PRO	2.4
2	E	71	LYS	2.4
1	A	60	VAL	2.4
3	D	111	GLU	2.4
2	E	117	VAL	2.4
2	E	80	LEU	2.3
3	F	18	ARG	2.3
3	F	181	LEU	2.3
2	E	197	THR	2.3
1	B	58	GLN	2.3
2	E	174	ALA	2.3
3	F	12	ALA	2.3
3	F	131	LEU	2.3
3	F	143	ASN	2.3
3	F	126	PRO	2.3
3	F	189	LYS	2.3
3	F	188	SER	2.3
1	A	65	VAL	2.3
2	E	180	GLY	2.3
3	D	148	ARG	2.3
3	F	214	SER	2.3
2	E	64	MET	2.3
2	E	130	LEU	2.3
3	F	120	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	220	LYS	2.2
3	F	75	THR	2.2
2	E	184	LEU	2.2
3	D	219	GLU	2.2
2	E	168	GLY	2.2
2	E	127	VAL	2.2
2	E	204	VAL	2.2
1	A	24	LEU	2.2
3	F	207	LEU	2.2
1	B	114	GLU	2.2
3	F	66	ASP	2.2
2	E	185	SER	2.2
1	A	28	ASN	2.1
3	F	133	SER	2.1
2	E	123	LYS	2.1
3	F	175	LYS	2.1
3	F	159	ALA	2.1
3	F	21	ILE	2.1
3	F	92	TYR	2.1
2	E	195	LEU	2.1
3	D	133	SER	2.1
3	F	69	SER	2.1
3	F	186	THR	2.1
2	E	88	VAL	2.1
2	E	217	VAL	2.1
3	F	202	VAL	2.1
1	B	112	ILE	2.0
2	E	152	PHE	2.0
2	E	207	LYS	2.0
3	F	194	LYS	2.0
2	E	42	GLY	2.0
3	F	46	PRO	2.0
2	C	146	CYS	2.0
2	E	166	THR	2.0
2	E	156	VAL	2.0

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

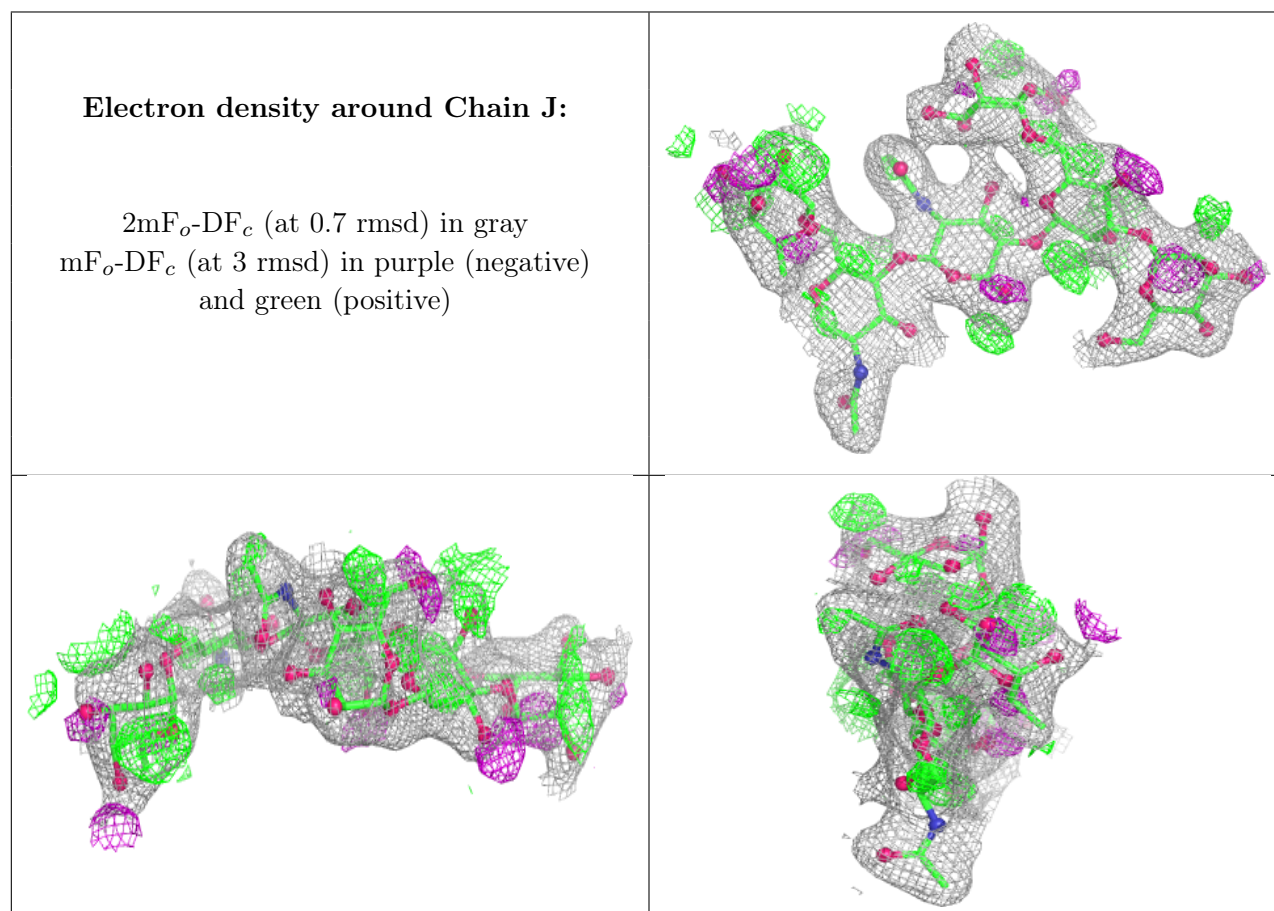
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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
4	NAG	J	1	14/15	-	-	31,36,42,45	0
4	NAG	J	2	14/15	-	-	31,38,43,46	0
4	MAN	J	3	11/12	-	-	50,53,55,58	0
4	MAN	J	4	11/12	-	-	61,63,64,64	0
4	MAN	J	5	11/12	-	-	52,53,54,55	0
4	FUC	J	6	10/11	-	-	49,52,53,54	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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
6	GOL	D	302	6/6	0.67	0.32	68,68,68,69	0
6	GOL	D	301	6/6	0.76	0.23	48,51,52,52	0
5	EDO	B	201	4/4	0.88	0.20	82,82,82,83	0
6	GOL	C	301	6/6	0.88	0.15	48,50,50,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.